Full wwPDB EM Validation Report ⓘ

Oct 25, 2024 – 05:27 pm BST

PDB ID	:	9H52
EMDB ID	:	EMD-51874
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit in complex with NOA1, ERAL1, METTL17, MCAT and TFB1M (state A1)
Deposited on	:	2024-10-22
Resolution	:	3.80 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ①) were used in the production of this report:

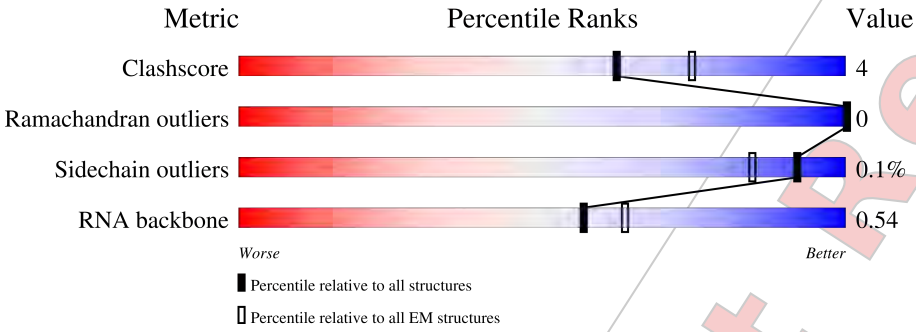
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	215	88% 10%
2	9	698	19% 50% 14% 36%
3	D	430	53% 46%
4	E	125	20% 76% 8% 16%
5	J	138	72% 6% 22%

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Mol	Chain	Length	Quality of chain
6	L	257	46% 52%
7	M	137	82% 16%
8	N	130	79% 5% 16%
9	O	258	70% 26%
10	P	142	10% 57% 8% 35%
11	Q	87	97%
12	R	360	78% 19%
13	S	190	12% 67% 30%
14	T	173	90% 5% 5%
15	U	205	7% 78% 6% 15%
16	a	437	52% 60% 40%
17	A	955	12% 52% 22% 22%
18	B	296	70% 26%
19	W	187	12% 42% 10% 48%
20	C	167	74% 60% 15% 25%
21	F	242	70% 77% 9% 14%
22	G	396	49% 62% 12% 26%
23	X	398	83% 84% 5% 12%
24	Y	395	27% 25% 73%
25	1	323	76% 70% 9% 21%
26	4	689	82% 77% 6% 18%
27	8	390	79% 78% 5% 16%
28	7	456	57% 83% 13%
29	5	346	12% 74% 18% 8%
30	V	414	63% 23% 13%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 127247 atoms, of which 59891 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	0	211	3513	1108	1759	333	308	5	0	0

- Molecule 2 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	9	446	7202	2271	3644	637	637	13	0	0

- Molecule 3 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	232	3705	1155	1867	345	329	9	0	0

- Molecule 4 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	E	105	1691	526	852	154	155	4	0	0

- Molecule 5 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	J	108	1730	521	891	169	143	6	0	0

- Molecule 6 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	L	124	2121	664	1081	182	188	6	0	0

- Molecule 7 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	M	115	1862	578	949	181	148	6	0	0

- Molecule 8 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	N	109	1785	557	926	155	144	3	0	0

- Molecule 9 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	O	190	3112	999	1542	291	274	6	0	0

- Molecule 10 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	P	92	1495	472	764	123	128	8	0	0

- Molecule 11 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	Q	3	35	10	15	4	5	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	variant	UNP P82921

- Molecule 12 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	R	291	4794	1518	2412	409	447	8	0	0

- Molecule 13 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	S	133	Total	C	H	N	O	S	0	0
			2204	709	1104	196	194	1		

- Molecule 14 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	T	164	Total	C	H	N	O	S	0	0
			2706	859	1362	234	240	11		

- Molecule 15 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	U	174	Total	C	H	N	O	S	0	0
			2951	905	1483	295	264	4		

- Molecule 16 is a protein called GTPase Era, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	a	263	Total	C	H	N	O	S	0	0
			3386	1121	1601	323	335	6		

- Molecule 17 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	A	747	Total	C	H	N	O	P	0	0
			23921	7114	8051	2859	5150	747		

- Molecule 18 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	B	220	Total	C	H	N	O	S	0	0
			3581	1142	1792	324	313	10		

- Molecule 19 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	W	98	Total	C	H	N	O	S	0	0
			1569	491	794	138	142	4		

- Molecule 20 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	C	126	Total	C	H	N	O	S	0	0
			2081	679	1039	181	177	5		

- Molecule 21 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	F	208	Total	C	H	N	O	S	0	0
			3498	1104	1774	312	297	11		

- Molecule 22 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	G	292	Total	C	H	N	O	S	0	0
			4767	1522	2372	418	441	14		

- Molecule 23 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	X	352	Total	C	H	N	O	S	0	0
			5706	1822	2857	499	517	11		

- Molecule 24 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Y	108	Total	C	H	N	O	S	0	0
			1777	593	863	150	169	2		

- Molecule 25 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	1	255	Total	C	H	N	O	S	0	0
			4154	1314	2089	346	395	10		

- Molecule 26 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	4	566	Total	C	H	N	O	S	0	0
			9194	2940	4609	774	843	28		

- Molecule 27 is a protein called Malonyl-CoA-acyl carrier protein transacylase, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	8	326	Total	C	H	N	O	S	0	0
			5119	1617	2576	463	446	17		

- Molecule 28 is a protein called Ribosome assembly protein METTL17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	7	398	Total	C	H	N	O	S	0	0
			6324	2006	3179	579	544	16		

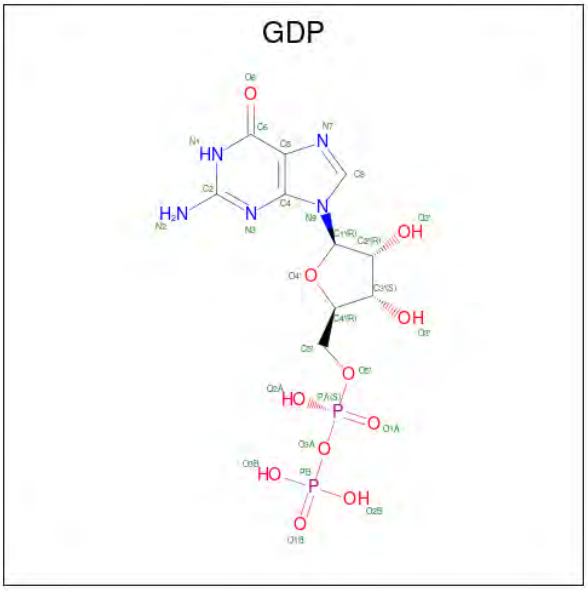
- Molecule 29 is a protein called Dimethyladenosine transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	5	319	Total	C	H	N	O	S	0	0
			5229	1648	2661	458	451	11		

- Molecule 30 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	V	359	Total	C	H	N	O	S	0	0
			5897	1891	2951	491	552	12		

- Molecule 31 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						AltConf
31	9	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

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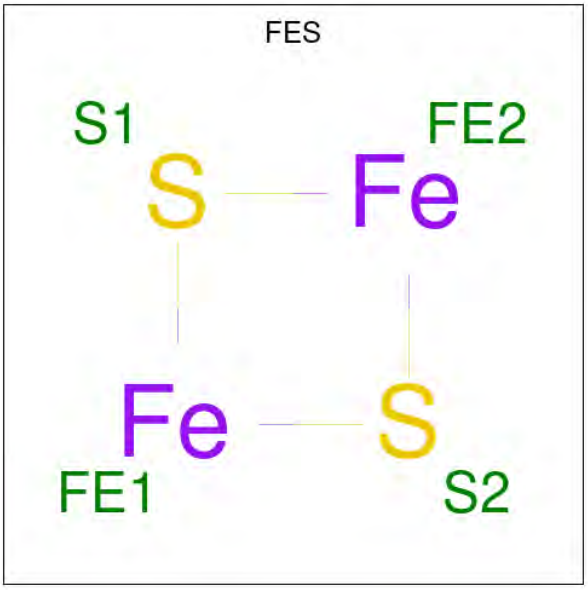
Mol	Chain	Residues	Atoms	AltConf
31	X	1	Total C H N O P 38 10 10 5 11 2	0

- Molecule 32 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
32	E	1	Total Fe S 4 2 2	0
32	T	1	Total Fe S 4 2 2	0

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

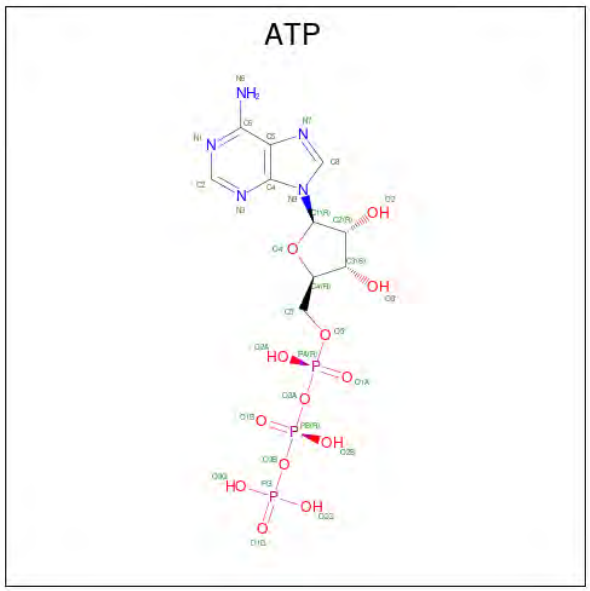
Mol	Chain	Residues	Atoms	AltConf
33	O	1	Total Zn 1 1	0

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
34	B	1	Total Mg 1 1	0
34	X	1	Total Mg 1 1	0

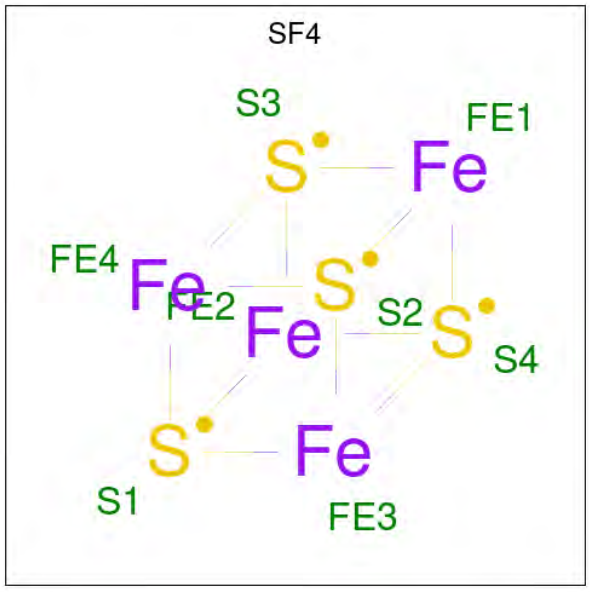
- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
35	X	1	43	10	12	5	13	3	0

- Molecule 36 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



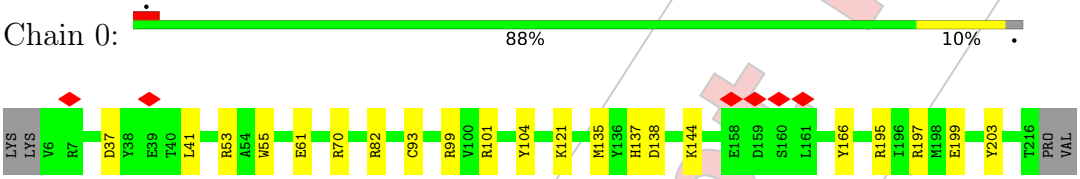
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
36	7	1	8	4	4	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

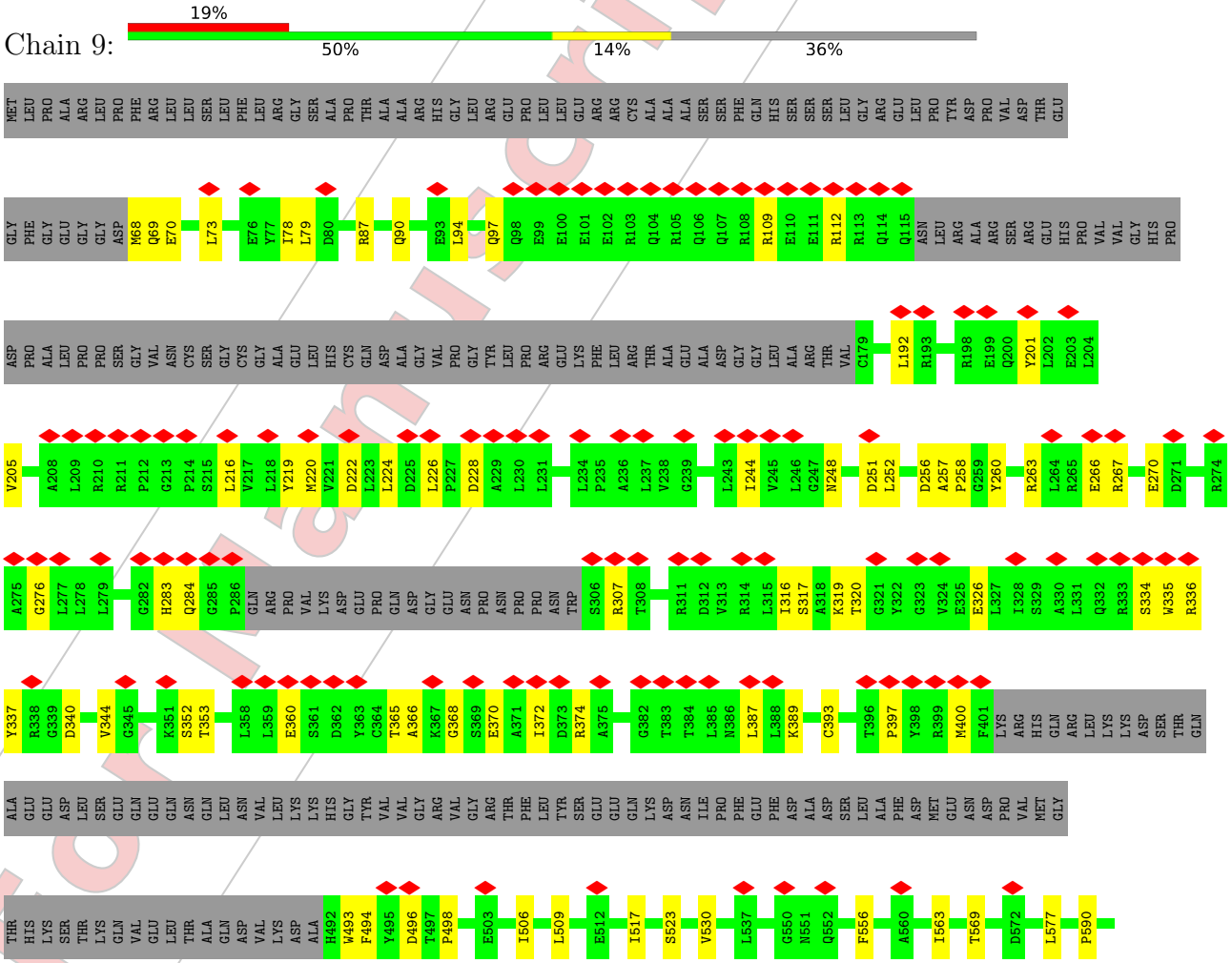
- Molecule 1: Small ribosomal subunit protein mS34

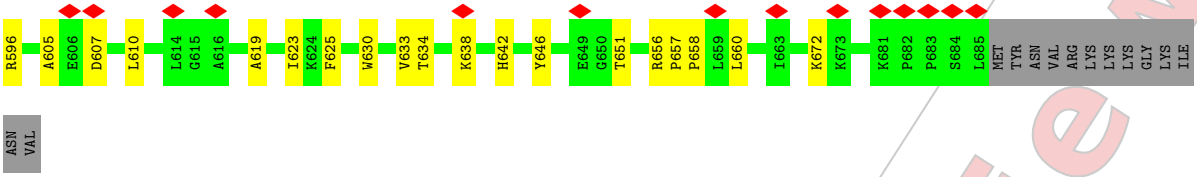
Chain 0:



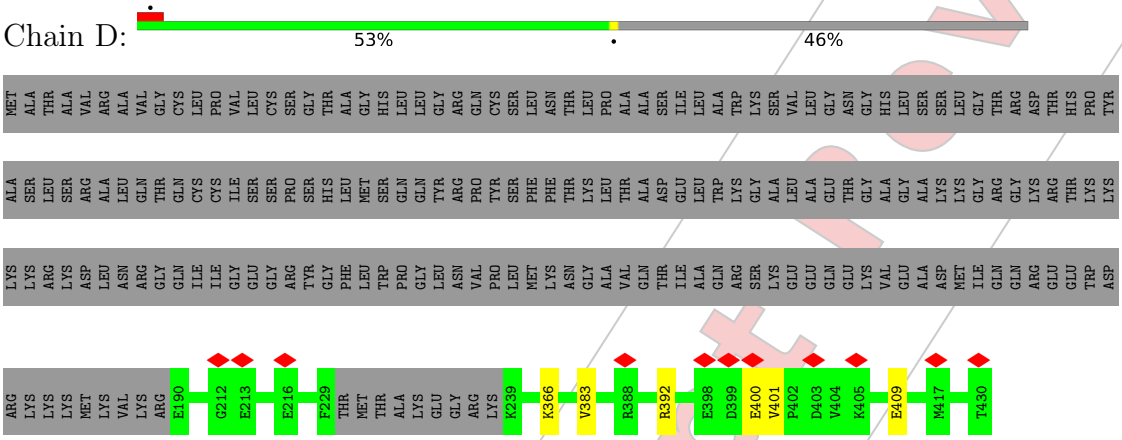
- Molecule 2: Nitric oxide-associated protein 1

Chain 9:

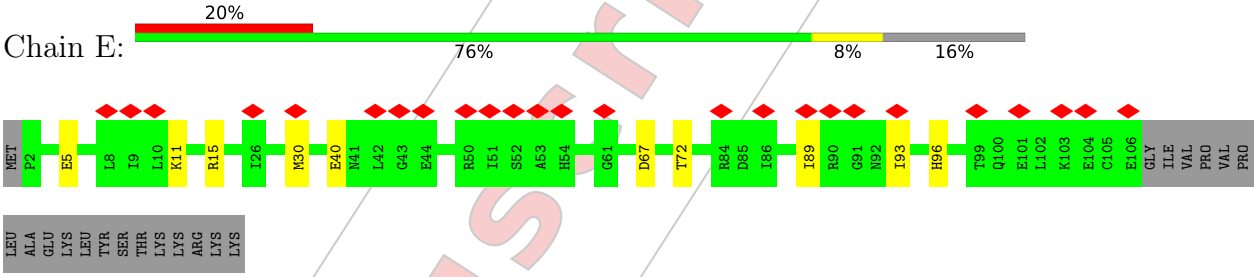




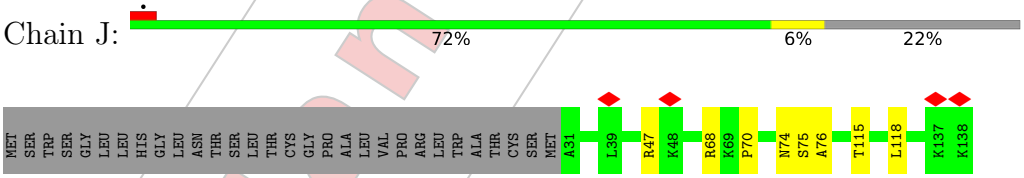
• Molecule 3: 28S ribosomal protein S5, mitochondrial



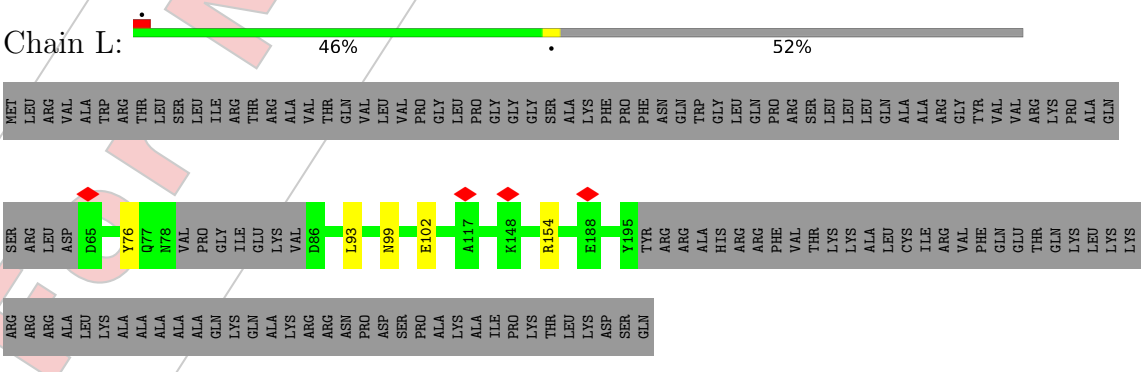
• Molecule 4: 28S ribosomal protein S6, mitochondrial



• Molecule 5: 28S ribosomal protein S12, mitochondrial

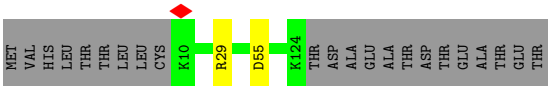


• Molecule 6: 28S ribosomal protein S15, mitochondrial



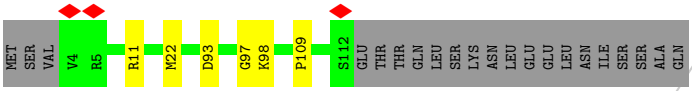
• Molecule 7: 28S ribosomal protein S16, mitochondrial

Chain M:



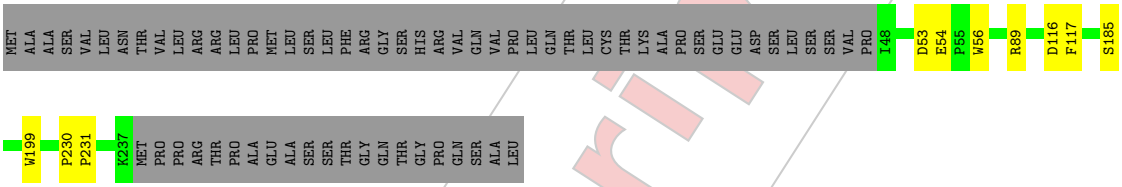
• Molecule 8: 28S ribosomal protein S17, mitochondrial

Chain N:



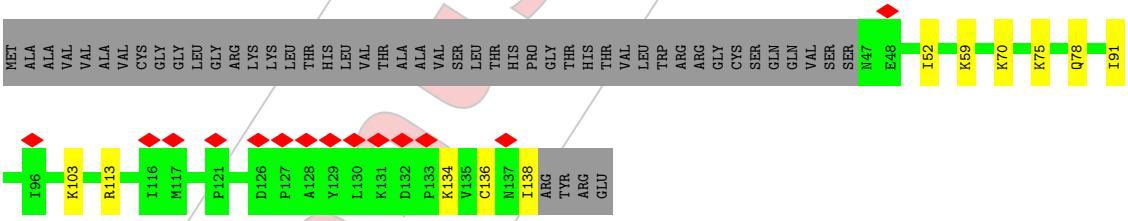
• Molecule 9: 28S ribosomal protein S18b, mitochondrial

Chain O:



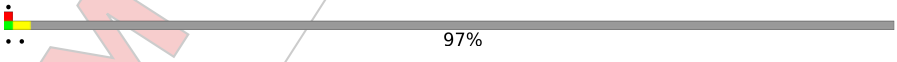
• Molecule 10: 28S ribosomal protein S18c, mitochondrial

Chain P:



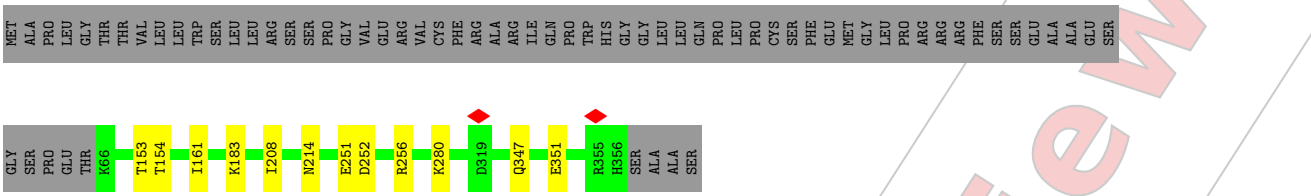
• Molecule 11: 28S ribosomal protein S21, mitochondrial

Chain Q:



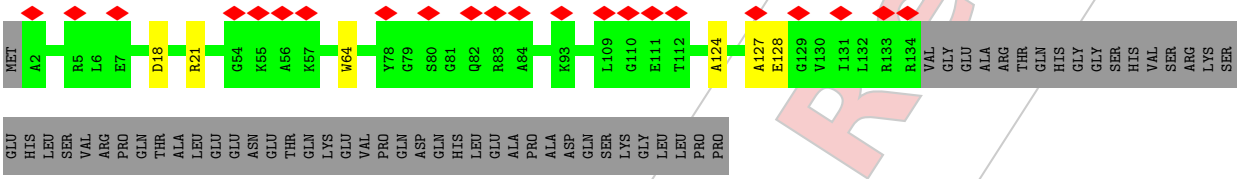
• Molecule 12: 28S ribosomal protein S22, mitochondrial

Chain R:



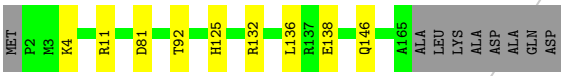
• Molecule 13: 28S ribosomal protein S23, mitochondrial

Chain S:



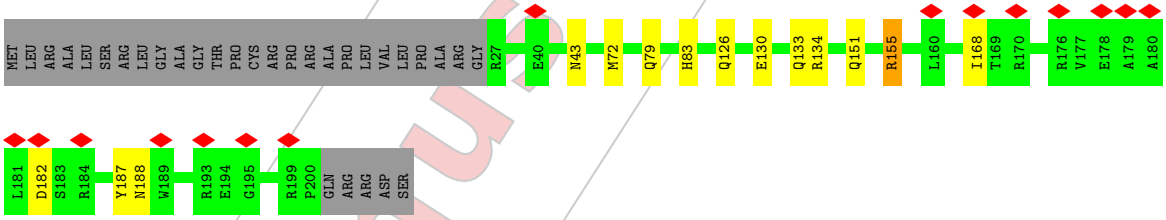
• Molecule 14: 28S ribosomal protein S25, mitochondrial

Chain T:



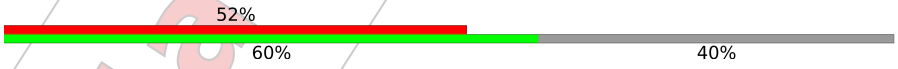
• Molecule 15: 28S ribosomal protein S26, mitochondrial

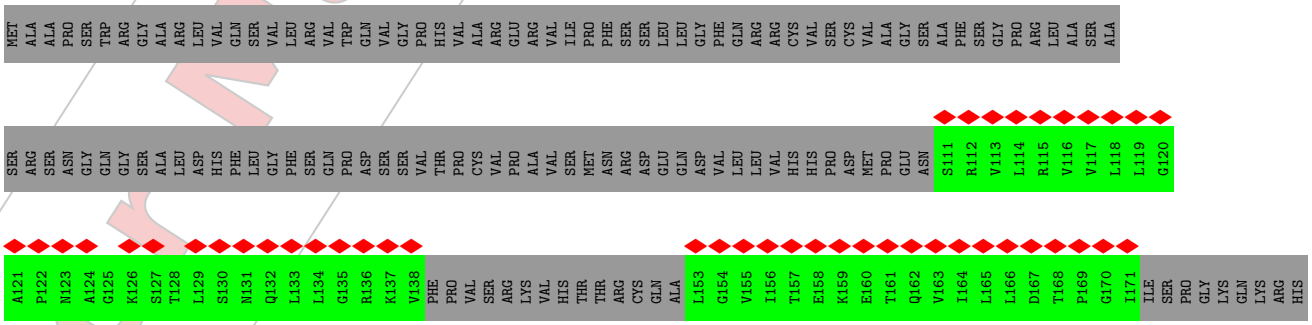
Chain U:



• Molecule 16: GTPase Era, mitochondrial

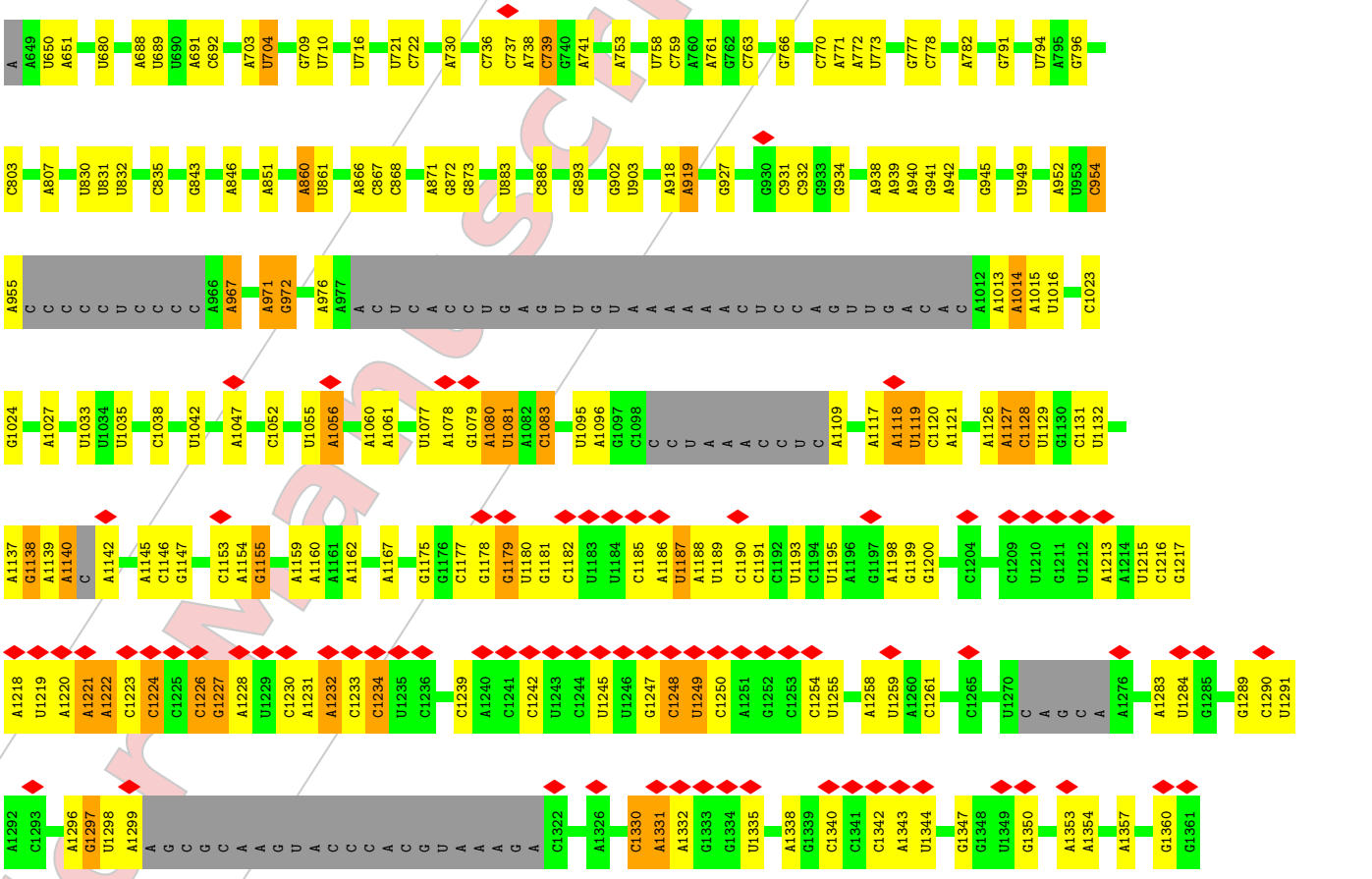
Chain a:

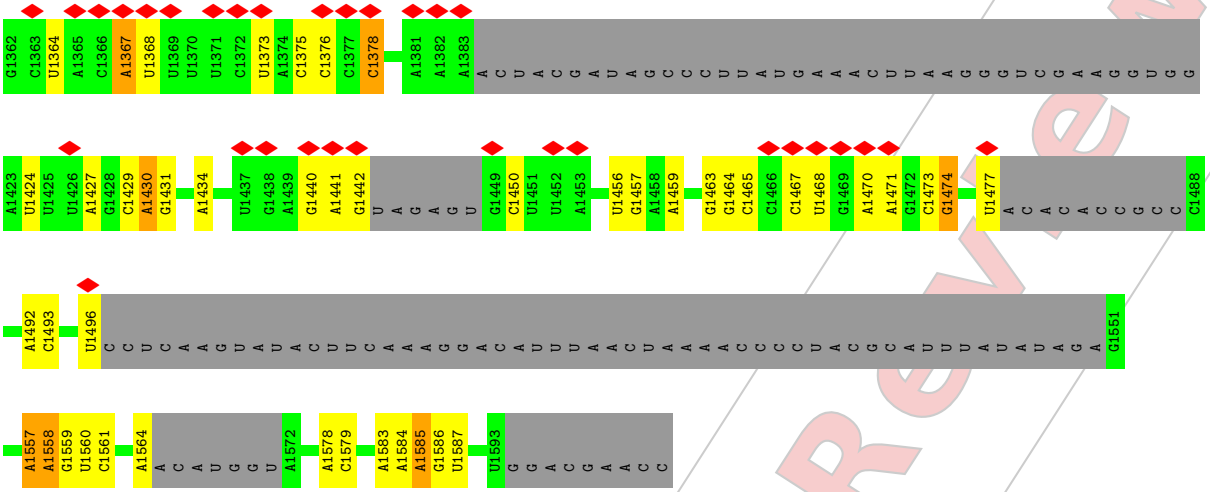




• Molecule 17: 12S mitochondrial rRNA

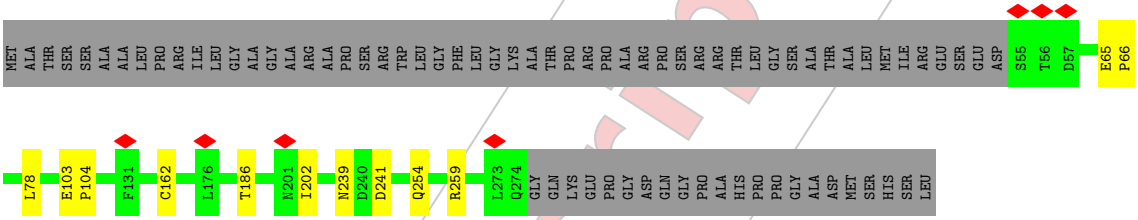
Chain A:





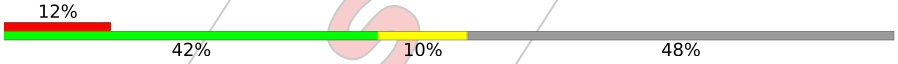
• Molecule 18: 28S ribosomal protein S2, mitochondrial

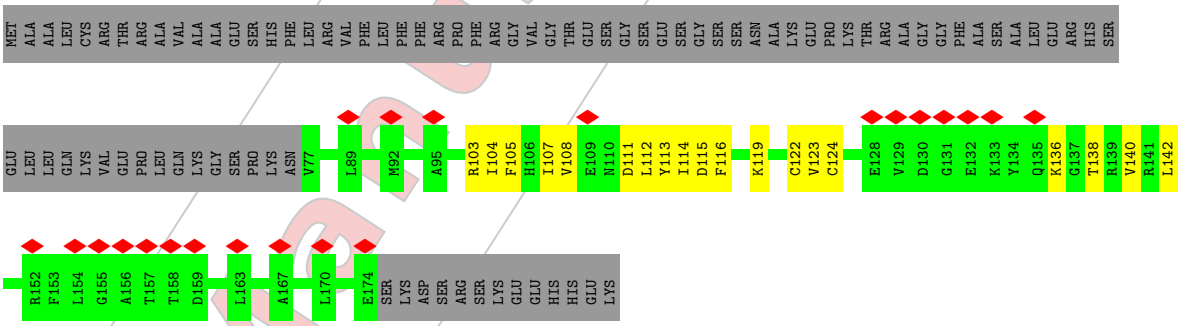
Chain B:



• Molecule 19: 28S ribosomal protein S28, mitochondrial

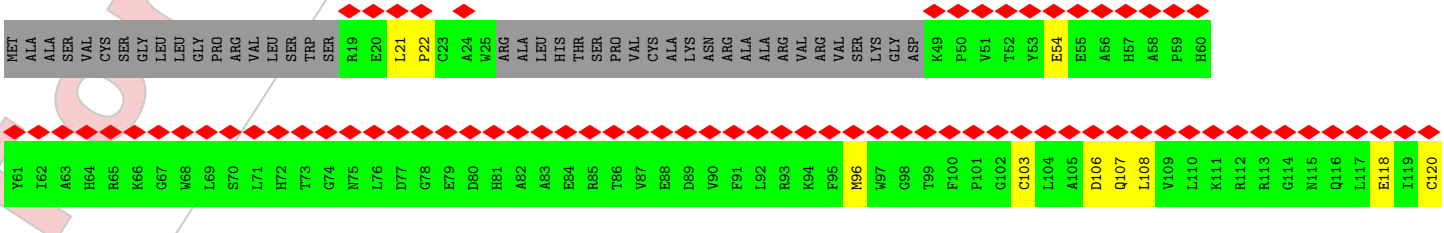
Chain W:

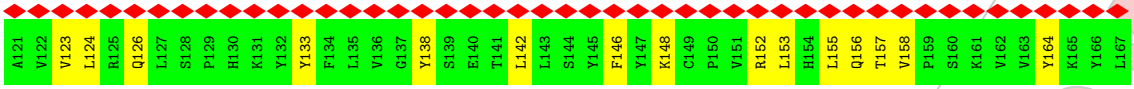




• Molecule 20: 28S ribosomal protein S24, mitochondrial

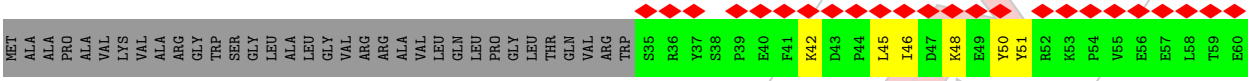
Chain C:

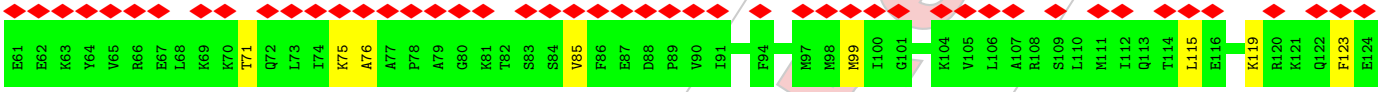


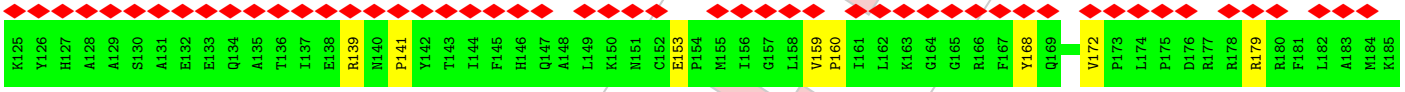


• Molecule 21: 28S ribosomal protein S7, mitochondrial

Chain F:

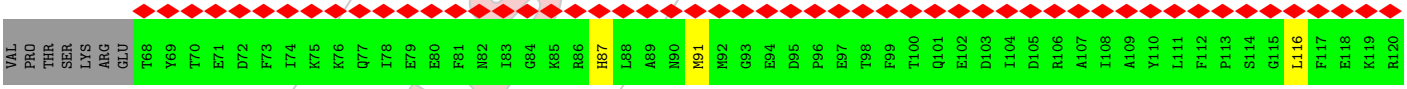


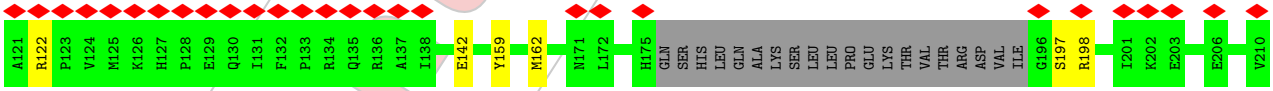


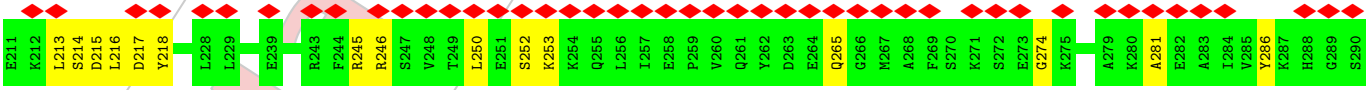


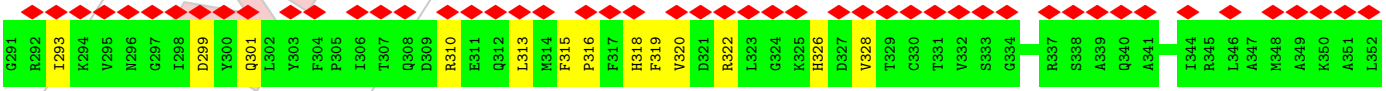
• Molecule 22: 28S ribosomal protein S9, mitochondrial

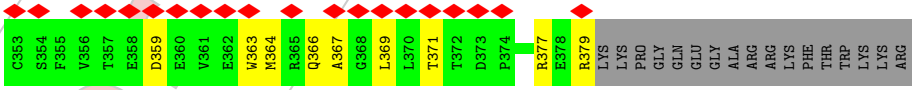
Chain G:





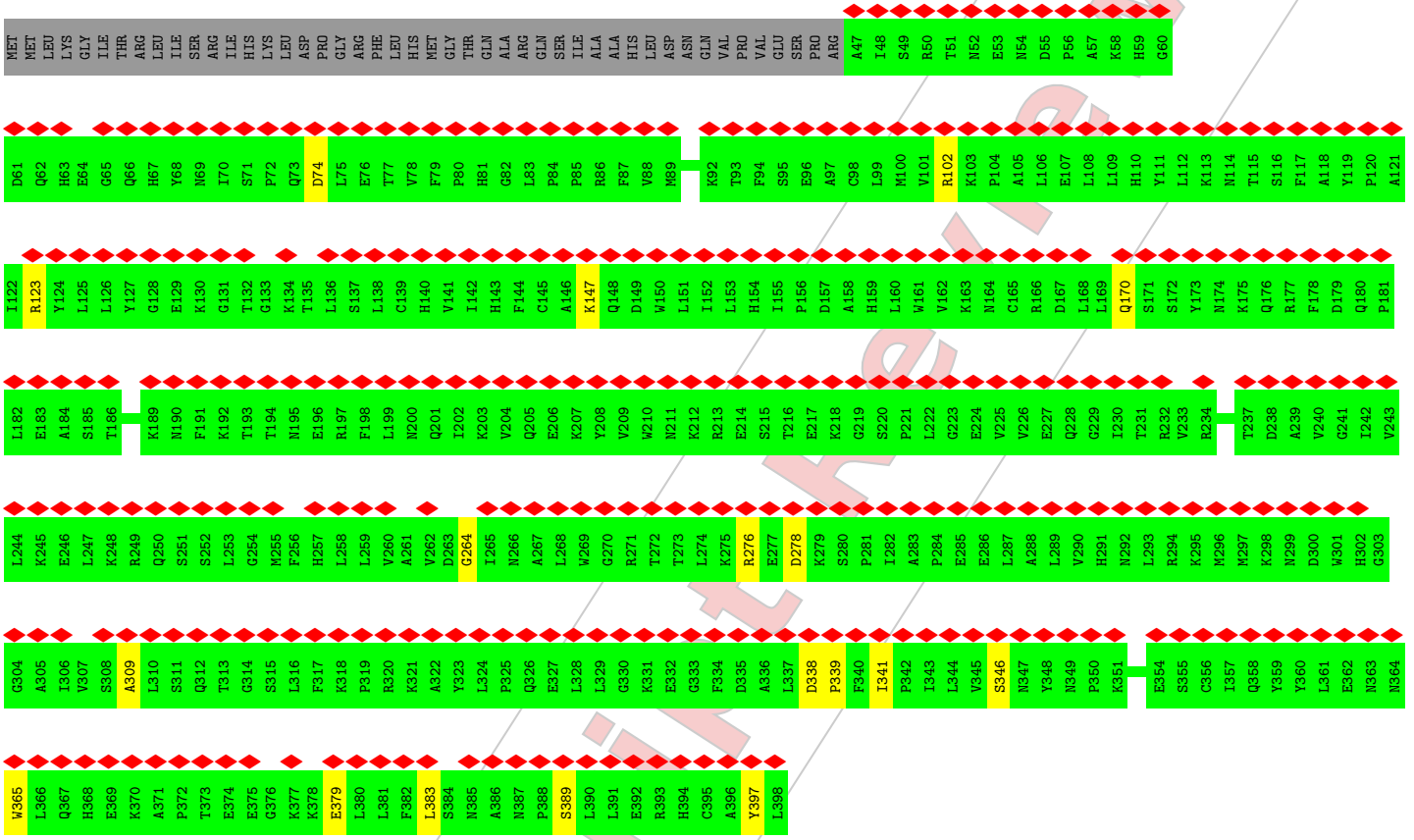






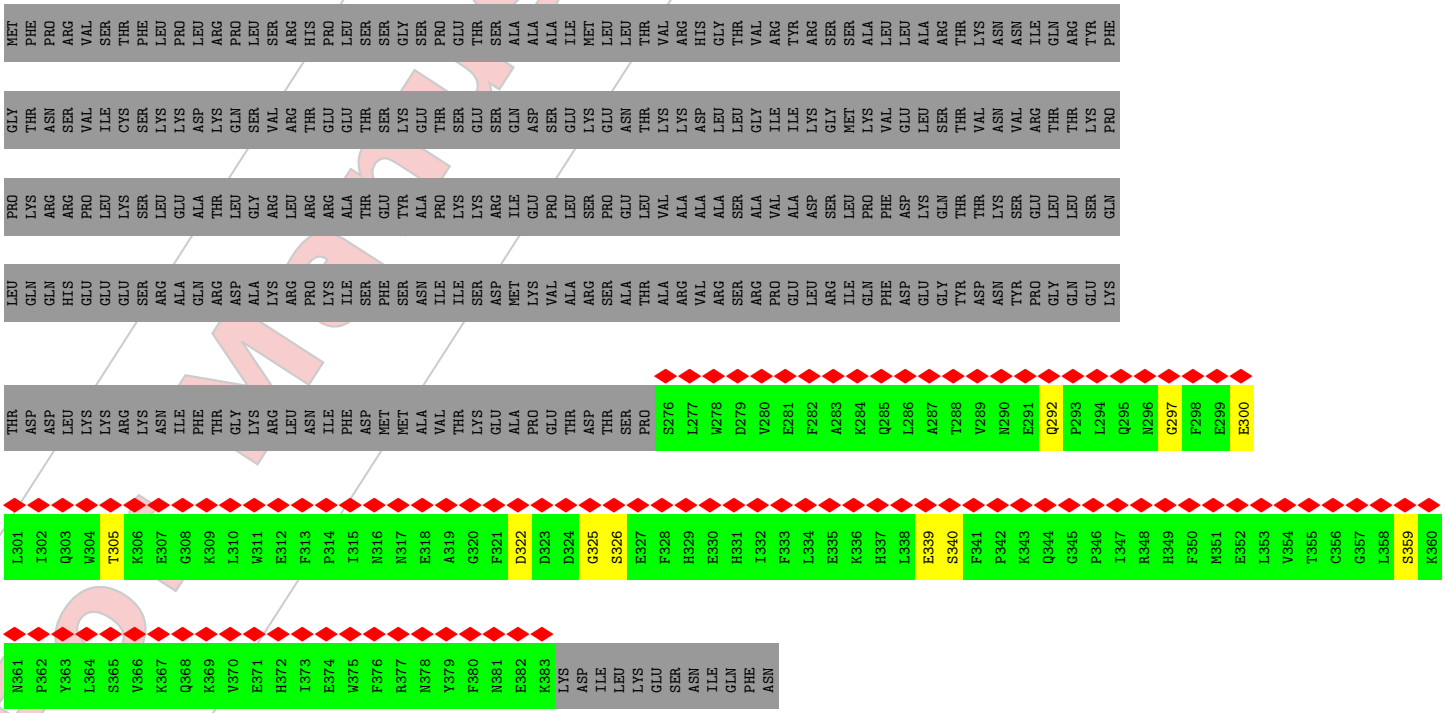
• Molecule 23: 28S ribosomal protein S29, mitochondrial

Chain X:



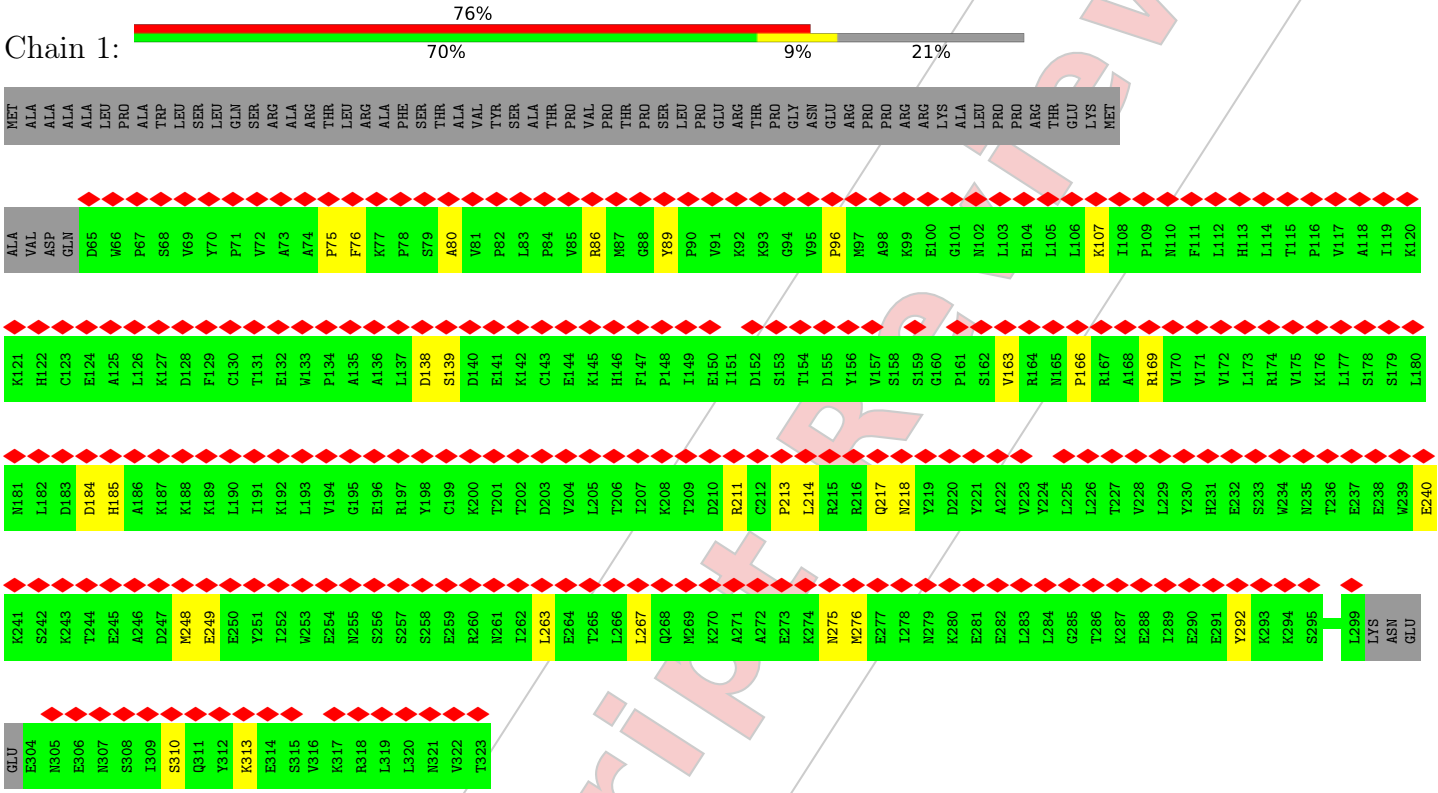
• Molecule 24: 28S ribosomal protein S31, mitochondrial

Chain Y:



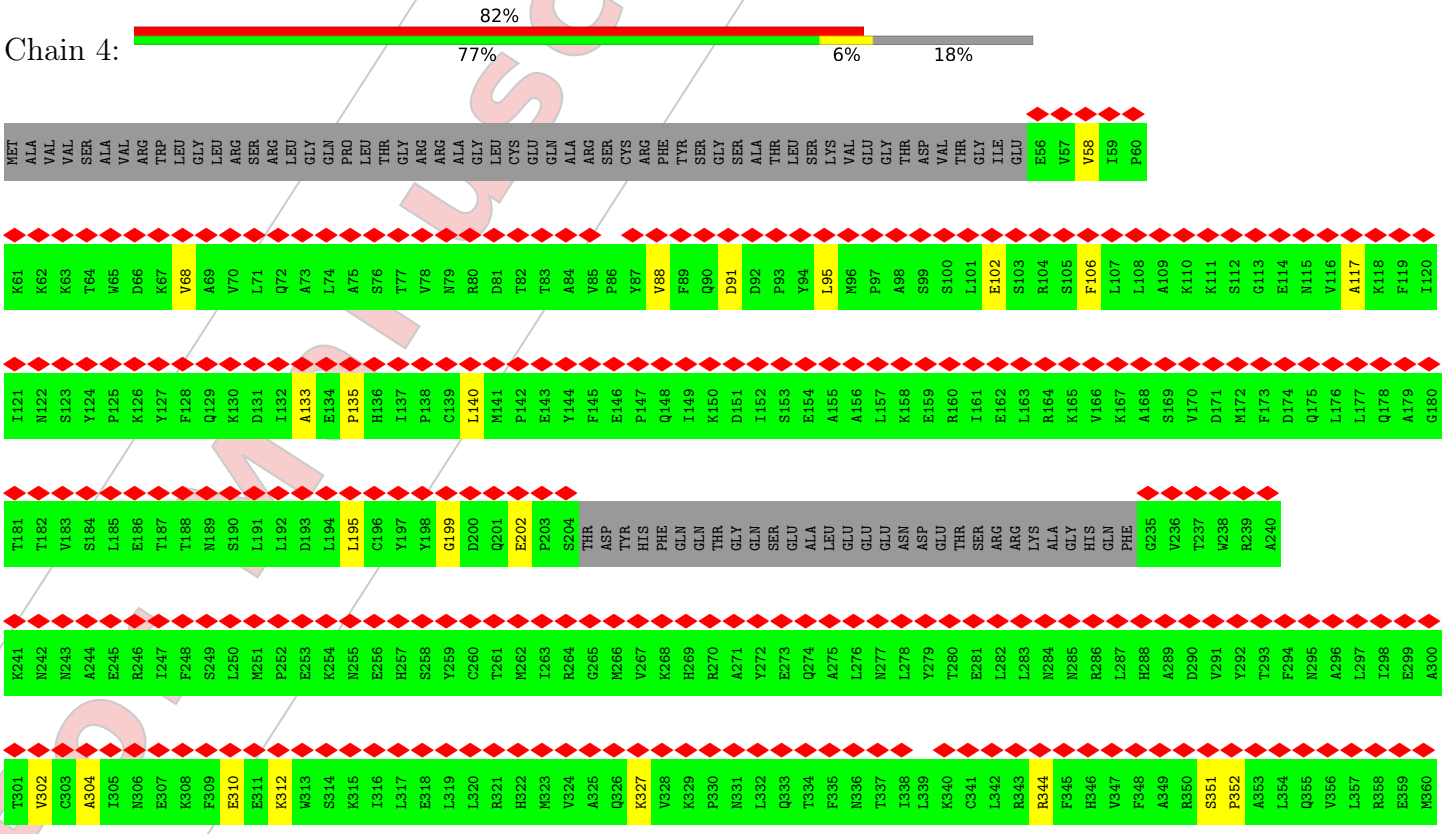
• Molecule 25: 28S ribosomal protein S35, mitochondrial

Chain 1:



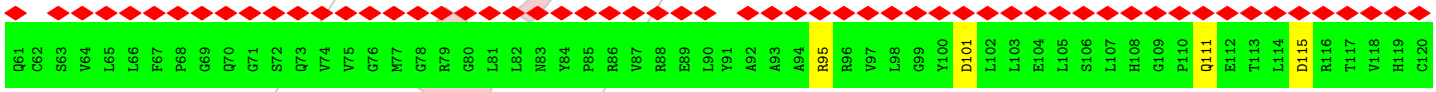
• Molecule 26: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

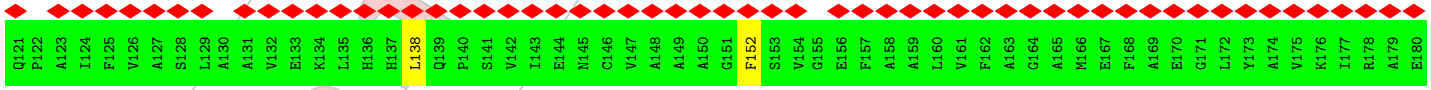
Chain 4:

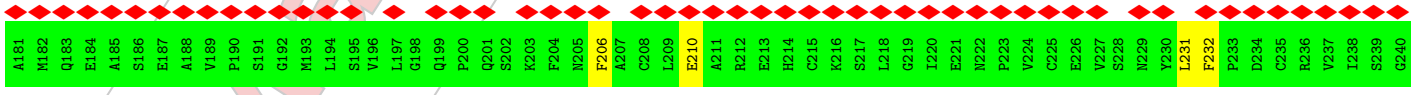


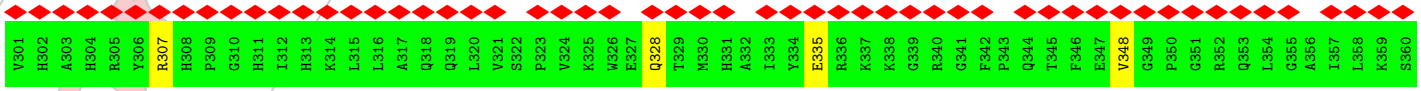
• Molecule 27: Malonyl-CoA-acyl carrier protein transacylase, mitochondrial

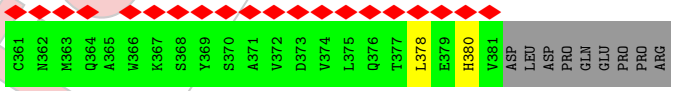
Chain 8:





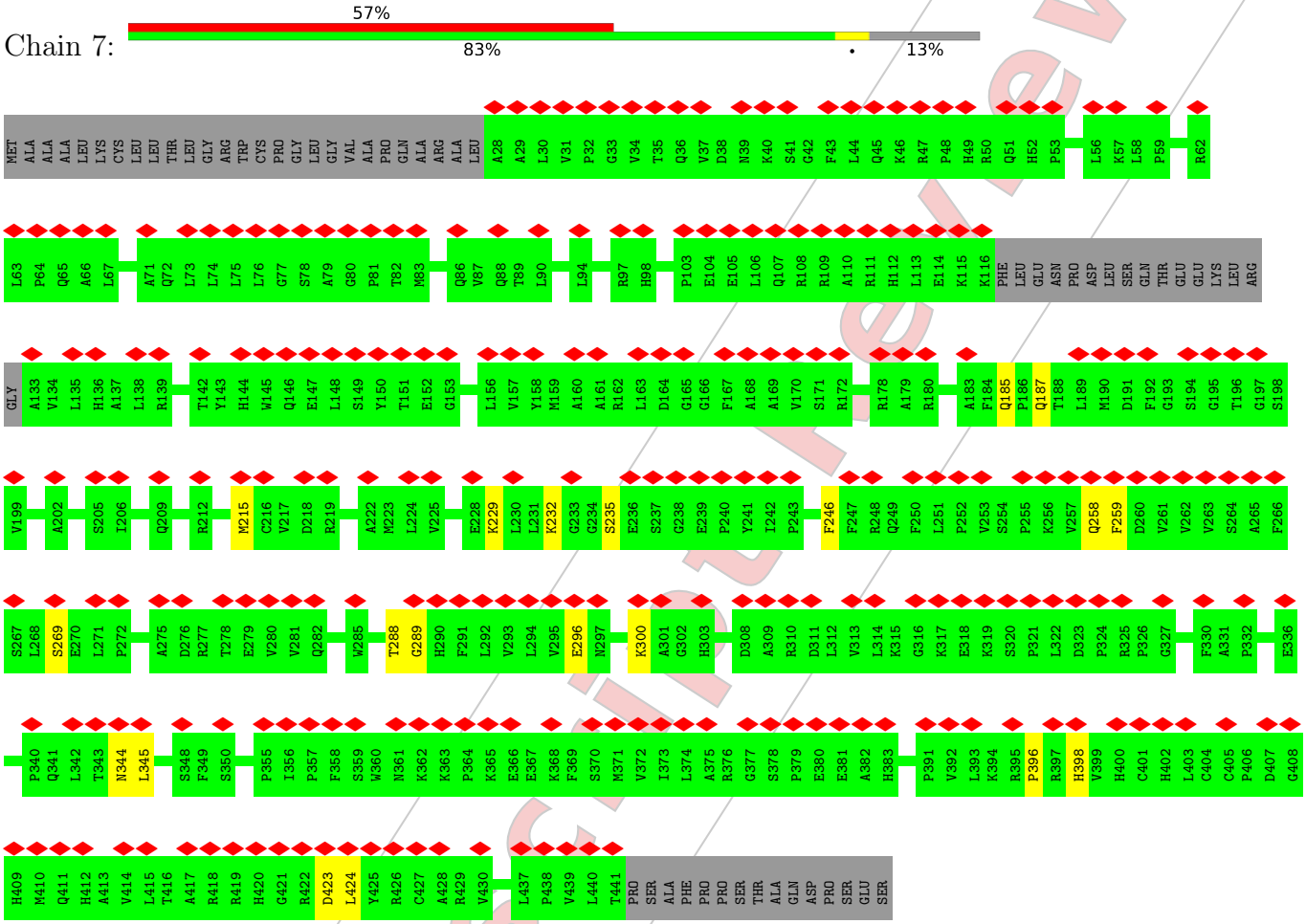






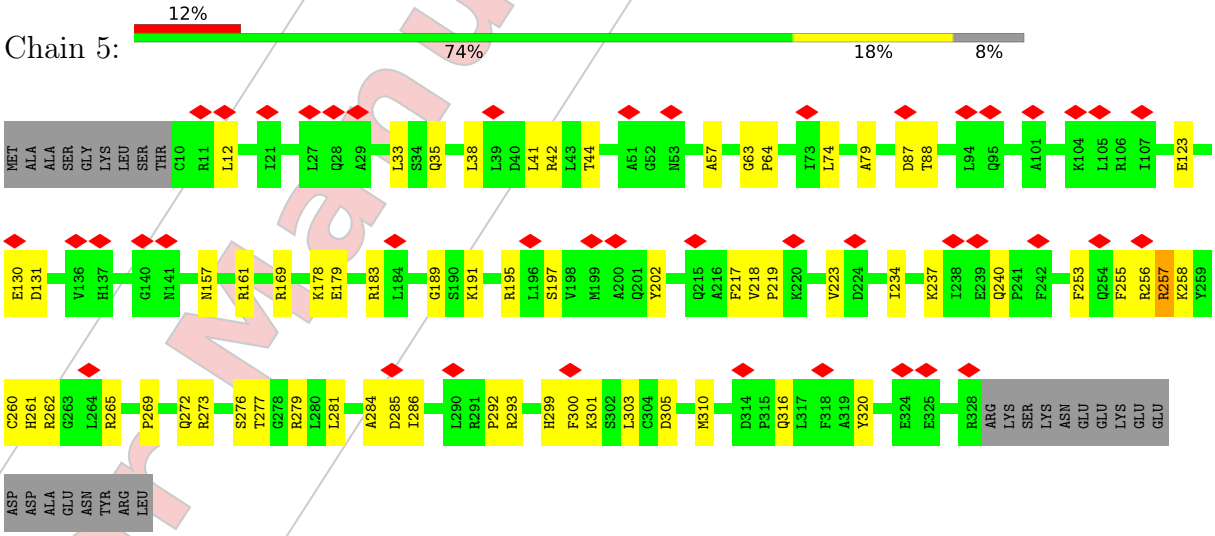
• Molecule 28: Ribosome assembly protein METTL17, mitochondrial

Chain 7:



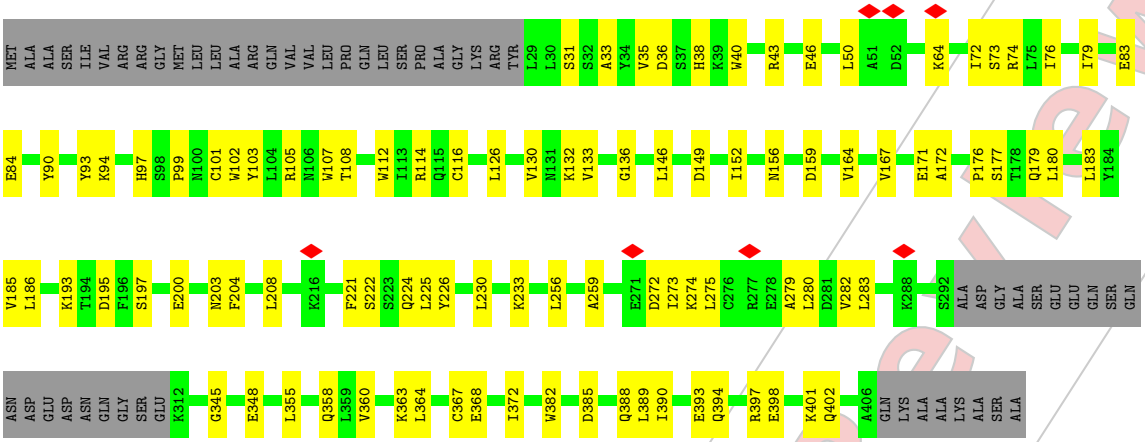
• Molecule 29: Dimethyladenosine transferase 1, mitochondrial

Chain 5:



• Molecule 30: 28S ribosomal protein S27, mitochondrial

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.009	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	609.12, 609.12, 609.12	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0152, 1.0152, 1.0152	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, SF4, FES, MG, ATP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.28	0/1800	0.55	0/2440
2	9	0.27	0/3637	0.54	0/4935
3	D	0.28	0/1877	0.53	0/2523
4	E	0.26	0/853	0.53	0/1151
5	J	0.29	0/855	0.56	0/1148
6	L	0.26	0/1058	0.45	0/1416
7	M	0.29	0/934	0.54	0/1255
8	N	0.27	0/877	0.50	0/1187
9	O	0.29	0/1624	0.49	0/2210
10	P	0.26	0/747	0.41	0/1004
11	Q	0.28	0/19	0.44	0/22
12	R	0.28	0/2429	0.46	0/3280
13	S	0.27	0/1127	0.53	0/1518
14	T	0.30	0/1375	0.47	0/1847
15	U	0.26	0/1490	0.54	0/1999
16	a	0.25	0/1801	0.46	0/2447
17	A	0.30	0/17742	0.70	0/27597
18	B	0.27	0/1832	0.51	0/2480
19	W	0.26	0/787	0.55	0/1060
20	C	0.26	0/1074	0.49	0/1456
21	F	0.25	0/1766	0.48	0/2373
22	G	0.27	0/2446	0.51	0/3283
23	X	0.25	0/2921	0.45	0/3954
24	Y	0.25	0/943	0.39	0/1274
25	1	0.25	0/2108	0.46	0/2852
26	4	0.25	0/4686	0.44	0/6335
27	8	0.25	0/2603	0.48	0/3520
28	7	0.25	0/3234	0.49	0/4390
29	5	0.27	0/2624	0.52	0/3552
30	V	0.29	0/3007	0.47	0/4062
All	All	0.27	0/70276	0.56	0/98570

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1754	1759	1754	16	0
2	9	3558	3644	3636	73	0
3	D	1838	1867	1858	4	0
4	E	839	852	848	9	0
5	J	839	891	887	5	0
6	L	1040	1081	1078	3	0
7	M	913	949	943	1	0
8	N	859	926	922	4	0
9	O	1570	1542	1533	7	0
10	P	731	764	761	8	0
11	Q	20	15	15	9	0
12	R	2382	2412	2405	7	0
13	S	1100	1104	1103	5	0
14	T	1344	1362	1359	8	0
15	U	1468	1483	1478	11	0
16	a	1785	1601	1599	0	0
17	A	15870	8051	8066	88	0
18	B	1789	1792	1781	10	0
19	W	775	794	791	23	0
20	C	1042	1039	1033	23	0
21	F	1724	1774	1769	20	0
22	G	2395	2372	2364	36	0
23	X	2849	2857	2843	15	0
24	Y	914	863	859	10	0
25	1	2065	2089	2086	25	0
26	4	4585	4609	4595	33	0
27	8	2543	2576	2561	14	0
28	7	3145	3179	3159	11	0
29	5	2568	2661	2655	44	0
30	V	2946	2951	2942	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	9	28	10	12	6	0
31	X	28	10	12	0	0
32	E	4	0	0	0	0
32	T	4	0	0	0	0
33	O	1	0	0	0	0
34	B	1	0	0	0	0
34	X	1	0	0	0	0
35	X	31	12	12	0	0
36	7	8	0	0	0	0
All	All	67356	59891	59719	491	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (491) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:78:LEU:HD11	18:B:259:ARG:NH2	1.96	0.80
24:Y:292:GLN:NE2	26:4:449:GLY:O	2.14	0.79
17:A:1456:U:O4	22:G:377:ARG:NH2	2.19	0.76
19:W:114:ILE:CG2	19:W:142:LEU:HD11	2.18	0.74
30:V:31:SER:OG	30:V:368:GLU:OE2	2.06	0.73
2:9:276:GLY:O	2:9:307:ARG:NH2	2.21	0.73
2:9:387:LEU:HD13	2:9:496:ASP:O	1.91	0.70
1:0:144:LYS:NZ	30:V:171:GLU:O	2.23	0.70
5:J:68:ARG:NH2	17:A:1496:U:OP1	2.25	0.70
27:8:95:ARG:NH2	27:8:101:ASP:OD1	2.25	0.70
22:G:197:SER:O	22:G:245:ARG:NH2	2.25	0.69
2:9:284:GLN:HA	29:5:299:HIS:CD2	2.28	0.68
26:4:612:ASN:OD1	26:4:648:ARG:NH1	2.27	0.68
2:9:340:ASP:OD1	2:9:493:TRP:N	2.26	0.68
21:F:119:LYS:NZ	23:X:365:TRP:O	2.24	0.67
11:Q:85:GLN:N	19:W:113:TYR:O	2.27	0.67
21:F:71:THR:HG23	22:G:250:LEU:HD11	1.76	0.67
17:A:1230:C:O2	27:8:307:ARG:NH2	2.28	0.67
11:Q:85:GLN:O	19:W:115:ASP:N	2.28	0.67
2:9:387:LEU:HD11	2:9:498:PRO:HG3	1.77	0.66
29:5:240:GLN:NE2	29:5:305:ASP:OD1	2.29	0.66
27:8:152:PHE:O	27:8:300:ASN:ND2	2.28	0.66
2:9:87:ARG:NH1	2:9:90:GLN:OE1	2.29	0.65
3:D:366:LYS:O	3:D:392:ARG:NH1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:115:ASP:OD1	19:W:116:PHE:N	2.30	0.65
22:G:116:LEU:O	22:G:122:ARG:NE	2.28	0.65
29:5:191:LYS:O	29:5:256:ARG:NH2	2.30	0.65
7:M:55:ASP:OD2	14:T:146:GLN:NE2	2.29	0.64
12:R:252:ASP:OD2	12:R:256:ARG:NH2	2.31	0.64
30:V:275:LEU:HD23	30:V:280:LEU:HD21	1.80	0.64
26:4:619:LYS:NZ	26:4:652:ASP:O	2.31	0.63
30:V:156:ASN:O	30:V:159:ASP:N	2.30	0.63
2:9:326:GLU:N	2:9:326:GLU:OE1	2.31	0.63
5:J:47:ARG:NH1	17:A:927:G:OP2	2.31	0.63
30:V:279:ALA:O	30:V:282:VAL:HG12	1.99	0.63
2:9:267:ARG:NH2	2:9:657:PRO:O	2.30	0.63
30:V:40:TRP:O	30:V:43:ARG:NH1	2.32	0.63
6:L:154:ARG:NH2	17:A:945:G:O2'	2.31	0.63
19:W:112:LEU:N	19:W:124:CYS:O	2.28	0.63
22:G:265:GLN:N	22:G:265:GLN:OE1	2.32	0.63
24:Y:326:SER:O	25:1:217:GLN:NE2	2.31	0.62
17:A:1561:C:O2'	29:5:42:ARG:NH1	2.32	0.62
30:V:193:LYS:NZ	30:V:195:ASP:O	2.33	0.62
19:W:114:ILE:HG21	19:W:142:LEU:HD11	1.81	0.62
18:B:241:ASP:OD2	19:W:119:LYS:NZ	2.32	0.61
2:9:69:GLN:NE2	2:9:70:GLU:O	2.33	0.61
15:U:43:ASN:ND2	17:A:703:A:OP2	2.34	0.60
2:9:672:LYS:N	17:A:692:C:OP2	2.35	0.59
9:O:185:SER:O	12:R:183:LYS:NZ	2.35	0.59
17:A:1429:C:OP1	17:A:1459:A:N6	2.32	0.59
2:9:220:MET:N	2:9:344:VAL:O	2.32	0.59
4:E:93:ILE:O	17:A:1033:U:O2'	2.20	0.59
2:9:506:ILE:HD12	2:9:625:PHE:O	2.02	0.59
29:5:218:VAL:HB	29:5:219:PRO:HD3	1.84	0.59
4:E:15:ARG:NH1	15:U:182:ASP:OD1	2.35	0.59
23:X:338:ASP:OD1	25:1:292:TYR:OH	2.15	0.59
30:V:364:LEU:O	30:V:368:GLU:N	2.36	0.59
2:9:256:ASP:OD1	2:9:257:ALA:N	2.35	0.58
28:7:423:ASP:OD1	28:7:424:LEU:N	2.36	0.58
29:5:41:LEU:O	29:5:44:THR:OG1	2.21	0.58
13:S:128:GLU:OE1	13:S:128:GLU:N	2.35	0.58
20:C:164:TYR:OH	25:1:89:TYR:O	2.19	0.58
20:C:142:LEU:HD21	26:4:117:ALA:HB1	1.85	0.58
2:9:70:GLU:HG2	30:V:103:TYR:HD2	1.69	0.58
27:8:328:GLN:OE1	27:8:328:GLN:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:157:ASN:O	29:5:161:ARG:N	2.37	0.58
22:G:217:ASP:OD1	22:G:218:TYR:N	2.37	0.58
28:7:185:GLN:O	28:7:187:GLN:NE2	2.37	0.58
25:1:166:PRO:O	25:1:169:ARG:NE	2.37	0.58
2:9:352:SER:OG	31:9:701:GDP:O3A	2.19	0.57
17:A:1227:G:N2	27:8:335:GLU:O	2.35	0.57
2:9:248:ASN:ND2	31:9:701:GDP:N7	2.52	0.57
23:X:102:ARG:NH2	23:X:346:SER:O	2.36	0.57
30:V:397:ARG:O	30:V:401:LYS:N	2.37	0.57
4:E:67:ASP:OD2	4:E:96:HIS:NE2	2.39	0.56
29:5:87:ASP:OD1	29:5:88:THR:N	2.38	0.56
25:1:185:HIS:NE2	25:1:240:GLU:OE2	2.38	0.56
29:5:57:ALA:O	29:5:79:ALA:N	2.37	0.56
4:E:72:THR:HG23	17:A:1035:U:H5"	1.85	0.56
29:5:130:GLU:HA	29:5:234:ILE:HG23	1.87	0.56
30:V:203:ASN:OD1	30:V:204:PHE:N	2.38	0.56
30:V:398:GLU:O	30:V:402:GLN:NE2	2.38	0.56
17:A:1578:A:O3'	29:5:257:ARG:NH1	2.39	0.56
4:E:40:GLU:OE1	15:U:187:TYR:OH	2.23	0.56
30:V:208:LEU:CD1	30:V:226:TYR:CD2	2.89	0.56
26:4:530:GLU:N	26:4:530:GLU:OE1	2.39	0.56
2:9:556:PHE:CE1	2:9:633:VAL:HG13	2.41	0.56
9:O:116:ASP:OD1	9:O:117:PHE:N	2.39	0.56
17:A:1289:G:O2'	17:A:1297:G:OP2	2.24	0.56
14:T:11:ARG:NH2	17:A:932:C:N3	2.54	0.55
29:5:269:PRO:O	29:5:273:ARG:N	2.39	0.55
1:0:197:ARG:NH1	1:0:199:GLU:OE1	2.39	0.55
20:C:138:TYR:CD1	26:4:117:ALA:HB2	2.42	0.55
30:V:274:LYS:NZ	30:V:345:GLY:O	2.37	0.55
25:1:138:ASP:OD1	25:1:139:SER:N	2.40	0.55
20:C:142:LEU:O	20:C:146:PHE:N	2.39	0.55
23:X:123:ARG:NH2	23:X:339:PRO:O	2.40	0.54
25:1:163:VAL:HG12	26:4:135:PRO:HD3	1.88	0.54
18:B:202:ILE:HG22	18:B:202:ILE:O	2.08	0.54
5:J:74:ASN:OD1	5:J:75:SER:N	2.40	0.54
11:Q:85:GLN:HA	19:W:105:PHE:H	1.73	0.54
20:C:118:GLU:OE2	20:C:152:ARG:NH2	2.41	0.54
28:7:300:LYS:NZ	28:7:344:ASN:O	2.38	0.54
3:D:409:GLU:N	3:D:409:GLU:OE1	2.38	0.54
14:T:132:ARG:NH1	14:T:136:LEU:O	2.41	0.54
17:A:843:G:N2	17:A:846:A:OP2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:1155:G:OP1	29:5:293:ARG:NH2	2.41	0.53
22:G:213:LEU:HD12	22:G:214:SER:O	2.08	0.53
20:C:106:ASP:OD1	20:C:107:GLN:N	2.37	0.53
29:5:38:LEU:HB2	29:5:217:PHE:CD1	2.44	0.53
2:9:256:ASP:HB3	2:9:660:LEU:HB3	1.91	0.53
12:R:251:GLU:OE2	12:R:280:LYS:NZ	2.41	0.53
2:9:283:HIS:O	29:5:299:HIS:NE2	2.41	0.53
27:8:111:GLN:NE2	27:8:115:ASP:OD1	2.41	0.52
17:A:1226:C:O2'	17:A:1227:G:OP1	2.23	0.52
28:7:259:PHE:O	28:7:289:GLY:N	2.43	0.52
4:E:5:GLU:OE1	10:P:75:LYS:NZ	2.40	0.52
17:A:1221:A:O2'	17:A:1222:A:OP2	2.25	0.52
17:A:1232:A:N6	17:A:1234:C:O4'	2.43	0.52
10:P:113:ARG:NH2	17:A:1033:U:OP1	2.39	0.52
25:1:263:LEU:O	25:1:267:LEU:HD23	2.09	0.52
21:F:45:LEU:O	22:G:367:ALA:HA	2.09	0.52
22:G:274:GLY:N	22:G:281:ALA:O	2.39	0.52
26:4:304:ALA:O	26:4:312:LYS:NZ	2.41	0.52
2:9:70:GLU:HA	30:V:103:TYR:CE2	2.44	0.52
2:9:335:TRP:CD1	2:9:397:PRO:HB3	2.44	0.52
8:N:11:ARG:NH1	14:T:81:ASP:OD1	2.43	0.52
17:A:1330:C:H4'	17:A:1331:A:O5'	2.10	0.52
26:4:195:LEU:O	26:4:199:GLY:N	2.43	0.51
2:9:226:LEU:O	2:9:656:ARG:NH1	2.38	0.51
2:9:353:THR:OG1	31:9:701:GDP:O2A	2.25	0.51
11:Q:85:GLN:HB2	19:W:114:ILE:HA	1.92	0.51
20:C:138:TYR:HD1	26:4:117:ALA:HB2	1.75	0.51
29:5:281:LEU:O	29:5:285:ASP:N	2.34	0.51
30:V:272:ASP:OD1	30:V:273:ILE:N	2.43	0.51
29:5:189:GLY:N	29:5:293:ARG:O	2.40	0.51
2:9:248:ASN:HA	2:9:316:ILE:O	2.10	0.51
30:V:105:ARG:O	30:V:108:THR:OG1	2.27	0.51
17:A:1179:G:H21	17:A:1180:U:H3'	1.75	0.51
17:A:1232:A:H2'	17:A:1232:A:N3	2.26	0.51
18:B:239:ASN:OD1	19:W:119:LYS:NZ	2.40	0.51
28:7:258:GLN:NE2	28:7:288:THR:O	2.37	0.51
20:C:133:TYR:OH	26:4:95:LEU:O	2.14	0.50
2:9:68:MET:SD	2:9:69:GLN:N	2.84	0.50
12:R:161:ILE:O	14:T:125:HIS:NE2	2.43	0.50
29:5:316:GLN:O	29:5:320:TYR:N	2.44	0.50
1:0:37:ASP:O	1:0:41:LEU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:216:LEU:N	2:9:340:ASP:O	2.44	0.50
11:Q:85:GLN:HB3	19:W:104:ILE:HA	1.94	0.50
2:9:607:ASP:OD1	2:9:642:HIS:NE2	2.45	0.50
24:Y:305:THR:HB	26:4:68:VAL:HG12	1.92	0.50
30:V:40:TRP:CZ2	30:V:114:ARG:HB2	2.47	0.50
12:R:208:ILE:O	12:R:214:ASN:ND2	2.44	0.50
17:A:1081:U:O2	17:A:1083:C:H2'	2.12	0.49
26:4:664:SER:O	26:4:667:THR:OG1	2.27	0.49
29:5:279:ARG:NH1	29:5:310:MET:SD	2.85	0.49
30:V:197:SER:O	30:V:200:GLU:N	2.45	0.49
2:9:251:ASP:OD2	2:9:317:SER:OG	2.29	0.49
2:9:506:ILE:HG12	2:9:651:THR:HG21	1.95	0.49
30:V:363:LYS:O	30:V:367:CYS:N	2.34	0.49
18:B:78:LEU:CD1	18:B:259:ARG:NH2	2.73	0.49
21:F:76:ALA:HA	22:G:371:THR:HB	1.95	0.49
17:A:770:C:H2'	17:A:771:A:O4'	2.12	0.49
30:V:256:LEU:O	30:V:259:ALA:N	2.44	0.49
20:C:148:LYS:HB2	26:4:133:ALA:HB3	1.94	0.49
23:X:276:ARG:HA	27:8:378:LEU:HD22	1.95	0.49
17:A:934:G:O2'	17:A:940:A:N1	2.41	0.49
19:W:114:ILE:HG22	19:W:142:LEU:HD11	1.95	0.48
20:C:148:LYS:HA	26:4:140:LEU:HD13	1.94	0.48
29:5:273:ARG:O	29:5:277:THR:N	2.39	0.48
30:V:208:LEU:HD12	30:V:226:TYR:CD2	2.48	0.48
2:9:192:LEU:HD22	2:9:352:SER:HB2	1.95	0.48
17:A:1120:C:N4	17:A:1283:A:O4'	2.46	0.48
18:B:186:THR:HG22	18:B:186:THR:O	2.13	0.48
21:F:153:GLU:HB3	21:F:179:ARG:HE	1.77	0.48
29:5:38:LEU:HB2	29:5:217:PHE:CE1	2.48	0.48
29:5:131:ASP:O	29:5:169:ARG:NH1	2.41	0.48
2:9:334:SER:OG	2:9:336:ARG:HG2	2.14	0.48
2:9:610:LEU:CD1	2:9:633:VAL:HG11	2.43	0.48
23:X:170:GLN:OE1	27:8:380:HIS:N	2.47	0.48
17:A:1139:A:H3'	17:A:1140:A:H5"	1.95	0.48
17:A:1231:A:H2'	17:A:1232:A:H4'	1.94	0.48
29:5:262:ARG:HA	29:5:265:ARG:HE	1.78	0.48
29:5:284:ALA:HB1	29:5:286:ILE:HD11	1.95	0.48
2:9:219:TYR:OH	2:9:228:ASP:OD2	2.29	0.48
4:E:30:MET:HE2	15:U:168:ILE:O	2.14	0.48
17:A:1457:G:O2'	21:F:99:MET:SD	2.69	0.48
15:U:126:GLN:O	15:U:130:GLU:OE1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:153:LEU:HD21	20:C:155:LEU:HG	1.95	0.48
2:9:222:ASP:OD1	2:9:224:LEU:N	2.47	0.47
17:A:967:A:O4'	17:A:1023:C:O2'	2.25	0.47
17:A:1024:G:N2	17:A:1027:A:OP2	2.42	0.47
26:4:591:GLU:OE1	26:4:591:GLU:N	2.45	0.47
21:F:115:LEU:HB2	23:X:397:TYR:HB2	1.96	0.47
2:9:258:PRO:HB3	17:A:1146:C:H4'	1.96	0.47
17:A:1226:C:OP1	27:8:57:ARG:NH2	2.47	0.47
22:G:215:ASP:OD1	22:G:216:LEU:N	2.47	0.47
30:V:83:GLU:OE1	30:V:83:GLU:N	2.40	0.47
14:T:92:THR:O	14:T:92:THR:HG22	2.14	0.47
17:A:1138:G:C6	17:A:1139:A:C6	3.02	0.47
3:D:400:GLU:OE1	3:D:401:VAL:HG23	2.14	0.47
23:X:74:ASP:OD1	23:X:147:LYS:NZ	2.36	0.47
24:Y:297:GLY:O	24:Y:300:GLU:HB3	2.15	0.47
30:V:208:LEU:HD12	30:V:226:TYR:HD2	1.80	0.47
5:J:70:PRO:HD3	5:J:76:ALA:O	2.14	0.47
17:A:1055:U:H2'	17:A:1056:A:O4'	2.15	0.47
20:C:96:MET:HB2	20:C:108:LEU:HD11	1.96	0.47
27:8:231:LEU:HD12	27:8:232:PHE:CD2	2.49	0.47
30:V:46:GLU:OE2	30:V:74:ARG:NE	2.48	0.47
20:C:54:GLU:OE2	25:1:107:LYS:NZ	2.43	0.47
22:G:252:SER:O	22:G:253:LYS:HB3	2.15	0.47
17:A:1378:C:O2	23:X:389:SER:OG	2.31	0.47
20:C:142:LEU:CD2	26:4:117:ALA:HB1	2.45	0.47
30:V:200:GLU:O	30:V:203:ASN:OD1	2.33	0.47
30:V:225:LEU:HD11	30:V:283:LEU:HD22	1.97	0.47
2:9:509:LEU:O	2:9:596:ARG:NH2	2.48	0.47
22:G:87:HIS:O	22:G:91:MET:HG3	2.15	0.47
25:1:275:ASN:OD1	25:1:276:MET:N	2.48	0.46
30:V:93:TYR:O	30:V:97:HIS:ND1	2.38	0.46
2:9:366:ALA:CB	2:9:374:ARG:HE	2.28	0.46
17:A:1248:C:H4'	17:A:1249:U:OP1	2.16	0.46
2:9:260:TYR:O	2:9:263:ARG:HG2	2.14	0.46
2:9:672:LYS:HA	17:A:692:C:H4'	1.96	0.46
17:A:758:U:O4	17:A:1159:A:H1'	2.16	0.46
19:W:104:ILE:CG2	19:W:136:LYS:HA	2.44	0.46
30:V:36:ASP:OD2	30:V:38:HIS:HB2	2.16	0.46
4:E:72:THR:HG21	17:A:1035:U:O3'	2.15	0.46
30:V:390:ILE:O	30:V:394:GLN:HG2	2.15	0.46
2:9:78:ILE:HG22	2:9:79:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:134:LYS:NZ	10:P:136:CYS:O	2.45	0.46
22:G:293:ILE:HG12	22:G:328:VAL:HB	1.97	0.46
23:X:264:GLY:N	23:X:309:ALA:O	2.48	0.46
1:0:61:GLU:HB2	1:0:137:HIS:O	2.16	0.46
24:Y:292:GLN:OE1	26:4:454:ARG:NH1	2.46	0.46
2:9:252:LEU:HA	2:9:523:SER:HA	1.97	0.46
2:9:352:SER:HG	31:9:701:GDP:PA	2.38	0.46
17:A:1558:A:H4'	17:A:1558:A:OP1	2.16	0.46
20:C:124:LEU:CD2	20:C:126:GLN:HB2	2.46	0.46
22:G:159:TYR:O	22:G:162:MET:N	2.49	0.46
30:V:176:PRO:O	30:V:180:LEU:N	2.49	0.46
30:V:179:GLN:O	30:V:183:LEU:N	2.37	0.46
17:A:971:A:H5'	17:A:972:G:OP2	2.16	0.46
30:V:275:LEU:CD2	30:V:280:LEU:HD21	2.46	0.46
10:P:70:LYS:O	10:P:103:LYS:NZ	2.49	0.46
30:V:64:LYS:O	30:V:64:LYS:HG3	2.16	0.46
30:V:126:LEU:O	30:V:130:VAL:N	2.48	0.46
1:0:70:ARG:HG2	30:V:133:VAL:HG22	1.98	0.45
22:G:359:ASP:O	22:G:363:TRP:CD1	2.69	0.45
23:X:341:ILE:HG23	25:1:313:LYS:HB2	1.98	0.45
1:0:53:ARG:NH1	17:A:704:U:OP1	2.48	0.45
2:9:530:VAL:O	2:9:530:VAL:HG13	2.17	0.45
17:A:1140:A:O4'	17:A:1142:A:O4'	2.34	0.45
25:1:248:MET:SD	25:1:249:GLU:N	2.90	0.45
25:1:86:ARG:NH1	25:1:96:PRO:O	2.44	0.45
30:V:385:ASP:HA	30:V:388:GLN:HB2	1.98	0.45
2:9:605:ALA:HA	2:9:646:TYR:CD1	2.51	0.45
19:W:114:ILE:N	19:W:122:CYS:O	2.49	0.45
30:V:167:VAL:HG13	30:V:172:ALA:HB3	1.99	0.45
2:9:109:ARG:O	2:9:112:ARG:HG2	2.16	0.45
4:E:11:LYS:HA	4:E:89:ILE:HD11	1.98	0.45
13:S:18:ASP:O	13:S:21:ARG:HG2	2.17	0.45
17:A:1429:C:H4'	17:A:1430:A:OP2	2.16	0.45
22:G:319:PHE:CZ	22:G:367:ALA:HB2	2.51	0.45
27:8:252:SER:O	27:8:256:HIS:N	2.49	0.45
22:G:299:ASP:HB3	22:G:301:GLN:OE1	2.17	0.45
25:1:214:LEU:O	25:1:218:ASN:ND2	2.50	0.45
26:4:538:ASP:OD1	26:4:539:LYS:N	2.46	0.45
17:A:1080:A:H3'	17:A:1081:U:C5'	2.47	0.45
18:B:78:LEU:HD11	18:B:259:ARG:HH21	1.79	0.45
30:V:114:ARG:HD3	30:V:146:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:1127:A:H3'	17:A:1128:C:H5"	1.98	0.45
22:G:364:MET:HG2	22:G:369:LEU:HD13	1.99	0.45
30:V:149:ASP:O	30:V:152:ILE:N	2.50	0.45
2:9:370:GLU:O	2:9:374:ARG:HG3	2.16	0.45
3:D:383:VAL:HG13	3:D:383:VAL:O	2.16	0.45
10:P:134:LYS:NZ	10:P:138:ILE:O	2.42	0.45
15:U:151:GLN:O	15:U:155:ARG:NE	2.48	0.45
19:W:111:ASP:OD1	19:W:112:LEU:N	2.49	0.45
22:G:198:ARG:O	22:G:246:ARG:N	2.50	0.45
24:Y:359:SER:OG	25:1:211:ARG:NH2	2.50	0.45
28:7:232:LYS:HB2	28:7:235:SER:O	2.17	0.45
30:V:107:TRP:HB3	30:V:382:TRP:CD2	2.52	0.45
17:A:1195:U:O2'	17:A:1459:A:N3	2.44	0.45
2:9:319:LYS:HG2	31:9:701:GDP:C6	2.53	0.44
26:4:58:VAL:HG23	26:4:58:VAL:O	2.16	0.44
30:V:101:CYS:SG	30:V:102:TRP:N	2.91	0.44
2:9:638:LYS:O	2:9:638:LYS:HG3	2.17	0.44
8:N:93:ASP:O	8:N:97:GLY:N	2.46	0.44
29:5:272:GLN:O	29:5:276:SER:N	2.24	0.44
30:V:108:THR:O	30:V:112:TRP:N	2.40	0.44
2:9:372:ILE:H	2:9:372:ILE:HD12	1.81	0.44
11:Q:86:GLY:HA2	19:W:103:ARG:N	2.32	0.44
17:A:1585:A:H4'	17:A:1585:A:OP1	2.16	0.44
27:8:348:VAL:HG23	27:8:348:VAL:O	2.17	0.44
29:5:12:LEU:HD21	29:5:74:LEU:HB2	1.98	0.44
17:A:1456:U:H2'	17:A:1457:G:O4'	2.17	0.44
17:A:1340:C:O4'	17:A:1344:U:C4	2.71	0.44
22:G:320:VAL:HG23	22:G:322:ARG:HG2	2.00	0.44
25:1:169:ARG:HB2	25:1:169:ARG:NH1	2.33	0.44
10:P:91:ILE:O	17:A:1016:U:O2'	2.31	0.44
1:0:41:LEU:HD13	1:0:55:TRP:CG	2.53	0.44
5:J:115:THR:HG21	5:J:118:LEU:HD12	2.00	0.44
23:X:276:ARG:HB2	23:X:278:ASP:OD1	2.16	0.44
26:4:88:VAL:HG12	26:4:88:VAL:O	2.18	0.44
1:0:104:TYR:CD2	30:V:99:PRO:HA	2.53	0.44
2:9:317:SER:HB3	2:9:320:THR:OG1	2.18	0.44
2:9:352:SER:OG	31:9:701:GDP:PA	2.76	0.44
2:9:109:ARG:NH2	17:A:763:C:H2'	2.33	0.44
2:9:619:ALA:HB3	2:9:658:PRO:HB3	2.00	0.44
17:A:1429:C:H3'	17:A:1430:A:H5"	1.99	0.44
29:5:237:LYS:O	29:5:301:LYS:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:35:VAL:HG23	30:V:36:ASP:N	2.33	0.44
8:N:98:LYS:HE3	8:N:109:PRO:HA	1.99	0.43
21:F:50:TYR:HD2	21:F:51:TYR:CD1	2.35	0.43
30:V:64:LYS:O	30:V:64:LYS:CG	2.65	0.43
1:0:195:ARG:NH1	15:U:72:MET:SD	2.91	0.43
2:9:201:TYR:CZ	2:9:205:VAL:HG11	2.53	0.43
1:0:166:TYR:O	9:O:199:TRP:NE1	2.48	0.43
11:Q:86:GLY:HA2	19:W:103:ARG:H	1.82	0.43
22:G:364:MET:HG2	22:G:369:LEU:CD1	2.48	0.43
30:V:90:TYR:O	30:V:94:LYS:HG2	2.19	0.43
9:O:54:GLU:HG3	9:O:56:TRP:CZ2	2.54	0.43
20:C:156:GLN:NE2	25:1:76:PHE:O	2.52	0.43
20:C:157:THR:HG22	20:C:158:VAL:N	2.34	0.43
29:5:286:ILE:HD11	29:5:303:LEU:HD21	1.99	0.43
12:R:347:GLN:NE2	12:R:351:GLU:OE2	2.50	0.43
8:N:22:MET:HE3	17:A:778:C:H5”	2.00	0.43
17:A:1579:C:OP1	29:5:257:ARG:HD2	2.19	0.43
21:F:48:LYS:NZ	22:G:318:HIS:O	2.34	0.43
27:8:206:PHE:O	27:8:210:GLU:OE1	2.36	0.43
17:A:1081:U:H1’	17:A:1083:C:OP2	2.18	0.43
22:G:315:PHE:CD2	22:G:369:LEU:CD2	3.02	0.43
22:G:364:MET:HA	22:G:367:ALA:HB3	2.01	0.43
25:1:163:VAL:CG1	26:4:135:PRO:HD3	2.48	0.43
17:A:1193:U:H5”	21:F:160:PRO:HG2	2.01	0.43
21:F:46:ILE:O	21:F:46:ILE:HG22	2.18	0.43
21:F:51:TYR:HB3	22:G:363:TRP:CD1	2.54	0.43
30:V:112:TRP:NE1	30:V:116:CYS:SG	2.92	0.43
30:V:275:LEU:O	30:V:348:GLU:N	2.35	0.43
11:Q:85:GLN:NE2	19:W:107:ILE:HG12	2.33	0.43
19:W:107:ILE:HG22	19:W:108:VAL:N	2.34	0.43
30:V:385:ASP:O	30:V:389:LEU:HB2	2.19	0.43
2:9:590:PRO:HB2	2:9:596:ARG:HG2	2.00	0.43
15:U:79:GLN:O	15:U:83:HIS:ND1	2.48	0.43
17:A:738:A:O2’	17:A:739:C:P	2.77	0.43
17:A:952:A:N3	17:A:954:C:N4	2.66	0.43
29:5:123:GLU:N	29:5:123:GLU:OE1	2.52	0.43
30:V:222:SER:HA	30:V:275:LEU:CD1	2.49	0.43
9:O:89:ARG:NH1	17:A:918:A:OP1	2.40	0.42
2:9:244:ILE:HD11	2:9:337:TYR:CE1	2.54	0.42
2:9:623:ILE:O	2:9:630:TRP:HA	2.19	0.42
18:B:103:GLU:N	18:B:104:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:114:ILE:HD12	19:W:140:VAL:HG21	2.01	0.42
30:V:355:LEU:O	30:V:358:GLN:HG2	2.20	0.42
26:4:310:GLU:OE1	26:4:310:GLU:N	2.52	0.42
30:V:390:ILE:O	30:V:393:GLU:HB3	2.18	0.42
2:9:73:LEU:HB3	2:9:78:ILE:HD11	2.02	0.42
2:9:569:THR:HG21	2:9:577:LEU:HD22	2.00	0.42
6:L:76:TYR:CD2	6:L:93:LEU:HD22	2.54	0.42
14:T:4:LYS:O	14:T:11:ARG:NH1	2.52	0.42
15:U:133:GLN:NE2	15:U:134:ARG:HG3	2.34	0.42
17:A:1585:A:C8	29:5:223:VAL:HG11	2.54	0.42
18:B:162:CYS:HB3	18:B:254:GLN:HG3	2.01	0.42
22:G:310:ARG:NE	23:X:383:LEU:O	2.52	0.42
2:9:517:ILE:HA	2:9:563:ILE:HD11	2.02	0.42
17:A:691:A:N7	17:A:716:U:O2'	2.50	0.42
22:G:313:LEU:O	22:G:316:PRO:HD2	2.19	0.42
26:4:641:ILE:O	26:4:641:ILE:HG22	2.19	0.42
29:5:63:GLY:N	29:5:64:PRO:HD3	2.34	0.42
29:5:179:GLU:OE1	29:5:179:GLU:N	2.46	0.42
30:V:230:LEU:O	30:V:233:LYS:HB3	2.19	0.42
1:0:99:ARG:CG	1:0:101:ARG:NH1	2.82	0.42
10:P:78:GLN:HB2	15:U:188:ASN:HB3	2.01	0.42
21:F:85:VAL:HG22	23:X:379:GLU:OE1	2.19	0.42
26:4:351:SER:HB2	26:4:352:PRO:HD3	2.02	0.42
26:4:622:ASN:ND2	26:4:622:ASN:O	2.52	0.42
29:5:33:LEU:HG	29:5:35:GLN:H	1.84	0.42
2:9:389:LYS:HB2	2:9:494:PHE:O	2.20	0.42
17:A:1131:C:H2'	17:A:1132:U:C6	2.55	0.42
28:7:215:MET:SD	28:7:246:PHE:HB2	2.60	0.42
12:R:153:THR:HG23	12:R:154:THR:HG23	2.01	0.42
30:V:132:LYS:O	30:V:136:GLY:N	2.53	0.42
1:0:135:MET:SD	1:0:135:MET:N	2.87	0.42
17:A:1187:U:O2'	17:A:1465:C:N4	2.53	0.42
21:F:159:VAL:HG23	21:F:172:VAL:HG11	2.02	0.42
24:Y:339:GLU:OE2	24:Y:340:SER:OG	2.38	0.42
30:V:79:ILE:HG23	30:V:84:GLU:HB2	2.01	0.42
30:V:152:ILE:HD11	30:V:185:VAL:CG2	2.49	0.42
11:Q:85:GLN:N	19:W:113:TYR:HB2	2.34	0.42
14:T:132:ARG:N	14:T:138:GLU:OE2	2.52	0.42
25:1:184:ASP:OD1	25:1:184:ASP:N	2.53	0.42
29:5:183:ARG:O	29:5:197:SER:HB3	2.20	0.42
29:5:300:PHE:HA	29:5:303:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:400:MET:SD	2:9:400:MET:N	2.93	0.41
17:A:1213:A:N3	17:A:1239:C:O2'	2.47	0.41
20:C:148:LYS:HA	26:4:140:LEU:CD1	2.50	0.41
21:F:123:PHE:CE1	21:F:139:ARG:HD2	2.55	0.41
21:F:160:PRO:HA	21:F:168:TYR:O	2.20	0.41
22:G:213:LEU:CD1	22:G:218:TYR:HB2	2.50	0.41
28:7:229:LYS:O	28:7:235:SER:N	2.54	0.41
30:V:394:GLN:O	30:V:398:GLU:HG2	2.19	0.41
6:L:99:ASN:OD1	6:L:102:GLU:OE1	2.38	0.41
17:A:1013:A:O2'	17:A:1014:A:O5'	2.34	0.41
17:A:1118:A:H3'	17:A:1119:U:H5"	2.01	0.41
20:C:124:LEU:O	20:C:126:GLN:N	2.52	0.41
24:Y:359:SER:O	25:1:211:ARG:HB3	2.20	0.41
25:1:80:ALA:HB2	26:4:91:ASP:OD2	2.19	0.41
30:V:50:LEU:HD22	30:V:84:GLU:HG2	2.02	0.41
30:V:149:ASP:O	30:V:152:ILE:HB	2.20	0.41
30:V:164:VAL:HG11	30:V:186:LEU:CD2	2.50	0.41
17:A:941:G:C6	17:A:1109:A:C5	3.09	0.41
21:F:42:LYS:O	21:F:75:LYS:N	2.32	0.41
29:5:202:TYR:HA	29:5:237:LYS:HD2	2.02	0.41
1:0:199:GLU:OE2	1:0:203:TYR:CD1	2.73	0.41
2:9:94:LEU:O	2:9:97:GLN:HG2	2.20	0.41
20:C:120:CYS:SG	25:1:75:PRO:HB3	2.60	0.41
29:5:255:PHE:HB3	29:5:258:LYS:CG	2.50	0.41
30:V:177:SER:HB3	30:V:367:CYS:HB3	2.01	0.41
30:V:221:PHE:HA	30:V:224:GLN:NE2	2.35	0.41
2:9:220:MET:CE	2:9:248:ASN:HD22	2.34	0.41
9:O:230:PRO:HA	9:O:231:PRO:HD3	1.96	0.41
17:A:1330:C:H1'	17:A:1331:A:OP2	2.20	0.41
29:5:284:ALA:CB	29:5:286:ILE:CD1	2.99	0.41
30:V:72:ILE:O	30:V:76:ILE:HG12	2.20	0.41
2:9:78:ILE:CG2	2:9:79:LEU:N	2.84	0.41
2:9:360:GLU:O	2:9:360:GLU:HG3	2.20	0.41
2:9:506:ILE:HA	2:9:651:THR:HG21	2.03	0.41
17:A:1145:A:N3	17:A:1147:G:C6	2.88	0.41
21:F:115:LEU:HD22	21:F:141:PRO:HB2	2.03	0.41
28:7:344:ASN:OD1	28:7:345:LEU:N	2.53	0.41
1:0:82:ARG:NE	1:0:138:ASP:OD2	2.49	0.41
2:9:365:THR:CG2	2:9:393:CYS:SG	3.09	0.41
2:9:672:LYS:HE3	17:A:803:C:H5'	2.03	0.41
17:A:1367:A:O2'	17:A:1368:U:O5'	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:142:GLU:OE1	22:G:142:GLU:N	2.40	0.41
25:1:169:ARG:HG2	25:1:213:PRO:O	2.20	0.41
25:1:310:SER:O	25:1:313:LYS:HG2	2.21	0.41
2:9:368:GLY:O	2:9:374:ARG:HG2	2.20	0.41
17:A:772:A:C5	17:A:773:U:H1'	2.55	0.41
17:A:1080:A:H3'	17:A:1081:U:H3'	2.02	0.41
19:W:112:LEU:O	19:W:123:VAL:HA	2.20	0.41
20:C:21:LEU:HB2	20:C:22:PRO:HD3	2.02	0.41
29:5:255:PHE:HB3	29:5:258:LYS:HB2	2.03	0.41
2:9:335:TRP:CD1	29:5:286:ILE:O	2.74	0.41
9:O:53:ASP:OD1	9:O:54:GLU:N	2.54	0.41
17:A:1080:A:H3'	17:A:1081:U:H5"	2.03	0.41
17:A:1179:G:H21	17:A:1180:U:C3'	2.34	0.41
17:A:1223:C:H2'	17:A:1224:C:O4'	2.21	0.41
17:A:1586:G:C2	17:A:1587:U:C2	3.09	0.41
24:Y:322:ASP:OD1	24:Y:325:GLY:N	2.54	0.41
26:4:102:GLU:HG2	26:4:106:PHE:CZ	2.56	0.41
26:4:327:LYS:HG3	26:4:327:LYS:O	2.20	0.41
28:7:396:PRO:O	28:7:398:HIS:HD2	2.04	0.41
30:V:360:VAL:O	30:V:364:LEU:HB3	2.20	0.41
2:9:266:GLU:O	2:9:270:GLU:OE1	2.39	0.41
13:S:124:ALA:O	13:S:127:ALA:N	2.54	0.41
15:U:151:GLN:C	15:U:155:ARG:HE	2.23	0.41
17:A:1139:A:OP2	17:A:1140:A:H3'	2.20	0.41
29:5:258:LYS:O	29:5:292:PRO:HD3	2.21	0.41
29:5:260:CYS:SG	29:5:261:HIS:N	2.93	0.41
22:G:286:TYR:O	22:G:326:HIS:ND1	2.53	0.40
22:G:364:MET:HB3	22:G:369:LEU:HB2	2.03	0.40
24:Y:359:SER:HB2	25:1:211:ARG:HH21	1.86	0.40
26:4:540:HIS:HB3	26:4:541:PRO:HD2	2.03	0.40
28:7:269:SER:OG	28:7:296:GLU:OE1	2.31	0.40
30:V:33:ALA:HB1	30:V:372:ILE:HD11	2.02	0.40
30:V:105:ARG:HD3	30:V:107:TRP:CH2	2.56	0.40
1:0:82:ARG:HB3	1:0:138:ASP:OD2	2.21	0.40
2:9:619:ALA:HA	2:9:634:THR:HG22	2.03	0.40
18:B:65:GLU:N	18:B:66:PRO:HD2	2.36	0.40
19:W:103:ARG:HA	19:W:138:THR:O	2.21	0.40
21:F:51:TYR:CD2	22:G:319:PHE:HZ	2.38	0.40
30:V:73:SER:HA	30:V:108:THR:HG21	2.03	0.40
17:A:758:U:O4	17:A:1145:A:C2	2.74	0.40
17:A:872:G:C6	17:A:873:G:C6	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:315:PHE:HB3	22:G:316:PRO:HD3	2.02	0.40
26:4:202:GLU:OE1	26:4:202:GLU:N	2.49	0.40
13:S:124:ALA:O	13:S:128:GLU:OE1	2.38	0.40
17:A:709:G:C6	17:A:710:U:C4	3.10	0.40
17:A:1473:C:H2'	17:A:1474:G:O4'	2.21	0.40
20:C:103:CYS:O	20:C:124:LEU:N	2.51	0.40
20:C:123:VAL:HG23	20:C:157:THR:HG23	2.03	0.40
22:G:197:SER:HB2	22:G:245:ARG:HG3	2.03	0.40
23:X:278:ASP:HB3	27:8:138:LEU:HB3	2.03	0.40
29:5:195:ARG:HG2	29:5:253:PHE:HB2	2.03	0.40
1:0:93:CYS:SG	1:0:121:LYS:N	2.83	0.40
10:P:52:ILE:O	13:S:64:TRP:HB2	2.22	0.40
17:A:860:A:N7	17:A:919:A:O2'	2.51	0.40
17:A:1557:A:H5'	17:A:1558:A:OP2	2.21	0.40
21:F:51:TYR:CZ	22:G:366:GLN:HB2	2.56	0.40
26:4:302:VAL:O	26:4:344:ARG:NH2	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
2	9	438/698 (63%)	428 (98%)	10 (2%)	0	100	100
3	D	228/430 (53%)	223 (98%)	5 (2%)	0	100	100
4	E	103/125 (82%)	100 (97%)	3 (3%)	0	100	100
5	J	106/138 (77%)	99 (93%)	7 (7%)	0	100	100
6	L	120/257 (47%)	119 (99%)	1 (1%)	0	100	100
7	M	113/137 (82%)	113 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	N	107/130 (82%)	106 (99%)	1 (1%)	0	100	100
9	O	188/258 (73%)	187 (100%)	1 (0%)	0	100	100
10	P	90/142 (63%)	89 (99%)	1 (1%)	0	100	100
11	Q	1/87 (1%)	0	1 (100%)	0	100	100
12	R	289/360 (80%)	287 (99%)	2 (1%)	0	100	100
13	S	131/190 (69%)	130 (99%)	1 (1%)	0	100	100
14	T	162/173 (94%)	160 (99%)	2 (1%)	0	100	100
15	U	172/205 (84%)	170 (99%)	2 (1%)	0	100	100
16	a	253/437 (58%)	249 (98%)	4 (2%)	0	100	100
18	B	218/296 (74%)	217 (100%)	1 (0%)	0	100	100
19	W	96/187 (51%)	92 (96%)	4 (4%)	0	100	100
20	C	122/167 (73%)	118 (97%)	4 (3%)	0	100	100
21	F	206/242 (85%)	201 (98%)	5 (2%)	0	100	100
22	G	288/396 (73%)	283 (98%)	5 (2%)	0	100	100
23	X	350/398 (88%)	342 (98%)	8 (2%)	0	100	100
24	Y	106/395 (27%)	106 (100%)	0	0	100	100
25	1	251/323 (78%)	242 (96%)	9 (4%)	0	100	100
26	4	558/689 (81%)	551 (99%)	7 (1%)	0	100	100
27	8	324/390 (83%)	318 (98%)	6 (2%)	0	100	100
28	7	394/456 (86%)	388 (98%)	6 (2%)	0	100	100
29	5	317/346 (92%)	305 (96%)	12 (4%)	0	100	100
30	V	355/414 (86%)	303 (85%)	52 (15%)	0	100	100
All	All	6295/8681 (72%)	6129 (97%)	166 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	184/188 (98%)	184 (100%)	0	100 100
2	9	388/600 (65%)	388 (100%)	0	100 100
3	D	196/357 (55%)	196 (100%)	0	100 100
4	E	89/107 (83%)	89 (100%)	0	100 100
5	J	93/118 (79%)	93 (100%)	0	100 100
6	L	117/226 (52%)	117 (100%)	0	100 100
7	M	94/113 (83%)	93 (99%)	1 (1%)	70 79
8	N	95/115 (83%)	95 (100%)	0	100 100
9	O	171/230 (74%)	171 (100%)	0	100 100
10	P	83/123 (68%)	82 (99%)	1 (1%)	67 77
11	Q	2/78 (3%)	2 (100%)	0	100 100
12	R	261/318 (82%)	261 (100%)	0	100 100
13	S	115/164 (70%)	115 (100%)	0	100 100
14	T	151/157 (96%)	151 (100%)	0	100 100
15	U	150/174 (86%)	149 (99%)	1 (1%)	81 86
16	a	151/386 (39%)	151 (100%)	0	100 100
18	B	194/249 (78%)	194 (100%)	0	100 100
19	W	85/158 (54%)	85 (100%)	0	100 100
20	C	111/143 (78%)	111 (100%)	0	100 100
21	F	185/209 (88%)	185 (100%)	0	100 100
22	G	254/342 (74%)	253 (100%)	1 (0%)	89 91
23	X	311/351 (89%)	311 (100%)	0	100 100
24	Y	99/357 (28%)	99 (100%)	0	100 100
25	1	235/291 (81%)	235 (100%)	0	100 100
26	4	506/609 (83%)	506 (100%)	0	100 100
27	8	270/317 (85%)	270 (100%)	0	100 100
28	7	339/385 (88%)	339 (100%)	0	100 100
29	5	286/309 (93%)	284 (99%)	2 (1%)	81 86
30	V	323/364 (89%)	323 (100%)	0	100 100
All	All	5538/7538 (74%)	5532 (100%)	6 (0%)	92 95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	M	29	ARG
10	P	59	LYS
15	U	155	ARG
22	G	379	ARG
29	5	178	LYS
29	5	257	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	9	69	GLN
2	9	106	GLN
2	9	187	HIS
2	9	283	HIS
2	9	348	ASN
2	9	551	ASN
2	9	584	HIS
3	D	280	HIS
3	D	341	ASN
3	D	424	ASN
12	R	278	ASN
12	R	308	HIS
13	S	47	GLN
15	U	62	HIS
16	a	301	HIS
19	W	106	HIS
20	C	57	HIS
20	C	72	HIS
20	C	130	HIS
20	C	156	GLN
21	F	146	HIS
21	F	238	HIS
22	G	82	ASN
23	X	63	HIS
23	X	110	HIS
23	X	114	ASN
23	X	140	HIS
23	X	235	ASN
26	4	577	ASN
27	8	70	GLN
27	8	108	HIS
27	8	121	GLN
27	8	251	ASN

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Mol	Chain	Res	Type
27	8	313	HIS
28	7	98	HIS
28	7	398	HIS
28	7	400	HIS
29	5	171	GLN
29	5	229	HIS
29	5	235	GLN
29	5	254	GLN
30	V	170	GLN
30	V	188	HIS
30	V	215	GLN
30	V	224	GLN
30	V	378	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	A	734/955 (76%)	180 (24%)	4 (0%)

All (180) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	A	650	U
17	A	651	A
17	A	680	U
17	A	688	A
17	A	689	U
17	A	704	U
17	A	721	U
17	A	722	C
17	A	730	A
17	A	736	C
17	A	737	C
17	A	739	C
17	A	741	A
17	A	753	A
17	A	759	C
17	A	761	A
17	A	766	G
17	A	777	G
17	A	782	A

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Mol	Chain	Res	Type
17	A	791	G
17	A	794	U
17	A	796	G
17	A	807	A
17	A	830	U
17	A	831	U
17	A	832	U
17	A	835	C
17	A	851	A
17	A	860	A
17	A	861	U
17	A	866	A
17	A	867	C
17	A	868	C
17	A	871	A
17	A	883	U
17	A	886	C
17	A	893	G
17	A	902	G
17	A	903	U
17	A	919	A
17	A	931	C
17	A	938	A
17	A	939	A
17	A	942	A
17	A	949	U
17	A	954	C
17	A	955	A
17	A	967	A
17	A	971	A
17	A	972	G
17	A	976	A
17	A	1014	A
17	A	1015	A
17	A	1038	C
17	A	1042	U
17	A	1047	A
17	A	1052	C
17	A	1056	A
17	A	1060	A
17	A	1061	A
17	A	1077	U

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Mol	Chain	Res	Type
17	A	1078	A
17	A	1079	G
17	A	1080	A
17	A	1081	U
17	A	1083	C
17	A	1095	U
17	A	1096	A
17	A	1117	A
17	A	1118	A
17	A	1119	U
17	A	1121	A
17	A	1126	A
17	A	1127	A
17	A	1128	C
17	A	1129	U
17	A	1137	A
17	A	1138	G
17	A	1140	A
17	A	1153	C
17	A	1154	A
17	A	1155	G
17	A	1160	A
17	A	1162	A
17	A	1167	A
17	A	1175	G
17	A	1177	C
17	A	1178	G
17	A	1179	G
17	A	1181	G
17	A	1182	C
17	A	1185	C
17	A	1186	A
17	A	1187	U
17	A	1188	A
17	A	1189	U
17	A	1190	C
17	A	1191	C
17	A	1198	A
17	A	1199	G
17	A	1200	G
17	A	1215	U
17	A	1216	C

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Mol	Chain	Res	Type
17	A	1217	G
17	A	1218	A
17	A	1219	U
17	A	1220	A
17	A	1221	A
17	A	1222	A
17	A	1224	C
17	A	1226	C
17	A	1227	G
17	A	1228	A
17	A	1232	A
17	A	1233	C
17	A	1234	C
17	A	1242	C
17	A	1245	U
17	A	1247	G
17	A	1248	C
17	A	1249	U
17	A	1250	C
17	A	1254	C
17	A	1255	U
17	A	1258	A
17	A	1259	U
17	A	1261	C
17	A	1284	U
17	A	1290	C
17	A	1291	U
17	A	1296	A
17	A	1297	G
17	A	1298	U
17	A	1299	A
17	A	1330	C
17	A	1331	A
17	A	1332	A
17	A	1335	U
17	A	1338	A
17	A	1342	C
17	A	1343	A
17	A	1347	G
17	A	1350	G
17	A	1353	A
17	A	1354	A

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Mol	Chain	Res	Type
17	A	1357	A
17	A	1360	G
17	A	1364	U
17	A	1367	A
17	A	1373	U
17	A	1375	C
17	A	1376	C
17	A	1378	C
17	A	1424	U
17	A	1427	A
17	A	1430	A
17	A	1431	G
17	A	1434	A
17	A	1440	G
17	A	1441	A
17	A	1442	G
17	A	1450	C
17	A	1463	G
17	A	1464	G
17	A	1467	C
17	A	1468	U
17	A	1470	A
17	A	1471	A
17	A	1474	G
17	A	1477	U
17	A	1492	A
17	A	1493	C
17	A	1557	A
17	A	1558	A
17	A	1559	G
17	A	1560	U
17	A	1564	A
17	A	1583	A
17	A	1584	A
17	A	1585	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	A	1078	A
17	A	1154	A
17	A	1226	C

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Mol	Chain	Res	Type
17	A	1330	C

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	ATP	X	501	34	26,33,33	0.73	0	31,52,52	0.68	0
31	GDP	X	503	-	24,30,30	0.88	1 (4%)	30,47,47	0.68	0
31	GDP	9	701	-	24,30,30	0.87	2 (8%)	30,47,47	0.73	0
32	FES	T	201	7,14	0,4,4	-	-	-		
36	SF4	7	501	28	0,12,12	-	-	-		
32	FES	E	201	4,10	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	X	501	34	-	2/18/38/38	0/3/3/3
31	GDP	X	503	-	-	6/12/32/32	0/3/3/3
31	GDP	9	701	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	FES	T	201	7,14	-	-	0/1/1/1
36	SF4	7	501	28	-	-	0/6/5/5
32	FES	E	201	4,10	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	503	GDP	C5-C6	-2.29	1.42	1.47
31	9	701	GDP	C5-C6	-2.15	1.43	1.47
31	9	701	GDP	C8-N7	-2.03	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	9	701	GDP	O4'-C4'-C5'-O5'
31	9	701	GDP	C3'-C4'-C5'-O5'
31	X	503	GDP	C5'-O5'-PA-O3A
31	X	503	GDP	PB-O3A-PA-O1A
35	X	501	ATP	PA-O3A-PB-O1B
31	X	503	GDP	C5'-O5'-PA-O1A
31	X	503	GDP	PB-O3A-PA-O2A
31	X	503	GDP	PA-O3A-PB-O1B
31	X	503	GDP	O4'-C4'-C5'-O5'
35	X	501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

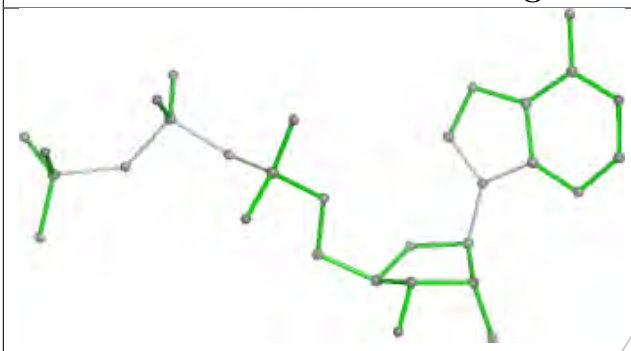
1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	9	701	GDP	6	0

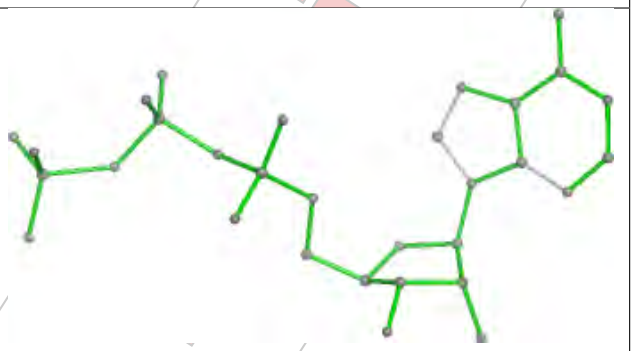
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

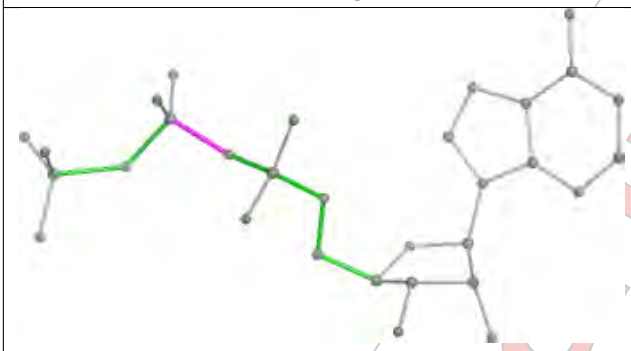
Ligand ATP X 501



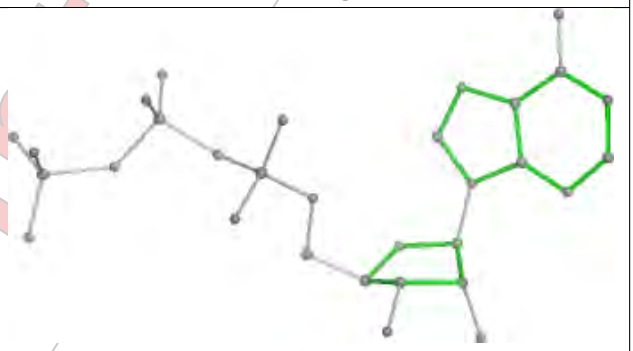
Bond lengths



Bond angles

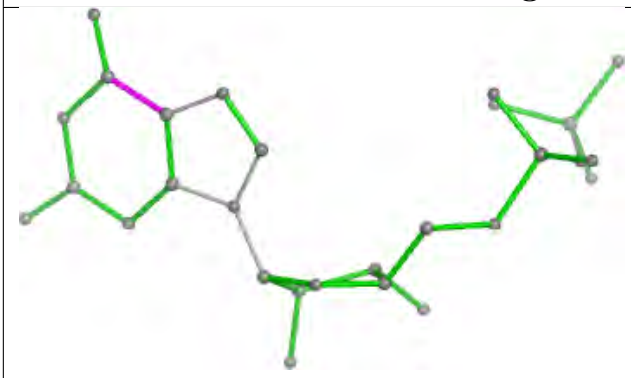


Torsions

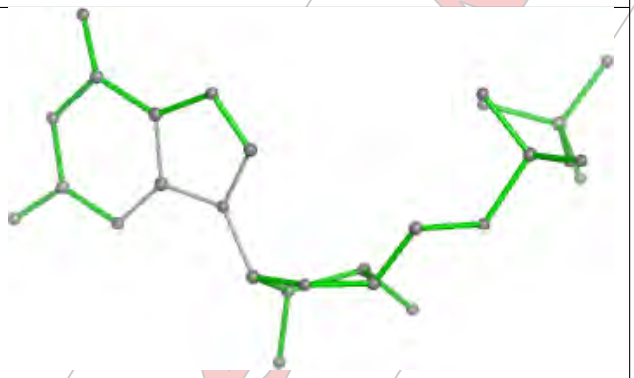


Rings

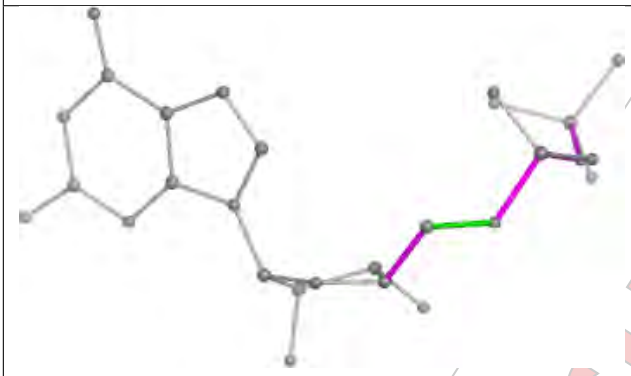
Ligand GDP X 503



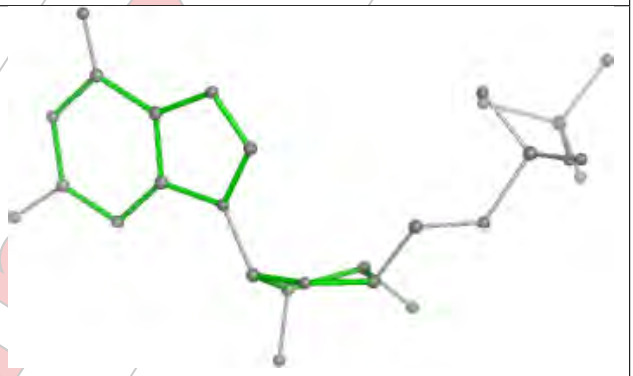
Bond lengths



Bond angles

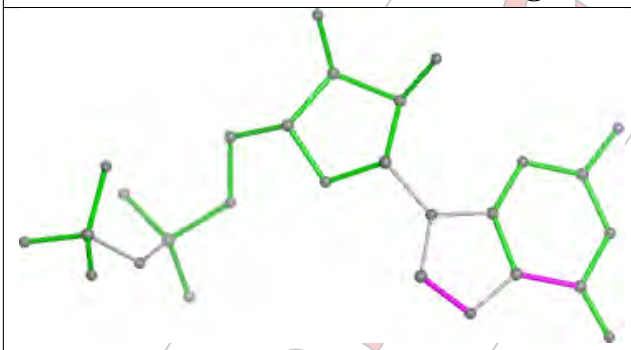


Torsions

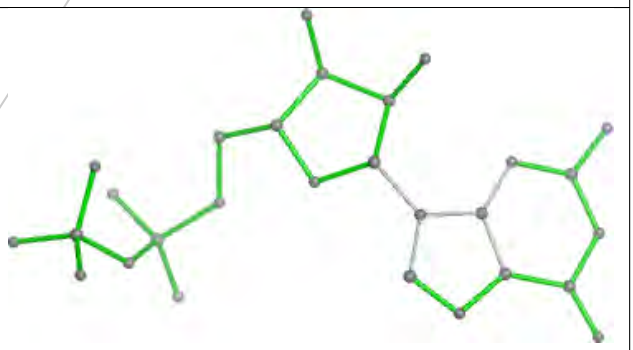


Rings

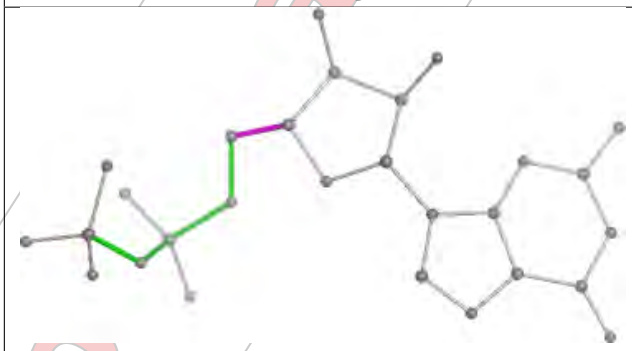
Ligand GDP 9 701



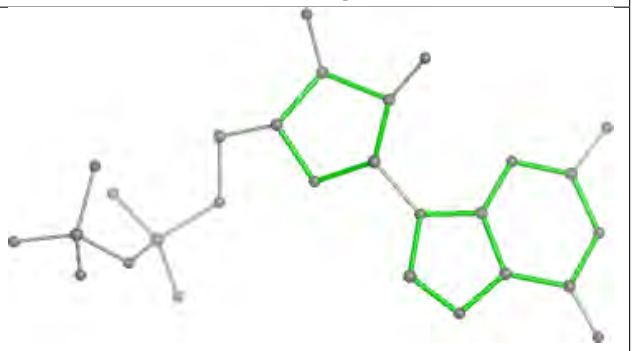
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1179:G	O3'	1180:U	P	6.84

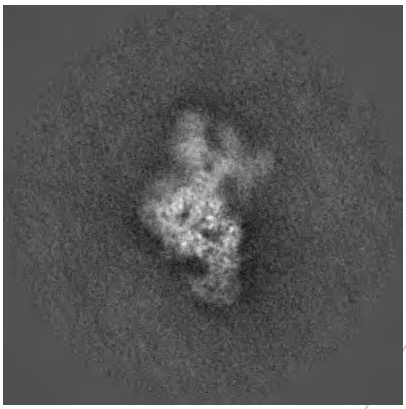
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51874. These allow visual inspection of the internal detail of the map and identification of artifacts.

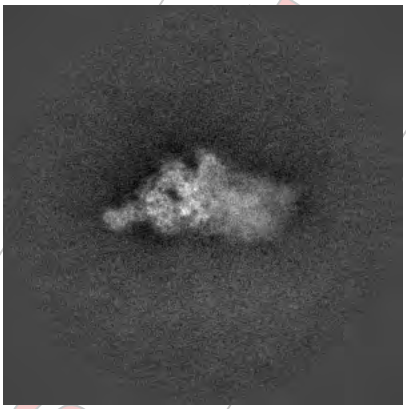
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

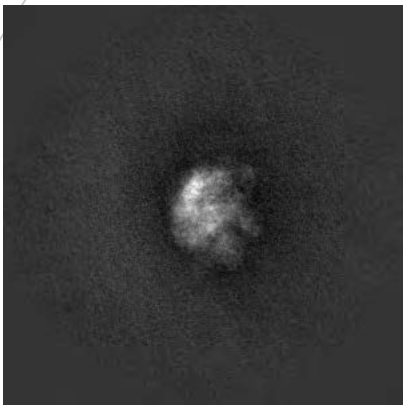
6.1.1 Primary map



X

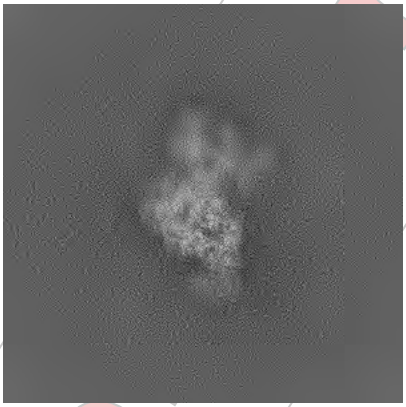


Y

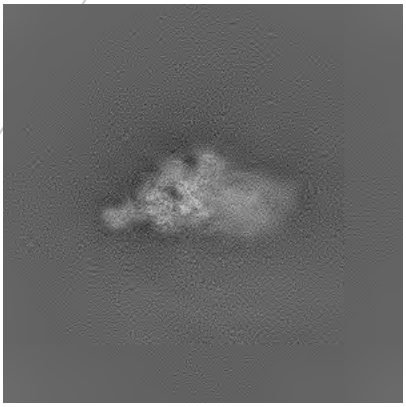


Z

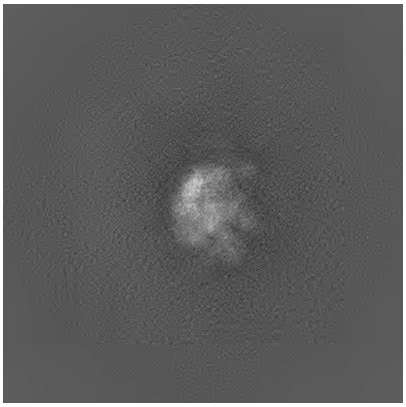
6.1.2 Raw map



X



Y

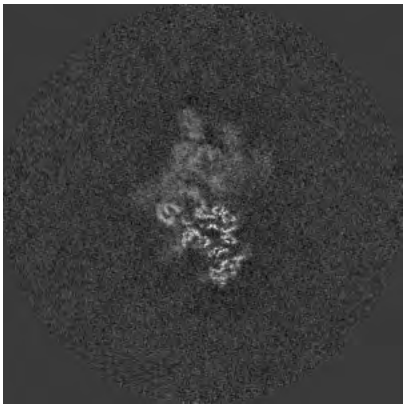


Z

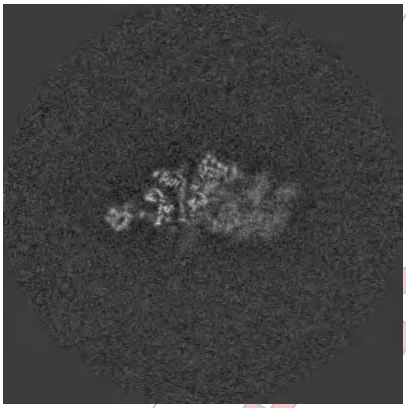
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

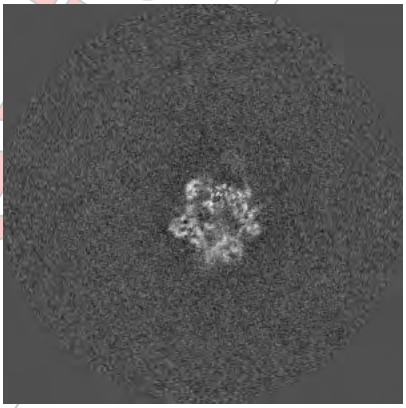
6.2.1 Primary map



X Index: 300

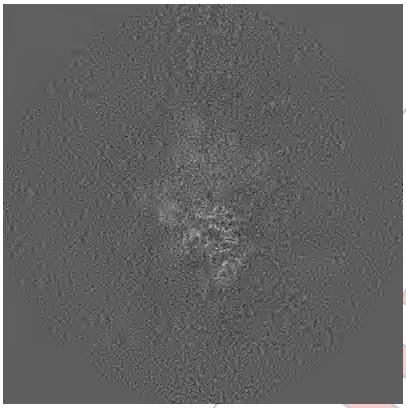


Y Index: 300

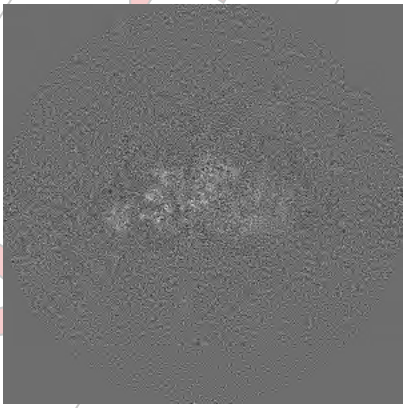


Z Index: 300

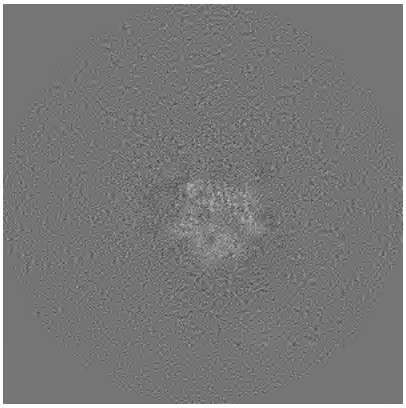
6.2.2 Raw map



X Index: 300



Y Index: 300

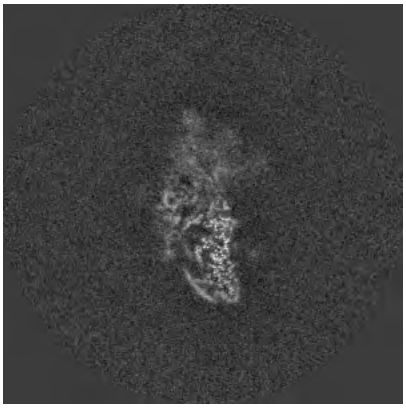


Z Index: 300

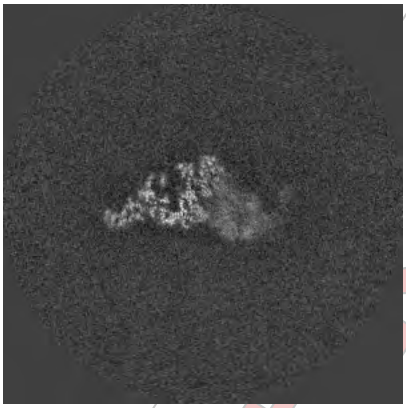
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

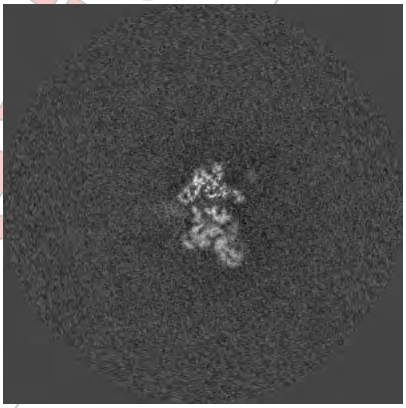
6.3.1 Primary map



X Index: 288

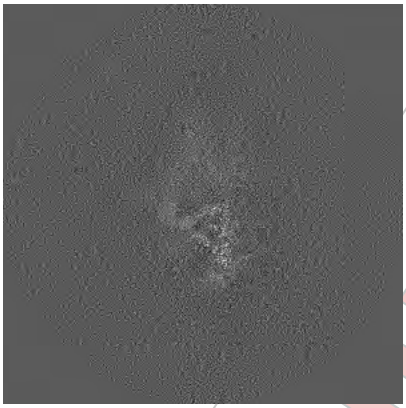


Y Index: 312

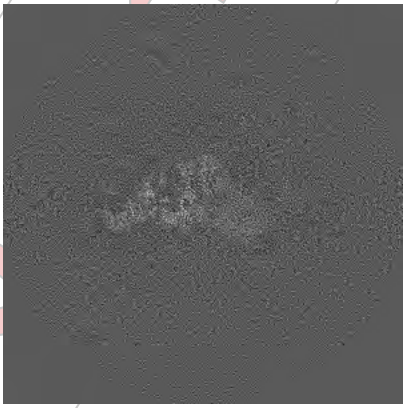


Z Index: 276

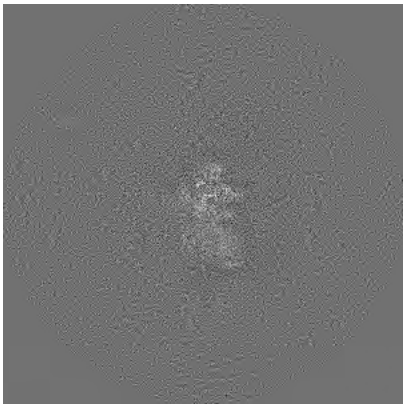
6.3.2 Raw map



X Index: 296



Y Index: 313

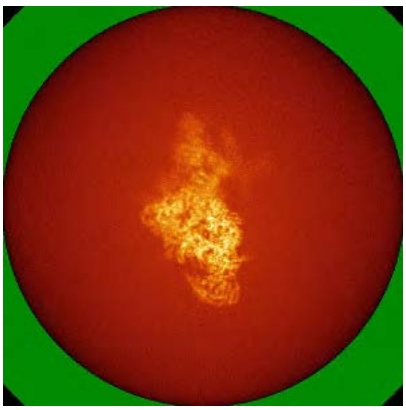


Z Index: 281

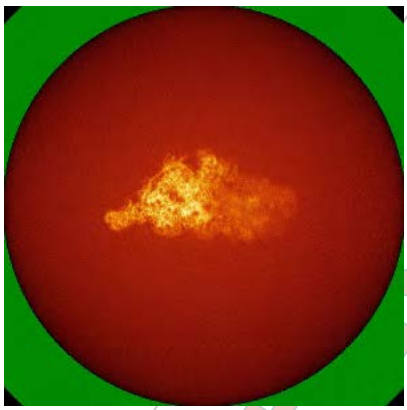
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

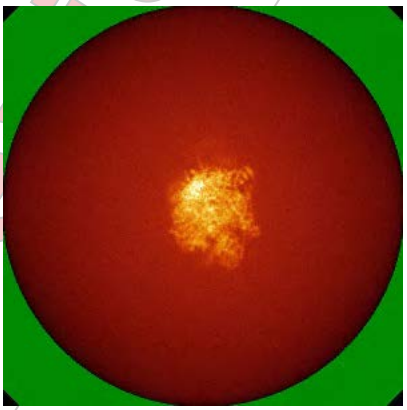
6.4.1 Primary map



X

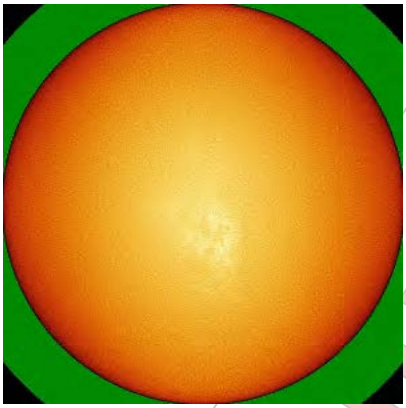


Y

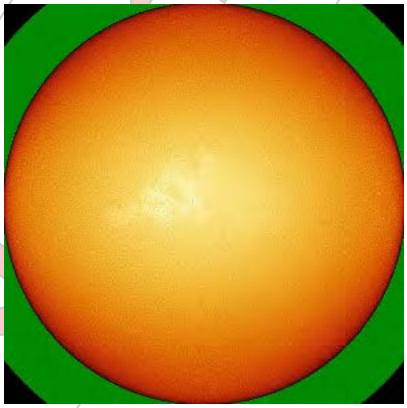


Z

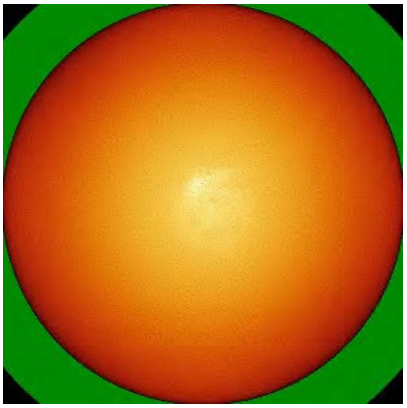
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

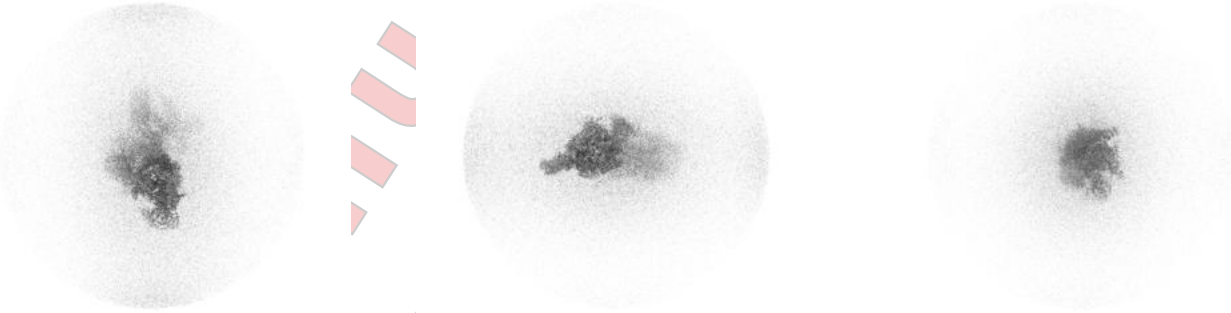
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

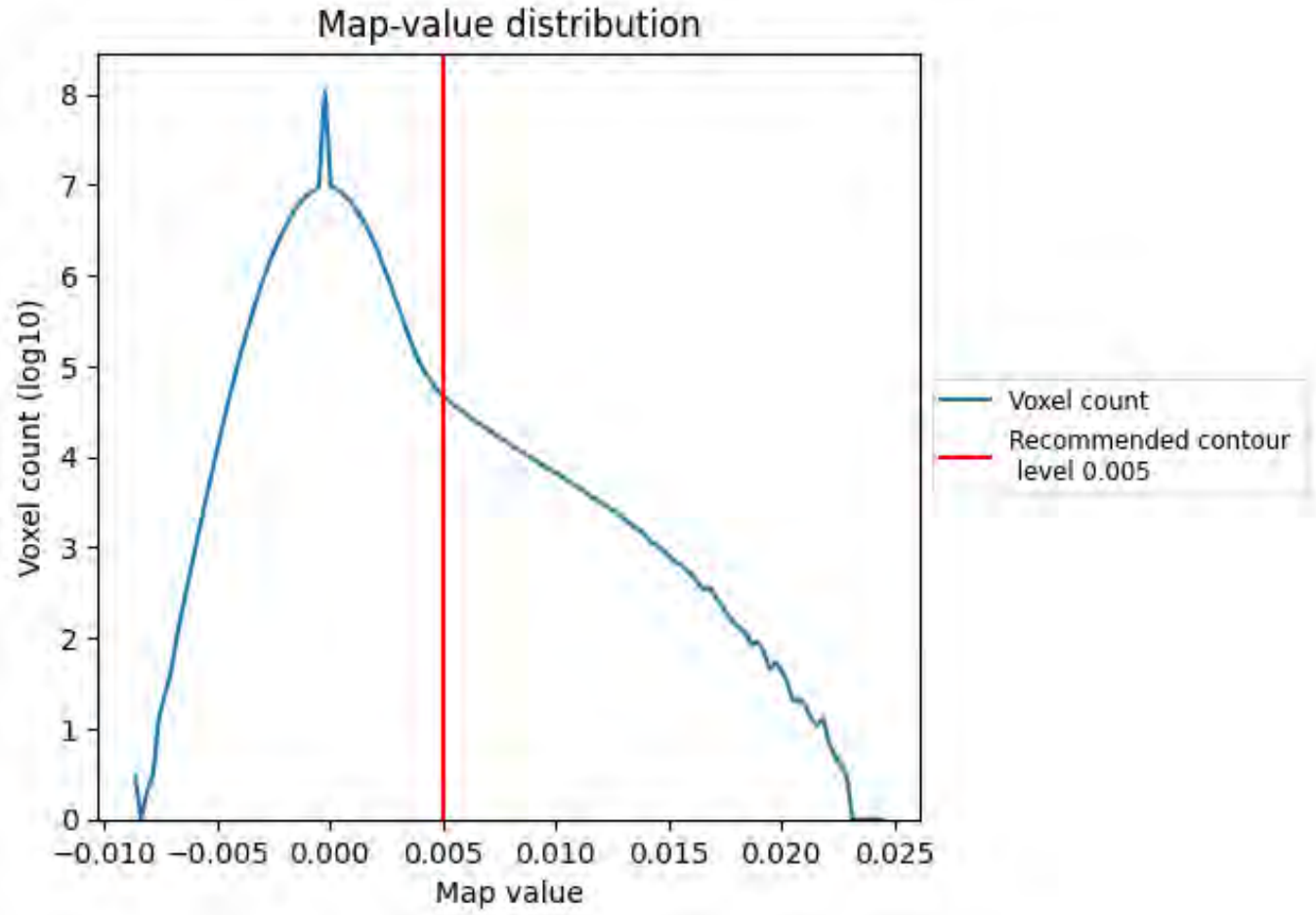
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

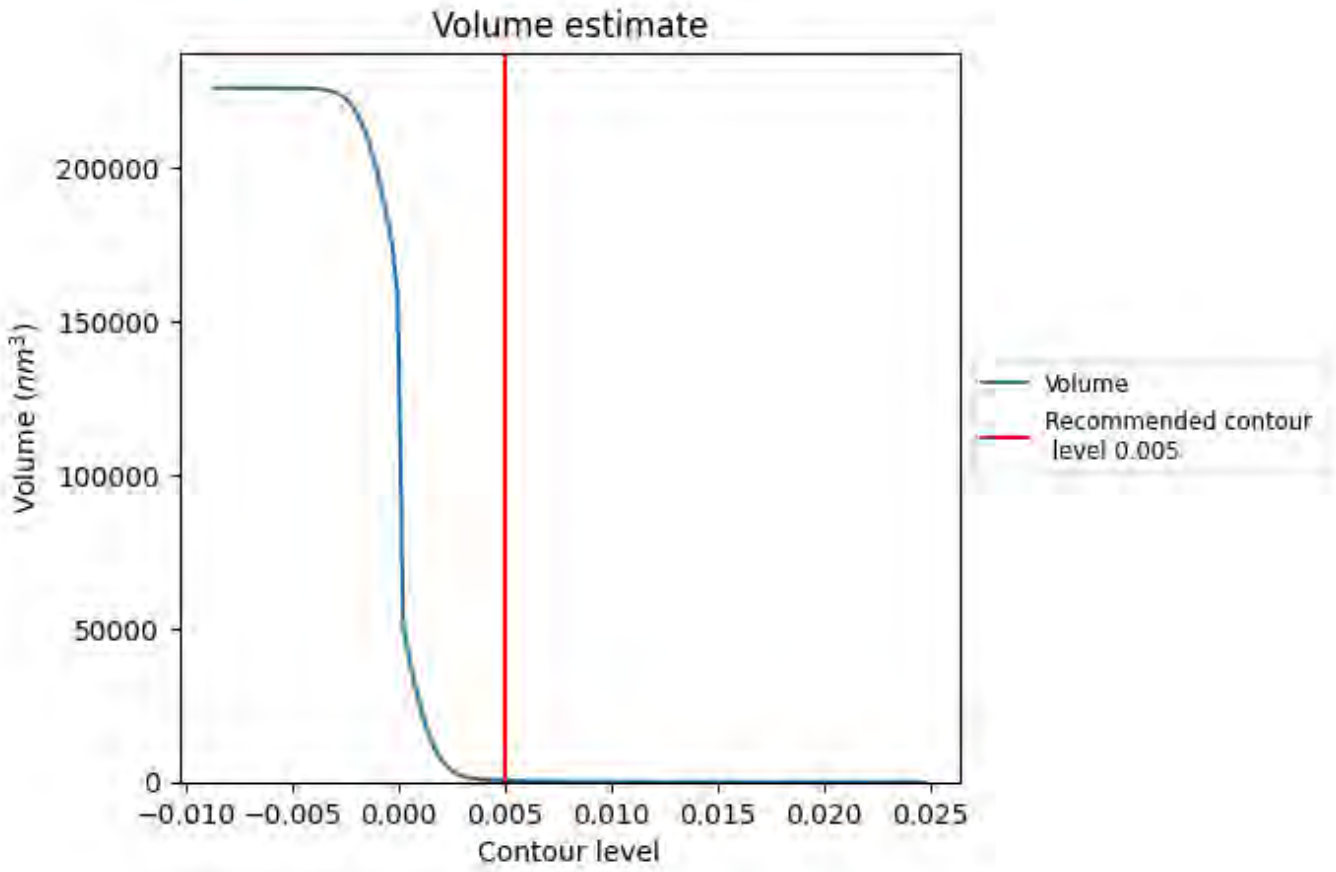
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

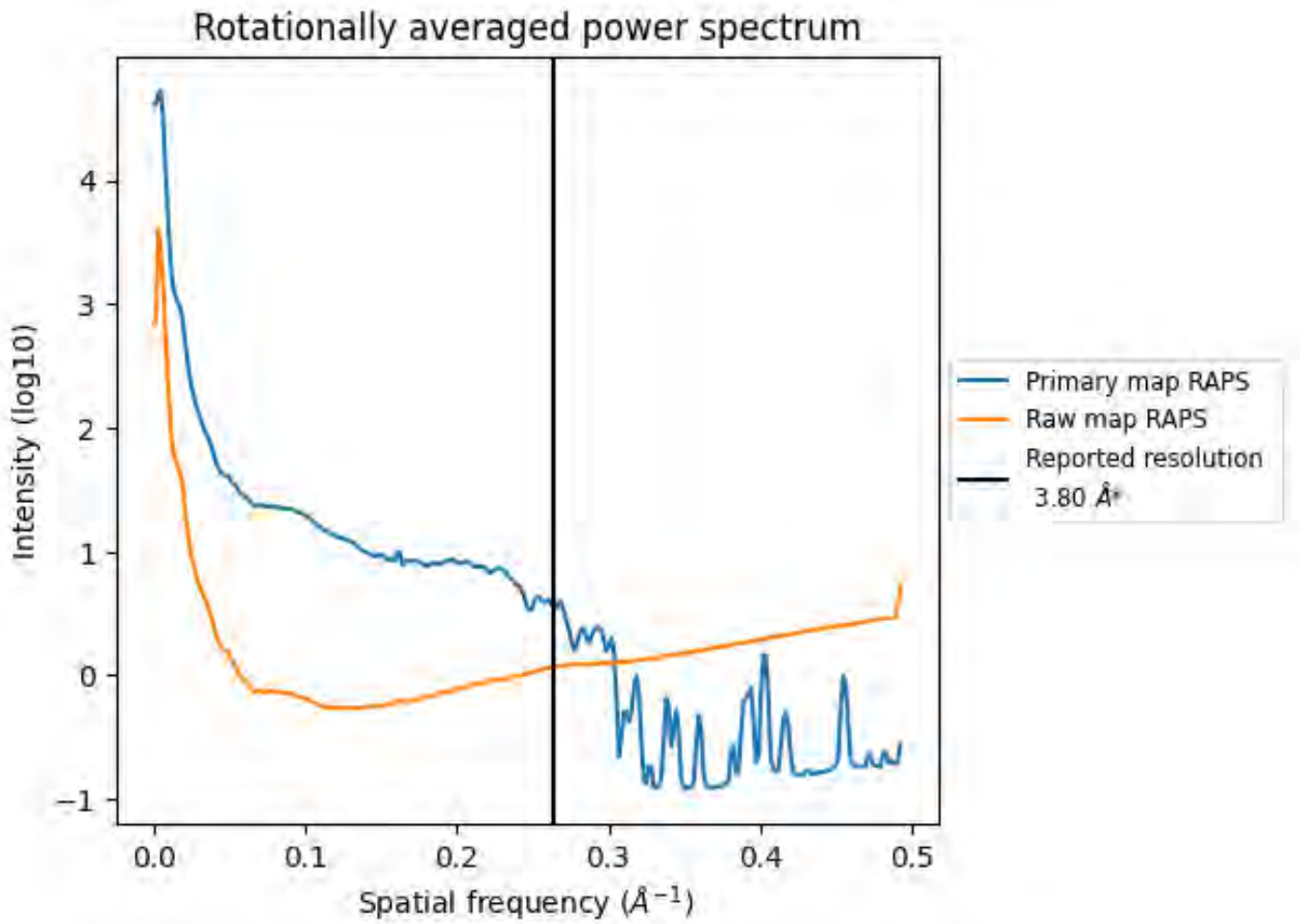
7.2 Volume estimate (i)



The volume at the recommended contour level is 479 nm^3; this corresponds to an approximate mass of 433 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

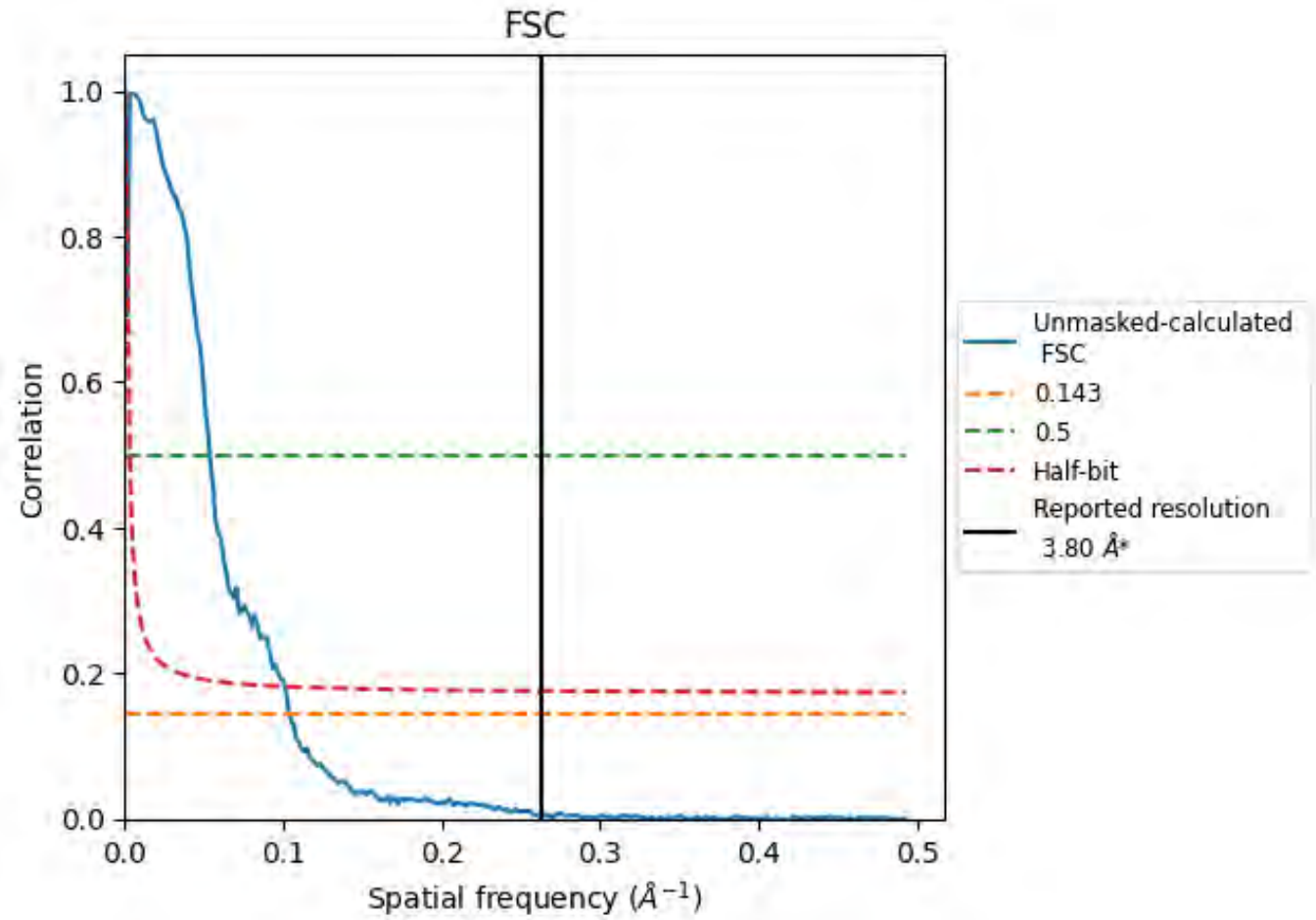


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.61	18.62	500.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.61 differs from the reported value 3.8 by more than 10 %

9 Map-model fit

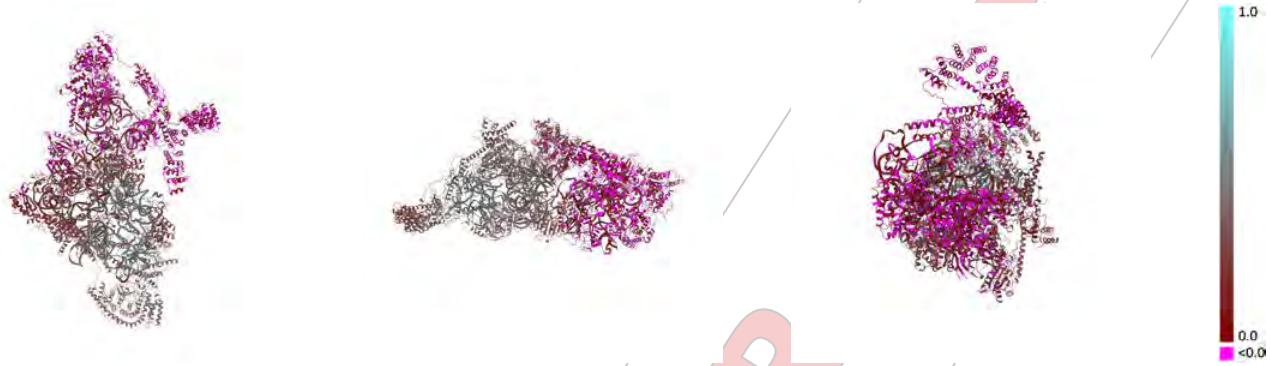
This section contains information regarding the fit between EMDB map EMD-51874 and PDB model 9H52. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

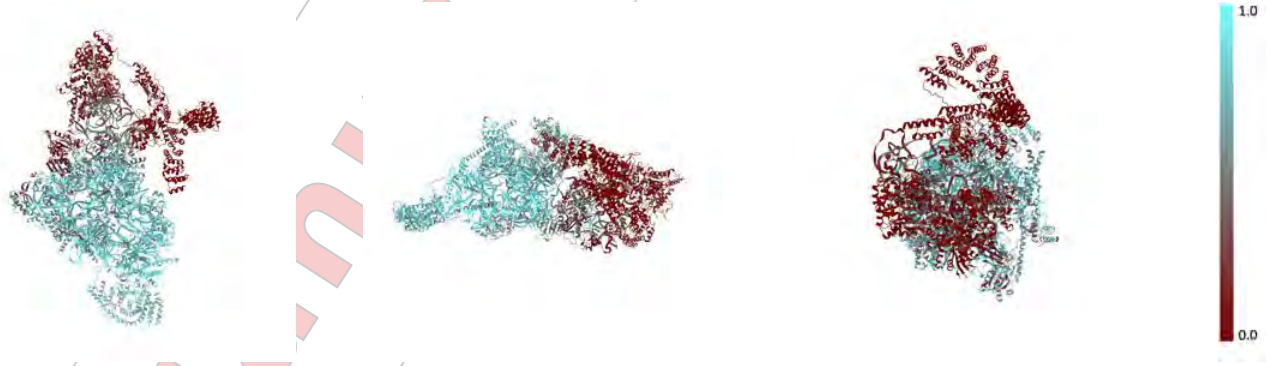
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

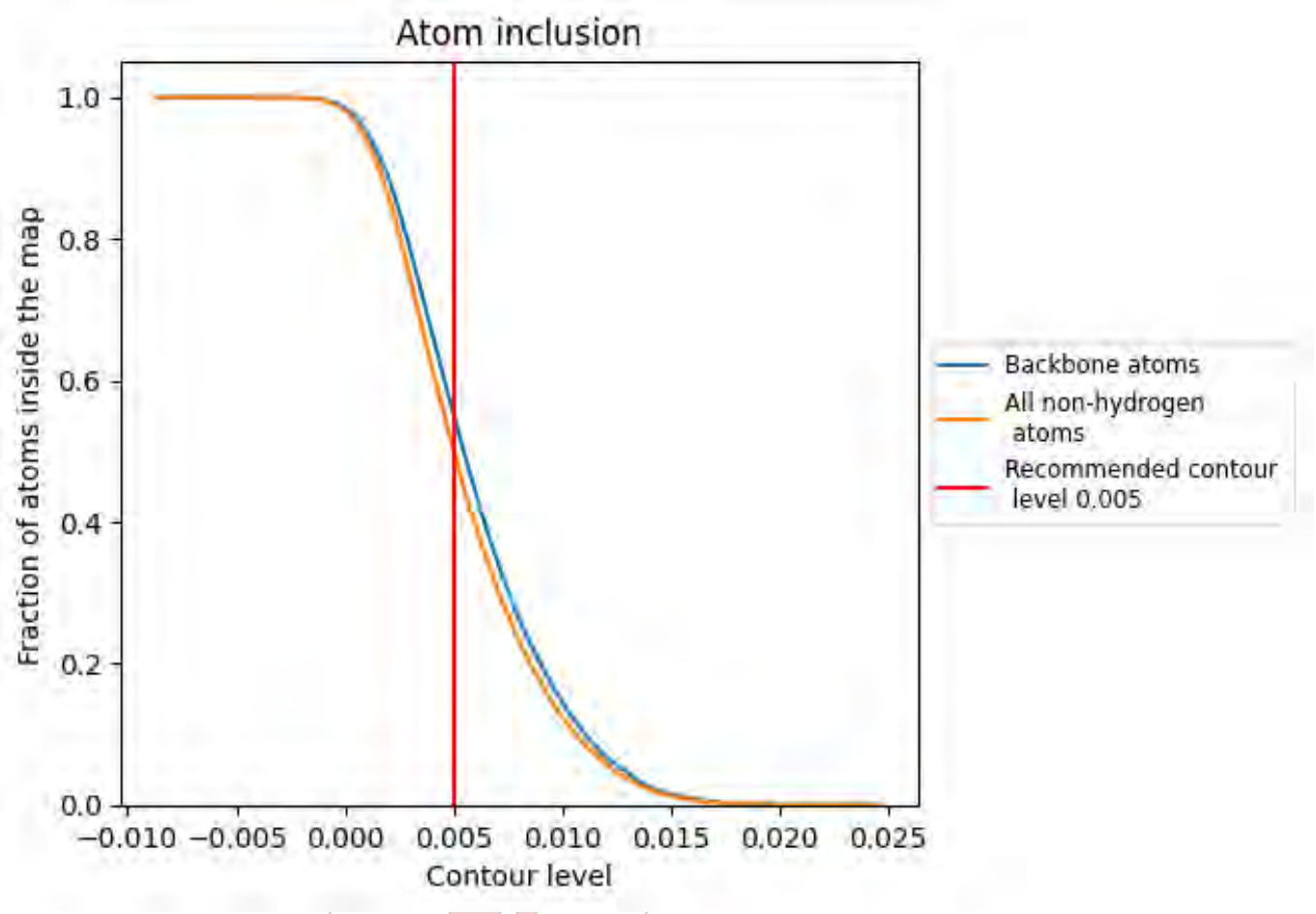
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5010	0.2410
0	0.8090	0.4110
1	0.0550	0.0600
4	0.0170	0.0540
5	0.6280	0.2640
7	0.3320	0.1350
8	0.1140	0.0450
9	0.5280	0.2720
A	0.7690	0.3020
B	0.7460	0.3300
C	0.0380	0.0450
D	0.7760	0.4270
E	0.5740	0.1910
F	0.2280	0.0880
G	0.3010	0.1130
J	0.7870	0.4110
L	0.7150	0.3050
M	0.8680	0.4830
N	0.8140	0.4210
O	0.8690	0.4420
P	0.6380	0.2110
Q	0.5500	0.1080
R	0.8200	0.4100
S	0.6640	0.2720
T	0.8170	0.4370
U	0.7270	0.3160
V	0.7500	0.3210
W	0.6240	0.2160
X	0.1160	0.0540
Y	0.0210	0.0520
a	0.1770	0.0910

Full wwPDB EM Validation Report ⓘ

Oct 25, 2024 – 12:03 pm BST

PDB ID	:	9H54
EMDB ID	:	EMD-51876
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit in complex with NOA1 and partial RBFA (state A2)
Deposited on	:	2024-10-22
Resolution	:	3.00 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

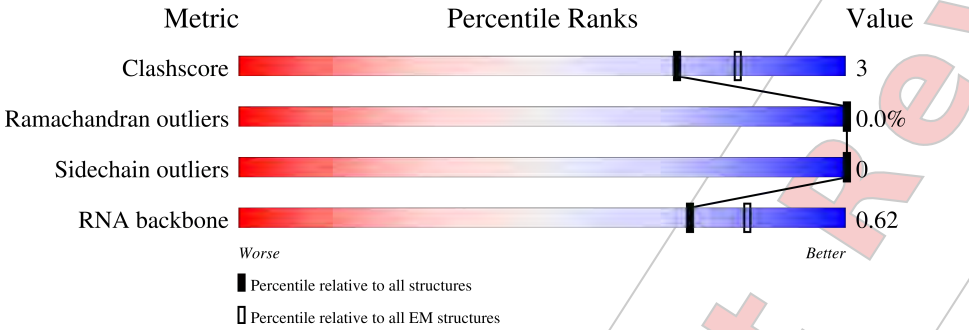
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	955	13% 67% 15% • 16%
2	B	296	• 73% • 24%
3	C	167	32% 65% 12% 23%
4	D	430	21% 73% 7% 21%
5	E	125	22% 70% 17% 13%

Continued on next page...

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Mol	Chain	Length	Quality of chain
6	F	242	51% 79% 19%
7	G	396	16% 74% 5% 21%
8	H	201	33% 65% 30%
9	I	194	41% 55% 12% 32%
10	J	138	71% 7% 22%
11	K	128	30% 70% 9% 21%
12	L	257	9% 56% 8% 36%
13	M	137	82% 13%
14	N	130	78% 6% 15%
15	O	258	72% 25%
16	P	142	18% 53% 15% 32%
17	Q	87	51% 84% 11% 5%
18	R	360	76% 6% 18%
19	S	190	66% 5% 29%
20	T	173	94%
21	U	205	79% 7% 14%
22	V	414	5% 81% 6% 13%
23	W	187	51% 47%
24	X	398	64% 81% 7% 12%
25	Y	395	27% 32% 65%
26	Z	106	62% 90% 5% 6%
27	0	215	5% 93% 7%
28	1	323	50% 82% 14%
29	4	689	71% 76% 10% 14%
30	9	698	31% 50% 9% 41%

Continued on next page...

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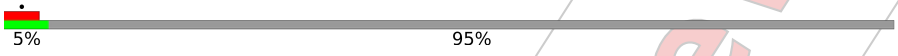
Mol	Chain	Length	Quality of chain
31	a	343	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	FES	P	201	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 122384 atoms, of which 57290 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	801	25644	7627	8633	3067	5516	801	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	225	3654	1164	1826	331	323	10	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	128	2099	677	1052	185	181	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	340	5479	1695	2775	512	484	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	109	1747	544	882	158	159	4	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	196	3296	1031	1677	292	285	11	1	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	313	5147	1637	2570	456	470	14	0	0

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	140	2343	745	1191	194	210	3	0	0

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	131	1964	609	998	178	175	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	108	1731	521	892	169	143	6	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	101	1751	537	889	179	141	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	164	2851	882	1467	256	239	7	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1914	594	972	185	157	6		

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	110	Total	C	H	N	O	S	0	0
			1801	562	933	156	147	3		

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	193	Total	C	H	N	O	S	0	0
			3158	1014	1566	294	277	7		

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	97	Total	C	H	N	O	S	0	0
			1590	501	809	134	138	8		

- Molecule 17 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	83	Total	C	H	N	O	S	0	0
			1425	431	723	145	118	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	295	Total	C	H	N	O	S	0	0
			4845	1533	2436	413	455	8		

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	135	Total	C	H	N	O	S	0	0
			2228	716	1117	198	196	1		

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	176	Total	C	H	N	O	S	0	0
			2993	916	1505	301	267	4		

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	362	Total	C	H	N	O	S	0	0
			5941	1904	2972	495	558	12		

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	100	Total	C	H	N	O	S	0	0
			1595	498	806	141	146	4		

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	352	Total	C	H	N	O	S	0	0
			5707	1822	2858	499	517	11		

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	138	Total	C	H	N	O	S	0	0
			2293	753	1127	195	214	4		

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	100	Total	C	H	N	O	S	0	0
			1701	534	862	153	148	4		

- Molecule 27 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	0	215	Total	C	H	N	O	S	0	0
			3589	1130	1802	339	313	5		

- Molecule 28 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	278	Total	C	H	N	O	S	0	0
			4550	1430	2294	386	429	11		

- Molecule 29 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	590	Total	C	H	N	O	S	0	0
			9572	3056	4797	809	882	28		

- Molecule 30 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	9	415	Total	C	H	N	O	S	0	0
			6647	2103	3374	576	582	12		

- Molecule 31 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	16	Total	C	H	N	O	0	0
			182	82	58	18	24		

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	40	Total	Mg	0
			40	40	
32	B	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
32	X	1	Total Mg 1 1	0

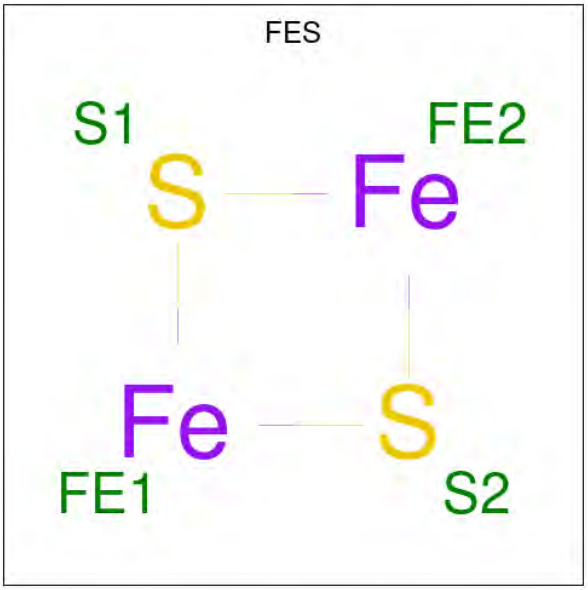
- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
33	A	11	Total K 11 11	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

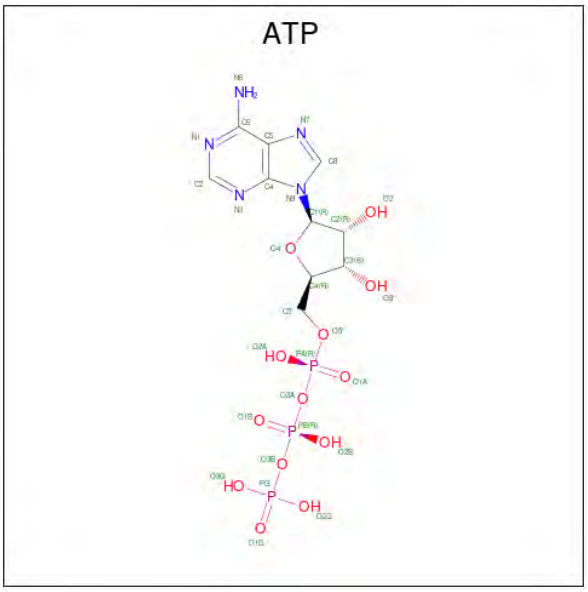
Mol	Chain	Residues	Atoms	AltConf
34	O	1	Total Zn 1 1	0

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



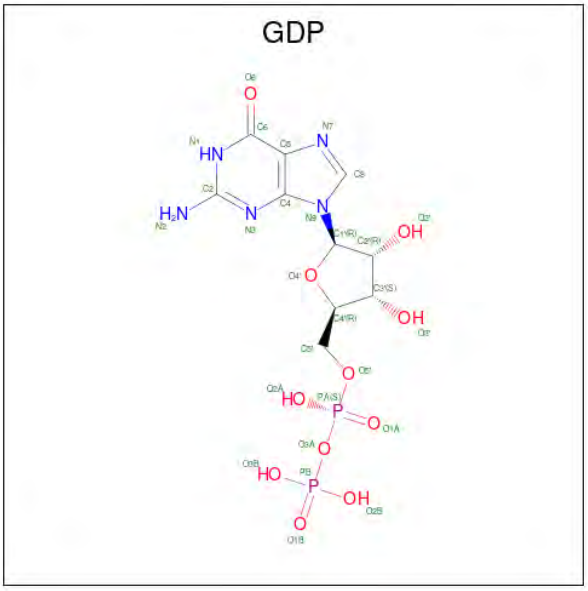
Mol	Chain	Residues	Atoms	AltConf
35	P	1	Total Fe S 4 2 2	0
35	T	1	Total Fe S 4 2 2	0

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
36	X	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 37 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



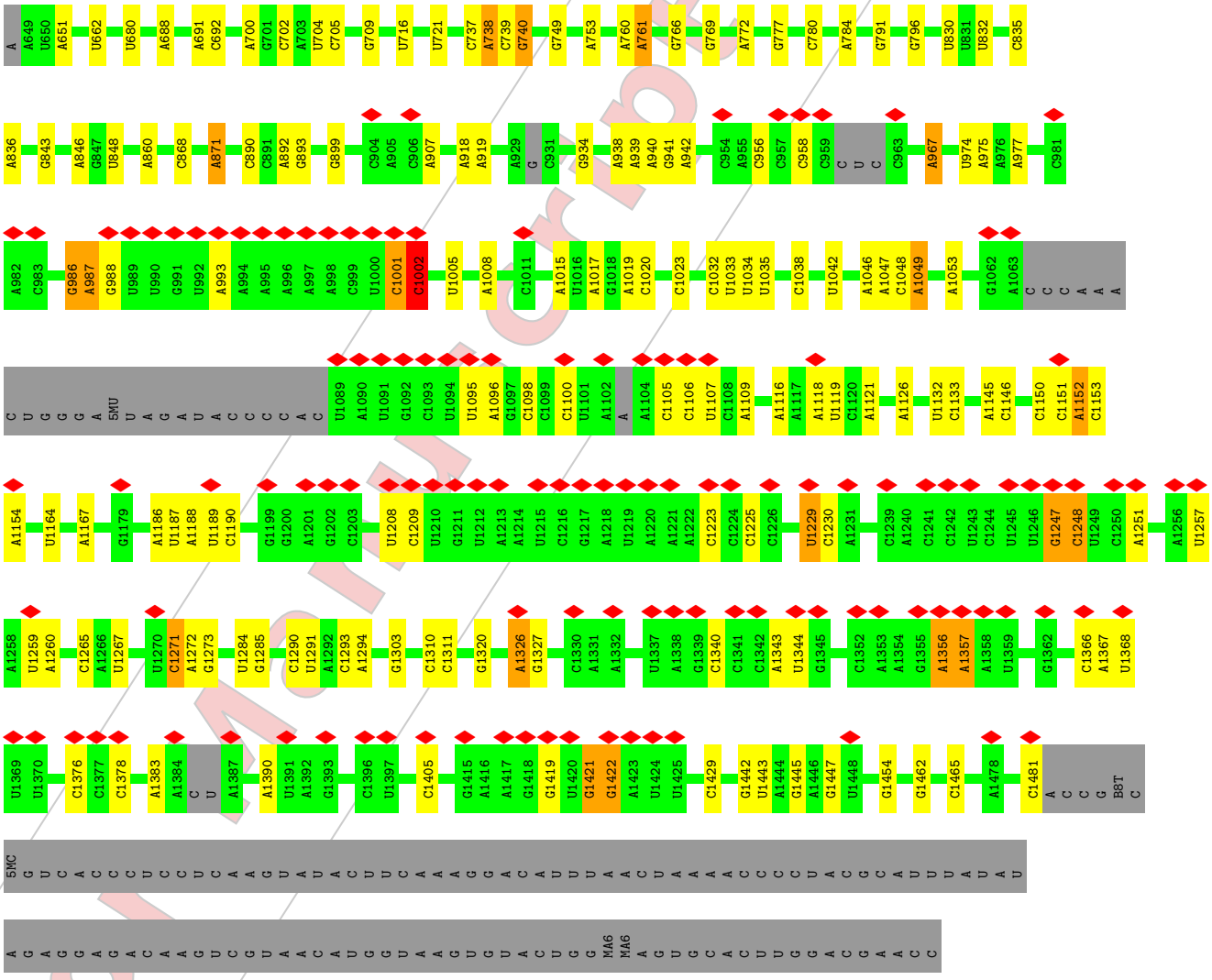
Mol	Chain	Residues	Atoms						AltConf
37	X	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	
37	9	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

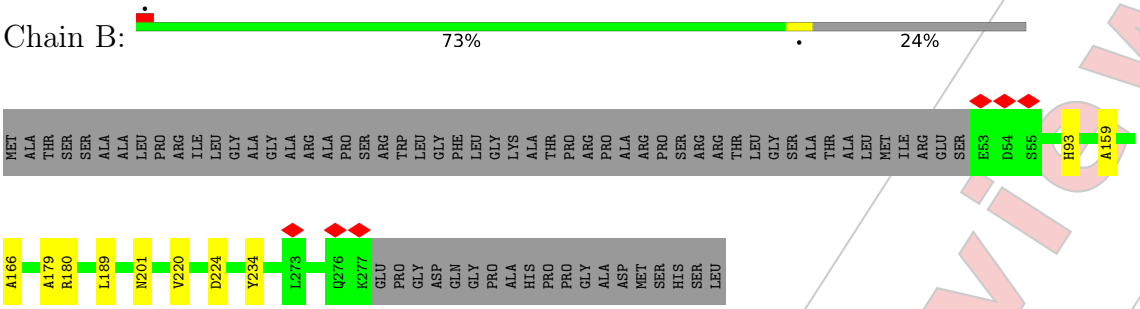
- Molecule 1: 12S mitochondrial rRNA

Chain A: 



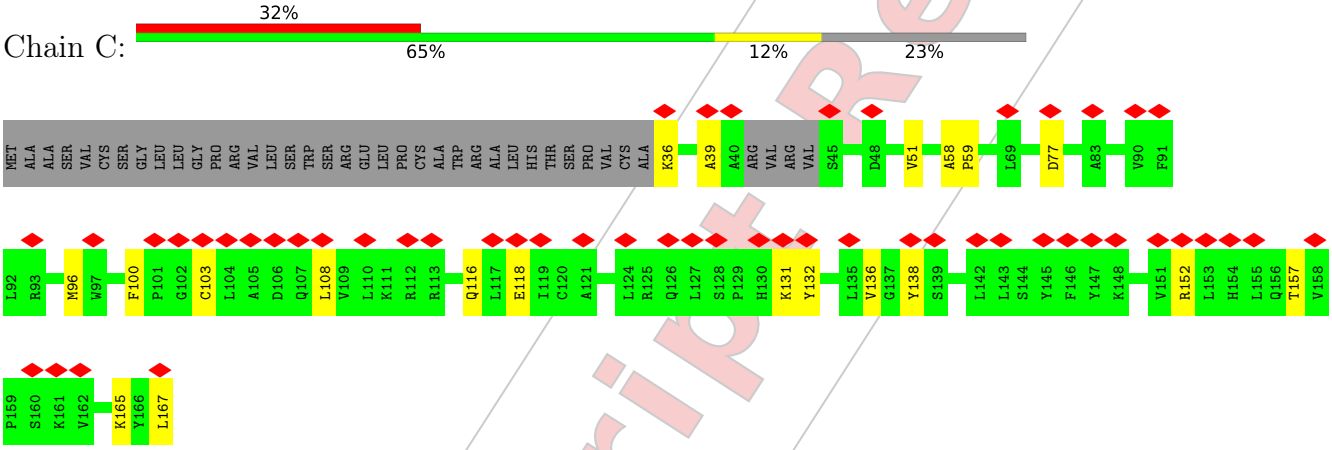
- Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:



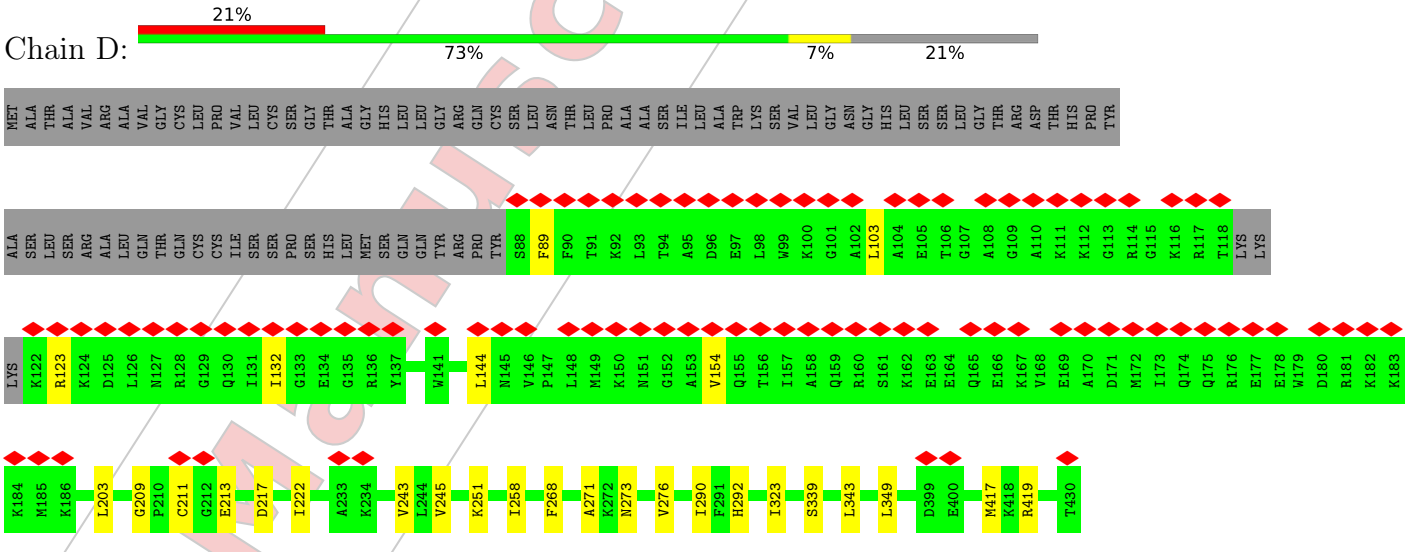
• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:



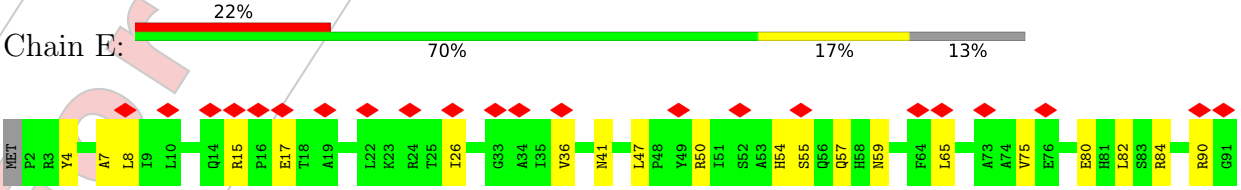
• Molecule 4: 28S ribosomal protein S5, mitochondrial

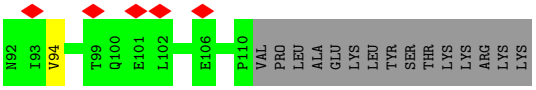
Chain D:



• Molecule 5: 28S ribosomal protein S6, mitochondrial

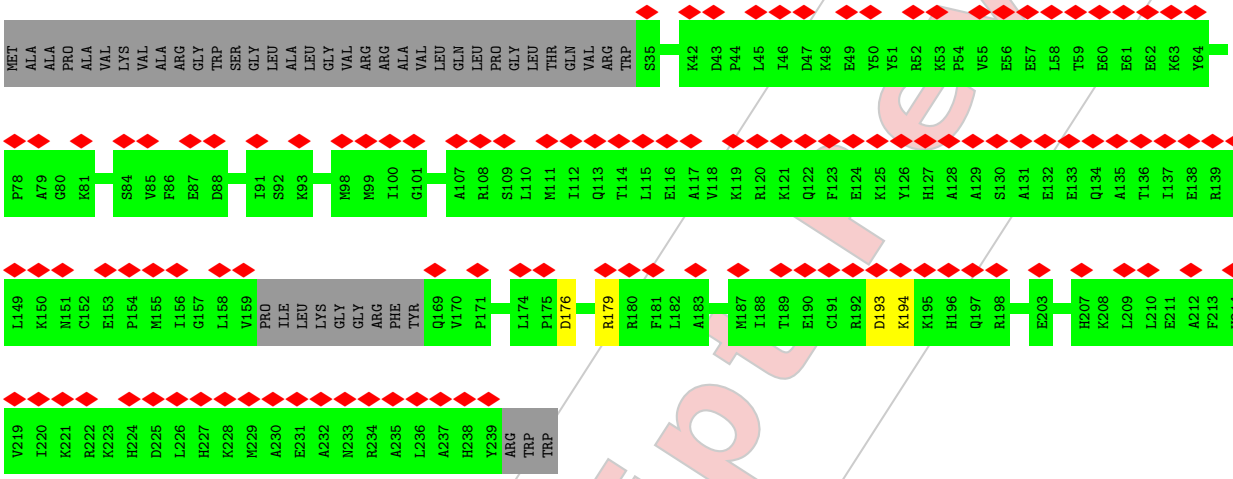
Chain E:





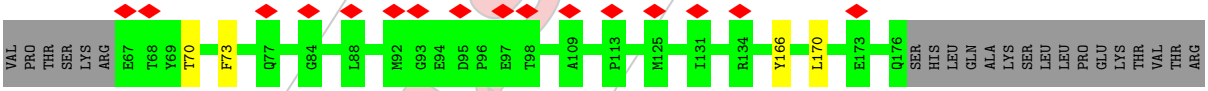
• Molecule 6: 28S ribosomal protein S7, mitochondrial

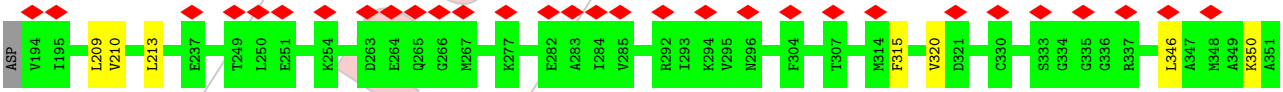
Chain F:



• Molecule 7: 28S ribosomal protein S9, mitochondrial

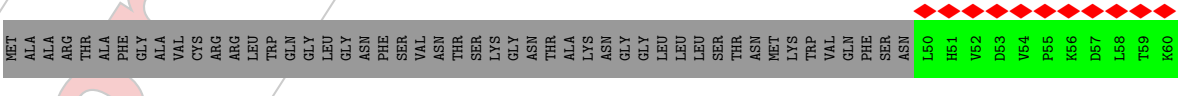
Chain G:

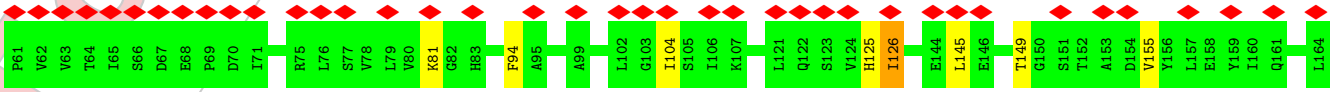


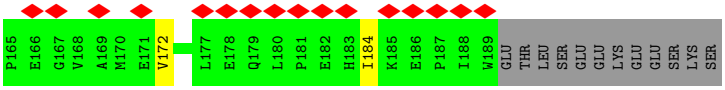


• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:

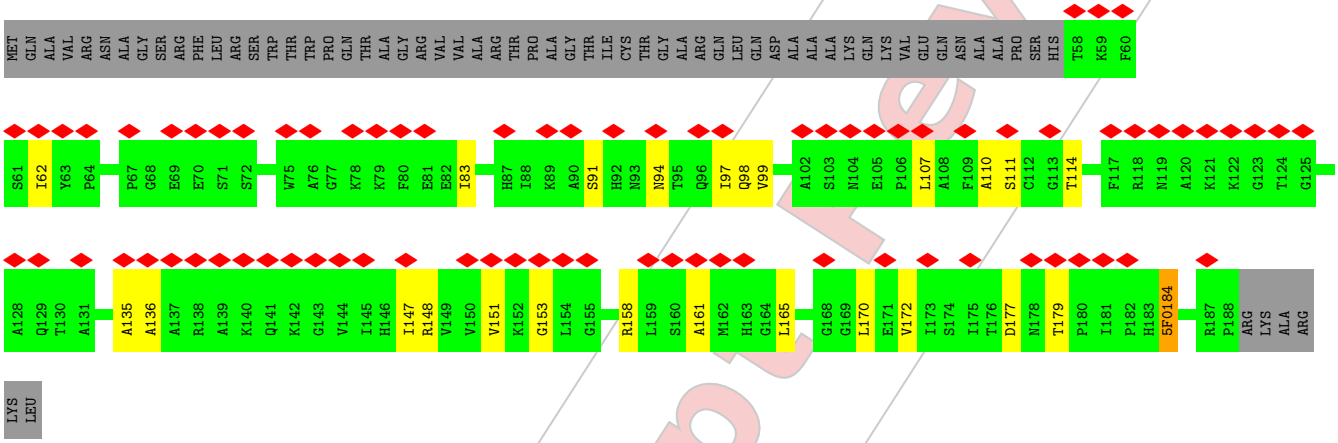






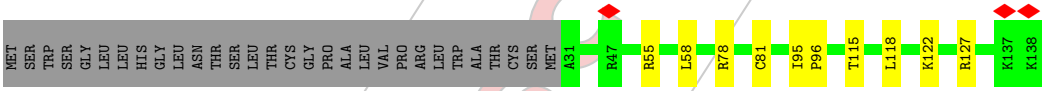
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



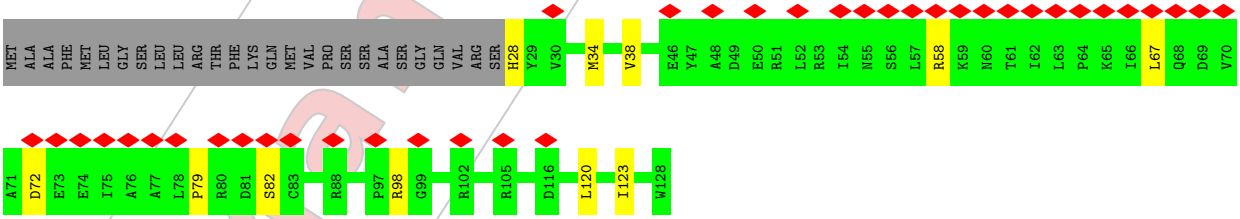
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:



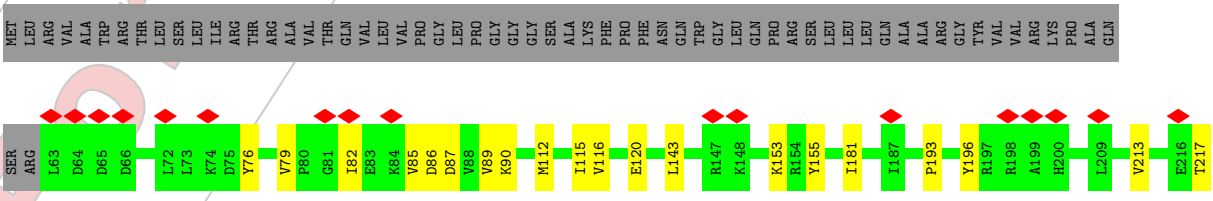
• Molecule 11: 28S ribosomal protein S14, mitochondrial

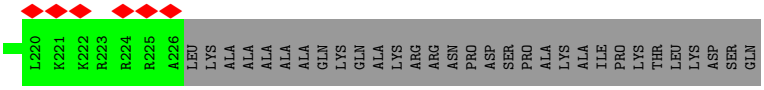
Chain K:



• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L:



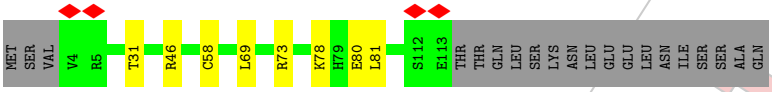


• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain M:

• Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain N:

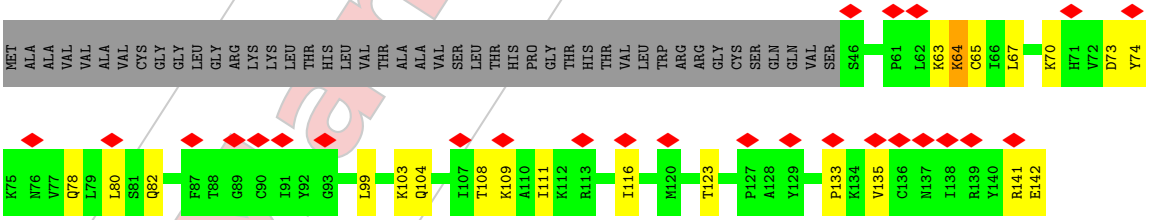


• Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain O:

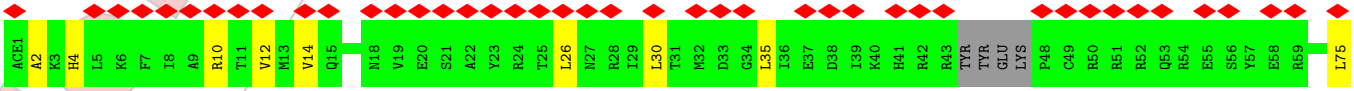
• Molecule 16: 28S ribosomal protein S18c, mitochondrial

Chain P:



• Molecule 17: Small ribosomal subunit protein bS21m

Chain Q:

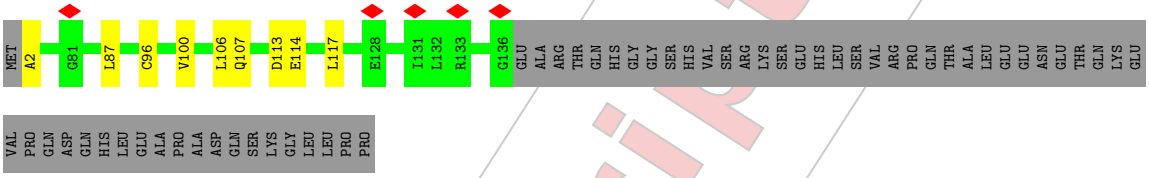


• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:

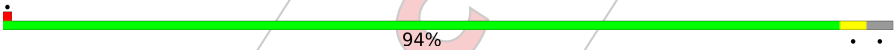
• Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S:



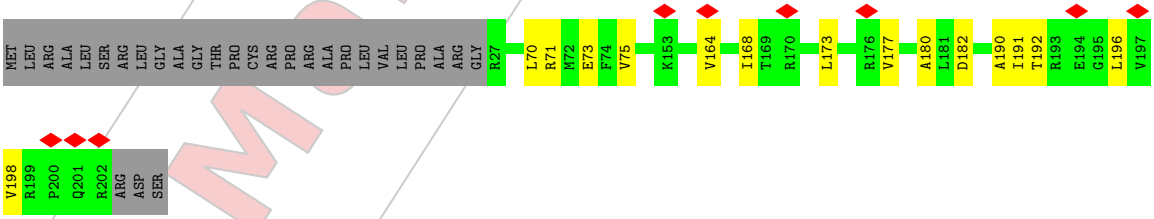
• Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T:



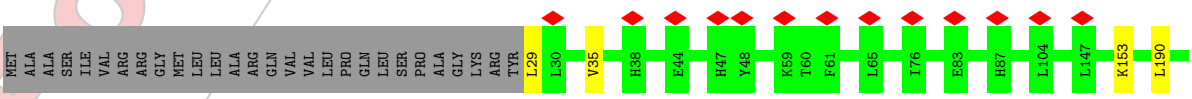
• Molecule 21: 28S ribosomal protein S26, mitochondrial

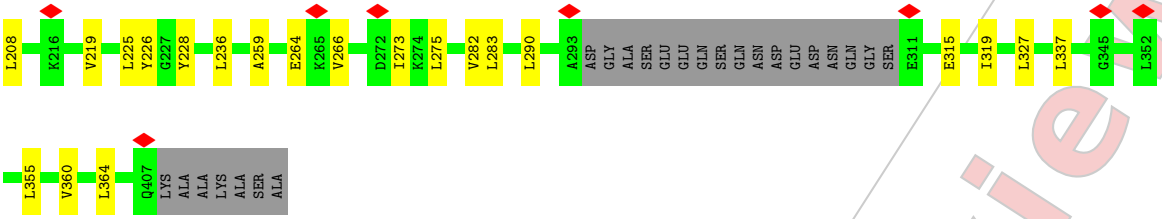
Chain U:



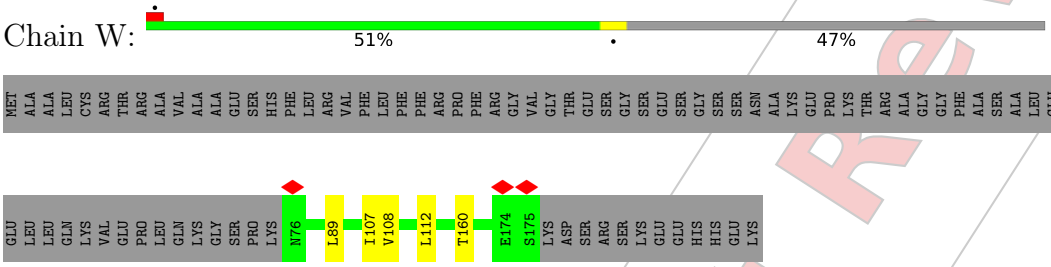
• Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V:



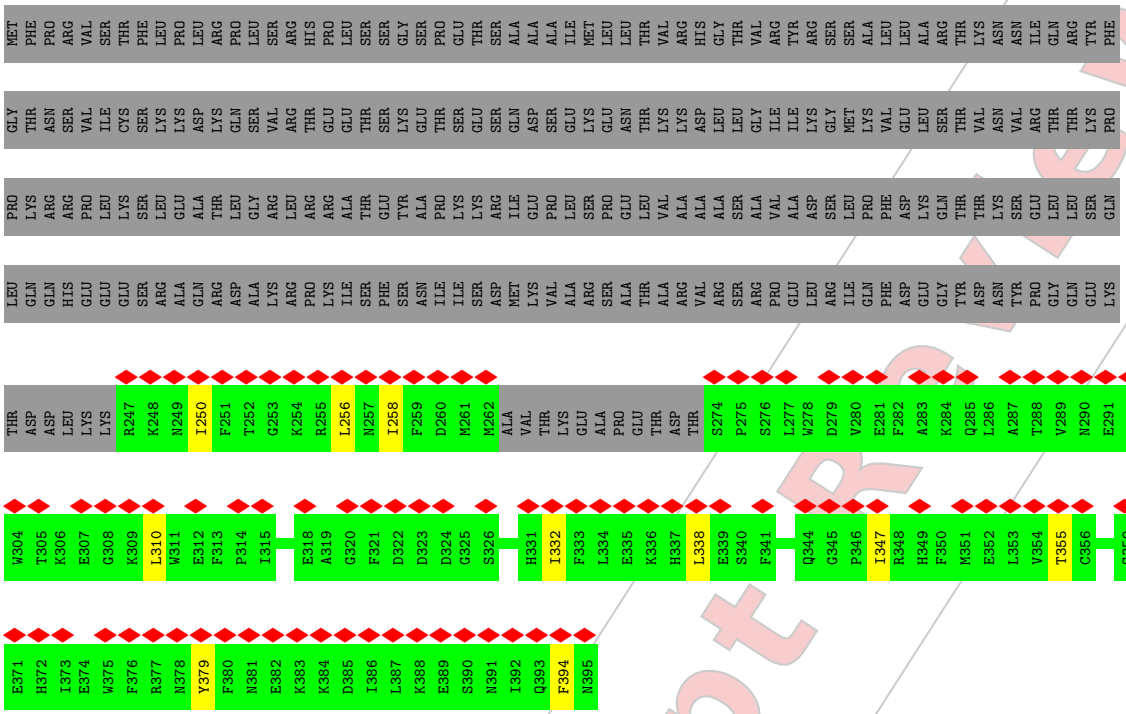


• Molecule 23: 28S ribosomal protein S28, mitochondrial



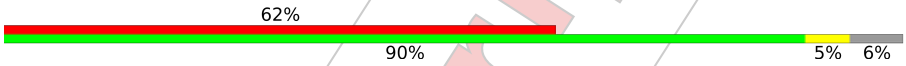
• Molecule 24: 28S ribosomal protein S29, mitochondrial

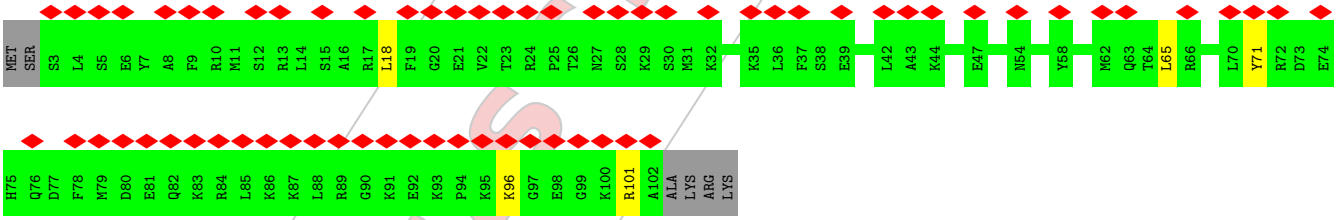
• Molecule 25: 28S ribosomal protein S31, mitochondrial



• Molecule 26: 28S ribosomal protein S33, mitochondrial

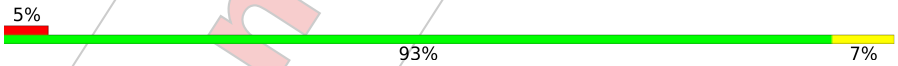
Chain Z:

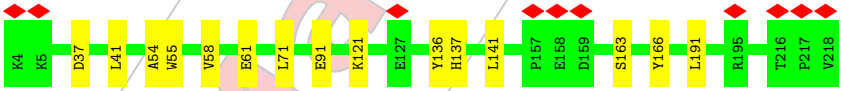




• Molecule 27: Small ribosomal subunit protein mS34

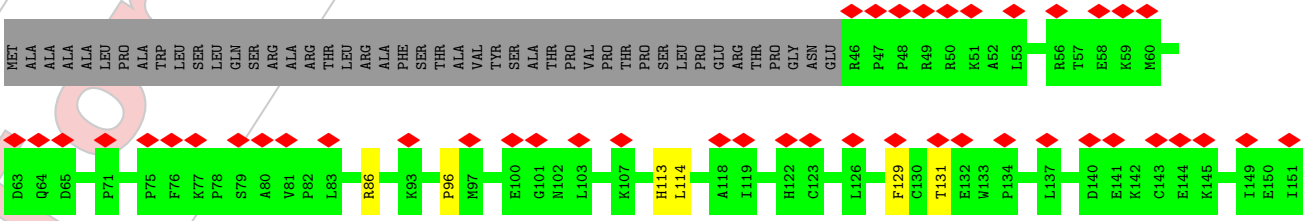
Chain 0:

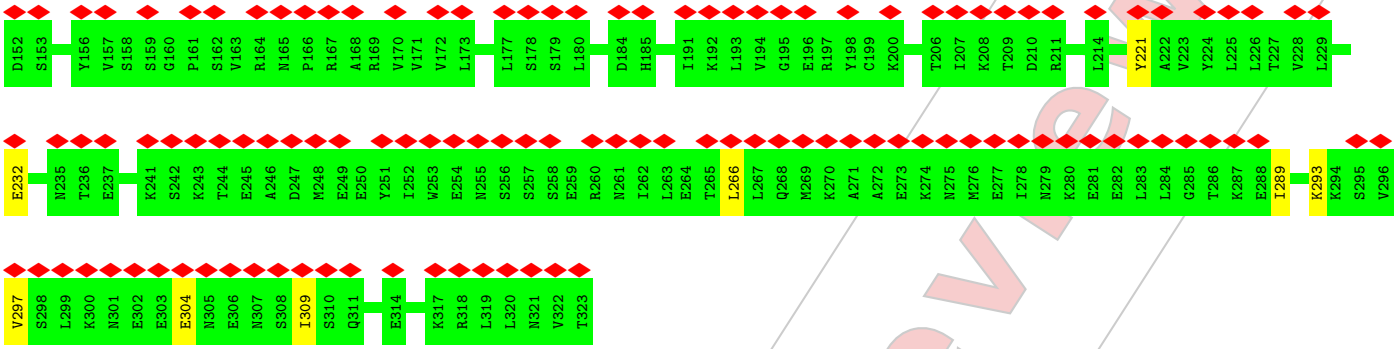




• Molecule 28: 28S ribosomal protein S35, mitochondrial

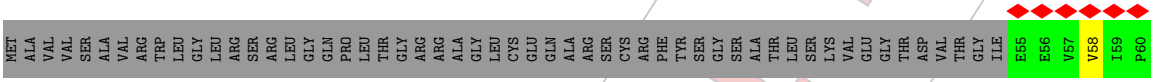
Chain 1:

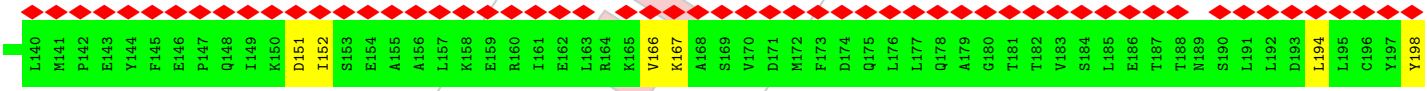


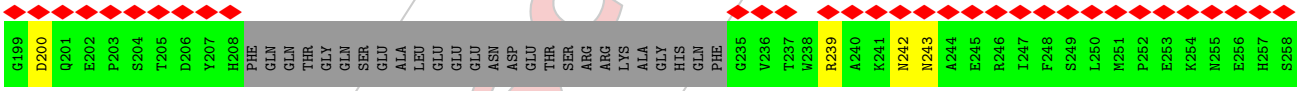


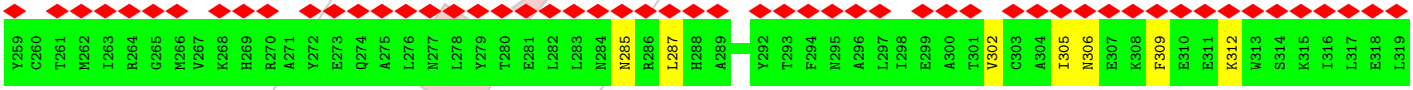
• Molecule 29: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

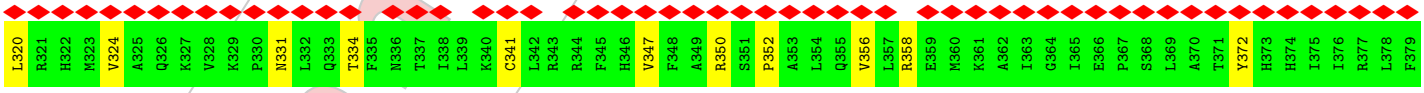
Chain 4:

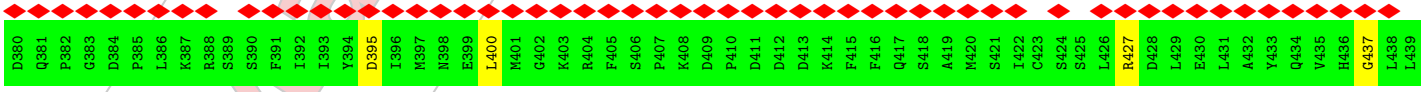


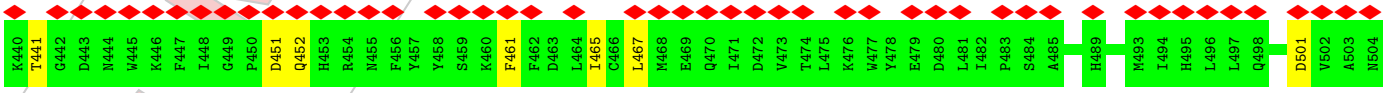


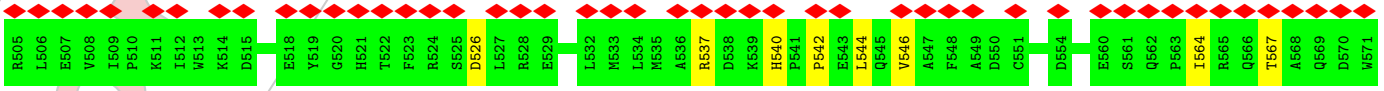


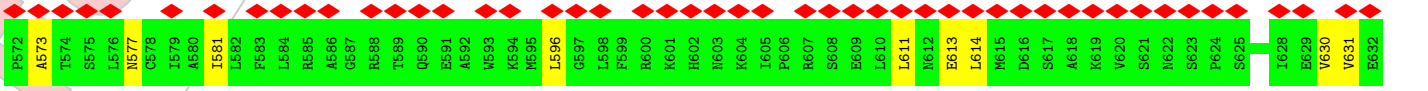


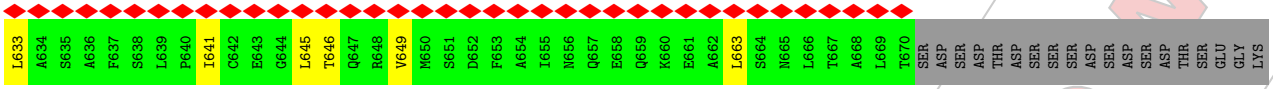






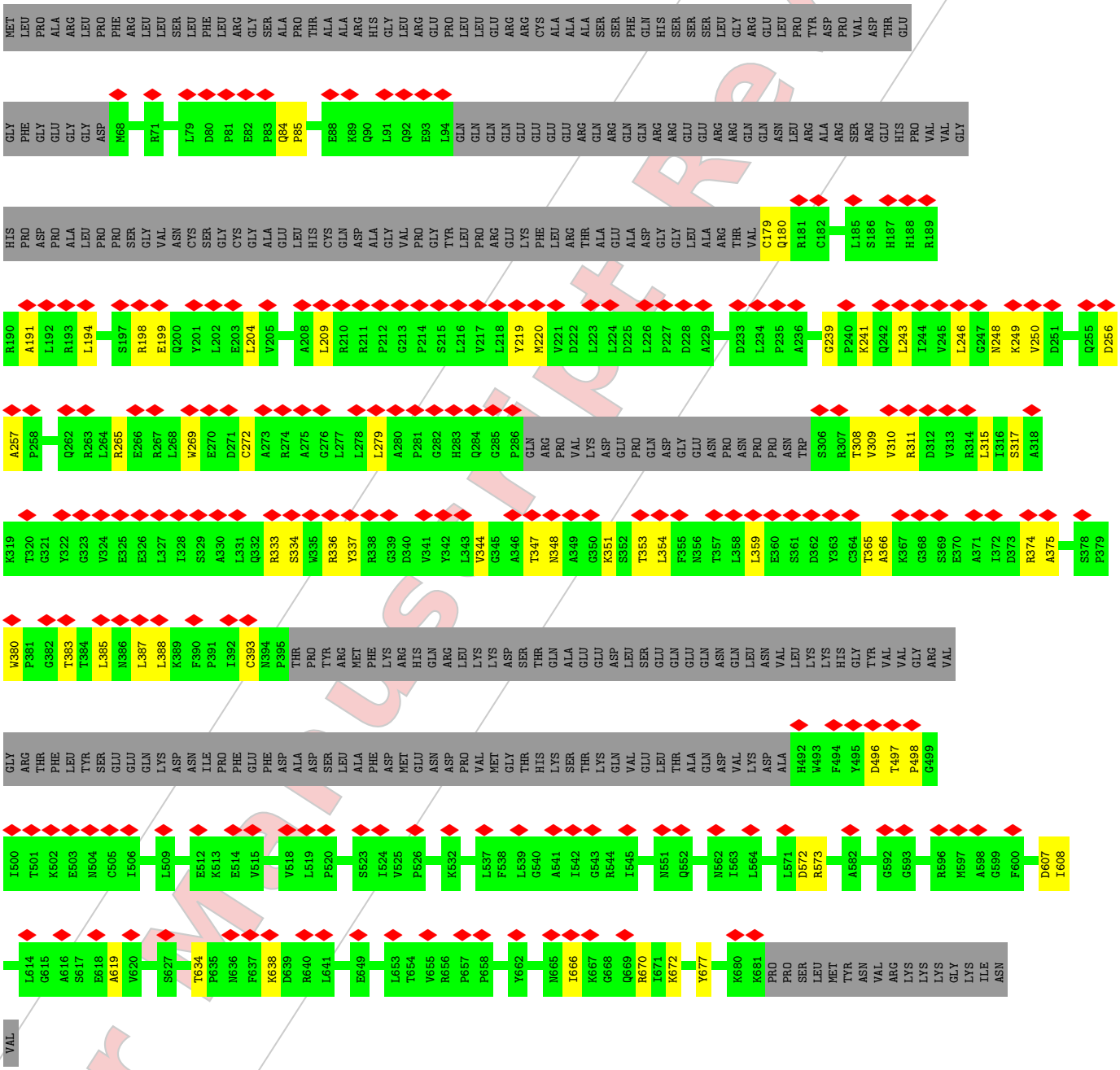






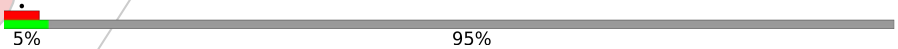
• Molecule 30: Nitric oxide-associated protein 1

Chain 9:



• Molecule 31: Putative ribosome-binding factor A, mitochondrial

Chain a:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33988	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, ATP, GDP, ACE, ZN, 5F0, MG, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/19025	0.69	1/29610 (0.0%)
2	B	0.25	0/1871	0.50	0/2531
3	C	0.26	0/1076	0.47	0/1454
4	D	0.26	0/2755	0.52	0/3688
5	E	0.24	0/880	0.53	0/1189
6	F	0.24	0/1653	0.45	0/2218
7	G	0.25	0/2632	0.48	0/3527
8	H	0.24	0/1178	0.47	0/1598
9	I	0.26	0/976	0.48	0/1318
10	J	0.25	0/855	0.55	0/1148
11	K	0.23	0/880	0.57	0/1182
12	L	0.24	0/1408	0.47	0/1882
13	M	0.26	0/963	0.55	0/1295
14	N	0.26	0/886	0.51	0/1199
15	O	0.26	0/1648	0.49	0/2243
16	P	0.25	0/798	0.45	0/1070
17	Q	0.25	0/709	0.58	0/940
18	R	0.26	0/2456	0.47	0/3317
19	S	0.26	0/1138	0.51	0/1533
20	T	0.26	0/1402	0.47	0/1883
21	U	0.24	0/1510	0.54	0/2025
22	V	0.24	0/3030	0.42	0/4093
23	W	0.25	0/801	0.52	0/1079
24	X	0.24	0/2921	0.45	0/3954
25	Y	0.25	0/1198	0.40	0/1610
26	Z	0.25	0/857	0.48	0/1141
27	0	0.26	0/1834	0.56	0/2484
28	1	0.24	0/2304	0.45	0/3117
29	4	0.24	0/4883	0.42	0/6608
30	9	0.25	0/3347	0.51	0/4548
31	a	0.23	0/123	0.33	0/164
All	All	0.25	0/67997	0.55	1/95648 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1002	C	O4'-C1'-N1	6.07	113.06	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	184	5F0	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17011	8633	8642	68	0
2	B	1828	1826	1815	8	0
3	C	1047	1052	1043	15	0
4	D	2704	2775	2764	22	0
5	E	865	882	878	17	0
6	F	1619	1677	1666	2	0
7	G	2577	2570	2560	11	0
8	H	1152	1191	1183	9	0
9	I	966	998	985	16	0
10	J	839	892	887	7	0
11	K	862	889	885	7	0
12	L	1384	1467	1462	12	0
13	M	942	972	965	4	0
14	N	868	933	928	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	1592	1566	1557	5	0
16	P	781	809	806	20	0
17	Q	702	723	721	9	0
18	R	2409	2436	2428	15	0
19	S	1111	1117	1115	6	0
20	T	1371	1396	1393	4	0
21	U	1488	1505	1499	23	0
22	V	2969	2972	2961	16	0
23	W	789	806	802	4	0
24	X	2849	2858	2843	16	0
25	Y	1166	1127	1120	11	0
26	Z	839	862	858	6	0
27	0	1787	1802	1796	11	0
28	1	2256	2294	2288	11	0
29	4	4775	4797	4779	47	0
30	9	3273	3374	3366	46	0
31	a	124	58	133	0	0
32	A	40	0	0	0	0
32	B	1	0	0	0	0
32	X	1	0	0	0	0
33	A	11	0	0	0	0
34	O	1	0	0	0	0
35	P	4	0	0	2	0
35	T	4	0	0	0	0
36	X	31	11	12	0	0
37	9	28	10	12	1	0
37	X	28	10	12	2	0
All	All	65094	57290	57164	377	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:O2'	1:A:1153:C:O4'	1.96	0.82
1:A:1230:C:O3'	11:K:98:ARG:NH1	2.16	0.78
1:A:1272:A:N1	1:A:1303:G:O2'	2.16	0.78
2:B:180:ARG:NH2	4:D:211:CYS:SG	2.58	0.77
12:L:112:MET:O	12:L:116:VAL:HG22	1.85	0.76
1:A:1265:C:OP2	3:C:39:ALA:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:C:OP1	16:P:109:LYS:NZ	2.20	0.74
29:4:200:ASP:OD2	29:4:243:ASN:N	2.21	0.73
30:9:209:LEU:O	30:9:241:LYS:NZ	2.15	0.72
29:4:596:LEU:HD21	29:4:614:LEU:HD11	1.72	0.71
16:P:70:LYS:O	16:P:103:LYS:NZ	2.25	0.70
17:Q:30:LEU:HD22	17:Q:35:LEU:HD22	1.72	0.69
9:I:111:SER:OG	9:I:114:THR:HG23	1.92	0.69
11:K:58:ARG:NE	11:K:72:ASP:OD1	2.26	0.69
16:P:133:PRO:HG2	21:U:198:VAL:HG21	1.76	0.68
9:I:97:ILE:HG21	9:I:165:LEU:HD21	1.74	0.67
1:A:986:G:O2'	1:A:987:A:OP1	2.14	0.65
6:F:176:ASP:OD1	6:F:179:ARG:NH2	2.29	0.65
1:A:977:A:OP2	17:Q:2:ALA:HB2	1.96	0.65
13:M:55:ASP:OD2	20:T:146:GLN:NE2	2.30	0.65
16:P:65:CYS:SG	35:P:201:FES:S1	2.94	0.65
7:G:320:VAL:HG21	7:G:352:LEU:HD21	1.79	0.65
1:A:1005:U:O4'	9:I:98:GLN:NE2	2.30	0.64
16:P:80:LEU:HD22	16:P:111:ILE:HG13	1.80	0.64
1:A:760:A:N1	1:A:780:C:O2'	2.29	0.63
3:C:118:GLU:OE2	3:C:152:ARG:NH2	2.31	0.62
3:C:157:THR:OG1	29:4:92:ASP:OD2	2.11	0.62
18:R:325:ILE:HG23	18:R:346:LEU:HD21	1.83	0.61
20:T:32:VAL:HG22	20:T:76:LEU:HD22	1.82	0.61
1:A:1267:U:O4	3:C:36:LYS:N	2.34	0.60
21:U:192:THR:CG2	21:U:198:VAL:HG23	2.31	0.60
29:4:564:ILE:HG22	29:4:567:THR:HB	1.81	0.60
29:4:501:ASP:OD2	29:4:537:ARG:NH1	2.34	0.60
1:A:843:G:N2	1:A:846:A:OP2	2.34	0.60
30:9:572:ASP:OD1	30:9:573:ARG:N	2.35	0.60
1:A:1164:U:OP1	10:J:122:LYS:NZ	2.31	0.60
9:I:110:ALA:HB3	9:I:135:ALA:HB2	1.83	0.60
3:C:131:LYS:NZ	4:D:144:LEU:O	2.35	0.60
30:9:256:ASP:OD1	30:9:257:ALA:N	2.34	0.60
1:A:769:G:OP2	14:N:73:ARG:NH2	2.35	0.60
1:A:749:G:O3'	14:N:78:LYS:NZ	2.35	0.59
1:A:1340:C:O2'	26:Z:101:ARG:NH2	2.35	0.59
18:R:162:SER:O	18:R:170:ARG:NH2	2.33	0.59
1:A:1152:A:OP1	1:A:1153:C:N4	2.36	0.59
29:4:631:VAL:CG2	29:4:649:VAL:HG21	2.32	0.59
12:L:86:ASP:OD1	12:L:87:ASP:N	2.35	0.59
16:P:133:PRO:CG	21:U:198:VAL:HG21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:A:N1	1:A:709:G:O2'	2.32	0.58
4:D:217:ASP:OD2	4:D:251:LYS:NZ	2.34	0.58
11:K:120:LEU:HB3	11:K:123:ILE:HD12	1.85	0.58
29:4:151:ASP:OD1	29:4:152:ILE:N	2.37	0.58
30:9:194:LEU:HD21	30:9:385:LEU:HB3	1.86	0.58
20:T:132:ARG:NH1	20:T:136:LEU:O	2.37	0.58
25:Y:258:ILE:HG21	29:4:320:LEU:CB	2.33	0.58
1:A:1344:U:OP1	26:Z:101:ARG:NH1	2.36	0.57
4:D:417:MET:O	4:D:419:ARG:NH1	2.37	0.57
19:S:106:LEU:HB2	19:S:117:LEU:HD11	1.87	0.57
3:C:58:ALA:HB1	3:C:59:PRO:CD	2.35	0.57
1:A:1008:A:OP2	5:E:50:ARG:NH2	2.38	0.57
5:E:47:LEU:HD12	5:E:59:ASN:HA	1.87	0.57
5:E:50:ARG:NH1	5:E:57:GLN:OE1	2.38	0.56
7:G:209:LEU:HD12	7:G:213:LEU:HD11	1.87	0.56
13:M:67:ALA:HB2	18:R:196:TYR:CE1	2.40	0.56
24:X:210:TRP:HE1	24:X:216:THR:HG1	1.54	0.56
25:Y:258:ILE:HG21	29:4:320:LEU:HB3	1.86	0.56
28:1:266:LEU:HD11	28:1:289:ILE:HD11	1.86	0.56
1:A:974:U:O2'	1:A:975:A:N7	2.32	0.56
5:E:54:HIS:O	5:E:55:SER:OG	2.22	0.56
18:R:302:GLN:O	18:R:306:VAL:HG23	2.05	0.56
29:4:302:VAL:HG21	29:4:341:CYS:HB3	1.86	0.55
1:A:1033:U:O3'	5:E:94:VAL:HG12	2.07	0.55
4:D:245:VAL:HG22	4:D:271:ALA:HB1	1.89	0.55
30:9:198:ARG:NH2	30:9:199:GLU:OE2	2.40	0.55
1:A:1272:A:N6	1:A:1320:G:O2'	2.37	0.55
3:C:51:VAL:HG11	3:C:167:LEU:HD12	1.89	0.55
4:D:273:ASN:O	4:D:276:VAL:HG12	2.07	0.54
21:U:173:LEU:O	21:U:177:VAL:HG23	2.07	0.54
22:V:190:LEU:HD11	22:V:208:LEU:HD11	1.88	0.54
1:A:941:G:O2'	1:A:1109:A:OP2	2.25	0.54
7:G:166:TYR:CE1	7:G:170:LEU:HD11	2.43	0.54
1:A:761:A:O2'	1:A:784:A:N1	2.32	0.54
24:X:268:LEU:HD21	24:X:293:LEU:HD23	1.89	0.54
4:D:203:LEU:HD21	4:D:222:ILE:HD11	1.89	0.53
5:E:8:LEU:HD11	5:E:82:LEU:HD22	1.89	0.53
7:G:315:PHE:CD2	7:G:369:LEU:HD21	2.42	0.53
16:P:63:LYS:O	16:P:64:LYS:HB2	2.08	0.53
24:X:206:GLU:OE2	24:X:249:ARG:NH2	2.41	0.53
1:A:986:G:O2'	1:A:987:A:P	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:115:THR:HG21	10:J:118:LEU:HD12	1.90	0.53
22:V:35:VAL:HG12	22:V:35:VAL:O	2.07	0.53
16:P:73:ASP:OD1	16:P:74:TYR:N	2.42	0.53
1:A:1248:C:O2	11:K:28:HIS:N	2.42	0.53
7:G:70:THR:HG23	7:G:73:PHE:H	1.73	0.53
29:4:573:ALA:O	29:4:577:ASN:ND2	2.42	0.53
12:L:85:VAL:HG23	12:L:90:LYS:HG3	1.91	0.52
21:U:192:THR:HG23	21:U:198:VAL:HG23	1.90	0.52
21:U:73:GLU:OE2	27:0:166:TYR:OH	2.26	0.52
7:G:210:VAL:HG12	7:G:210:VAL:O	2.09	0.52
3:C:100:PHE:HB3	3:C:103:CYS:SG	2.50	0.52
9:I:97:ILE:HD11	9:I:161:ALA:HB1	1.90	0.52
15:O:182:GLY:O	18:R:183:LYS:NZ	2.41	0.52
5:E:90:ARG:NH1	16:P:116:ILE:O	2.43	0.52
18:R:208:ILE:O	18:R:214:ASN:ND2	2.39	0.52
29:4:645:LEU:O	29:4:649:VAL:HG23	2.10	0.52
29:4:451:ASP:OD1	29:4:452:GLN:N	2.43	0.51
29:4:611:LEU:HD21	29:4:633:LEU:HD23	1.91	0.51
16:P:82:GLN:NE2	21:U:190:ALA:HB1	2.25	0.51
25:Y:332:ILE:HD13	28:1:221:TYR:CD1	2.44	0.51
11:K:34:MET:O	11:K:38:VAL:HG23	2.09	0.51
29:4:372:TYR:CE2	29:4:400:LEU:HD21	2.46	0.51
5:E:80:GLU:OE1	5:E:84:ARG:NE	2.44	0.51
21:U:192:THR:HG23	21:U:196:LEU:O	2.10	0.51
29:4:166:VAL:HG12	29:4:194:LEU:HG	1.91	0.51
24:X:242:ILE:HD11	37:X:502:GDP:N3	2.26	0.51
29:4:239:ARG:O	29:4:242:ASN:ND2	2.38	0.51
1:A:662:U:OP2	4:D:339:SER:OG	2.29	0.50
1:A:1186:A:N6	1:A:1465:C:O2	2.44	0.50
29:4:630:VAL:HG12	29:4:645:LEU:HD21	1.92	0.50
1:A:967:A:O4'	1:A:1023:C:O2'	2.24	0.50
9:I:83:ILE:O	9:I:148:ARG:NH2	2.41	0.50
12:L:120:GLU:N	12:L:120:GLU:OE1	2.44	0.50
17:Q:12:VAL:HG23	17:Q:26:LEU:HD13	1.94	0.50
30:9:194:LEU:HD23	30:9:387:LEU:HG	1.94	0.50
1:A:934:G:O2'	1:A:940:A:N1	2.30	0.50
1:A:1001:C:H5"	1:A:1002:C:H5"	1.93	0.50
29:4:305:ILE:O	29:4:312:LYS:NZ	2.43	0.50
17:Q:75:LEU:HD21	23:W:160:THR:HG21	1.93	0.50
22:V:225:LEU:HD11	22:V:283:LEU:HD22	1.93	0.50
27:0:54:ALA:O	27:0:58:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:86:ARG:NH1	28:1:96:PRO:O	2.43	0.50
30:9:220:MET:CE	30:9:354:LEU:HD23	2.42	0.50
5:E:7:ALA:HA	5:E:65:LEU:HD23	1.93	0.50
30:9:309:VAL:HG21	30:9:311:ARG:HH21	1.76	0.50
4:D:243:VAL:HG11	4:D:268:PHE:CD1	2.46	0.49
1:A:1257:U:O2'	1:A:1260:A:OP2	2.21	0.49
1:A:1095:U:O4	1:A:1096:A:N6	2.45	0.49
18:R:82:MET:HE1	18:R:300:LEU:HD13	1.93	0.49
9:I:158:ARG:NH2	9:I:177:ASP:OD2	2.45	0.49
1:A:1048:C:HO2'	1:A:1049:A:C5'	2.25	0.49
1:A:1259:U:H6	1:A:1326:A:HO2'	1.60	0.49
10:J:55:ARG:HD3	10:J:58:LEU:HD21	1.94	0.49
21:U:70:LEU:CD2	27:0:191:LEU:HD11	2.42	0.49
25:Y:250:ILE:O	29:4:358:ARG:NH2	2.46	0.49
4:D:103:LEU:HD11	4:D:123:ARG:HB2	1.95	0.49
1:A:705:C:H2'	27:0:136:TYR:CE1	2.47	0.49
1:A:899:G:O2'	1:A:907:A:N1	2.26	0.49
1:A:1053:A:N6	1:A:1100:C:O2'	2.45	0.49
1:A:1150:C:H2'	1:A:1152:A:N7	2.27	0.49
3:C:138:TYR:OH	26:Z:65:LEU:HD22	2.12	0.49
24:X:242:ILE:HD11	37:X:502:GDP:C2	2.47	0.49
1:A:1366:C:O2'	1:A:1419:G:N3	2.46	0.48
25:Y:338:LEU:HD11	25:Y:355:THR:HG21	1.95	0.48
1:A:1229:U:O2'	1:A:1442:G:O4'	2.31	0.48
16:P:78:GLN:HE21	21:U:190:ALA:HB2	1.77	0.48
27:0:71:LEU:HD11	27:0:141:LEU:HD22	1.94	0.48
1:A:1247:G:N7	26:Z:96:LYS:NZ	2.54	0.48
25:Y:256:LEU:HD11	29:4:356:VAL:HG22	1.94	0.48
28:1:304:GLU:OE2	28:1:309:ILE:HD11	2.13	0.48
29:4:437:GLY:O	29:4:441:THR:HG23	2.13	0.48
30:9:317:SER:OG	30:9:354:LEU:HD22	2.13	0.48
1:A:702:C:OP1	1:A:848:U:O2'	2.24	0.48
12:L:115:ILE:HG21	12:L:181:ILE:HD13	1.95	0.48
2:B:93:HIS:CD2	2:B:224:ASP:OD2	2.66	0.48
3:C:132:TYR:O	3:C:136:VAL:HG23	2.13	0.48
4:D:132:ILE:HG22	4:D:144:LEU:HD11	1.94	0.48
9:I:62:ILE:HG23	16:P:141:ARG:NH2	2.28	0.48
30:9:619:ALA:HA	30:9:634:THR:HG22	1.95	0.48
19:S:87:LEU:HD13	23:W:89:LEU:HD13	1.94	0.48
29:4:540:HIS:HB3	29:4:544:LEU:HD23	1.96	0.48
12:L:143:LEU:HD11	12:L:153:LYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:366:ALA:HB1	30:9:374:ARG:NE	2.29	0.48
1:A:1145:A:H2'	1:A:1146:C:O4'	2.13	0.48
3:C:77:ASP:O	8:H:81:LYS:NZ	2.40	0.48
12:L:76:TYR:O	12:L:79:VAL:HG22	2.14	0.48
29:4:461:PHE:CZ	29:4:465:ILE:HD11	2.49	0.48
12:L:89:VAL:HG22	21:U:164:VAL:HG21	1.95	0.48
1:A:871:A:N1	1:A:918:A:O2'	2.41	0.47
30:9:666:ILE:HG23	30:9:666:ILE:O	2.13	0.47
9:I:91:SER:N	9:I:94:ASN:O	2.47	0.47
24:X:108:LEU:HD21	24:X:307:VAL:CG1	2.44	0.47
5:E:36:VAL:HG12	21:U:168:ILE:HD12	1.95	0.47
30:9:239:GLY:O	30:9:308:THR:OG1	2.24	0.47
1:A:1294:A:OP1	2:B:201:ASN:ND2	2.46	0.47
30:9:387:LEU:HD11	30:9:498:PRO:HG3	1.97	0.47
29:4:581:ILE:HG23	29:4:613:GLU:OE2	2.15	0.47
21:U:70:LEU:HD21	27:0:191:LEU:HD11	1.96	0.47
10:J:96:PRO:O	10:J:127:ARG:NH1	2.43	0.47
22:V:266:VAL:HG13	22:V:273:ILE:HG22	1.96	0.47
22:V:315:GLU:O	22:V:315:GLU:HG2	2.14	0.47
5:E:26:ILE:HG21	21:U:173:LEU:HD13	1.98	0.46
8:H:125:HIS:CD2	8:H:126:ILE:HG23	2.50	0.46
29:4:58:VAL:HG23	29:4:58:VAL:O	2.15	0.46
2:B:179:ALA:CB	2:B:189:LEU:HD21	2.45	0.46
4:D:89:PHE:HE1	26:Z:71:TYR:HH	1.62	0.46
4:D:213:GLU:OE2	19:S:2:ALA:N	2.48	0.46
14:N:31:THR:HG22	14:N:46:ARG:HB3	1.97	0.46
16:P:103:LYS:HG2	35:P:201:FES:S1	2.56	0.46
30:9:670:ARG:HA	30:9:677:TYR:HA	1.98	0.46
1:A:738:A:H2'	1:A:740:G:C5	2.50	0.46
9:I:179:THR:O	17:Q:10:ARG:NH1	2.48	0.46
18:R:273:TRP:CZ3	18:R:307:LEU:HD11	2.50	0.46
14:N:69:LEU:HD21	14:N:80:GLU:HB3	1.97	0.46
18:R:162:SER:O	18:R:170:ARG:NH1	2.49	0.46
1:A:1443:U:O2'	1:A:1445:G:N7	2.34	0.46
2:B:220:VAL:HG22	2:B:234:TYR:HB2	1.98	0.46
30:9:220:MET:SD	30:9:248:ASN:ND2	2.87	0.46
9:I:147:ILE:HD13	9:I:170:LEU:HD13	1.98	0.46
29:4:611:LEU:HA	29:4:614:LEU:HD12	1.96	0.46
23:W:107:ILE:HG23	23:W:112:LEU:HD23	1.98	0.45
30:9:334:SER:HB3	30:9:337:TYR:CD2	2.52	0.45
30:9:366:ALA:HB1	30:9:374:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:84:GLN:N	30:9:85:PRO:HD3	2.30	0.45
21:U:190:ALA:HB3	21:U:198:VAL:HB	1.98	0.45
22:V:228:TYR:HB3	22:V:259:ALA:HB2	1.97	0.45
29:4:631:VAL:HG23	29:4:649:VAL:HG21	1.97	0.45
15:O:208:PRO:HG2	15:O:213:LEU:HD21	1.99	0.45
29:4:347:VAL:HG22	29:4:350:ARG:NH1	2.31	0.45
18:R:325:ILE:CG2	18:R:346:LEU:HD21	2.47	0.45
27:0:41:LEU:HD13	27:0:55:TRP:CG	2.52	0.45
29:4:305:ILE:HG22	29:4:306:ASN:N	2.32	0.45
30:9:607:ASP:OD1	30:9:608:ILE:N	2.49	0.45
4:D:243:VAL:HG11	4:D:268:PHE:HD1	1.81	0.45
19:S:107:GLN:HB2	19:S:117:LEU:HD21	1.98	0.45
1:A:1038:C:HO2'	12:L:155:TYR:HH	1.63	0.44
8:H:149:THR:OG1	28:1:131:THR:OG1	1.99	0.44
30:9:191:ALA:HB3	30:9:388:LEU:HD21	1.99	0.44
1:A:1034:U:O2'	5:E:75:VAL:HG11	2.17	0.44
30:9:243:LEU:O	30:9:311:ARG:N	2.48	0.44
30:9:638:LYS:O	30:9:638:LYS:HG3	2.17	0.44
8:H:94:PHE:CD1	28:1:114:LEU:HD13	2.52	0.44
17:Q:10:ARG:HB3	17:Q:30:LEU:HD21	2.00	0.44
24:X:50:ARG:NH2	24:X:96:GLU:OE2	2.47	0.44
30:9:265:ARG:O	30:9:269:TRP:CD1	2.71	0.44
24:X:276:ARG:NH2	24:X:286:GLU:OE1	2.51	0.44
25:Y:258:ILE:O	29:4:324:VAL:HG21	2.17	0.44
22:V:264:GLU:HG3	22:V:337:LEU:HD21	1.99	0.44
30:9:219:TYR:O	30:9:246:LEU:N	2.43	0.44
30:9:359:LEU:HD11	30:9:375:ALA:HB2	1.99	0.44
1:A:986:G:HO2'	1:A:987:A:P	2.39	0.44
1:A:1429:C:OP1	7:G:388:ARG:NH1	2.50	0.44
5:E:26:ILE:HG21	21:U:173:LEU:CD1	2.47	0.44
6:F:193:ASP:OD1	6:F:194:LYS:N	2.51	0.44
29:4:331:ASN:OD1	29:4:334:THR:OG1	2.35	0.44
30:9:336:ARG:NH1	30:9:337:TYR:CE1	2.86	0.44
11:K:67:LEU:HD11	25:Y:379:TYR:HE2	1.83	0.44
27:0:163:SER:HA	27:0:191:LEU:O	2.18	0.44
29:4:285:ASN:HB2	29:4:287:LEU:HD12	1.99	0.44
29:4:646:THR:HG23	29:4:663:LEU:HD22	1.99	0.44
2:B:159:ALA:CB	2:B:166:ALA:HB2	2.48	0.44
7:G:346:LEU:HD11	7:G:350:LYS:HE3	2.00	0.44
28:1:293:LYS:O	28:1:297:VAL:HG23	2.17	0.44
9:I:153:GLY:O	9:I:158:ARG:NH1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:93:THR:HG21	24:X:365:TRP:CZ3	2.53	0.43
13:M:19:ILE:HB	13:M:83:LEU:HD23	2.00	0.43
24:X:151:LEU:CD2	24:X:247:LEU:HD22	2.48	0.43
29:4:131:ASP:OD2	29:4:136:HIS:ND1	2.50	0.43
10:J:78:ARG:CB	10:J:118:LEU:HD11	2.48	0.43
29:4:320:LEU:O	29:4:324:VAL:HG23	2.18	0.43
30:9:220:MET:HE2	30:9:354:LEU:HD23	1.99	0.43
14:N:58:CYS:SG	14:N:81:LEU:HD22	2.57	0.43
30:9:191:ALA:HB3	30:9:388:LEU:CD2	2.49	0.43
20:T:92:THR:O	20:T:92:THR:HG22	2.19	0.43
3:C:96:MET:HB2	3:C:108:LEU:HD11	2.00	0.43
5:E:15:ARG:NH2	21:U:182:ASP:OD1	2.52	0.43
5:E:17:GLU:OE1	5:E:17:GLU:N	2.48	0.43
11:K:79:PRO:O	11:K:82:SER:OG	2.32	0.43
22:V:208:LEU:HD13	22:V:226:TYR:CD1	2.54	0.43
1:A:1017:A:O3'	16:P:104:GLN:NE2	2.52	0.43
3:C:116:GLN:HE21	25:Y:310:LEU:HD11	1.82	0.43
9:I:151:VAL:HG22	9:I:158:ARG:NH1	2.33	0.43
30:9:351:LYS:NZ	30:9:497:THR:O	2.45	0.43
9:I:99:VAL:HG12	9:I:107:LEU:HD12	2.01	0.42
22:V:360:VAL:HG13	22:V:364:LEU:HD22	2.01	0.42
30:9:194:LEU:HD23	30:9:387:LEU:CD2	2.49	0.42
4:D:243:VAL:HG12	4:D:245:VAL:HG13	2.01	0.42
9:I:172:VAL:O	17:Q:14:VAL:HG21	2.18	0.42
21:U:71:ARG:O	21:U:75:VAL:HG23	2.20	0.42
24:X:126:LEU:HD23	24:X:343:ILE:HB	2.00	0.42
1:A:691:A:N7	1:A:716:U:O2'	2.51	0.42
16:P:135:VAL:HG11	21:U:191:ILE:O	2.18	0.42
27:0:61:GLU:HB2	27:0:137:HIS:O	2.20	0.42
1:A:769:G:N2	1:A:772:A:OP2	2.50	0.42
18:R:209:ILE:HD12	18:R:214:ASN:HB3	2.01	0.42
30:9:380:TRP:HB2	30:9:387:LEU:HD12	2.01	0.42
30:9:365:THR:HG22	30:9:393:CYS:SG	2.59	0.42
8:H:155:VAL:HG21	28:1:129:PHE:CB	2.49	0.42
15:O:137:ALA:HB3	15:O:138:PRO:HD3	2.01	0.42
21:U:190:ALA:O	21:U:198:VAL:N	2.53	0.42
30:9:315:LEU:N	30:9:315:LEU:HD12	2.35	0.42
12:L:82:ILE:O	12:L:85:VAL:HG22	2.19	0.42
30:9:204:LEU:HB3	30:9:383:THR:HG21	2.02	0.42
13:M:29:ARG:CD	13:M:57:LEU:HD12	2.49	0.42
19:S:96:CYS:O	19:S:100:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:236:LEU:CD1	22:V:327:LEU:HD21	2.49	0.42
27:0:37:ASP:O	27:0:41:LEU:N	2.48	0.42
29:4:427:ARG:NE	29:4:467:LEU:HD21	2.34	0.42
29:4:542:PRO:O	29:4:546:VAL:HG23	2.20	0.42
1:A:1421:G:H5"	1:A:1422:G:OP1	2.19	0.42
3:C:51:VAL:HG22	3:C:165:LYS:O	2.20	0.42
3:C:58:ALA:HB1	3:C:59:PRO:HD2	2.00	0.42
8:H:172:VAL:HG13	8:H:172:VAL:O	2.20	0.42
24:X:75:LEU:HD11	24:X:97:ALA:HB3	2.02	0.42
29:4:461:PHE:CE2	29:4:465:ILE:HD11	2.54	0.42
1:A:1017:A:O2'	16:P:108:THR:OG1	2.34	0.41
4:D:323:ILE:HG21	4:D:349:LEU:HD23	2.02	0.41
9:I:136:ALA:HB2	9:I:165:LEU:HA	2.02	0.41
10:J:78:ARG:HB2	10:J:118:LEU:HD11	2.02	0.41
22:V:226:TYR:CE2	22:V:282:VAL:HG21	2.55	0.41
24:X:138:LEU:O	24:X:142:ILE:HG12	2.20	0.41
26:Z:18:LEU:HD21	28:1:232:GLU:HG3	2.02	0.41
8:H:184:ILE:O	8:H:184:ILE:HG22	2.19	0.41
19:S:113:ASP:OD1	19:S:114:GLU:N	2.54	0.41
22:V:266:VAL:HG11	22:V:275:LEU:HG	2.02	0.41
29:4:166:VAL:HG23	29:4:167:LYS:N	2.34	0.41
30:9:250:VAL:HG23	30:9:315:LEU:HD23	2.02	0.41
30:9:347:THR:O	30:9:348:ASN:CB	2.68	0.41
1:A:692:C:H4'	30:9:672:LYS:HB2	2.02	0.41
7:G:353:CYS:SG	7:G:370:LEU:HD21	2.60	0.41
8:H:104:ILE:HG21	8:H:145:LEU:HD23	2.00	0.41
12:L:193:PRO:HG2	12:L:196:TYR:CE1	2.55	0.41
22:V:219:VAL:HG22	22:V:355:LEU:HD23	2.02	0.41
30:9:248:ASN:OD1	30:9:249:LYS:N	2.53	0.41
30:9:387:LEU:HD13	30:9:496:ASP:O	2.20	0.41
1:A:1132:U:H2'	1:A:1133:C:C6	2.55	0.41
15:O:185:SER:O	18:R:183:LYS:NZ	2.52	0.41
16:P:123:THR:HG23	17:Q:4:HIS:CE1	2.55	0.41
29:4:631:VAL:HG21	29:4:649:VAL:HG21	2.02	0.41
1:A:1035:U:OP1	5:E:4:TYR:OH	2.24	0.41
1:A:1368:U:O4	1:A:1383:A:O2'	2.20	0.41
18:R:191:ARG:HG3	18:R:204:ILE:HG23	2.01	0.41
4:D:209:GLY:HA3	4:D:213:GLU:HB2	2.03	0.41
24:X:142:ILE:HD13	24:X:259:LEU:HD21	2.03	0.41
24:X:394:HIS:CE1	24:X:398:LEU:HD11	2.56	0.41
1:A:986:G:H2'	1:A:987:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:356:VAL:HG23	7:G:361:VAL:HG23	2.01	0.41
16:P:78:GLN:NE2	21:U:190:ALA:HB2	2.35	0.41
21:U:192:THR:HG22	21:U:198:VAL:HG23	1.99	0.41
28:1:113:HIS:CD2	28:1:114:LEU:HG	2.55	0.41
1:A:1271:C:N4	1:A:1320:G:O2'	2.54	0.41
2:B:159:ALA:HB2	2:B:166:ALA:HB2	2.02	0.41
2:B:179:ALA:HB2	2:B:189:LEU:HD21	2.03	0.41
4:D:154:VAL:HG21	29:4:108:LEU:HD22	2.03	0.41
5:E:41:ASN:HB3	21:U:180:ALA:O	2.20	0.41
16:P:67:LEU:HD12	16:P:99:LEU:CD1	2.51	0.41
29:4:641:ILE:O	29:4:645:LEU:N	2.44	0.41
30:9:333:ARG:O	30:9:333:ARG:HG2	2.21	0.41
30:9:353:THR:OG1	37:9:801:GDP:H5"	2.21	0.41
1:A:1208:U:H2'	1:A:1209:C:O4'	2.20	0.41
12:L:213:VAL:O	12:L:217:THR:HG23	2.21	0.41
27:0:91:GLU:HB2	27:0:121:LYS:HA	2.02	0.41
29:4:309:PHE:CZ	29:4:352:PRO:HG2	2.56	0.41
4:D:290:ILE:HD12	4:D:292:HIS:O	2.20	0.41
18:R:238:ASP:OD1	18:R:238:ASP:N	2.47	0.41
25:Y:347:ILE:HD13	25:Y:394:PHE:HD2	1.85	0.41
30:9:219:TYR:HA	30:9:344:VAL:O	2.21	0.41
1:A:1356:A:H2'	1:A:1357:A:O5'	2.20	0.40
4:D:258:ILE:HD11	4:D:343:LEU:CD1	2.51	0.40
10:J:81:CYS:HB3	10:J:95:ILE:HD11	2.02	0.40
22:V:29:LEU:N	22:V:153:LYS:HZ3	2.19	0.40
1:A:1310:C:HO2'	1:A:1311:C:H5	1.66	0.40
4:D:132:ILE:CG2	4:D:144:LEU:HD11	2.52	0.40
16:P:141:ARG:O	16:P:142:GLU:C	2.59	0.40
18:R:219:TYR:O	18:R:256:ARG:NH2	2.53	0.40
29:4:526:ASP:N	29:4:526:ASP:OD1	2.55	0.40
30:9:272:CYS:CB	30:9:279:LEU:HD21	2.51	0.40
1:A:1053:A:N1	1:A:1100:C:O2'	2.42	0.40
1:A:1454:G:OP2	7:G:377:ARG:NH1	2.54	0.40
4:D:203:LEU:HD11	4:D:222:ILE:HG12	2.04	0.40
15:O:214:SER:OG	22:V:319:ILE:HG23	2.20	0.40
22:V:236:LEU:HD12	22:V:290:LEU:HD13	2.02	0.40
25:Y:250:ILE:HG23	29:4:395:ASP:OD2	2.21	0.40
30:9:179:CYS:SG	30:9:180:GLN:N	2.92	0.40
30:9:309:VAL:HG22	30:9:310:VAL:N	2.37	0.40
17:Q:83:PRO:HA	23:W:108:VAL:HG21	2.03	0.40
24:X:81:HIS:CD2	24:X:156:PRO:HD3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:194:LEU:HD12	29:4:198:TYR:CD2	2.56	0.40
8:H:155:VAL:HG21	28:1:129:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
3	C	124/167 (74%)	122 (98%)	2 (2%)	0	100	100
4	D	336/430 (78%)	330 (98%)	6 (2%)	0	100	100
5	E	107/125 (86%)	106 (99%)	1 (1%)	0	100	100
6	F	193/242 (80%)	191 (99%)	2 (1%)	0	100	100
7	G	309/396 (78%)	306 (99%)	3 (1%)	0	100	100
8	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	19	54
9	I	128/194 (66%)	123 (96%)	5 (4%)	0	100	100
10	J	106/138 (77%)	105 (99%)	1 (1%)	0	100	100
11	K	99/128 (77%)	99 (100%)	0	0	100	100
12	L	162/257 (63%)	160 (99%)	2 (1%)	0	100	100
13	M	117/137 (85%)	117 (100%)	0	0	100	100
14	N	108/130 (83%)	108 (100%)	0	0	100	100
15	O	191/258 (74%)	190 (100%)	1 (0%)	0	100	100
16	P	95/142 (67%)	92 (97%)	2 (2%)	1 (1%)	12	44
17	Q	79/87 (91%)	77 (98%)	2 (2%)	0	100	100
18	R	293/360 (81%)	289 (99%)	4 (1%)	0	100	100
19	S	133/190 (70%)	132 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
21	U	174/205 (85%)	174 (100%)	0	0	100	100
22	V	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
23	W	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
24	X	350/398 (88%)	348 (99%)	2 (1%)	0	100	100
25	Y	134/395 (34%)	133 (99%)	1 (1%)	0	100	100
26	Z	98/106 (92%)	98 (100%)	0	0	100	100
27	0	213/215 (99%)	212 (100%)	1 (0%)	0	100	100
28	1	276/323 (85%)	274 (99%)	2 (1%)	0	100	100
29	4	586/689 (85%)	581 (99%)	5 (1%)	0	100	100
30	9	407/698 (58%)	399 (98%)	8 (2%)	0	100	100
31	a	12/343 (4%)	12 (100%)	0	0	100	100
All	All	5813/8024 (72%)	5752 (99%)	59 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	126	ILE
16	P	64	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	198/249 (80%)	198 (100%)	0	100	100
3	C	111/143 (78%)	111 (100%)	0	100	100
4	D	283/357 (79%)	283 (100%)	0	100	100
5	E	92/107 (86%)	92 (100%)	0	100	100
6	F	176/209 (84%)	176 (100%)	0	100	100
7	G	272/342 (80%)	272 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	99/146 (68%)	99 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	153/226 (68%)	153 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	174/230 (76%)	174 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100
17	Q	74/78 (95%)	74 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100
19	S	116/164 (71%)	116 (100%)	0	100	100
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	V	325/364 (89%)	325 (100%)	0	100	100
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	311 (100%)	0	100	100
25	Y	128/357 (36%)	128 (100%)	0	100	100
26	Z	90/95 (95%)	90 (100%)	0	100	100
27	0	188/188 (100%)	188 (100%)	0	100	100
28	1	256/291 (88%)	256 (100%)	0	100	100
29	4	527/609 (86%)	527 (100%)	0	100	100
30	9	357/600 (60%)	357 (100%)	0	100	100
31	a	14/288 (5%)	14 (100%)	0	100	100
All	All	5195/6963 (75%)	5195 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	201	ASN
3	C	116	GLN

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Mol	Chain	Res	Type
4	D	415	GLN
7	G	77	GLN
9	I	104	ASN
9	I	141	GLN
12	L	162	GLN
15	O	160	HIS
16	P	78	GLN
17	Q	4	HIS
20	T	101	HIS
22	V	145	ASN
24	X	164	ASN
30	9	492	HIS
30	9	636	ASN
30	9	669	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	795/955 (83%)	89 (11%)	3 (0%)

All (89) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	651	A
1	A	680	U
1	A	688	A
1	A	704	U
1	A	721	U
1	A	737	C
1	A	738	A
1	A	739	C
1	A	740	G
1	A	753	A
1	A	761	A
1	A	766	G
1	A	777	G
1	A	791	G
1	A	796	G
1	A	830	U
1	A	832	U
1	A	835	C

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Mol	Chain	Res	Type
1	A	836	A
1	A	860	A
1	A	868	C
1	A	871	A
1	A	890	C
1	A	892	A
1	A	893	G
1	A	919	A
1	A	938	A
1	A	939	A
1	A	942	A
1	A	956	C
1	A	958	C
1	A	967	A
1	A	987	A
1	A	988	G
1	A	993	A
1	A	1001	C
1	A	1002	C
1	A	1015	A
1	A	1019	A
1	A	1020	C
1	A	1042	U
1	A	1046	A
1	A	1047	A
1	A	1049	A
1	A	1098	C
1	A	1105	C
1	A	1106	C
1	A	1107	U
1	A	1116	A
1	A	1118	A
1	A	1119	U
1	A	1121	A
1	A	1126	A
1	A	1151	C
1	A	1152	A
1	A	1154	A
1	A	1167	A
1	A	1187	U
1	A	1188	A
1	A	1189	U

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Mol	Chain	Res	Type
1	A	1190	C
1	A	1223	C
1	A	1225	C
1	A	1229	U
1	A	1247	G
1	A	1248	C
1	A	1251	A
1	A	1271	C
1	A	1273	G
1	A	1284	U
1	A	1285	G
1	A	1290	C
1	A	1291	U
1	A	1293	C
1	A	1326	A
1	A	1327	G
1	A	1343	A
1	A	1356	A
1	A	1357	A
1	A	1367	A
1	A	1376	C
1	A	1378	C
1	A	1390	A
1	A	1405	C
1	A	1421	G
1	A	1422	G
1	A	1447	G
1	A	1462	G
1	A	1481	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	986	G
1	A	1046	A
1	A	1152	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	5F0	I	184	9	8,8,9	0.58	0	7,9,11	1.13	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	5F0	I	184	9	-	1/9/9/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	184	5F0	O-C-CB	-2.70	117.55	125.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	184	5F0	OD1-C1-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 59 ligands modelled in this entry, 54 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	ATP	X	501	32	26,33,33	0.76	0	31,52,52	0.70	0
37	GDP	X	502	-	24,30,30	0.90	2 (8%)	30,47,47	0.60	0
37	GDP	9	801	-	24,30,30	0.88	1 (4%)	30,47,47	0.71	0
35	FES	T	201	20,13	0,4,4	-	-	-		
35	FES	P	201	16,5	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	X	501	32	-	0/18/38/38	0/3/3/3
37	GDP	X	502	-	-	1/12/32/32	0/3/3/3
37	GDP	9	801	-	-	4/12/32/32	0/3/3/3
35	FES	T	201	20,13	-	-	0/1/1/1
35	FES	P	201	16,5	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	502	GDP	C5-C6	-2.25	1.42	1.47
37	9	801	GDP	C5-C6	-2.24	1.42	1.47
37	X	502	GDP	C8-N7	-2.02	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	9	801	GDP	C5'-O5'-PA-O1A
37	9	801	GDP	C4'-C5'-O5'-PA
37	9	801	GDP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
37	9	801	GDP	O4'-C4'-C5'-O5'
37	X	502	GDP	C4'-C5'-O5'-PA

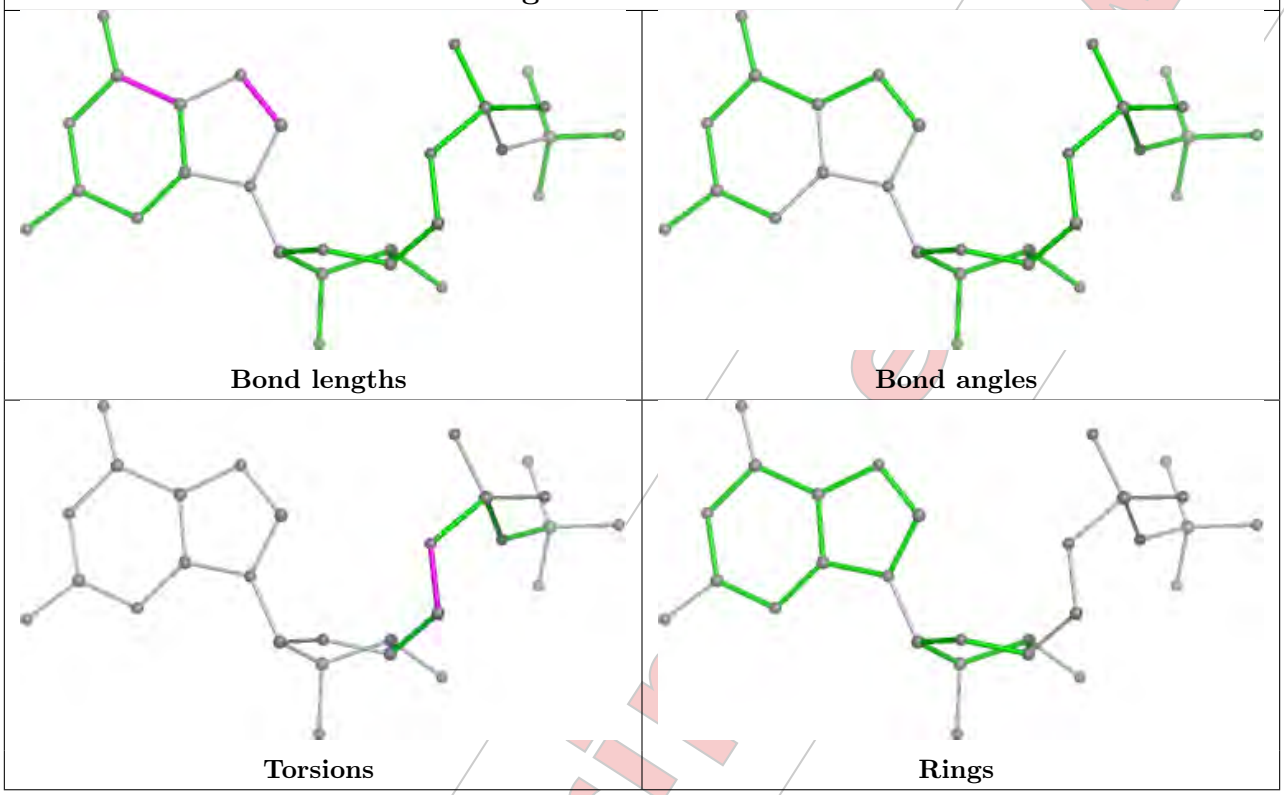
There are no ring outliers.

3 monomers are involved in 5 short contacts:

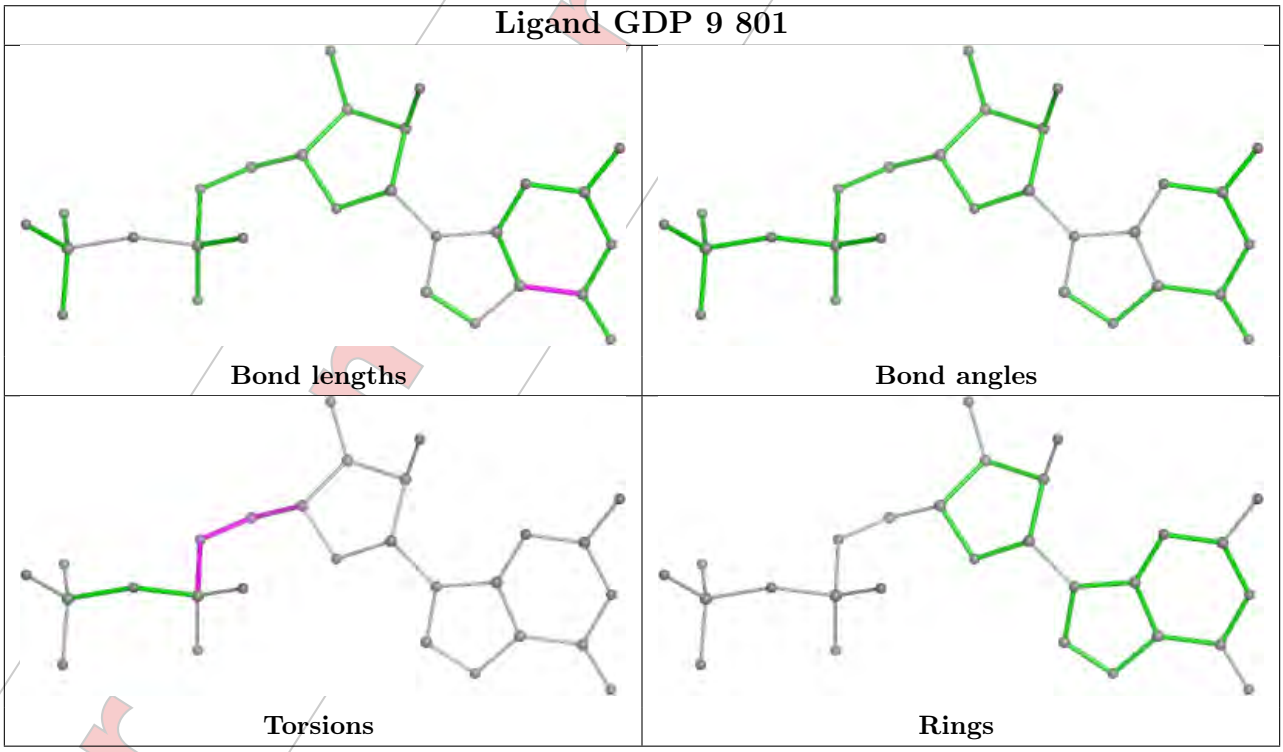
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	X	502	GDP	2	0
37	9	801	GDP	1	0
35	P	201	FES	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP X 502



Ligand GDP 9 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

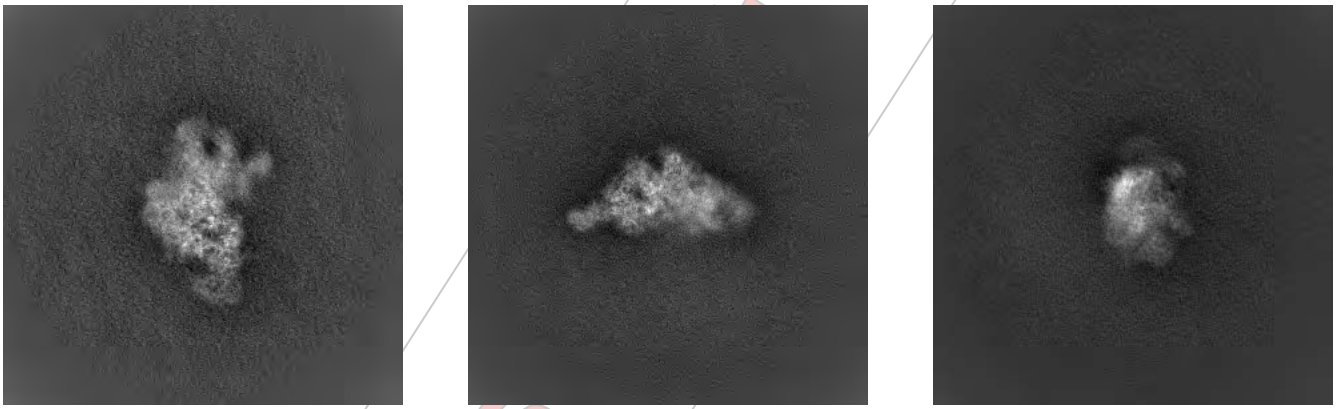
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51876. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

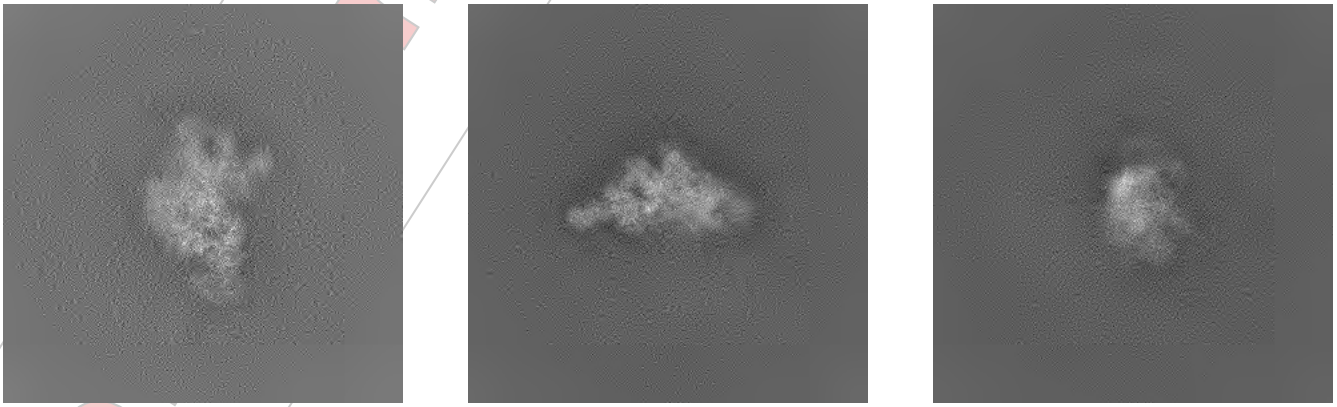
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

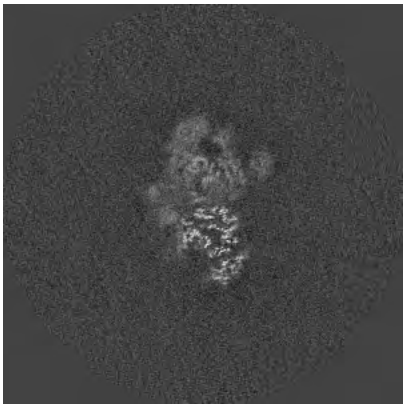


X Y Z

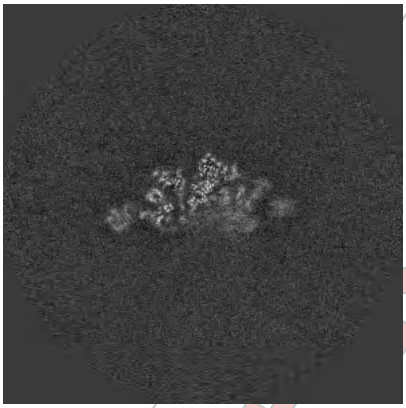
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

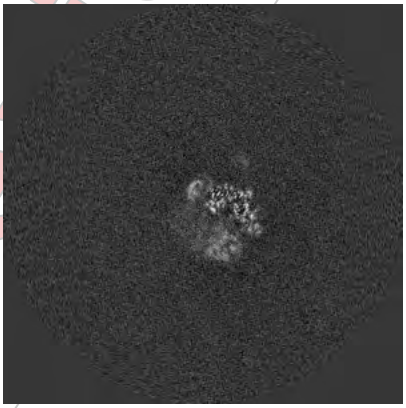
6.2.1 Primary map



X Index: 300

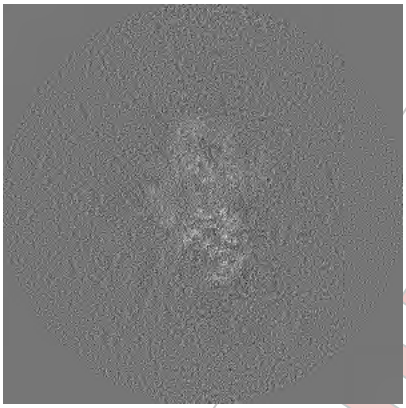


Y Index: 300

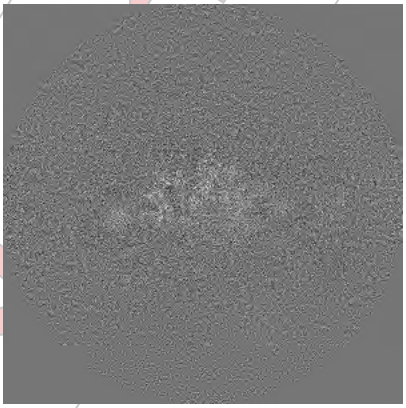


Z Index: 300

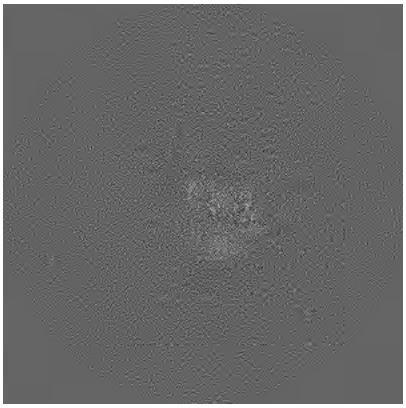
6.2.2 Raw map



X Index: 300



Y Index: 300

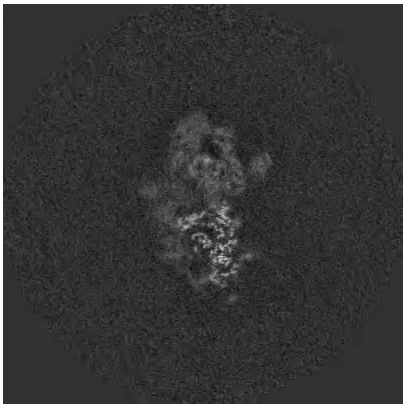


Z Index: 300

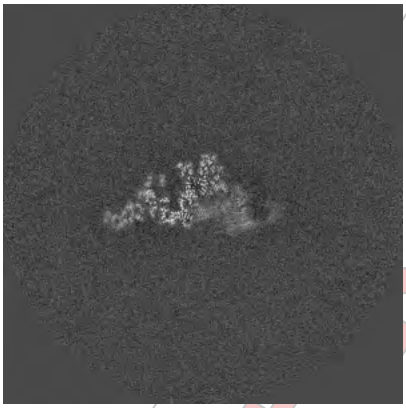
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

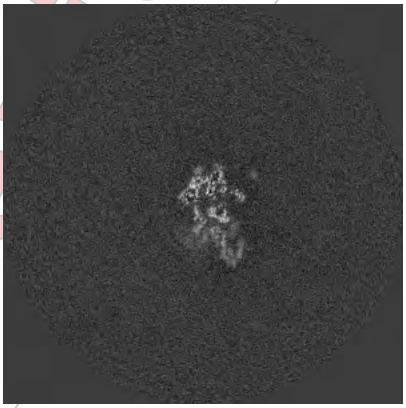
6.3.1 Primary map



X Index: 294

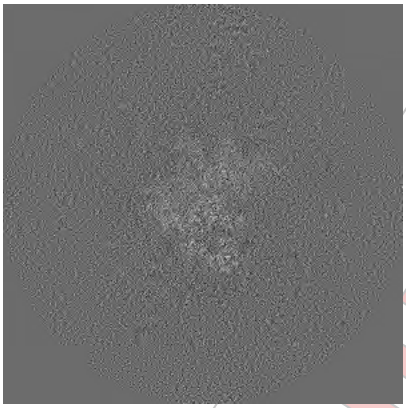


Y Index: 313

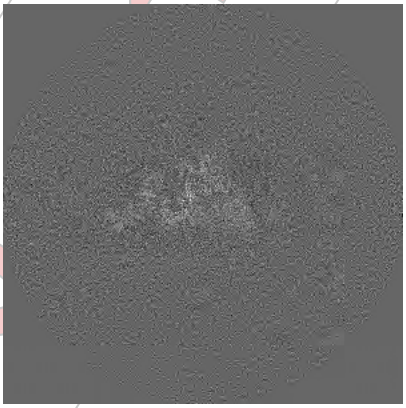


Z Index: 273

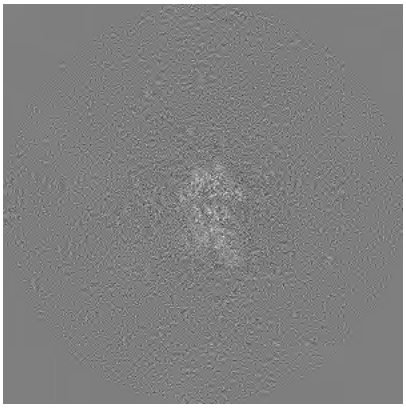
6.3.2 Raw map



X Index: 319



Y Index: 312

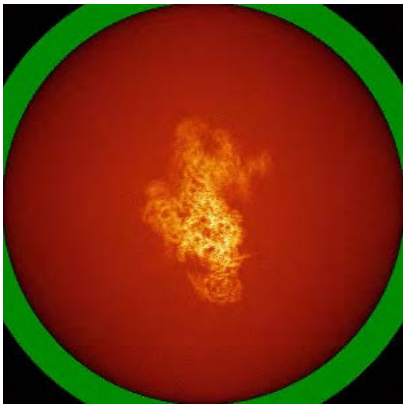


Z Index: 276

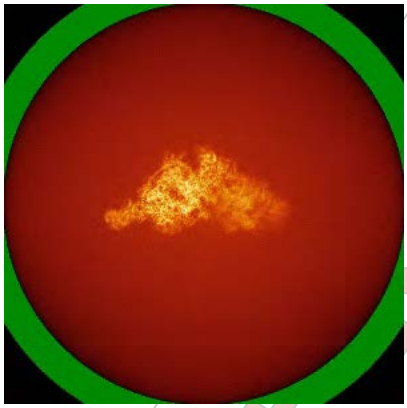
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

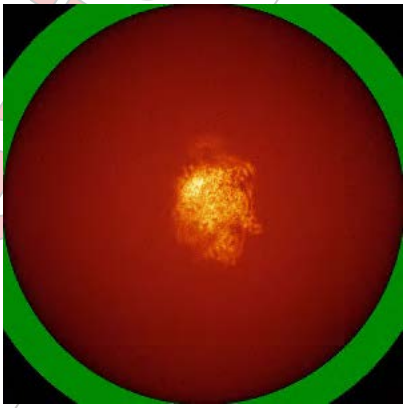
6.4.1 Primary map



X

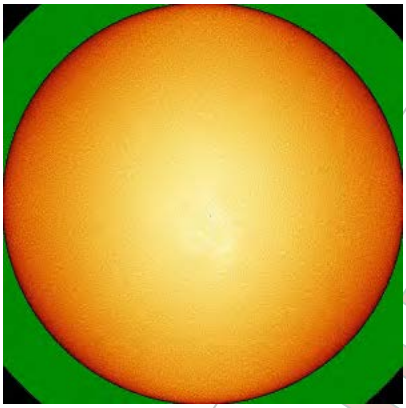


Y

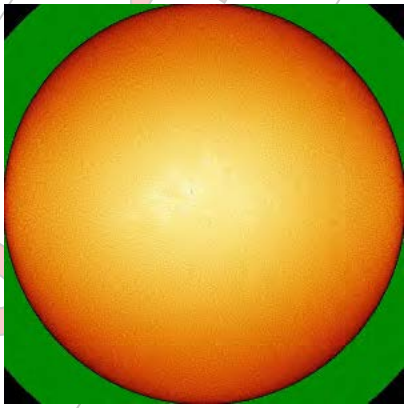


Z

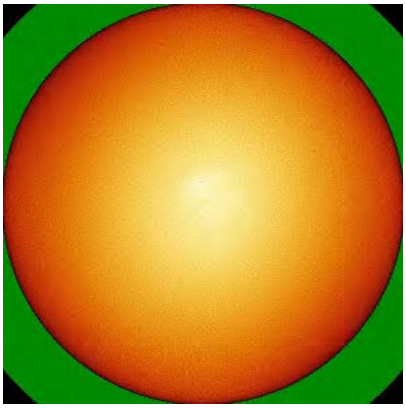
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

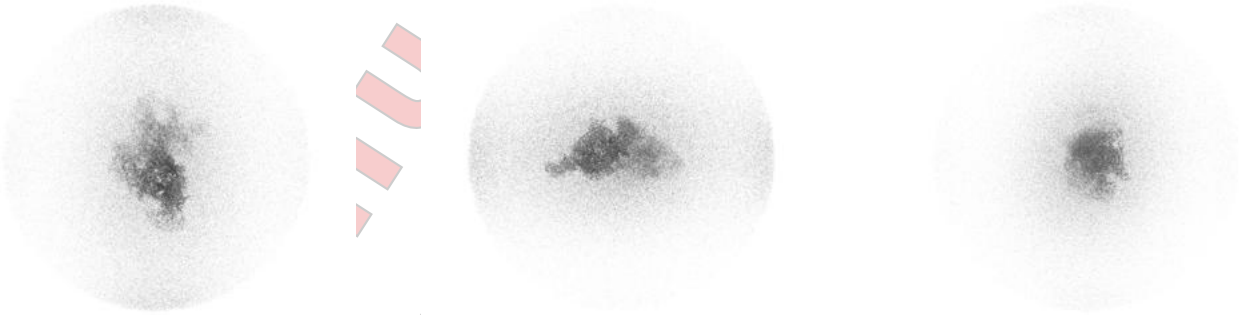
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

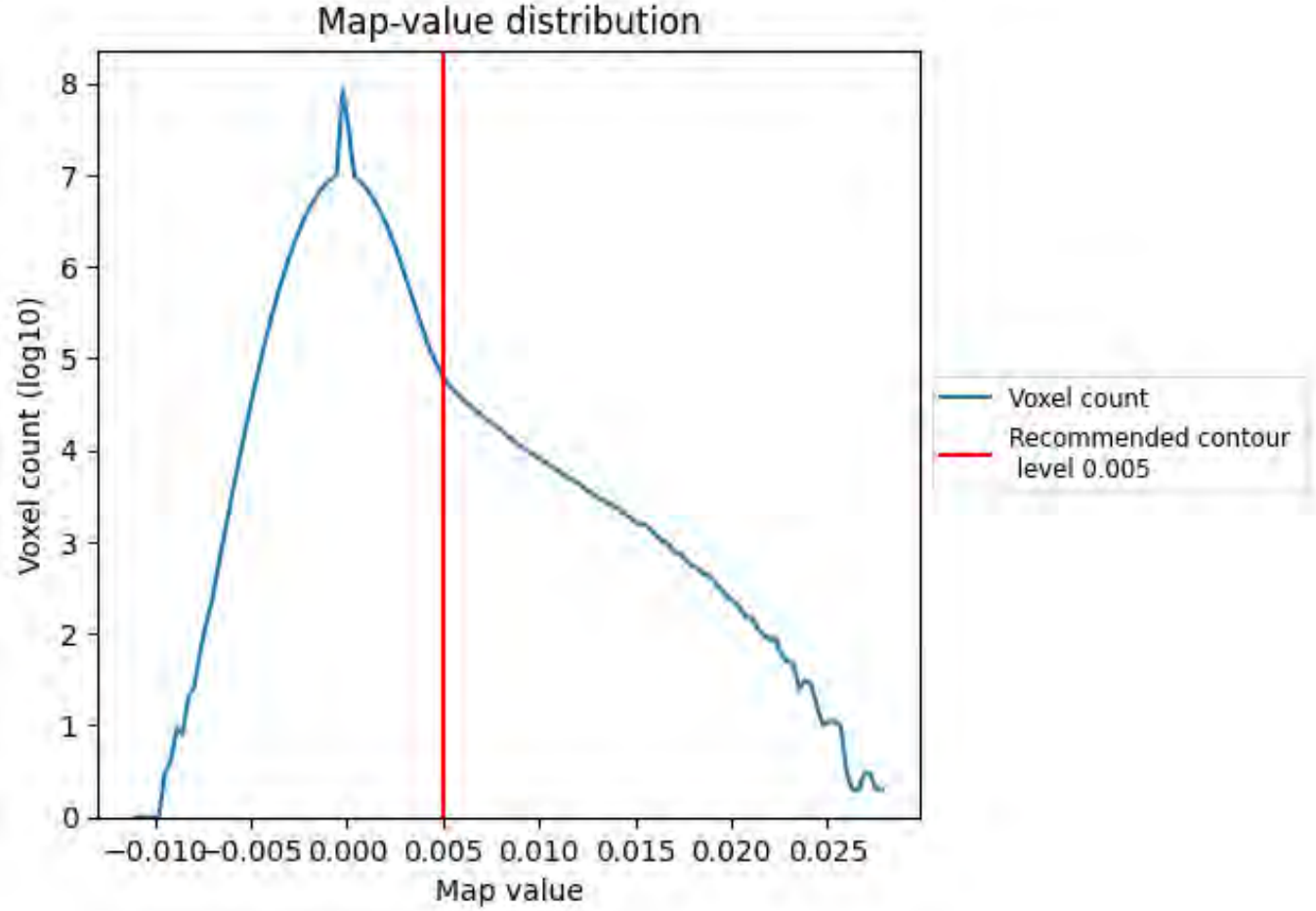
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

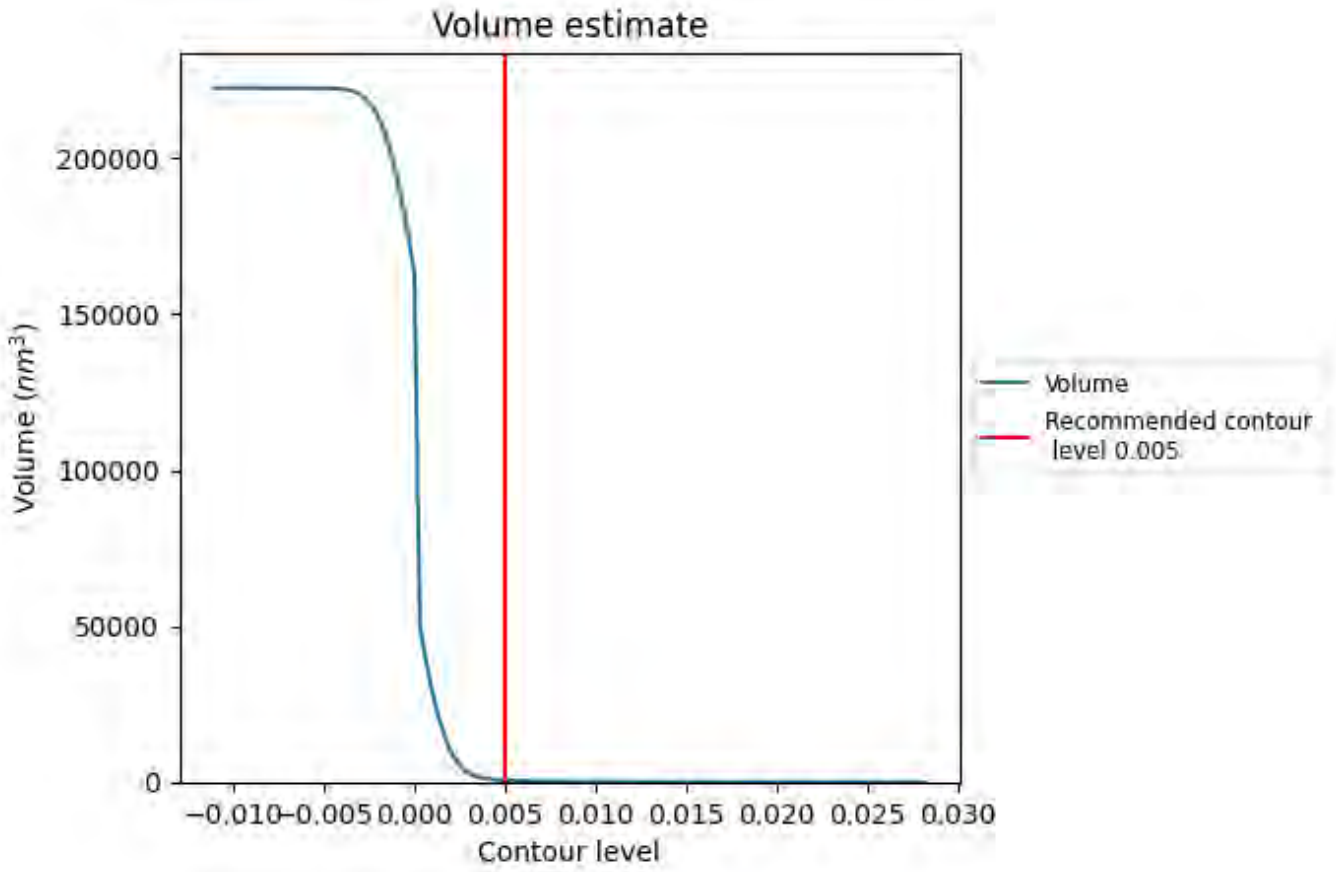
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

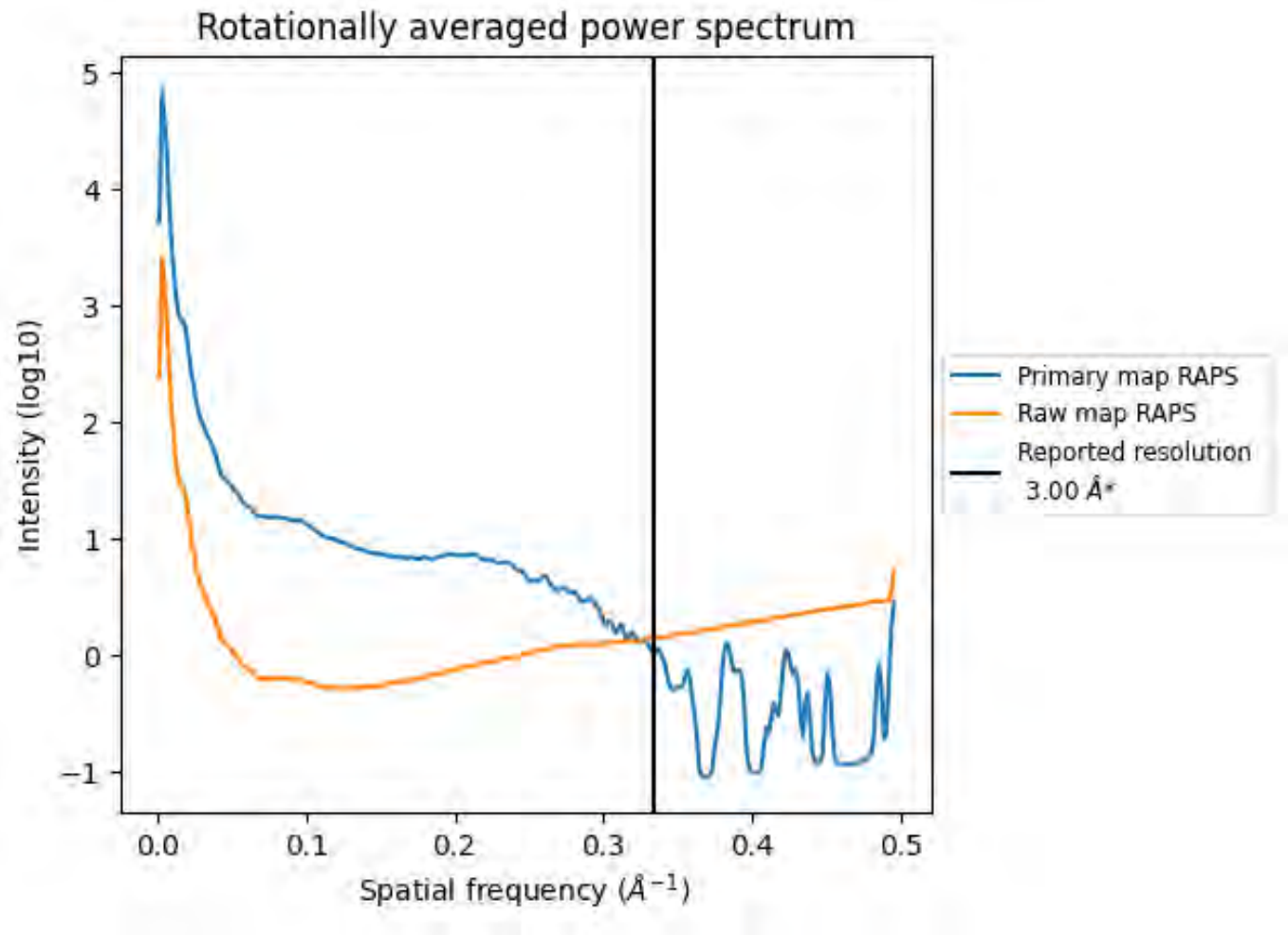
7.2 Volume estimate (i)



The volume at the recommended contour level is 524 nm^3; this corresponds to an approximate mass of 473 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

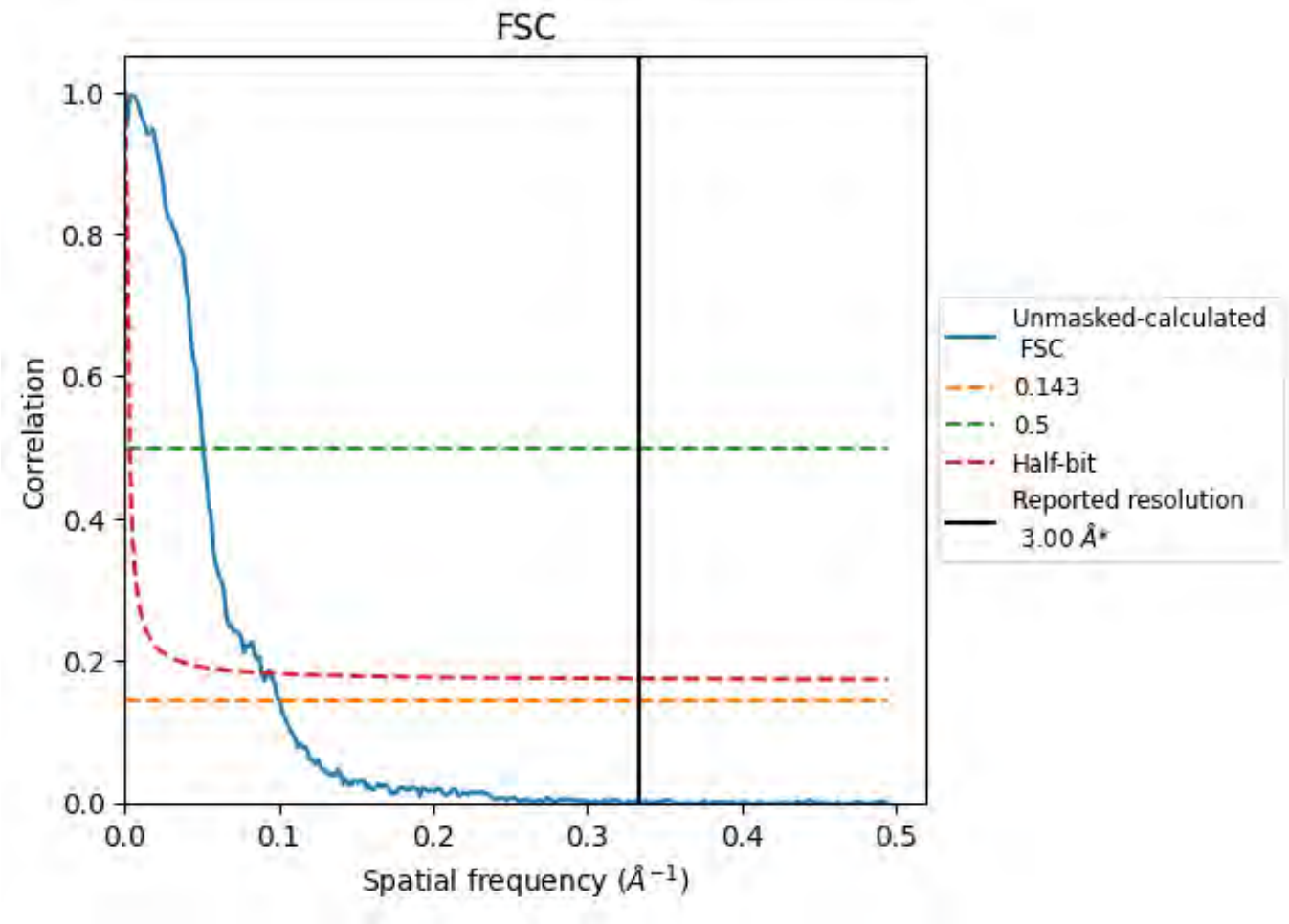


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

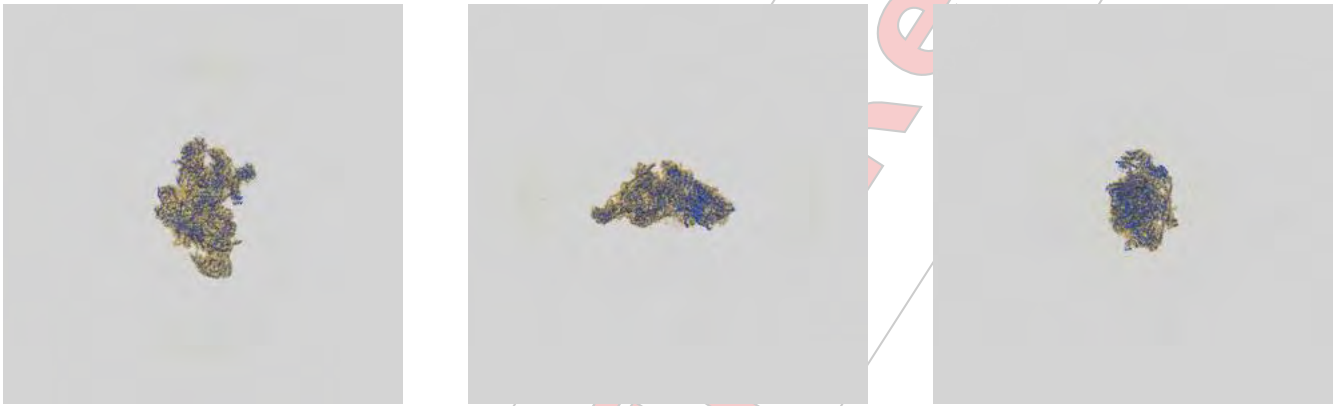
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.93	19.72	11.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.93 differs from the reported value 3.0 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51876 and PDB model 9H54. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay



X Y Z

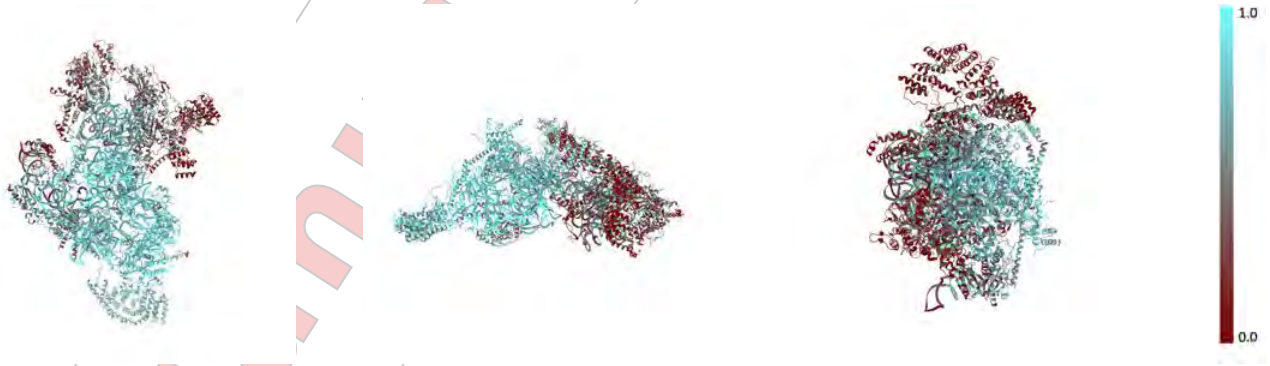
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

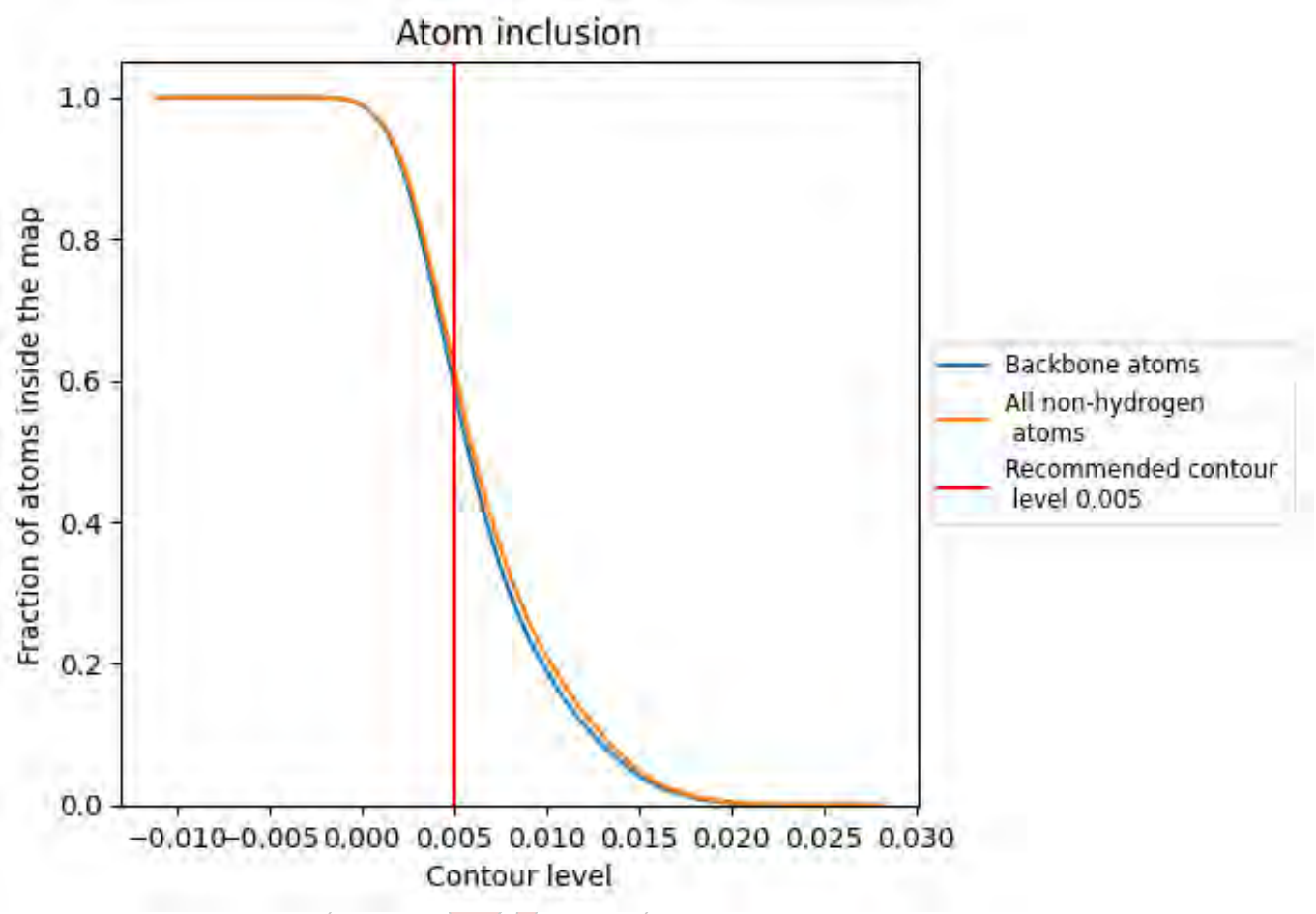
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6190	0.2570
0	0.8020	0.4130
1	0.3710	0.0920
4	0.2030	0.0480
9	0.3870	0.1340
A	0.7740	0.3100
B	0.8330	0.4570
C	0.4890	0.1950
D	0.6430	0.3690
E	0.5620	0.1470
F	0.3420	0.1070
G	0.5900	0.2190
H	0.4320	0.1430
I	0.3470	0.0650
J	0.7680	0.4050
K	0.4980	0.1520
L	0.6420	0.2710
M	0.8740	0.4970
N	0.8270	0.4510
O	0.8700	0.4720
P	0.5660	0.1690
Q	0.4230	0.1520
R	0.8380	0.4430
S	0.7680	0.3680
T	0.8330	0.4600
U	0.7290	0.3000
V	0.6920	0.2570
W	0.7560	0.3800
X	0.2770	0.0850
Y	0.2430	0.0890
Z	0.3300	0.0690
a	0.1300	-0.0010

Full wwPDB EM Validation Report ⓘ

Oct 25, 2024 – 01:16 pm BST

PDB ID	:	9H55
EMDB ID	:	EMD-51877
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit in complex with NOA1 and TFB1M (state A3)
Deposited on	:	2024-10-22
Resolution	:	3.40 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

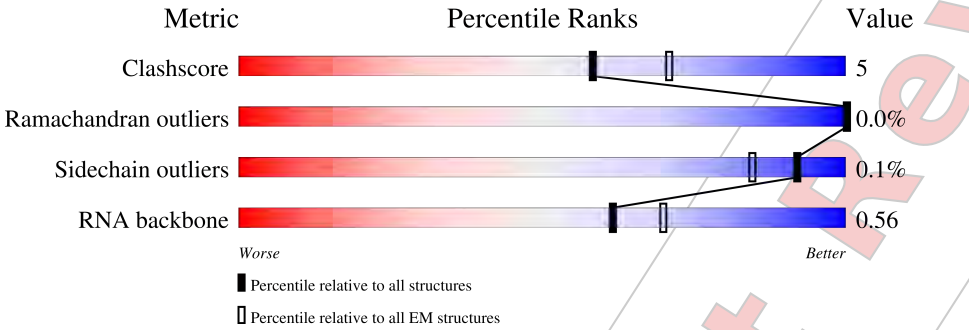
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	955	20% 63% 23% • 11%
2	B	296	• 68% 8% 24%
3	C	167	61% 65% 14% 21%
4	D	430	21% 69% 8% 23%
5	E	125	6% 75% 12% 13%

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Mol	Chain	Length	Quality of chain
6	F	242	78% 77% 6% 17%
7	G	396	45% 73% 6% 21%
8	H	201	57% 62% 8% 30%
9	I	194	27% 61% 9% 29%
10	J	138	72% 6% 22%
11	K	128	61% 71% 8% 21%
12	L	257	6% 57% 7% 36%
13	M	137	81% 6% 13%
14	N	130	72% 13% 15%
15	O	258	71% 25%
16	P	142	6% 61% 7% 32%
17	Q	87	21% 95% 5%
18	R	360	76% 6% 18%
19	S	190	62% 9% 29%
20	T	173	90% 7%
21	U	205	78% 8% 14%
22	V	414	74% 14% 13%
23	W	187	44% 10% 47%
24	X	398	84% 77% 11% 12%
25	Y	395	32% 29% 5% 66%
26	Z	106	77% 86% 5% 9%
27	0	215	5% 87% 13%
28	1	323	80% 78% 8% 14%
29	4	689	83% 73% 12% 15%
30	9	698	21% 46% 13% 41%

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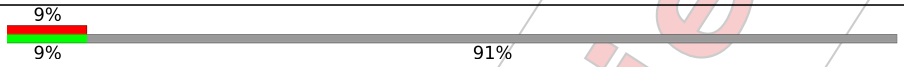
Mol	Chain	Length	Quality of chain
31	5	346	
32	a	343	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 129555 atoms, of which 60710 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	850	27223	8095	9165	3258	5855	850	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	225	3654	1164	1826	331	323	10	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	132	2179	699	1096	195	185	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	332	5349	1660	2705	496	475	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	109	1747	544	882	158	159	4	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	201	3405	1071	1733	298	292	11	2	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	313	5147	1637	2570	456	470	14	0	0

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	140	2343	745	1191	194	210	3	0	0

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	137	2086	642	1066	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	108	1731	521	892	169	143	6	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	101	1751	537	889	179	141	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	164	2851	882	1467	256	239	7	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1914	594	972	185	157	6		

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	110	Total	C	H	N	O	S	0	0
			1801	562	933	156	147	3		

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	193	Total	C	H	N	O	S	0	0
			3158	1014	1566	294	277	7		

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	97	Total	C	H	N	O	S	0	0
			1590	501	809	134	138	8		

- Molecule 17 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	87	Total	C	H	N	O	S	0	0
			1504	460	760	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	295	Total	C	H	N	O	S	0	0
			4845	1533	2436	413	455	8		

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	135	Total	C	H	N	O	S	0	0
			2228	716	1117	198	196	1		

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	176	Total	C	H	N	O	S	0	0
			2993	916	1505	301	267	4		

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	362	Total	C	H	N	O	S	0	0
			5941	1904	2972	495	558	12		

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	100	Total	C	H	N	O	S	0	0
			1595	498	806	141	146	4		

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	350	Total	C	H	N	O	S	0	0
			5678	1813	2842	497	515	11		

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	134	Total	C	H	N	O	S	0	0
			2236	736	1100	191	207	2		

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	96	Total	C	H	N	O	S	0	0
			1638	517	828	145	144	4		

- Molecule 27 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	0	215	Total	C	H	N	O	S	0	0
			3589	1130	1802	339	313	5		

- Molecule 28 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	277	Total	C	H	N	O	S	0	0
			4526	1424	2281	382	428	11		

- Molecule 29 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	586	Total	C	H	N	O	S	0	0
			9502	3035	4761	803	875	28		

- Molecule 30 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	9	415	Total	C	H	N	O	S	0	0
			6656	2108	3378	574	584	12		

- Molecule 31 is a protein called Dimethyladenosine transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	5	319	Total	C	H	N	O	S	0	0
			5229	1648	2661	458	451	11		

- Molecule 32 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	32	Total	C	H	N	O	0	0
			520	162	271	42	45		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
33	A	39	Total Mg 39 39	0
33	B	1	Total Mg 1 1	0
33	X	1	Total Mg 1 1	0

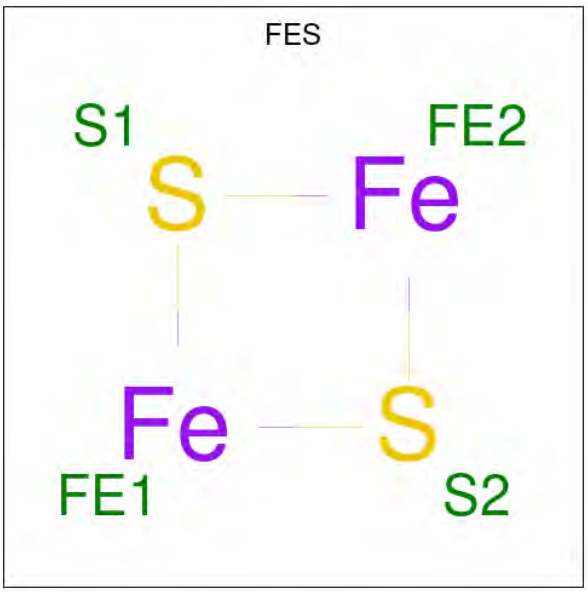
- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
34	A	10	Total K 10 10	0

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

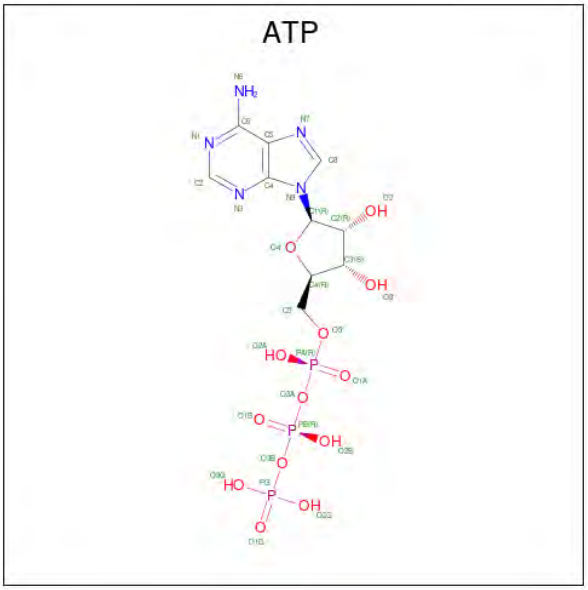
Mol	Chain	Residues	Atoms	AltConf
35	O	1	Total Zn 1 1	0

- Molecule 36 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



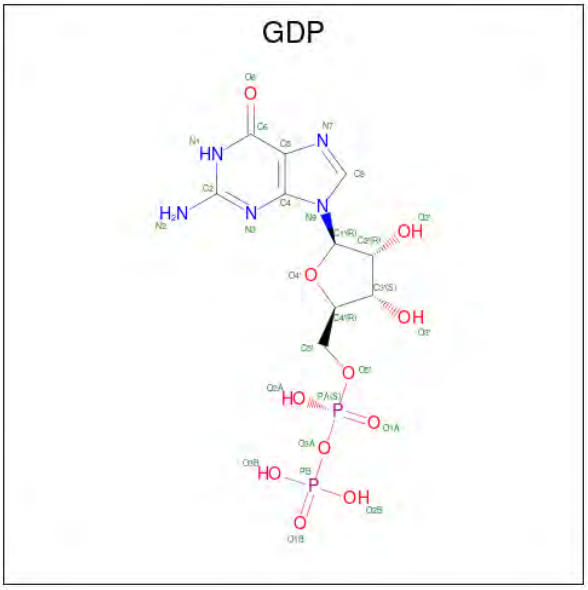
Mol	Chain	Residues	Atoms	AltConf
36	P	1	Total Fe S 4 2 2	0
36	T	1	Total Fe S 4 2 2	0

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
37	X	1	43	10	12	5	13	3	0

- Molecule 38 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
38	X	1	38	10	10	5	11	2	0

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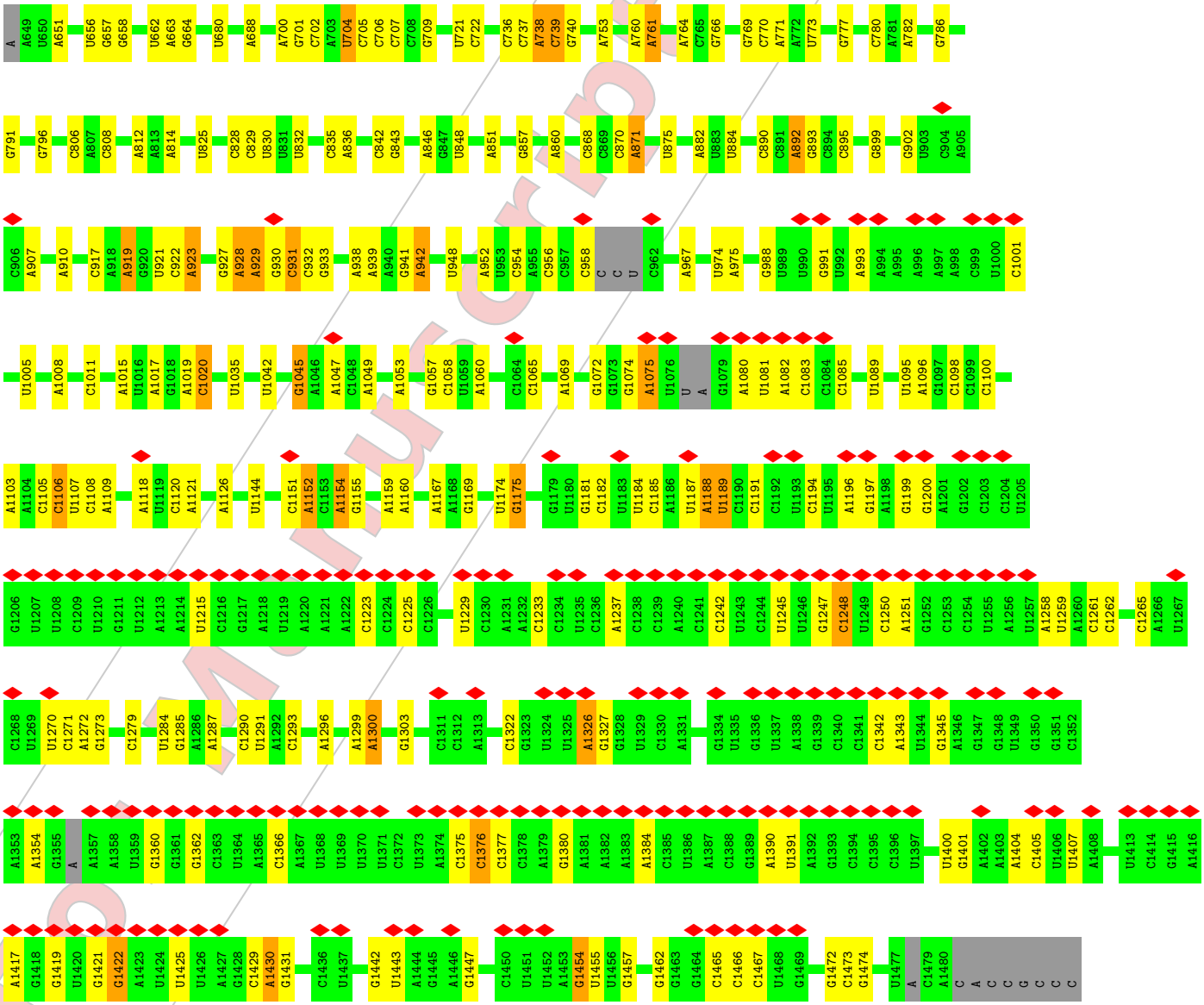
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
38	9	1	38	10	10	5	11	2	0

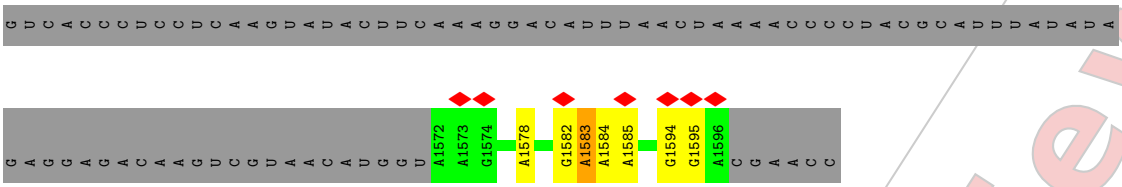
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 12S mitochondrial rRNA

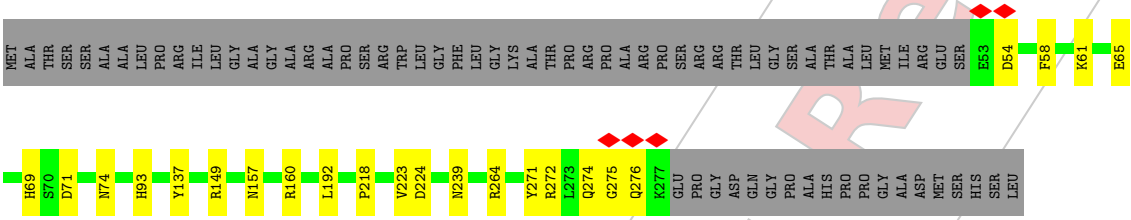
Chain A:





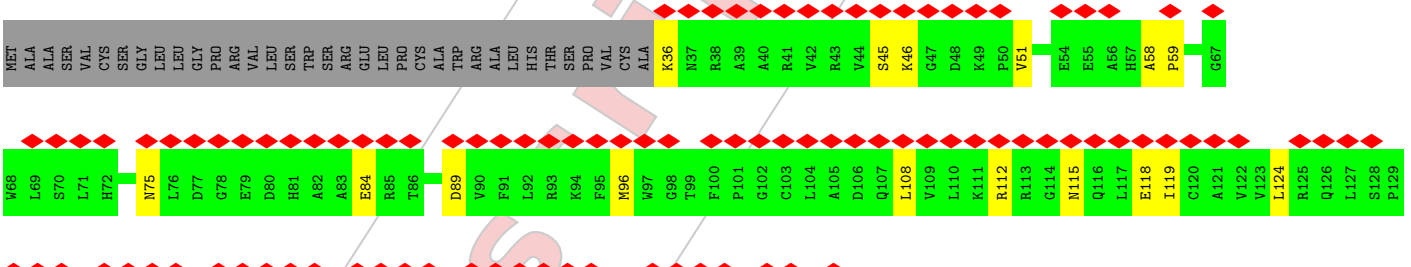
• Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:



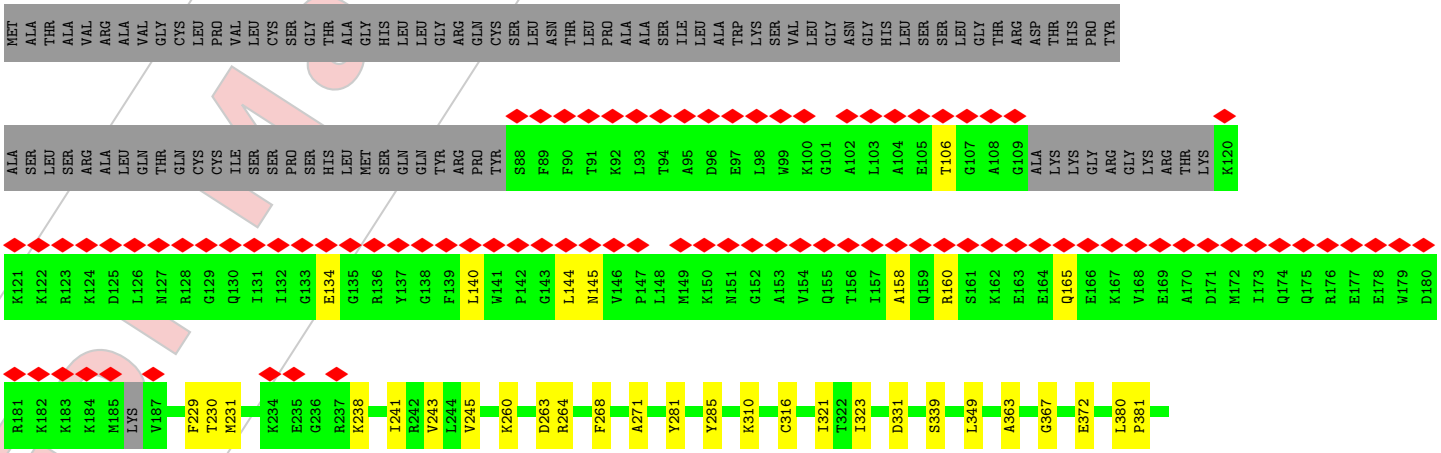
• Molecule 3: 28S ribosomal protein S24, mitochondrial

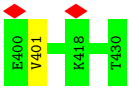
Chain C:



• Molecule 4: 28S ribosomal protein S5, mitochondrial

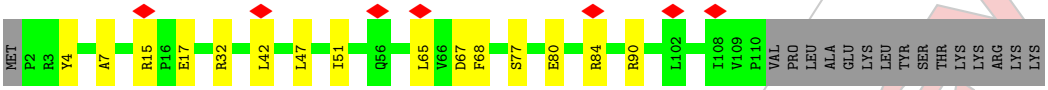
Chain D:





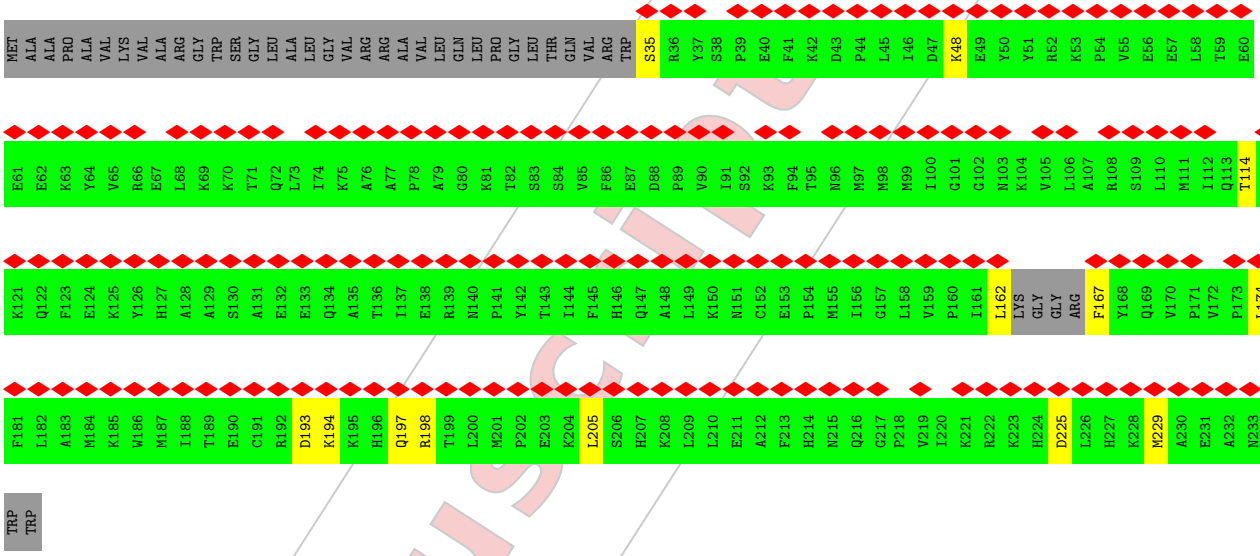
• Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain E:



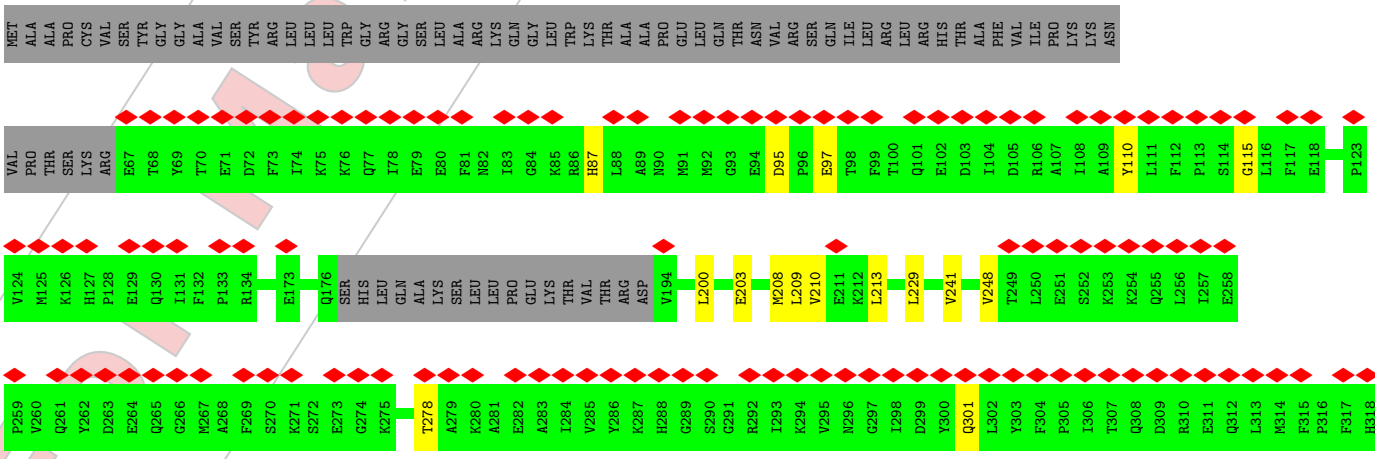
• Molecule 6: 28S ribosomal protein S7, mitochondrial

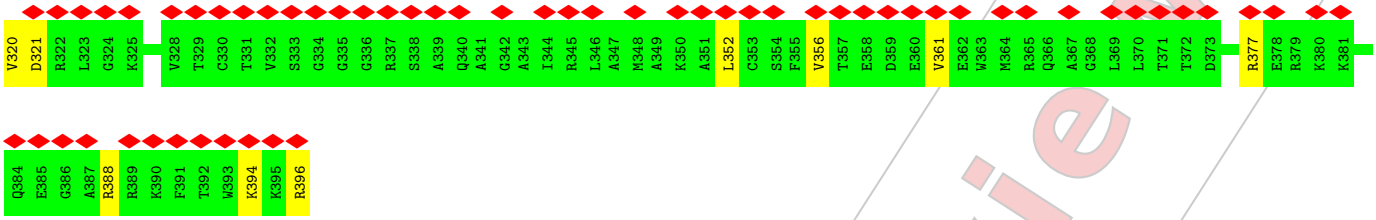
Chain F:



• Molecule 7: 28S ribosomal protein S9, mitochondrial

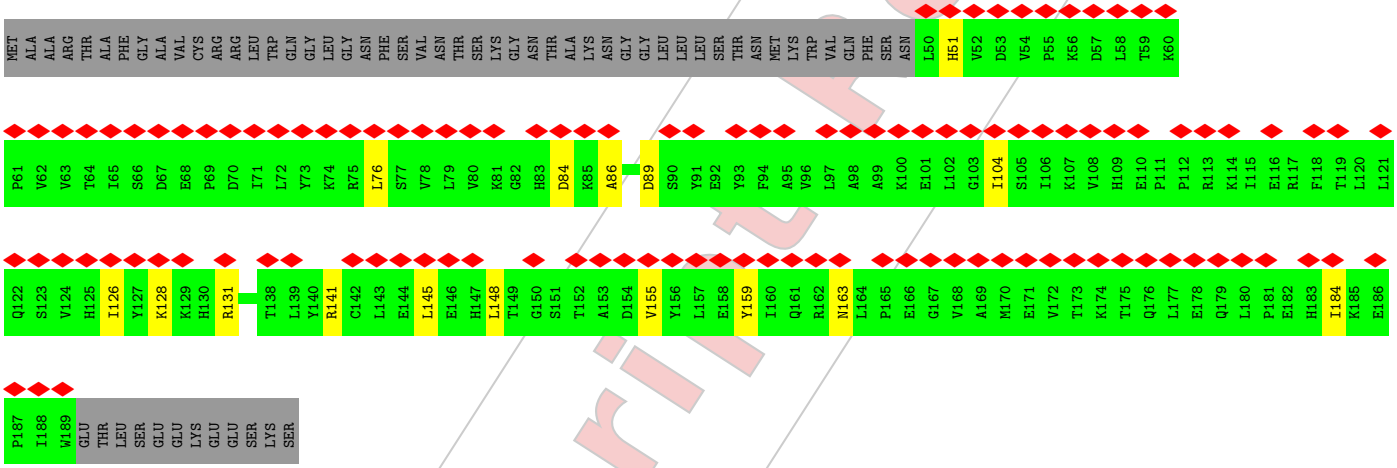
Chain G:





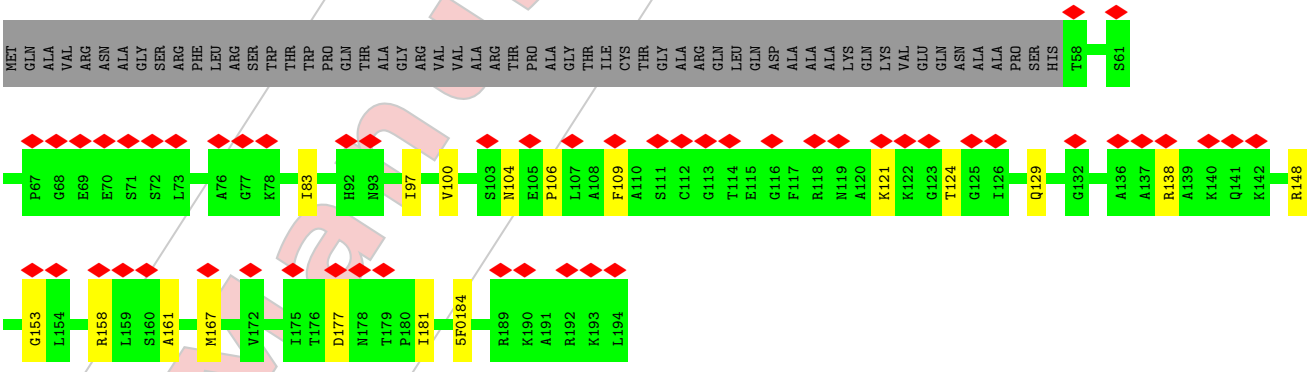
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



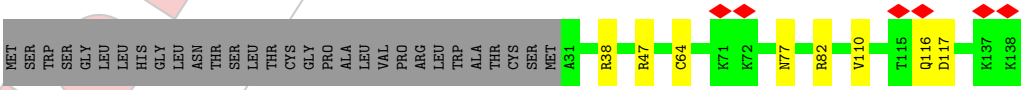
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



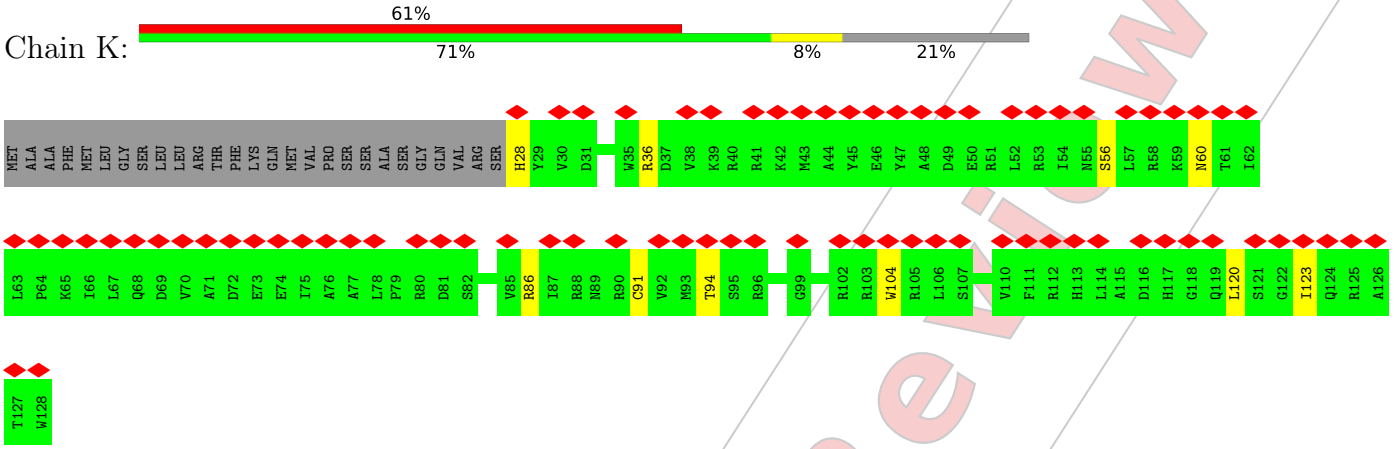
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:



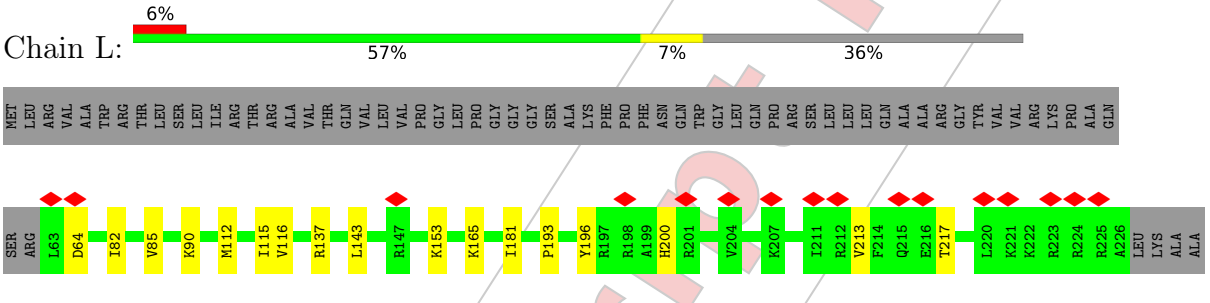
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:



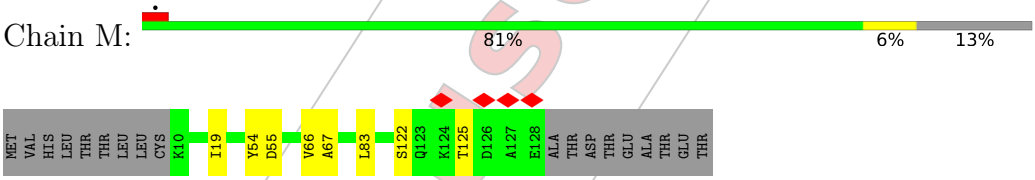
• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L:



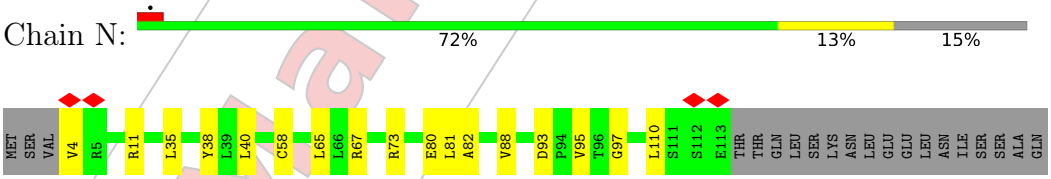
• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain M:



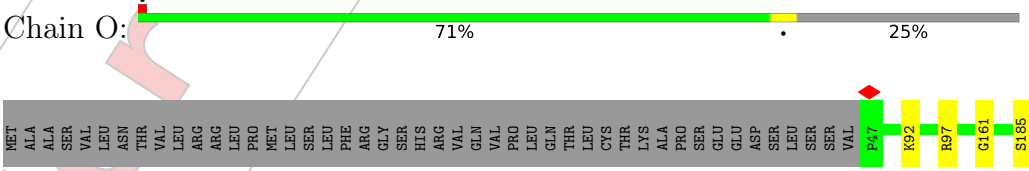
• Molecule 14: 28S ribosomal protein S17, mitochondrial

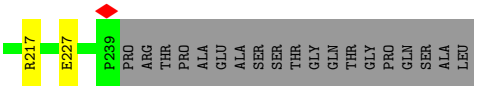
Chain N:



• Molecule 15: 28S ribosomal protein S18b, mitochondrial

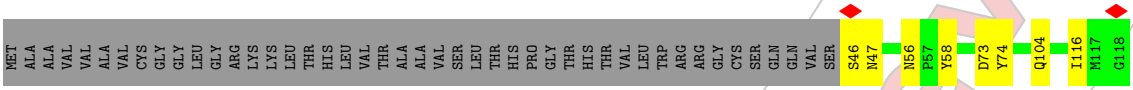
Chain O:

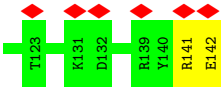




• Molecule 16: 28S ribosomal protein S18c, mitochondrial

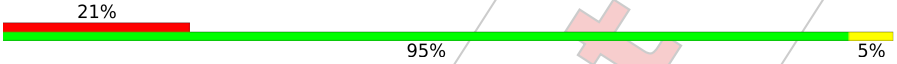
Chain P:

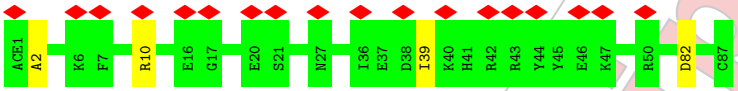




• Molecule 17: Small ribosomal subunit protein bS21m

Chain Q:



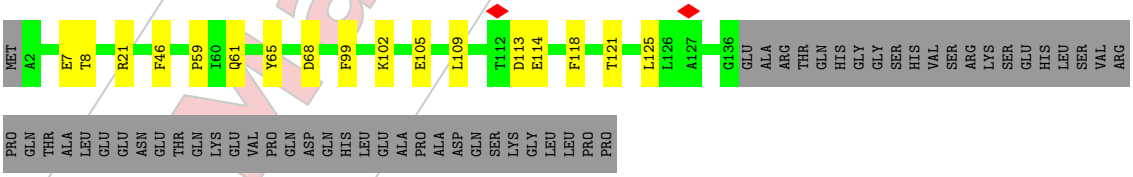


• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:

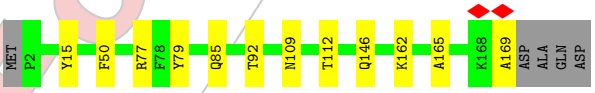
• Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S:



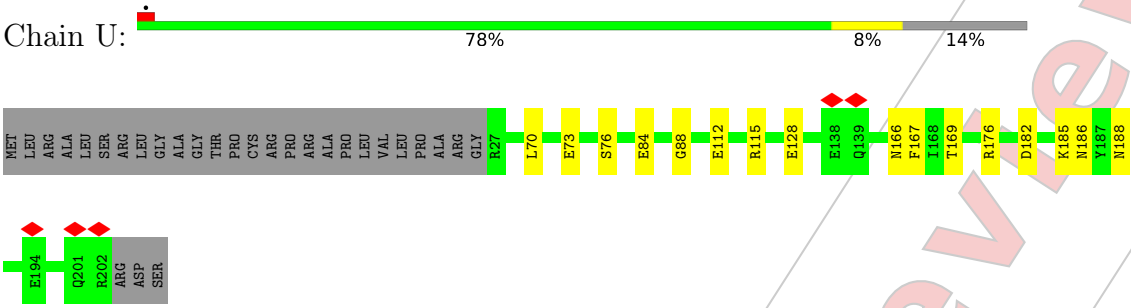
• Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T:



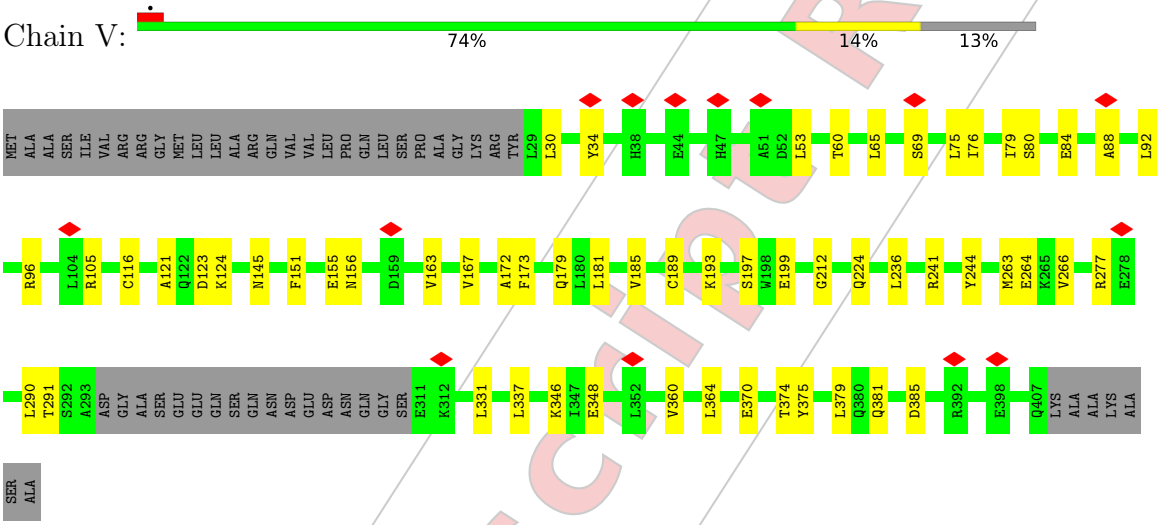
• Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U:



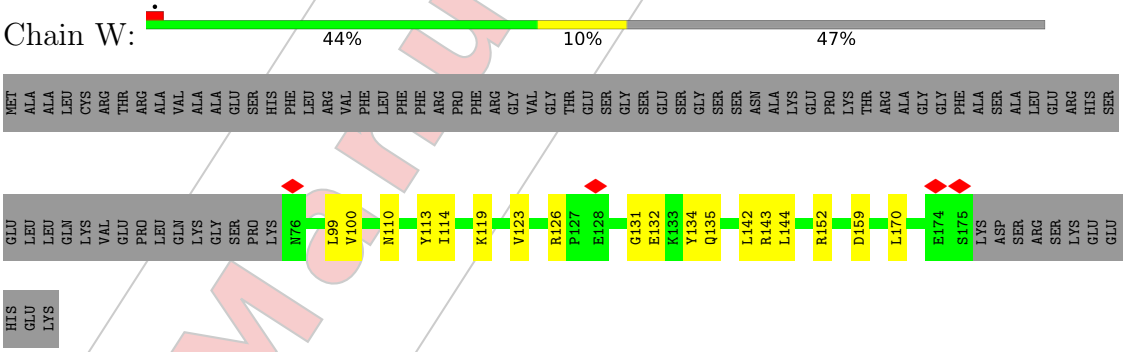
• Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V:



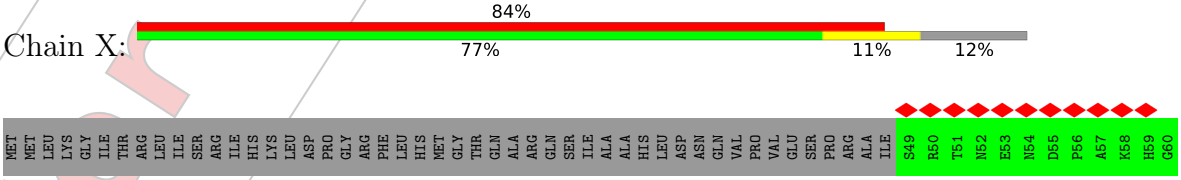
• Molecule 23: 28S ribosomal protein S28, mitochondrial

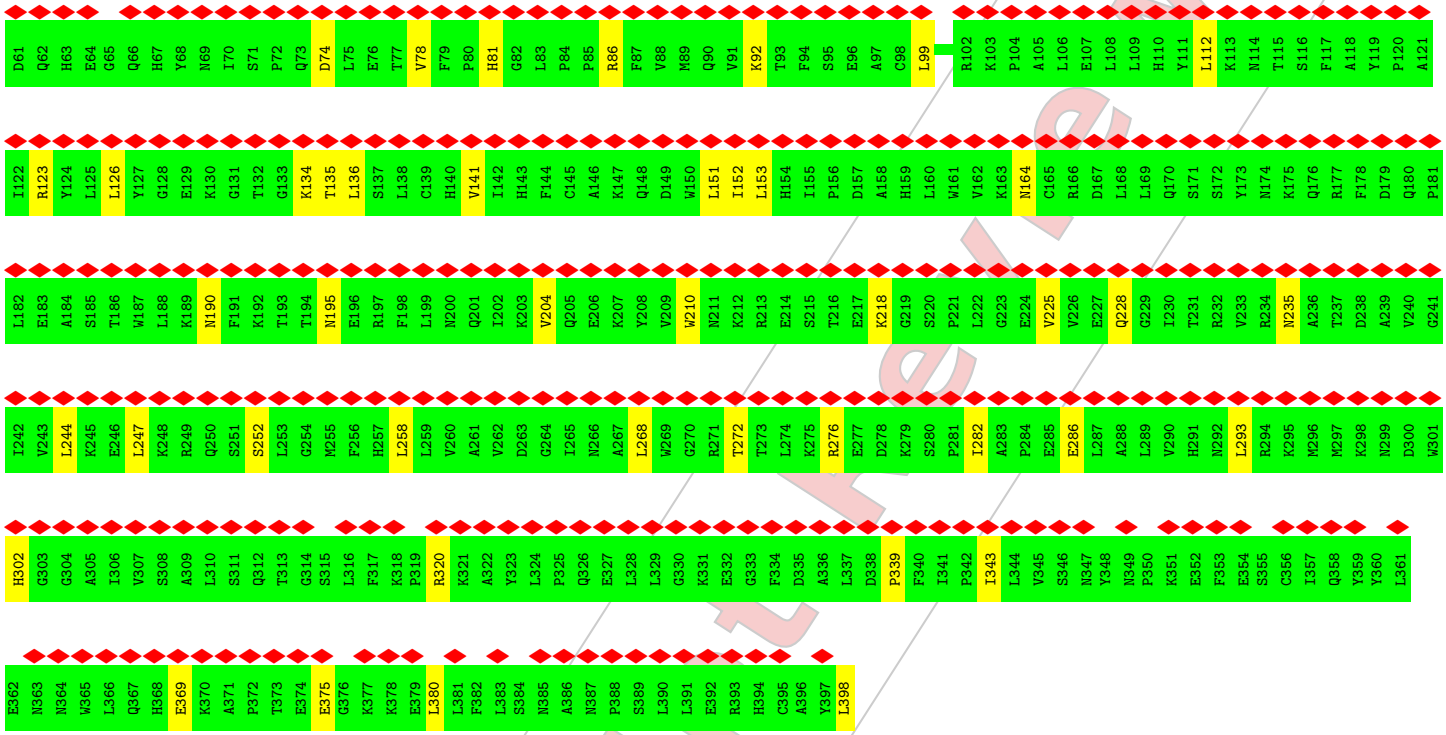
Chain W:



• Molecule 24: 28S ribosomal protein S29, mitochondrial

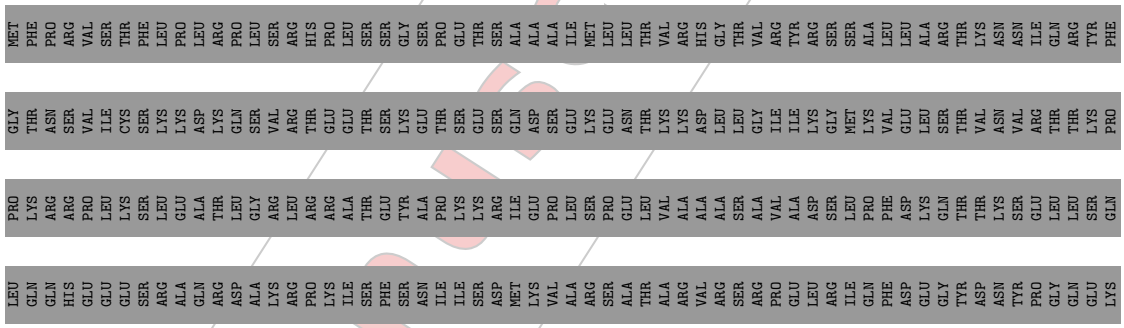
Chain X:

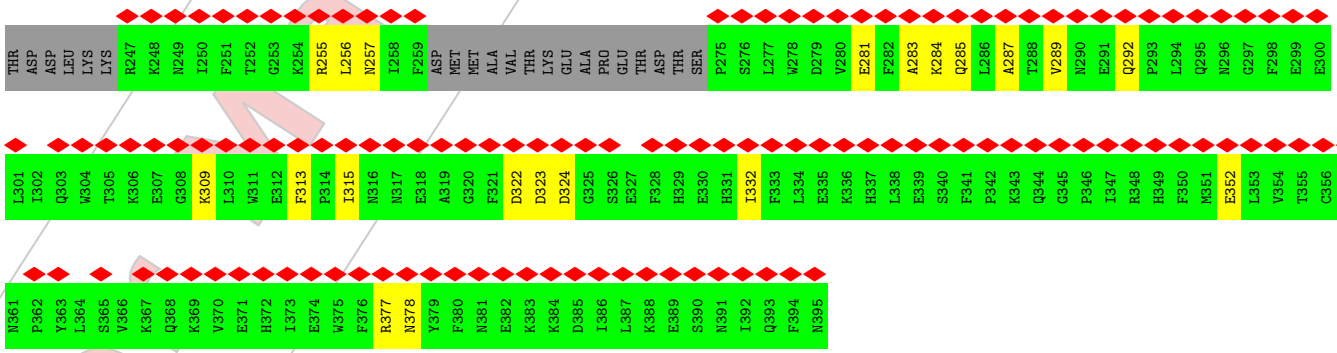




- Molecule 25: 28S ribosomal protein S31, mitochondrial

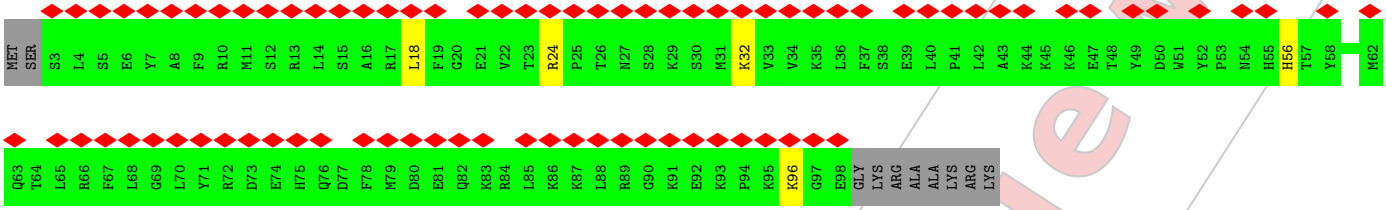
Chain Y:





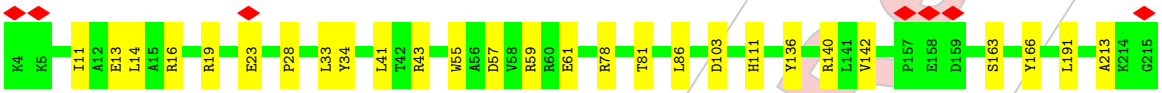
- Molecule 26: 28S ribosomal protein S33, mitochondrial

Chain Z:



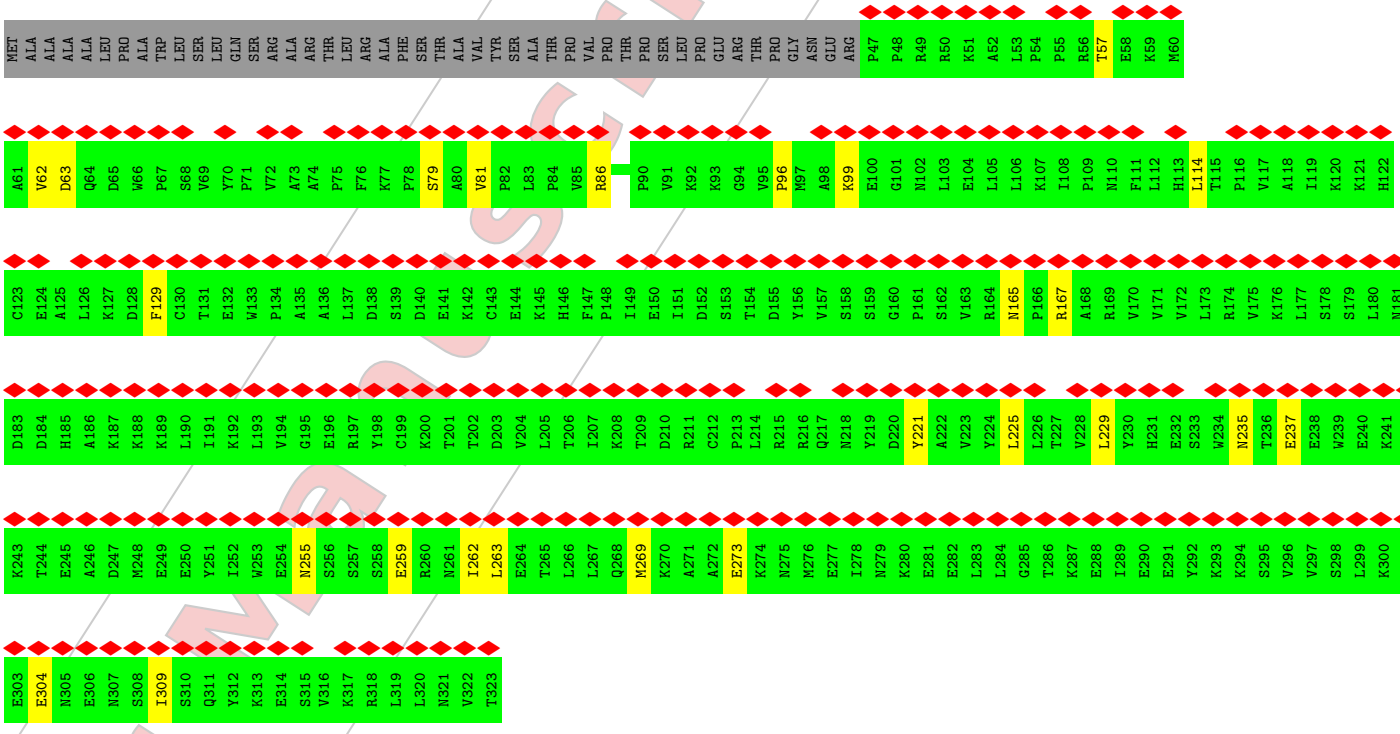
• Molecule 27: Small ribosomal subunit protein mS34

Chain 0:



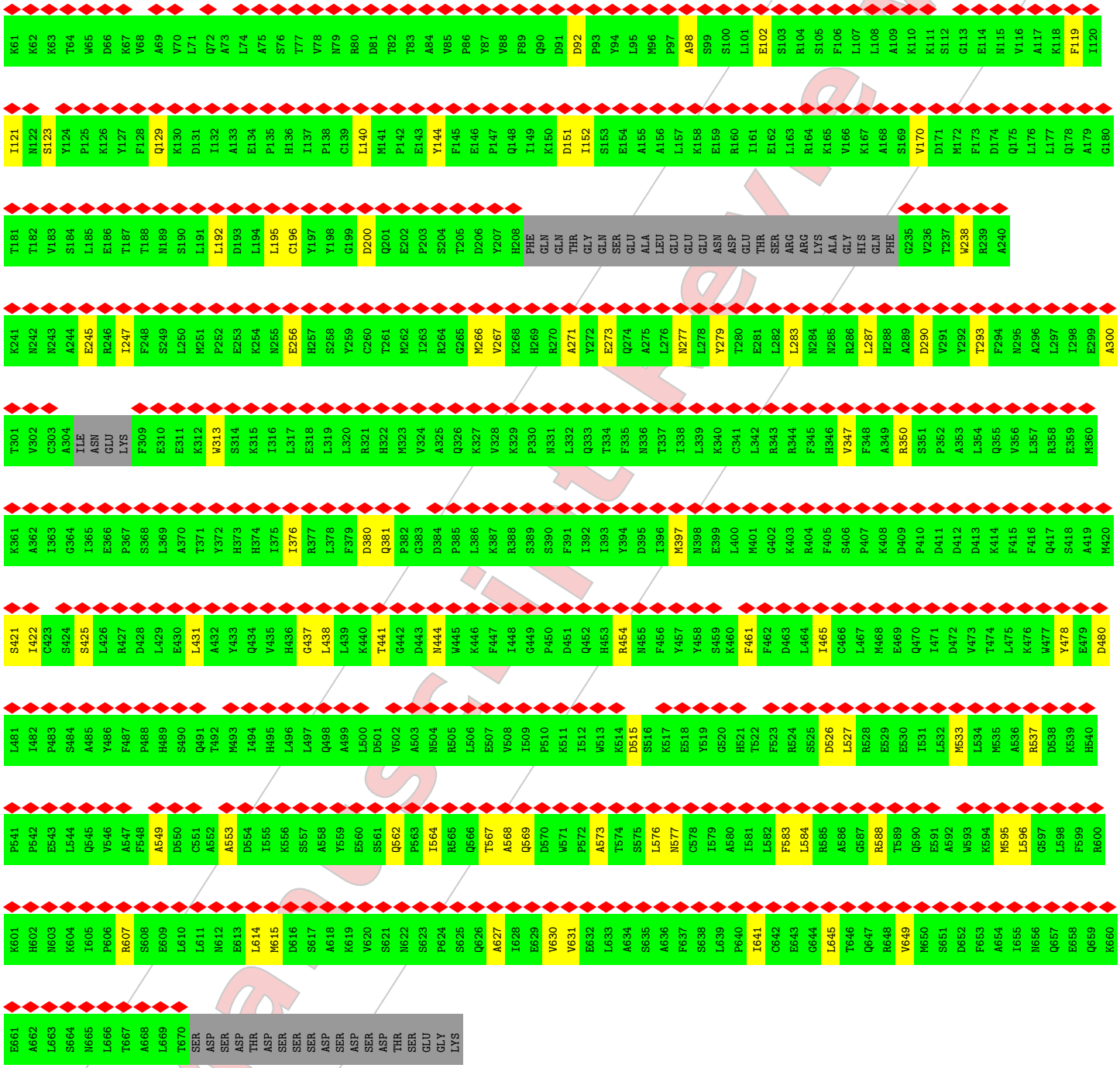
• Molecule 28: 28S ribosomal protein S35, mitochondrial

Chain 1:



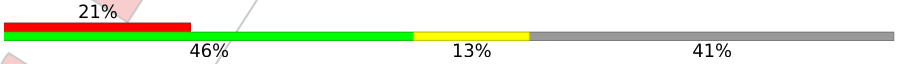
• Molecule 29: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

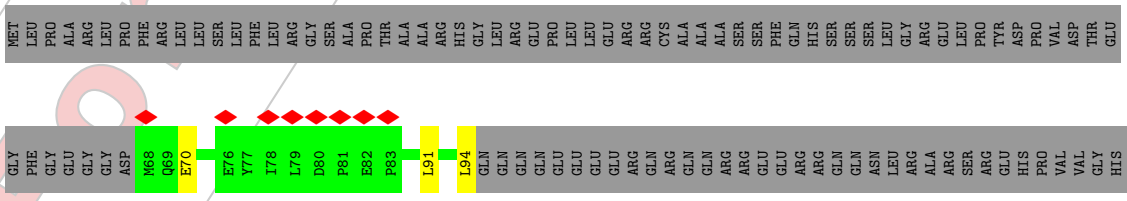
Chain 4:

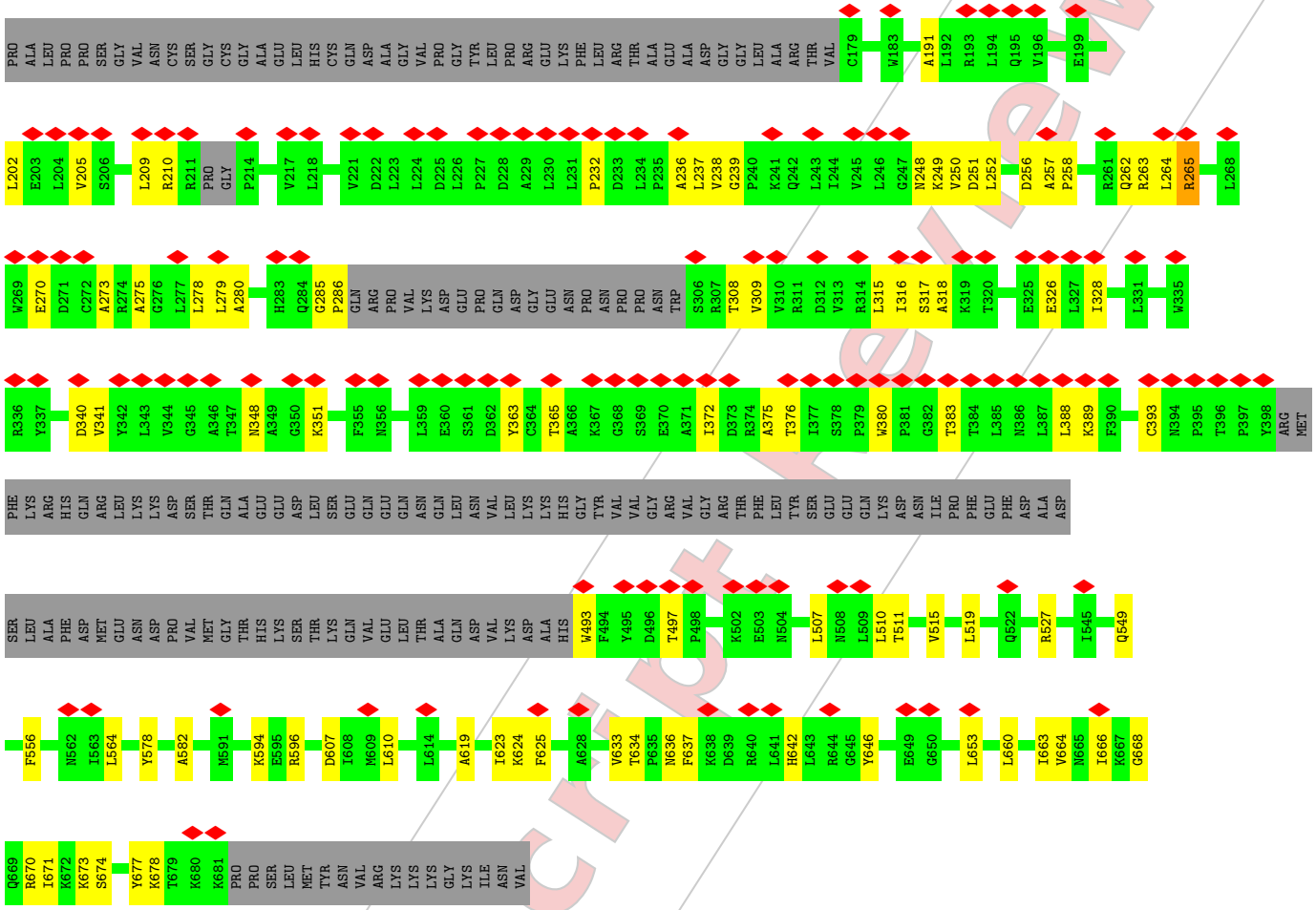


• Molecule 30: Nitric oxide-associated protein 1

Chain 9:

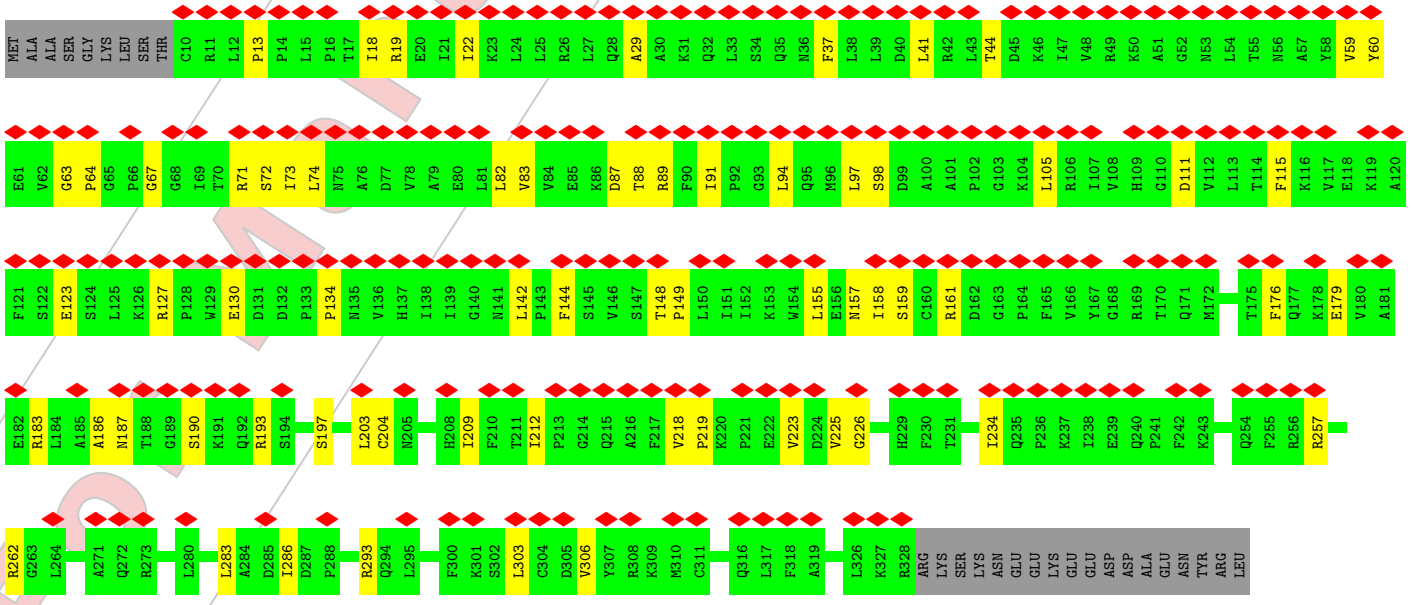






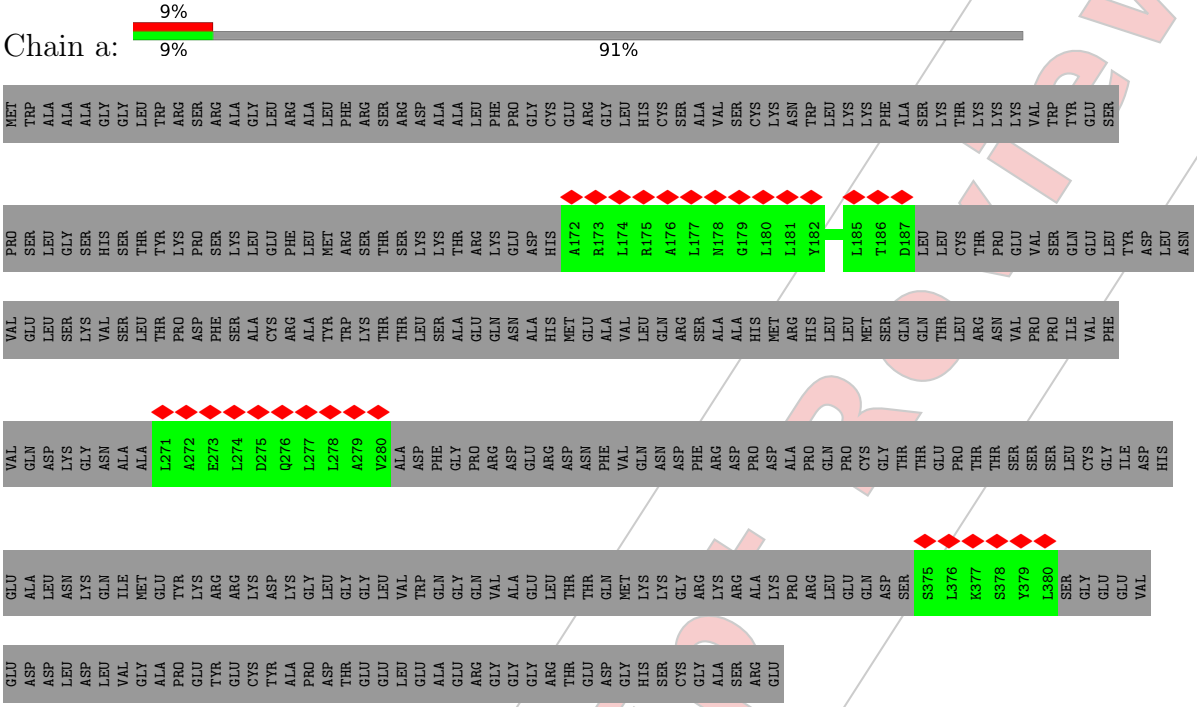
• Molecule 31: Dimethyladenosine transferase 1, mitochondrial

Chain 5:



• Molecule 32: Putative ribosome-binding factor A, mitochondrial

Chain a:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16018	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0054	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ATP, ACE, MG, K, 5F0, FES, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.37	0/20197	0.69	0/31437
2	B	0.30	0/1871	0.50	0/2531
3	C	0.30	0/1113	0.48	0/1505
4	D	0.29	0/2694	0.51	0/3608
5	E	0.27	0/880	0.53	0/1189
6	F	0.25	0/1709	0.46	0/2297
7	G	0.28	0/2632	0.49	0/3527
8	H	0.28	0/1178	0.47	0/1598
9	I	0.26	0/1030	0.50	0/1386
10	J	0.28	0/855	0.55	0/1148
11	K	0.25	0/880	0.57	0/1182
12	L	0.27	0/1408	0.48	0/1882
13	M	0.30	0/963	0.55	0/1295
14	N	0.31	0/886	0.51	0/1199
15	O	0.31	0/1648	0.49	0/2243
16	P	0.27	0/798	0.45	0/1070
17	Q	0.26	0/754	0.56	0/1003
18	R	0.30	0/2456	0.46	0/3317
19	S	0.29	0/1138	0.52	0/1533
20	T	0.31	0/1402	0.45	0/1883
21	U	0.26	0/1510	0.54	0/2025
22	V	0.25	0/3030	0.41	0/4093
23	W	0.28	0/801	0.52	0/1079
24	X	0.27	0/2908	0.45	0/3936
25	Y	0.27	0/1168	0.42	0/1570
26	Z	0.28	0/828	0.47	0/1104
27	0	0.26	0/1834	0.55	0/2484
28	1	0.27	0/2293	0.44	0/3102
29	4	0.25	0/4848	0.42	0/6560
30	9	0.26	0/3350	0.51	0/4549
31	5	0.26	0/2624	0.51	0/3552
32	a	0.26	0/248	0.47	0/331

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.30	0/71934	0.56	0/101218

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18058	9165	9171	106	0
2	B	1828	1826	1815	14	0
3	C	1083	1096	1088	17	0
4	D	2644	2705	2693	25	0
5	E	865	882	878	11	0
6	F	1672	1733	1722	14	0
7	G	2577	2570	2560	18	0
8	H	1152	1191	1183	11	0
9	I	1020	1066	1053	10	0
10	J	839	892	887	7	0
11	K	862	889	885	7	0
12	L	1384	1467	1462	10	0
13	M	942	972	965	5	0
14	N	868	933	928	13	0
15	O	1592	1566	1557	8	0
16	P	781	809	806	6	0
17	Q	744	760	758	3	0
18	R	2409	2436	2428	13	0
19	S	1111	1117	1115	11	0
20	T	1371	1396	1393	9	0
21	U	1488	1505	1499	11	0
22	V	2969	2972	2961	36	0
23	W	789	806	802	11	0
24	X	2836	2842	2827	27	0
25	Y	1136	1100	1094	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Z	810	828	824	5	0
27	0	1787	1802	1796	21	0
28	1	2245	2281	2276	16	0
29	4	4741	4761	4742	52	0
30	9	3278	3378	3371	69	0
31	5	2568	2661	2655	46	0
32	a	249	271	270	0	0
33	A	39	0	0	0	0
33	B	1	0	0	0	0
33	X	1	0	0	0	0
34	A	10	0	0	0	0
35	O	1	0	0	0	0
36	P	4	0	0	0	0
36	T	4	0	0	0	0
37	X	31	12	12	2	0
38	9	28	10	12	1	0
38	X	28	10	12	0	0
All	All	68845	60710	60500	543	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (543) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:623:ILE:HG22	30:9:653:LEU:HD11	1.46	0.94
1:A:1237:A:OP1	11:K:36:ARG:NH2	2.07	0.87
1:A:1429:C:OP1	7:G:388:ARG:NH1	2.12	0.83
30:9:624:LYS:O	30:9:653:LEU:HD12	1.89	0.72
22:V:167:VAL:HG13	22:V:172:ALA:HB3	1.72	0.71
1:A:1181:G:O4'	1:A:1474:G:N2	2.24	0.70
31:5:157:ASN:O	31:5:161:ARG:N	2.26	0.69
1:A:952:A:N3	1:A:954:C:N4	2.42	0.68
1:A:1035:U:OP1	5:E:4:TYR:OH	2.11	0.67
24:X:272:THR:OG1	24:X:282:ILE:O	2.11	0.67
1:A:1262:C:OP1	4:D:106:THR:OG1	2.12	0.67
1:A:899:G:O2'	1:A:907:A:N1	2.25	0.67
2:B:239:ASN:OD1	23:W:119:LYS:NZ	2.28	0.67
4:D:281:TYR:OH	19:S:21:ARG:NH2	2.28	0.66
30:9:250:VAL:CG1	30:9:318:ALA:HB2	2.25	0.66
1:A:895:C:N4	10:J:117:ASP:OD2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:C:O2	11:K:28:HIS:N	2.28	0.65
24:X:252:SER:O	24:X:302:HIS:NE2	2.30	0.65
27:0:41:LEU:HD13	27:0:55:TRP:CG	2.31	0.65
3:C:118:GLU:OE2	3:C:152:ARG:NH2	2.30	0.64
31:5:283:LEU:HD23	31:5:306:VAL:HG13	1.80	0.64
7:G:229:LEU:HD21	7:G:241:VAL:HG11	1.79	0.64
29:4:238:TRP:NE1	29:4:245:GLU:OE2	2.30	0.64
1:A:1287:A:N7	4:D:260:LYS:NZ	2.45	0.64
12:L:112:MET:O	12:L:116:VAL:HG22	1.97	0.64
18:R:187:GLU:N	18:R:187:GLU:OE1	2.30	0.64
2:B:271:TYR:O	2:B:275:GLY:N	2.29	0.64
19:S:59:PRO:O	19:S:61:GLN:NE2	2.31	0.64
1:A:902:G:OP2	1:A:902:G:N2	2.32	0.63
22:V:381:GLN:NE2	22:V:385:ASP:OD1	2.32	0.63
29:4:577:ASN:OD1	29:4:607:ARG:N	2.31	0.63
30:9:351:LYS:NZ	30:9:497:THR:O	2.24	0.63
19:S:102:LYS:HG3	19:S:121:THR:HG23	1.80	0.63
1:A:1199:G:N1	1:A:1422:G:OP2	2.30	0.63
31:5:44:THR:OG1	31:5:72:SER:OG	2.15	0.62
7:G:301:GLN:N	7:G:301:GLN:OE1	2.31	0.62
22:V:189:CYS:O	22:V:193:LYS:N	2.31	0.62
1:A:1245:U:O2	26:Z:96:LYS:NZ	2.33	0.62
3:C:51:VAL:HG11	3:C:167:LEU:HD12	1.80	0.62
31:5:13:PRO:O	31:5:71:ARG:NH2	2.31	0.62
22:V:197:SER:OG	22:V:199:GLU:OE1	2.18	0.62
31:5:212:ILE:N	31:5:225:VAL:O	2.32	0.62
31:5:148:THR:HB	31:5:149:PRO:HD3	1.81	0.62
1:A:700:A:N1	1:A:709:G:O2'	2.30	0.62
29:4:129:GLN:NE2	29:4:144:TYR:OH	2.33	0.62
22:V:116:CYS:HA	22:V:121:ALA:HB3	1.82	0.62
23:W:132:GLU:N	23:W:132:GLU:OE1	2.31	0.61
1:A:704:U:N3	27:0:57:ASP:OD2	2.30	0.61
25:Y:377:ARG:NH2	25:Y:378:ASN:OD1	2.34	0.61
28:1:81:VAL:O	28:1:99:LYS:NZ	2.33	0.61
31:5:144:PHE:HZ	31:5:225:VAL:HG13	1.64	0.61
1:A:1189:U:O2	1:A:1191:C:N4	2.33	0.61
1:A:737:C:O2'	1:A:739:C:N4	2.32	0.61
7:G:320:VAL:HG21	7:G:352:LEU:HD21	1.83	0.61
22:V:151:PHE:O	22:V:156:ASN:N	2.34	0.60
21:U:185:LYS:NZ	21:U:186:ASN:O	2.34	0.60
1:A:843:G:N2	1:A:846:A:OP2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:ARG:NH2	16:P:116:ILE:O	2.34	0.60
30:9:663:ILE:O	30:9:666:ILE:HG22	2.02	0.60
3:C:157:THR:OG1	29:4:92:ASP:OD1	2.19	0.59
28:1:269:MET:O	28:1:273:GLU:N	2.32	0.59
7:G:115:GLY:N	8:H:84:ASP:OD2	2.34	0.59
4:D:134:GLU:OE1	4:D:160:ARG:NH2	2.36	0.59
10:J:116:GLN:OE1	10:J:116:GLN:N	2.34	0.59
21:U:186:ASN:OD1	21:U:188:ASN:N	2.35	0.58
24:X:74:ASP:O	24:X:78:VAL:N	2.33	0.58
1:A:941:G:O2'	1:A:1109:A:OP2	2.15	0.58
30:9:670:ARG:NH2	30:9:674:SER:O	2.36	0.58
4:D:160:ARG:NE	4:D:165:GLN:OE1	2.34	0.58
7:G:95:ASP:OD1	7:G:97:GLU:N	2.37	0.58
7:G:203:GLU:N	7:G:203:GLU:OE1	2.34	0.58
26:Z:18:LEU:HD13	28:1:229:LEU:HD23	1.86	0.58
14:N:4:VAL:O	14:N:11:ARG:NH2	2.36	0.58
18:R:325:ILE:HG23	18:R:346:LEU:HD21	1.86	0.58
30:9:191:ALA:HB3	30:9:388:LEU:CD2	2.33	0.58
29:4:192:LEU:O	29:4:196:CYS:N	2.34	0.58
3:C:84:GLU:OE1	3:C:84:GLU:N	2.36	0.58
2:B:93:HIS:CD2	2:B:224:ASP:OD2	2.56	0.57
6:F:48:LYS:NZ	7:G:321:ASP:OD1	2.35	0.57
30:9:380:TRP:CH2	30:9:497:THR:HG22	2.39	0.57
29:4:615:MET:HE1	29:4:649:VAL:HG22	1.85	0.57
1:A:928:A:O2'	1:A:929:A:P	2.62	0.57
30:9:634:THR:HG21	30:9:664:VAL:HG21	1.85	0.57
1:A:1248:C:O2	26:Z:56:HIS:NE2	2.37	0.57
29:4:631:VAL:HG22	29:4:645:LEU:HG	1.86	0.57
31:5:179:GLU:OE1	31:5:179:GLU:N	2.37	0.57
1:A:738:A:H2'	1:A:740:G:C5	2.40	0.57
1:A:1401:G:N1	1:A:1404:A:OP2	2.38	0.57
23:W:110:ASN:O	23:W:126:ARG:N	2.37	0.57
30:9:250:VAL:HG12	30:9:318:ALA:HB2	1.86	0.57
30:9:578:TYR:O	30:9:582:ALA:N	2.38	0.57
1:A:760:A:N1	1:A:780:C:O2'	2.32	0.57
1:A:948:U:OP2	1:A:1045:G:N1	2.38	0.57
19:S:114:GLU:O	19:S:118:PHE:N	2.32	0.57
1:A:1582:G:N3	31:5:144:PHE:HB2	2.20	0.56
1:A:871:A:OP2	15:O:97:ARG:NH1	2.38	0.56
25:Y:292:GLN:OE1	29:4:454:ARG:NH1	2.38	0.56
29:4:615:MET:CE	29:4:649:VAL:HG22	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:151:ASP:OD1	29:4:152:ILE:N	2.39	0.56
18:R:162:SER:O	18:R:170:ARG:NH2	2.36	0.56
29:4:573:ALA:O	29:4:577:ASN:ND2	2.39	0.56
30:9:607:ASP:OD2	30:9:642:HIS:NE2	2.39	0.56
5:E:17:GLU:OE1	5:E:17:GLU:N	2.33	0.56
7:G:248:VAL:O	7:G:248:VAL:HG13	2.04	0.56
22:V:212:GLY:O	22:V:224:GLN:NE2	2.37	0.56
9:I:153:GLY:O	9:I:158:ARG:NH1	2.37	0.56
1:A:1188:A:N6	1:A:1194:C:O2	2.34	0.56
2:B:157:ASN:OD1	2:B:160:ARG:NH2	2.36	0.56
31:5:59:VAL:HG11	31:5:73:ILE:HG21	1.88	0.56
7:G:394:LYS:O	7:G:396:ARG:NH1	2.39	0.55
7:G:209:LEU:HD12	7:G:213:LEU:HD11	1.87	0.55
12:L:213:VAL:O	12:L:217:THR:HG23	2.06	0.55
29:4:347:VAL:HG23	29:4:381:GLN:OE1	2.06	0.55
8:H:84:ASP:OD1	8:H:86:ALA:N	2.39	0.55
12:L:82:ILE:O	12:L:85:VAL:HG22	2.06	0.55
22:V:291:THR:HG21	22:V:331:LEU:HD22	1.87	0.55
30:9:634:THR:CG2	30:9:664:VAL:HG21	2.36	0.55
22:V:105:ARG:NH2	30:9:70:GLU:OE1	2.39	0.55
2:B:54:ASP:OD1	2:B:271:TYR:OH	2.24	0.55
30:9:666:ILE:HG23	30:9:666:ILE:O	2.06	0.55
23:W:126:ARG:NH1	23:W:131:GLY:O	2.39	0.55
30:9:251:ASP:OD1	30:9:252:LEU:N	2.40	0.55
1:A:1454:G:OP2	7:G:377:ARG:NH1	2.39	0.55
22:V:80:SER:OG	22:V:84:GLU:OE2	2.24	0.55
31:5:158:ILE:HD13	31:5:204:CYS:SG	2.46	0.55
24:X:134:LYS:NZ	37:X:501:ATP:O2B	2.39	0.55
5:E:15:ARG:NH2	21:U:182:ASP:OD1	2.40	0.55
30:9:239:GLY:O	30:9:308:THR:OG1	2.20	0.55
1:A:662:U:OP2	4:D:339:SER:OG	2.25	0.54
22:V:76:ILE:HD11	22:V:92:LEU:HD11	1.89	0.54
30:9:273:ALA:N	30:9:279:LEU:HD12	2.22	0.54
22:V:264:GLU:HG3	22:V:337:LEU:HD11	1.89	0.54
1:A:917:C:O2'	1:A:921:U:OP1	2.22	0.54
3:C:124:LEU:O	3:C:132:TYR:OH	2.16	0.54
22:V:53:LEU:HD13	22:V:75:LEU:HA	1.89	0.54
30:9:610:LEU:CD1	30:9:633:VAL:HG11	2.37	0.54
1:A:1095:U:O4	1:A:1096:A:N6	2.40	0.54
27:0:78:ARG:NH2	27:0:142:VAL:O	2.39	0.54
8:H:89:ASP:OD1	8:H:141:ARG:NH1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:352:GLU:OE1	26:Z:24:ARG:NE	2.41	0.54
1:A:1259:U:OP2	1:A:1327:G:P	2.66	0.54
30:9:341:VAL:HG21	30:9:363:TYR:OH	2.08	0.54
30:9:623:ILE:CG2	30:9:653:LEU:HD11	2.29	0.54
1:A:1229:U:O2'	1:A:1442:G:O4'	2.25	0.53
1:A:927:G:OP1	10:J:47:ARG:NH1	2.41	0.53
29:4:526:ASP:OD1	29:4:527:LEU:N	2.41	0.53
4:D:243:VAL:HG11	4:D:268:PHE:CD1	2.43	0.53
29:4:347:VAL:HG22	29:4:350:ARG:CZ	2.37	0.53
1:A:702:C:OP1	1:A:848:U:O2'	2.24	0.53
4:D:380:LEU:HD12	4:D:381:PRO:HD2	1.91	0.53
1:A:1380:G:O2'	24:X:164:ASN:ND2	2.41	0.53
13:M:122:SER:O	13:M:125:THR:OG1	2.23	0.53
24:X:204:VAL:HG23	24:X:218:LYS:HA	1.89	0.53
1:A:705:C:H2'	27:0:136:TYR:CE1	2.44	0.53
12:L:115:ILE:HG21	12:L:181:ILE:HD13	1.90	0.53
2:B:192:LEU:HD12	2:B:218:PRO:O	2.09	0.53
30:9:365:THR:HG22	30:9:393:CYS:SG	2.49	0.53
4:D:134:GLU:OE2	4:D:145:ASN:ND2	2.43	0.52
28:1:304:GLU:OE2	28:1:309:ILE:HD11	2.10	0.52
5:E:7:ALA:HA	5:E:65:LEU:HD23	1.90	0.52
22:V:116:CYS:CA	22:V:121:ALA:HB3	2.40	0.52
22:V:375:TYR:CZ	22:V:379:LEU:HD11	2.44	0.52
31:5:87:ASP:OD1	31:5:89:ARG:N	2.43	0.52
1:A:875:U:O2'	1:A:882:A:N1	2.37	0.52
1:A:974:U:O2'	1:A:975:A:N7	2.30	0.52
3:C:96:MET:HB2	3:C:108:LEU:HD11	1.90	0.52
1:A:1184:U:H2'	1:A:1185:C:O4'	2.10	0.52
31:5:218:VAL:HB	31:5:219:PRO:HD3	1.92	0.52
1:A:1259:U:H6	1:A:1326:A:HO2'	1.57	0.52
4:D:230:THR:O	4:D:238:LYS:N	2.40	0.52
7:G:110:TYR:OH	28:1:114:LEU:O	2.24	0.52
8:H:128:LYS:O	8:H:131:ARG:NE	2.39	0.52
9:I:177:ASP:OD1	17:Q:10:ARG:NH1	2.43	0.52
2:B:71:ASP:OD1	2:B:74:ASN:N	2.43	0.52
18:R:145:ASP:OD2	18:R:175:ARG:NH1	2.37	0.52
19:S:99:PHE:HA	19:S:125:LEU:HD11	1.91	0.52
22:V:69:SER:N	30:9:70:GLU:OE2	2.42	0.52
31:5:144:PHE:CZ	31:5:225:VAL:HG13	2.44	0.52
1:A:1429:C:H4'	1:A:1430:A:O5'	2.10	0.52
19:S:113:ASP:OD1	19:S:114:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:A:N6	1:A:1100:C:O2'	2.42	0.51
29:4:421:SER:O	29:4:425:SER:OG	2.23	0.51
20:T:165:ALA:O	20:T:169:ALA:N	2.42	0.51
22:V:173:PHE:O	22:V:179:GLN:NE2	2.43	0.51
1:A:1005:U:O2	9:I:104:ASN:ND2	2.39	0.51
5:E:80:GLU:OE2	5:E:84:ARG:NE	2.38	0.51
12:L:143:LEU:HD11	12:L:153:LYS:HA	1.93	0.51
29:4:266:MET:O	29:4:271:ALA:N	2.43	0.51
29:4:267:VAL:HG22	29:4:300:ALA:HB2	1.92	0.51
1:A:1174:U:O2'	4:D:231:MET:O	2.27	0.51
7:G:210:VAL:HG12	7:G:210:VAL:O	2.10	0.51
5:E:42:LEU:HD11	5:E:65:LEU:HD11	1.93	0.51
29:4:119:PHE:O	29:4:123:SER:OG	2.22	0.51
1:A:761:A:OP2	12:L:200:HIS:NE2	2.44	0.51
28:1:86:ARG:NH1	28:1:96:PRO:O	2.44	0.51
1:A:806:C:C4	27:0:11:ILE:HD12	2.46	0.51
24:X:151:LEU:CD2	24:X:247:LEU:HD22	2.39	0.51
25:Y:332:ILE:HD13	28:1:221:TYR:CD1	2.45	0.51
29:4:195:LEU:HD22	29:4:200:ASP:OD1	2.11	0.51
30:9:91:LEU:O	30:9:94:LEU:N	2.44	0.51
2:B:65:GLU:OE2	2:B:69:HIS:NE2	2.44	0.50
24:X:369:GLU:OE1	24:X:369:GLU:N	2.38	0.50
29:4:58:VAL:HG23	29:4:58:VAL:O	2.11	0.50
30:9:326:GLU:N	30:9:326:GLU:OE1	2.43	0.50
28:1:165:ASN:OD1	28:1:167:ARG:NH1	2.44	0.50
29:4:461:PHE:CZ	29:4:465:ILE:HD11	2.46	0.50
31:5:41:LEU:O	31:5:44:THR:OG1	2.29	0.50
19:S:7:GLU:N	19:S:7:GLU:OE1	2.44	0.50
24:X:268:LEU:HD21	24:X:293:LEU:HD23	1.92	0.50
30:9:328:ILE:HG23	30:9:363:TYR:HB2	1.94	0.50
30:9:660:LEU:HD13	30:9:663:ILE:HD13	1.93	0.50
1:A:1045:G:O6	12:L:165:LYS:NZ	2.44	0.50
3:C:115:ASN:ND2	25:Y:309:LYS:O	2.44	0.50
30:9:210:ARG:NH2	30:9:236:ALA:O	2.44	0.50
1:A:702:C:O2'	1:A:842:C:O2	2.29	0.50
1:A:1582:G:C4	31:5:144:PHE:HB2	2.46	0.50
24:X:210:TRP:HZ2	24:X:225:VAL:HG22	1.76	0.50
1:A:942:A:N6	1:A:1047:A:OP2	2.45	0.49
25:Y:322:ASP:O	25:Y:323:ASP:OD1	2.30	0.49
30:9:380:TRP:HD1	30:9:383:THR:HG1	1.58	0.49
30:9:549:GLN:HB3	30:9:642:HIS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:88:VAL:O	14:N:88:VAL:HG13	2.11	0.49
30:9:372:ILE:H	30:9:372:ILE:HD12	1.77	0.49
31:5:176:PHE:O	31:5:226:GLY:N	2.38	0.49
1:A:1057:G:H4'	1:A:1578:A:H4'	1.94	0.49
9:I:181:ILE:HD11	17:Q:39:ILE:HD11	1.94	0.49
22:V:277:ARG:N	22:V:348:GLU:O	2.45	0.49
25:Y:281:GLU:OE1	25:Y:284:LYS:NZ	2.35	0.49
27:0:13:GLU:OE1	27:0:16:ARG:NH1	2.45	0.49
29:4:630:VAL:HG12	29:4:645:LEU:HD21	1.94	0.49
30:9:507:LEU:HD23	30:9:510:LEU:HD12	1.93	0.49
8:H:76:LEU:HD12	8:H:148:LEU:HD11	1.95	0.49
24:X:276:ARG:NH2	24:X:286:GLU:OE1	2.46	0.49
1:A:769:G:OP2	14:N:73:ARG:NH2	2.46	0.49
18:R:239:SER:OG	18:R:241:GLU:OE1	2.30	0.49
1:A:656:U:O2'	1:A:658:G:N7	2.36	0.49
1:A:782:A:OP2	10:J:38:ARG:NH2	2.40	0.49
22:V:69:SER:OG	30:9:70:GLU:OE1	2.26	0.49
18:R:176:GLU:OE2	18:R:182:ARG:NE	2.35	0.49
31:5:111:ASP:O	31:5:115:PHE:N	2.42	0.49
9:I:100:VAL:HG12	9:I:106:PRO:HA	1.94	0.48
9:I:129:GLN:NE2	9:I:167:MET:SD	2.85	0.48
19:S:65:TYR:N	19:S:68:ASP:OD2	2.46	0.48
30:9:507:LEU:HD21	30:9:519:LEU:HD21	1.95	0.48
20:T:15:TYR:OH	20:T:50:PHE:O	2.24	0.48
23:W:114:ILE:HG21	23:W:142:LEU:HD11	1.95	0.48
25:Y:255:ARG:O	25:Y:257:ASN:ND2	2.46	0.48
30:9:205:VAL:HG12	30:9:209:LEU:HD13	1.95	0.48
3:C:58:ALA:HB1	3:C:59:PRO:CD	2.43	0.48
22:V:123:ASP:OD1	22:V:124:LYS:N	2.46	0.48
4:D:263:ASP:OD1	4:D:264:ARG:N	2.46	0.48
21:U:73:GLU:OE1	27:0:166:TYR:OH	2.28	0.48
22:V:181:LEU:O	22:V:185:VAL:HG23	2.13	0.48
29:4:564:ILE:HG22	29:4:567:THR:HB	1.96	0.48
6:F:114:THR:HG21	6:F:205:LEU:HG	1.95	0.48
6:F:174:LEU:HD22	6:F:178:ARG:HG2	1.94	0.48
1:A:1430:A:OP2	6:F:35:SER:N	2.46	0.48
22:V:360:VAL:HG13	22:V:364:LEU:HD22	1.96	0.48
22:V:370:GLU:O	22:V:374:THR:HG23	2.13	0.48
28:1:235:ASN:ND2	28:1:237:GLU:OE2	2.37	0.48
30:9:375:ALA:HB1	30:9:388:LEU:HD12	1.96	0.48
2:B:61:LYS:NZ	2:B:274:GLN:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5:155:LEU:HA	31:5:158:ILE:HD12	1.96	0.48
2:B:54:ASP:O	2:B:58:PHE:N	2.42	0.48
27:0:81:THR:HG21	27:0:86:LEU:HD11	1.96	0.48
30:9:636:ASN:OD1	30:9:637:PHE:N	2.47	0.48
22:V:34:TYR:OH	22:V:145:ASN:ND2	2.41	0.47
29:4:170:VAL:CG2	29:4:195:LEU:HD21	2.44	0.47
31:5:37:PHE:O	31:5:219:PRO:HD2	2.14	0.47
3:C:45:SER:OG	3:C:46:LYS:N	2.46	0.47
11:K:120:LEU:HB3	11:K:123:ILE:HD12	1.96	0.47
14:N:93:ASP:OD1	14:N:95:VAL:N	2.45	0.47
16:P:56:ASN:OD1	16:P:58:TYR:N	2.47	0.47
4:D:285:TYR:OH	4:D:372:GLU:OE2	2.26	0.47
31:5:186:ALA:O	31:5:193:ARG:NH1	2.46	0.47
31:5:186:ALA:O	31:5:197:SER:OG	2.29	0.47
16:P:46:SER:OG	16:P:47:ASN:N	2.45	0.47
29:4:441:THR:OG1	29:4:444:ASN:ND2	2.46	0.47
30:9:250:VAL:HG13	30:9:318:ALA:HB2	1.94	0.47
2:B:137:TYR:O	2:B:264:ARG:NH1	2.45	0.47
13:M:55:ASP:OD2	20:T:146:GLN:NE2	2.45	0.47
14:N:67:ARG:NE	14:N:80:GLU:OE2	2.45	0.47
23:W:99:LEU:HD22	23:W:170:LEU:HD11	1.96	0.47
31:5:159:SER:HB3	31:5:203:LEU:HD11	1.97	0.47
8:H:104:ILE:HG21	8:H:145:LEU:HD23	1.97	0.47
14:N:4:VAL:O	14:N:4:VAL:HG12	2.14	0.47
21:U:112:GLU:OE2	21:U:115:ARG:NH2	2.48	0.47
30:9:232:PRO:HA	30:9:275:ALA:HB1	1.97	0.47
30:9:248:ASN:OD1	30:9:249:LYS:N	2.46	0.47
30:9:256:ASP:OD1	30:9:257:ALA:N	2.48	0.47
30:9:340:ASP:OD1	30:9:493:TRP:N	2.48	0.47
30:9:376:THR:O	30:9:389:LYS:N	2.44	0.47
6:F:225:ASP:O	6:F:229:MET:N	2.36	0.47
14:N:110:LEU:HD12	21:U:128:GLU:CD	2.34	0.47
29:4:256:GLU:HG2	29:4:287:LEU:HD22	1.95	0.47
31:5:74:LEU:HD13	31:5:97:LEU:HD22	1.96	0.47
1:A:1472:G:H2'	1:A:1473:C:O4'	2.15	0.47
1:A:1582:G:H2'	1:A:1583:A:O4'	2.15	0.47
11:K:91:CYS:SG	11:K:94:THR:OG1	2.56	0.47
22:V:121:ALA:HB1	22:V:124:LYS:HB2	1.96	0.47
30:9:348:ASN:N	38:9:801:GDP:O1B	2.34	0.47
1:A:1074:G:H2'	1:A:1075:A:H5"	1.97	0.47
1:A:1366:C:O2'	1:A:1419:G:N3	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:641:ILE:O	29:4:641:ILE:HG22	2.15	0.47
31:5:63:GLY:HA3	31:5:142:LEU:HG	1.97	0.46
1:A:1583:A:O2'	31:5:223:VAL:HG21	2.15	0.46
12:L:85:VAL:HG23	12:L:90:LYS:HG3	1.98	0.46
29:4:397:MET:HG3	29:4:431:LEU:HD11	1.97	0.46
3:C:145:TYR:CG	29:4:121:ILE:HD13	2.50	0.46
22:V:263:MET:HB2	22:V:337:LEU:HD13	1.98	0.46
29:4:376:ILE:HG23	29:4:422:ILE:HD12	1.97	0.46
30:9:280:ALA:N	30:9:309:VAL:HG23	2.30	0.46
1:A:706:C:OP1	27:0:43:ARG:NE	2.46	0.46
6:F:48:LYS:NZ	24:X:375:GLU:OE2	2.49	0.46
15:O:185:SER:O	18:R:183:LYS:NZ	2.45	0.46
28:1:255:ASN:N	28:1:259:GLU:OE1	2.39	0.46
31:5:22:ILE:HD12	31:5:29:ALA:O	2.14	0.46
29:4:567:THR:HG22	29:4:568:ALA:N	2.30	0.46
1:A:812:A:O2'	1:A:814:A:N1	2.44	0.46
29:4:279:TYR:CZ	29:4:283:LEU:HD11	2.50	0.46
30:9:596:ARG:O	30:9:596:ARG:NH1	2.43	0.46
31:5:130:GLU:HA	31:5:234:ILE:HG23	1.96	0.46
8:H:159:TYR:O	8:H:163:ASN:ND2	2.49	0.46
24:X:81:HIS:CD2	24:X:190:ASN:HB3	2.51	0.46
24:X:228:GLN:NE2	24:X:235:ASN:OD1	2.48	0.46
31:5:123:GLU:N	31:5:123:GLU:OE1	2.48	0.46
1:A:825:U:O4	1:A:828:C:N4	2.49	0.46
18:R:252:ASP:OD1	18:R:256:ARG:NH1	2.48	0.46
23:W:100:VAL:HG11	23:W:144:LEU:HD11	1.98	0.46
24:X:126:LEU:HD23	24:X:343:ILE:HB	1.98	0.46
29:4:627:ALA:HB1	29:4:649:VAL:HG13	1.98	0.46
1:A:1431:G:O2'	1:A:1457:G:O6	2.25	0.46
6:F:116:GLU:OE2	24:X:86:ARG:NH2	2.42	0.46
23:W:99:LEU:HD23	23:W:143:ARG:HG3	1.98	0.46
24:X:380:LEU:HD21	24:X:398:LEU:CD1	2.47	0.45
30:9:278:LEU:O	30:9:280:ALA:N	2.49	0.45
30:9:556:PHE:CE1	30:9:633:VAL:HG13	2.51	0.45
1:A:1106:C:H2'	1:A:1108:C:OP2	2.16	0.45
27:0:34:TYR:O	27:0:43:ARG:NH1	2.49	0.45
29:4:273:GLU:O	29:4:277:ASN:N	2.41	0.45
1:A:1455:U:OP1	7:G:278:THR:OG1	2.23	0.45
24:X:123:ARG:NH2	24:X:339:PRO:O	2.47	0.45
4:D:401:VAL:HG21	20:T:50:PHE:CD1	2.51	0.45
9:I:83:ILE:O	9:I:148:ARG:NE	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:478:TYR:OH	29:4:515:ASP:OD2	2.34	0.45
6:F:193:ASP:OD1	6:F:194:LYS:N	2.49	0.45
24:X:151:LEU:HD23	24:X:247:LEU:HD22	1.97	0.45
30:9:670:ARG:NH2	30:9:671:ILE:O	2.46	0.45
4:D:140:LEU:N	4:D:158:ALA:O	2.47	0.45
29:4:438:LEU:O	29:4:441:THR:OG1	2.28	0.45
29:4:576:LEU:HD23	29:4:595:MET:CE	2.47	0.45
31:5:64:PRO:HG2	31:5:83:VAL:HG13	1.99	0.45
1:A:928:A:H3'	1:A:929:A:C5	2.52	0.45
1:A:1299:A:H2'	1:A:1300:A:C8	2.52	0.45
15:O:214:SER:OG	15:O:217:ARG:NH2	2.50	0.45
3:C:89:ASP:OD1	3:C:112:ARG:NH2	2.45	0.44
9:I:109:PHE:O	9:I:138:ARG:NH2	2.50	0.44
22:V:92:LEU:O	22:V:96:ARG:N	2.47	0.44
31:5:18:ILE:HG23	31:5:19:ARG:N	2.31	0.44
1:A:938:A:O2'	1:A:1169:G:O2'	2.34	0.44
2:B:149:ARG:NH2	17:Q:82:ASP:OD1	2.43	0.44
15:O:208:PRO:HG2	15:O:213:LEU:HD21	1.99	0.44
22:V:266:VAL:O	22:V:346:LYS:HE2	2.17	0.44
29:4:98:ALA:N	29:4:102:GLU:OE1	2.39	0.44
29:4:170:VAL:HG13	29:4:247:ILE:HD11	1.99	0.44
7:G:356:VAL:HG23	7:G:361:VAL:HG23	1.99	0.44
19:S:102:LYS:CG	19:S:121:THR:HG23	2.48	0.44
1:A:928:A:HO2'	1:A:929:A:P	2.38	0.44
1:A:1233:C:O2	11:K:86:ARG:NH1	2.50	0.44
29:4:562:GLN:NE2	29:4:569:GLN:OE1	2.51	0.44
30:9:210:ARG:O	30:9:210:ARG:HG2	2.17	0.44
30:9:670:ARG:HA	30:9:677:TYR:HA	1.99	0.44
13:M:19:ILE:HB	13:M:83:LEU:HD23	2.00	0.44
27:0:163:SER:HA	27:0:191:LEU:O	2.17	0.44
30:9:668:GLY:N	30:9:678:LYS:O	2.42	0.44
4:D:245:VAL:HG22	4:D:271:ALA:HB1	2.00	0.44
25:Y:283:ALA:O	25:Y:287:ALA:N	2.47	0.44
24:X:112:LEU:HD12	24:X:141:VAL:HG13	2.00	0.44
25:Y:256:LEU:HD21	29:4:313:TRP:HZ2	1.81	0.44
30:9:671:ILE:HG22	30:9:673:LYS:HG2	1.99	0.44
31:5:88:THR:HG23	31:5:89:ARG:HD3	1.99	0.44
1:A:1152:A:H2'	1:A:1152:A:N3	2.32	0.44
1:A:1272:A:N1	1:A:1303:G:O2'	2.26	0.44
13:M:54:TYR:CD1	13:M:66:VAL:HG22	2.52	0.44
21:U:166:ASN:O	21:U:176:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5:187:ASN:OD1	31:5:190:SER:OG	2.36	0.44
8:H:184:ILE:O	8:H:184:ILE:HG22	2.18	0.43
27:0:41:LEU:HD11	27:0:59:ARG:NH1	2.33	0.43
31:5:13:PRO:HG2	31:5:97:LEU:HD23	1.99	0.43
4:D:241:ILE:HG21	4:D:264:ARG:HG3	2.00	0.43
11:K:56:SER:O	11:K:60:ASN:ND2	2.51	0.43
16:P:73:ASP:OD1	16:P:74:TYR:N	2.51	0.43
19:S:8:THR:HG22	19:S:46:PHE:CG	2.53	0.43
30:9:209:LEU:HD23	30:9:238:VAL:HG12	2.00	0.43
1:A:808:C:OP2	27:0:19:ARG:NH2	2.50	0.43
22:V:76:ILE:HD13	22:V:88:ALA:HB1	2.01	0.43
30:9:262:GLN:HA	30:9:265:ARG:HE	1.84	0.43
28:1:63:ASP:OD1	28:1:63:ASP:N	2.45	0.43
1:A:1060:A:OP2	31:5:262:ARG:NH2	2.51	0.43
27:0:103:ASP:N	27:0:111:HIS:O	2.41	0.43
3:C:58:ALA:HB1	3:C:59:PRO:HD2	2.01	0.43
4:D:243:VAL:HG11	4:D:268:PHE:HD1	1.81	0.43
10:J:64:CYS:SG	10:J:82:ARG:NH1	2.92	0.43
27:0:19:ARG:O	27:0:23:GLU:N	2.50	0.43
6:F:174:LEU:HD22	6:F:178:ARG:CG	2.49	0.43
7:G:200:LEU:CD1	7:G:208:MET:SD	3.07	0.43
9:I:121:LYS:O	9:I:124:THR:OG1	2.28	0.43
14:N:93:ASP:O	14:N:97:GLY:N	2.47	0.43
31:5:87:ASP:OD2	31:5:89:ARG:NH2	2.49	0.43
22:V:151:PHE:HE2	22:V:163:VAL:HG21	1.84	0.43
24:X:152:ILE:O	24:X:195:ASN:ND2	2.49	0.43
13:M:67:ALA:HB2	18:R:196:TYR:CE1	2.53	0.43
24:X:151:LEU:O	24:X:258:LEU:HD12	2.18	0.43
30:9:527:ARG:NH1	30:9:564:LEU:O	2.47	0.43
31:5:91:ILE:HD13	31:5:94:LEU:HD12	2.01	0.43
2:B:272:ARG:O	2:B:276:GLN:N	2.52	0.43
5:E:32:ARG:NE	5:E:77:SER:OG	2.45	0.43
6:F:114:THR:HG21	6:F:205:LEU:CD2	2.48	0.43
14:N:58:CYS:SG	14:N:81:LEU:HD22	2.58	0.43
27:0:81:THR:CG2	27:0:86:LEU:HD11	2.49	0.43
30:9:258:PRO:O	30:9:263:ARG:NH2	2.52	0.43
30:9:270:GLU:O	30:9:273:ALA:HB3	2.19	0.43
31:5:127:ARG:CG	31:5:134:PRO:HA	2.49	0.43
16:P:141:ARG:HG2	16:P:142:GLU:HG2	2.01	0.42
18:R:274:TYR:O	18:R:278:ASN:ND2	2.46	0.42
20:T:92:THR:O	20:T:92:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:376:ILE:HG23	29:4:422:ILE:CD1	2.49	0.42
1:A:919:A:OP1	15:O:92:LYS:NZ	2.33	0.42
30:9:273:ALA:CA	30:9:279:LEU:HD12	2.49	0.42
31:5:209:ILE:HD12	31:5:209:ILE:H	1.84	0.42
1:A:931:C:C4	14:N:38:TYR:CD2	3.07	0.42
1:A:1053:A:N6	1:A:1100:C:HO2'	2.16	0.42
20:T:77:ARG:HG2	20:T:79:TYR:CE1	2.54	0.42
1:A:941:G:H4'	1:A:942:A:OP1	2.19	0.42
14:N:65:LEU:O	14:N:82:ALA:N	2.51	0.42
24:X:135:THR:N	37:X:501:ATP:O1B	2.43	0.42
30:9:316:ILE:HG12	30:9:317:SER:N	2.35	0.42
29:4:533:MET:O	29:4:537:ARG:N	2.53	0.42
30:9:619:ALA:HA	30:9:634:THR:HG22	2.02	0.42
1:A:1199:G:N2	1:A:1422:G:O5'	2.52	0.42
19:S:105:GLU:O	19:S:109:LEU:N	2.46	0.42
23:W:152:ARG:NE	23:W:159:ASP:OD1	2.51	0.42
28:1:262:ILE:HG23	28:1:263:LEU:N	2.35	0.42
31:5:286:ILE:HD13	31:5:303:LEU:HD21	2.00	0.42
1:A:1019:A:H3'	1:A:1020:C:H5'	2.02	0.42
1:A:1465:C:O2	1:A:1467:C:N4	2.52	0.42
20:T:79:TYR:CD1	20:T:85:GLN:HG2	2.54	0.42
25:Y:285:GLN:O	25:Y:289:VAL:HG13	2.20	0.42
2:B:223:VAL:O	2:B:223:VAL:HG23	2.20	0.42
8:H:145:LEU:N	8:H:145:LEU:HD12	2.34	0.42
15:O:161:GLY:O	18:R:223:ARG:NH1	2.52	0.42
29:4:583:PHE:O	29:4:588:ARG:N	2.53	0.42
29:4:584:LEU:HD11	29:4:614:LEU:HG	2.00	0.42
31:5:183:ARG:O	31:5:197:SER:HB2	2.20	0.42
1:A:1375:C:H2'	1:A:1376:C:O4'	2.20	0.42
1:A:1377:C:OP1	24:X:320:ARG:NE	2.53	0.42
8:H:51:HIS:N	29:4:480:ASP:OD2	2.53	0.42
22:V:236:LEU:HD12	22:V:290:LEU:HD13	2.02	0.42
25:Y:323:ASP:O	25:Y:324:ASP:HB2	2.20	0.42
29:4:376:ILE:O	29:4:380:ASP:N	2.52	0.42
29:4:437:GLY:O	29:4:441:THR:HG23	2.19	0.42
1:A:1058:C:OP1	31:5:257:ARG:NE	2.53	0.42
18:R:352:ALA:O	18:R:356:HIS:ND1	2.52	0.42
22:V:30:LEU:HD21	22:V:181:LEU:HD11	2.02	0.42
31:5:67:GLY:O	31:5:71:ARG:N	2.50	0.42
1:A:1017:A:O2'	16:P:104:GLN:NE2	2.53	0.41
3:C:75:ASN:OD1	11:K:104:TRP:NE1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:70:LEU:HD21	27:0:191:LEU:HD11	2.02	0.41
27:0:28:PRO:CG	27:0:33:LEU:HD21	2.50	0.41
29:4:549:ALA:O	29:4:553:ALA:N	2.38	0.41
30:9:202:LEU:HD12	30:9:237:LEU:HD21	2.02	0.41
1:A:707:C:OP1	27:0:213:ALA:N	2.51	0.41
3:C:134:PHE:CD2	4:D:144:LEU:HD13	2.55	0.41
4:D:323:ILE:HG21	4:D:349:LEU:HD23	2.02	0.41
15:O:213:LEU:HD13	15:O:227:GLU:OE2	2.21	0.41
21:U:73:GLU:O	21:U:76:SER:OG	2.27	0.41
24:X:380:LEU:HD21	24:X:398:LEU:HD11	2.02	0.41
27:0:61:GLU:OE2	27:0:140:ARG:NH2	2.48	0.41
1:A:1154:A:OP1	31:5:293:ARG:NH1	2.52	0.41
6:F:197:GLN:N	6:F:197:GLN:OE1	2.52	0.41
21:U:167:PHE:O	21:U:169:THR:HG23	2.20	0.41
22:V:79:ILE:HD11	22:V:88:ALA:CB	2.50	0.41
30:9:264:LEU:HD12	30:9:315:LEU:CD2	2.51	0.41
30:9:265:ARG:HD3	30:9:315:LEU:HD13	2.01	0.41
30:9:625:PHE:CD2	30:9:653:LEU:HD13	2.56	0.41
1:A:1196:A:H2'	1:A:1197:G:O4'	2.20	0.41
3:C:148:LYS:HA	29:4:140:LEU:HD13	2.02	0.41
21:U:84:GLU:O	21:U:88:GLY:N	2.53	0.41
1:A:663:A:H2'	1:A:664:G:C8	2.56	0.41
5:E:47:LEU:HD13	5:E:51:ILE:HD12	2.01	0.41
10:J:110:VAL:O	10:J:110:VAL:HG23	2.21	0.41
23:W:134:TYR:O	23:W:135:GLN:NE2	2.54	0.41
31:5:60:TYR:CD1	31:5:82:LEU:HD22	2.56	0.41
31:5:98:SER:HB2	31:5:105:LEU:HD23	2.01	0.41
1:A:857:G:OP1	20:T:162:LYS:NZ	2.25	0.41
4:D:363:ALA:O	4:D:367:GLY:N	2.53	0.41
22:V:151:PHE:O	22:V:155:GLU:N	2.54	0.41
1:A:922:C:O2'	1:A:923:A:OP2	2.28	0.41
1:A:1322:C:OP2	3:C:36:LYS:NZ	2.48	0.41
4:D:316:CYS:O	4:D:321:ILE:HD11	2.21	0.41
9:I:97:ILE:HD11	9:I:161:ALA:HB1	2.02	0.41
15:O:208:PRO:CG	15:O:213:LEU:HD21	2.51	0.41
22:V:241:ARG:HA	22:V:244:TYR:CE2	2.55	0.41
23:W:113:TYR:CD2	23:W:123:VAL:HG22	2.56	0.41
29:4:596:LEU:HD21	29:4:614:LEU:HD11	2.01	0.41
1:A:892:A:OP1	10:J:77:ASN:HB2	2.21	0.41
1:A:1174:U:H2'	1:A:1175:G:O4'	2.21	0.41
1:A:1384:A:OP2	6:F:198:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:U:OP1	26:Z:32:LYS:NZ	2.45	0.41
4:D:229:PHE:HA	4:D:238:LYS:O	2.20	0.41
5:E:67:ASP:OD1	5:E:68:PHE:N	2.54	0.41
6:F:114:THR:HG21	6:F:205:LEU:HD23	2.02	0.41
12:L:64:ASP:OD2	12:L:137:ARG:NH2	2.54	0.41
14:N:35:LEU:HD11	14:N:40:LEU:HA	2.03	0.41
14:N:67:ARG:NH2	14:N:80:GLU:OE2	2.54	0.41
27:0:14:LEU:HB2	30:9:91:LEU:HD13	2.02	0.41
30:9:646:TYR:N	30:9:646:TYR:CD1	2.87	0.41
20:T:109:ASN:OD1	20:T:112:THR:N	2.37	0.41
25:Y:323:ASP:OD1	25:Y:323:ASP:C	2.59	0.41
6:F:162:LEU:HD13	6:F:167:PHE:CE1	2.57	0.40
8:H:155:VAL:HG21	28:1:129:PHE:CB	2.51	0.40
29:4:290:ASP:OD1	29:4:293:THR:OG1	2.32	0.40
1:A:974:U:H4'	5:E:90:ARG:HH12	1.85	0.40
1:A:991:G:O2'	1:A:1085:C:H4'	2.21	0.40
4:D:310:LYS:HA	4:D:331:ASP:OD2	2.21	0.40
28:1:57:THR:HG23	28:1:79:SER:O	2.22	0.40
1:A:1279:C:O2'	1:A:1296:A:N1	2.39	0.40
3:C:119:ILE:O	3:C:153:LEU:HD12	2.22	0.40
24:X:99:LEU:HD11	24:X:136:LEU:HB3	2.03	0.40
24:X:153:LEU:HD21	24:X:244:LEU:HD22	2.04	0.40
1:A:770:C:H2'	1:A:771:A:O4'	2.21	0.40
1:A:1159:A:C2'	1:A:1160:A:O5'	2.70	0.40
18:R:160:ASP:O	18:R:170:ARG:NH1	2.54	0.40
22:V:60:THR:HG22	22:V:65:LEU:O	2.21	0.40
25:Y:313:PHE:CE2	25:Y:315:ILE:HD11	2.57	0.40
30:9:285:GLY:N	30:9:286:PRO:CD	2.85	0.40
30:9:511:THR:O	30:9:515:VAL:HG23	2.21	0.40
1:A:700:A:H4'	1:A:701:G:O5'	2.22	0.40
1:A:1181:G:H2'	1:A:1182:C:C6	2.56	0.40
4:D:243:VAL:HG12	4:D:245:VAL:HG13	2.03	0.40
7:G:87:HIS:CD2	28:1:62:VAL:HG12	2.56	0.40
12:L:193:PRO:HG2	12:L:196:TYR:CE1	2.57	0.40
28:1:221:TYR:CZ	28:1:225:LEU:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	223/296 (75%)	220 (99%)	3 (1%)	0	100	100
3	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
4	D	326/430 (76%)	320 (98%)	6 (2%)	0	100	100
5	E	107/125 (86%)	104 (97%)	3 (3%)	0	100	100
6	F	199/242 (82%)	198 (100%)	1 (0%)	0	100	100
7	G	309/396 (78%)	303 (98%)	6 (2%)	0	100	100
8	H	138/201 (69%)	135 (98%)	2 (1%)	1 (1%)	19	47
9	I	134/194 (69%)	132 (98%)	2 (2%)	0	100	100
10	J	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
11	K	99/128 (77%)	99 (100%)	0	0	100	100
12	L	162/257 (63%)	160 (99%)	2 (1%)	0	100	100
13	M	117/137 (85%)	117 (100%)	0	0	100	100
14	N	108/130 (83%)	108 (100%)	0	0	100	100
15	O	191/258 (74%)	188 (98%)	3 (2%)	0	100	100
16	P	95/142 (67%)	92 (97%)	3 (3%)	0	100	100
17	Q	85/87 (98%)	82 (96%)	2 (2%)	1 (1%)	11	35
18	R	293/360 (81%)	289 (99%)	4 (1%)	0	100	100
19	S	133/190 (70%)	128 (96%)	5 (4%)	0	100	100
20	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
22	V	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
23	W	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
24	X	348/398 (87%)	342 (98%)	6 (2%)	0	100	100
25	Y	130/395 (33%)	128 (98%)	2 (2%)	0	100	100
26	Z	94/106 (89%)	94 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	0	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
28	1	275/323 (85%)	273 (99%)	2 (1%)	0	100	100
29	4	580/689 (84%)	570 (98%)	10 (2%)	0	100	100
30	9	403/698 (58%)	385 (96%)	18 (4%)	0	100	100
31	5	317/346 (92%)	313 (99%)	4 (1%)	0	100	100
32	a	26/343 (8%)	26 (100%)	0	0	100	100
All	All	6137/8370 (73%)	6030 (98%)	105 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	126	ILE
17	Q	2	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	198/249 (80%)	198 (100%)	0	100	100
3	C	115/143 (80%)	115 (100%)	0	100	100
4	D	278/357 (78%)	278 (100%)	0	100	100
5	E	92/107 (86%)	92 (100%)	0	100	100
6	F	182/209 (87%)	182 (100%)	0	100	100
7	G	272/342 (80%)	272 (100%)	0	100	100
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	104/146 (71%)	104 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	153/226 (68%)	153 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	174/230 (76%)	174 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100
17	Q	78/78 (100%)	78 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100
19	S	116/164 (71%)	116 (100%)	0	100	100
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	V	325/364 (89%)	325 (100%)	0	100	100
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	310/351 (88%)	309 (100%)	1 (0%)	91	95
25	Y	124/357 (35%)	124 (100%)	0	100	100
26	Z	88/95 (93%)	88 (100%)	0	100	100
27	0	188/188 (100%)	188 (100%)	0	100	100
28	1	255/291 (88%)	255 (100%)	0	100	100
29	4	523/609 (86%)	523 (100%)	0	100	100
30	9	358/600 (60%)	356 (99%)	2 (1%)	84	90
31	5	286/309 (93%)	286 (100%)	0	100	100
32	a	26/288 (9%)	26 (100%)	0	100	100
All	All	5496/7272 (76%)	5493 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	X	92	LYS
30	9	265	ARG
30	9	594	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	201	ASN
4	D	151	ASN
4	D	415	GLN

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Mol	Chain	Res	Type
5	E	81	HIS
6	F	147	GLN
6	F	151	ASN
7	G	82	ASN
7	G	87	HIS
7	G	175	HIS
8	H	51	HIS
8	H	163	ASN
13	M	82	HIS
15	O	160	HIS
16	P	104	GLN
22	V	131	ASN
22	V	396	GLN
23	W	135	GLN
24	X	110	HIS
24	X	140	HIS
24	X	164	ASN
24	X	228	GLN
24	X	394	HIS
25	Y	257	ASN
25	Y	290	ASN
25	Y	337	HIS
25	Y	395	ASN
26	Z	55	HIS
27	0	111	HIS
29	4	129	GLN
29	4	189	ASN
29	4	562	GLN
30	9	516	ASN
30	9	551	ASN
30	9	669	GLN
31	5	137	HIS
31	5	171	GLN
31	5	235	GLN
31	5	299	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	844/955 (88%)	132 (15%)	4 (0%)

All (132) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	651	A
1	A	657	G
1	A	680	U
1	A	688	A
1	A	704	U
1	A	721	U
1	A	722	C
1	A	736	C
1	A	738	A
1	A	739	C
1	A	753	A
1	A	761	A
1	A	764	A
1	A	766	G
1	A	773	U
1	A	777	G
1	A	786	G
1	A	791	G
1	A	796	G
1	A	829	C
1	A	830	U
1	A	832	U
1	A	835	C
1	A	836	A
1	A	851	A
1	A	860	A
1	A	868	C
1	A	870	C
1	A	871	A
1	A	884	U
1	A	890	C
1	A	892	A
1	A	893	G
1	A	910	A
1	A	919	A
1	A	923	A
1	A	929	A
1	A	930	G
1	A	931	C
1	A	932	C
1	A	933	G
1	A	939	A
1	A	942	A

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Mol	Chain	Res	Type
1	A	956	C
1	A	958	C
1	A	967	A
1	A	988	G
1	A	993	A
1	A	1001	C
1	A	1008	A
1	A	1011	C
1	A	1015	A
1	A	1020	C
1	A	1042	U
1	A	1045	G
1	A	1049	A
1	A	1065	C
1	A	1069	A
1	A	1072	G
1	A	1075	A
1	A	1080	A
1	A	1081	U
1	A	1082	A
1	A	1083	C
1	A	1089	U
1	A	1098	C
1	A	1103	A
1	A	1105	C
1	A	1106	C
1	A	1107	U
1	A	1118	A
1	A	1120	C
1	A	1121	A
1	A	1126	A
1	A	1144	U
1	A	1151	C
1	A	1152	A
1	A	1154	A
1	A	1155	G
1	A	1167	A
1	A	1175	G
1	A	1187	U
1	A	1188	A
1	A	1189	U
1	A	1200	G

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Mol	Chain	Res	Type
1	A	1215	U
1	A	1223	C
1	A	1225	C
1	A	1242	C
1	A	1247	G
1	A	1248	C
1	A	1250	C
1	A	1251	A
1	A	1258	A
1	A	1261	C
1	A	1265	C
1	A	1270	U
1	A	1271	C
1	A	1273	G
1	A	1284	U
1	A	1285	G
1	A	1290	C
1	A	1291	U
1	A	1293	C
1	A	1300	A
1	A	1326	A
1	A	1342	C
1	A	1343	A
1	A	1345	G
1	A	1354	A
1	A	1360	G
1	A	1362	G
1	A	1376	C
1	A	1390	A
1	A	1391	U
1	A	1405	C
1	A	1407	U
1	A	1417	A
1	A	1421	G
1	A	1422	G
1	A	1425	U
1	A	1430	A
1	A	1443	U
1	A	1447	G
1	A	1454	G
1	A	1462	G
1	A	1466	C

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Mol	Chain	Res	Type
1	A	1583	A
1	A	1584	A
1	A	1585	A
1	A	1594	G
1	A	1595	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	928	A
1	A	930	G
1	A	931	C
1	A	1154	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	5F0	I	184	9	8,8,9	0.58	0	7,9,11	1.09	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	5F0	I	184	9	-	0/9/9/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	184	5F0	O-C-CB	-2.54	118.01	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 52 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
38	GDP	X	502	-	24,30,30	0.91	2 (8%)	30,47,47	0.62	0
36	FES	P	201	16,5	0,4,4	-	-	-		
36	FES	T	201	13,20	0,4,4	-	-	-		
38	GDP	9	801	-	24,30,30	0.88	1 (4%)	30,47,47	0.71	0
37	ATP	X	501	33	26,33,33	0.76	0	31,52,52	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GDP	X	502	-	-	3/12/32/32	0/3/3/3
36	FES	P	201	16,5	-	-	0/1/1/1
36	FES	T	201	13,20	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GDP	9	801	-	-	0/12/32/32	0/3/3/3
37	ATP	X	501	33	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	502	GDP	C5-C6	-2.42	1.42	1.47
38	9	801	GDP	C5-C6	-2.22	1.42	1.47
38	X	502	GDP	C8-N7	-2.03	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	X	502	GDP	C5'-O5'-PA-O1A
38	X	502	GDP	C5'-O5'-PA-O3A
38	X	502	GDP	C4'-C5'-O5'-PA

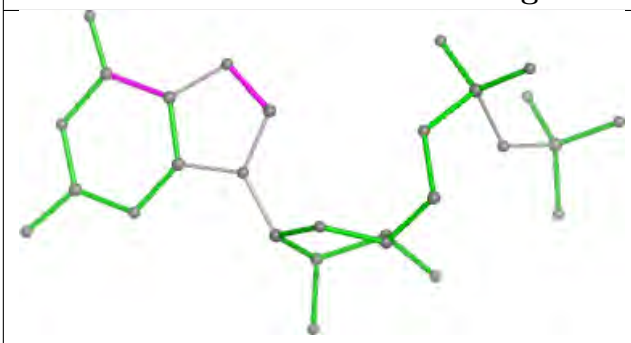
There are no ring outliers.

2 monomers are involved in 3 short contacts:

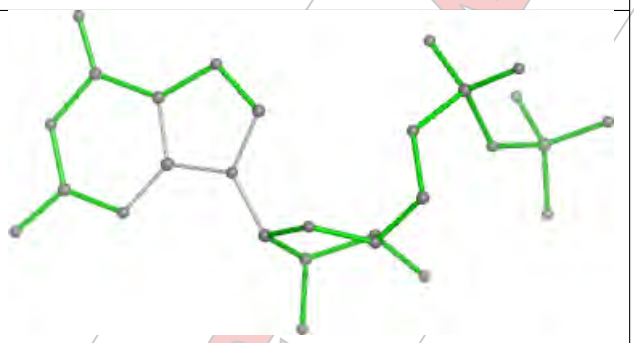
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	9	801	GDP	1	0
37	X	501	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

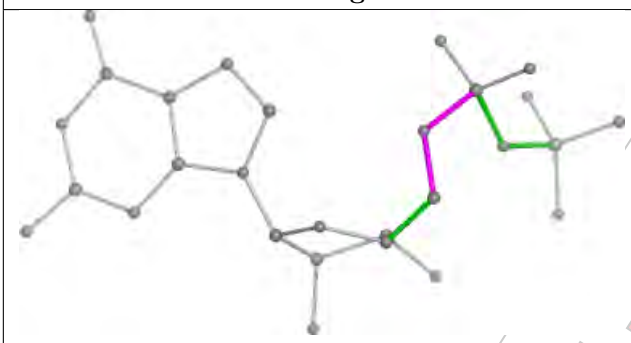
Ligand GDP X 502



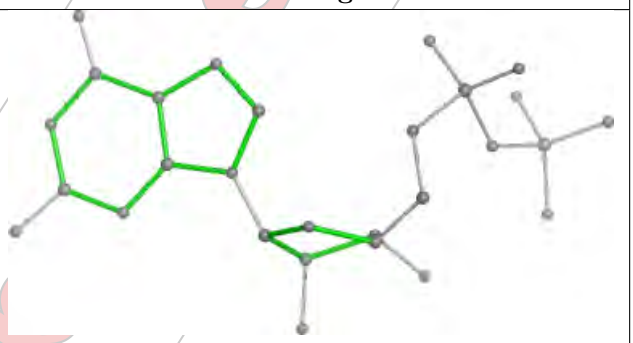
Bond lengths



Bond angles

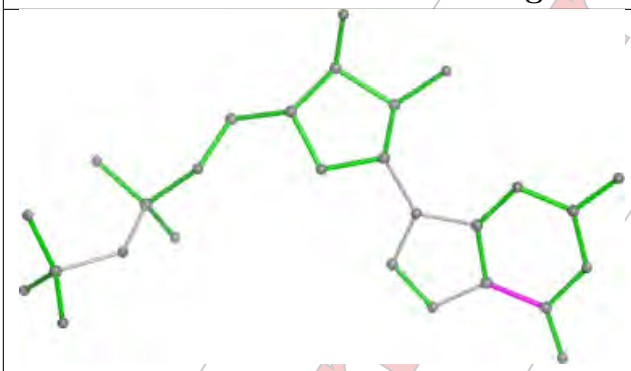


Torsions

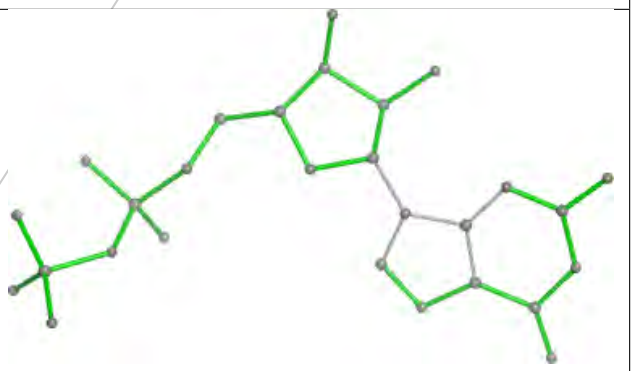


Rings

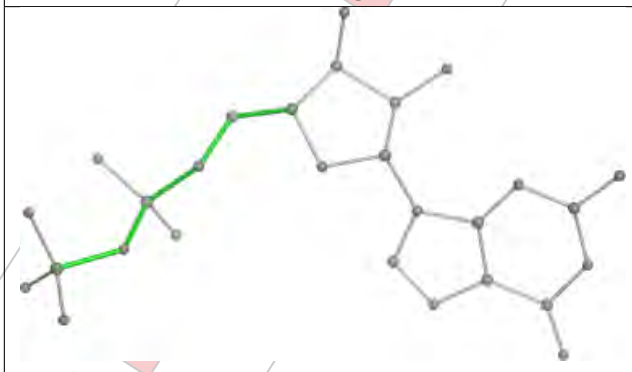
Ligand GDP 9 801



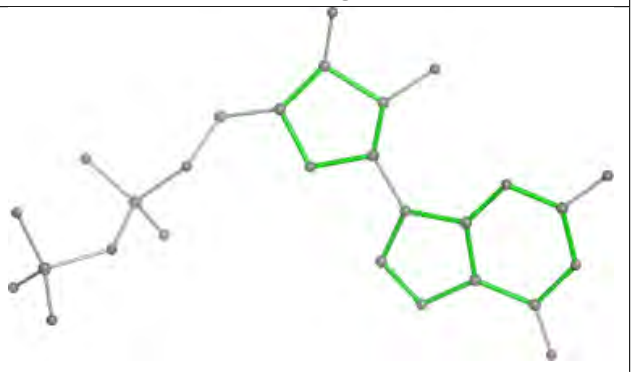
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	9	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	279:LEU	C	280:ALA	N	4.87

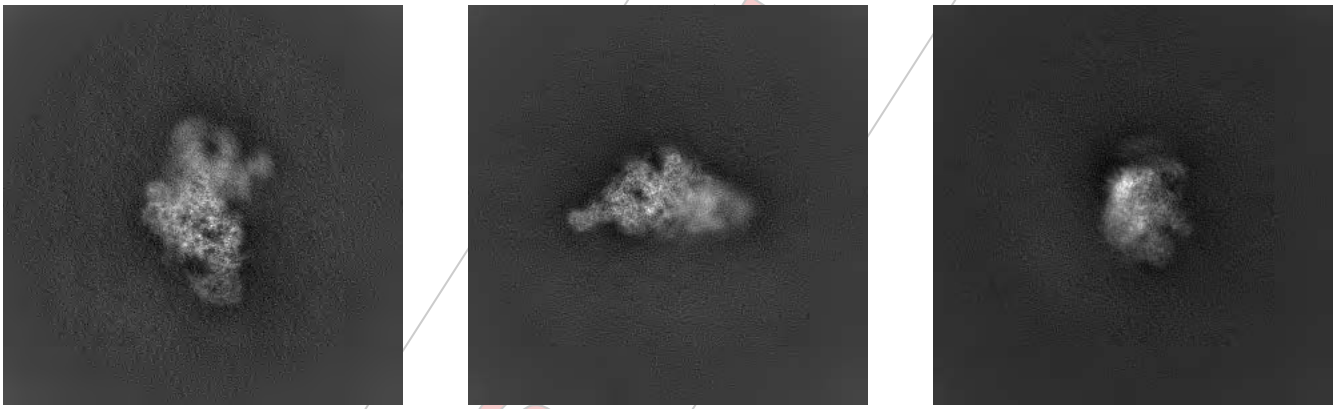
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51877. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

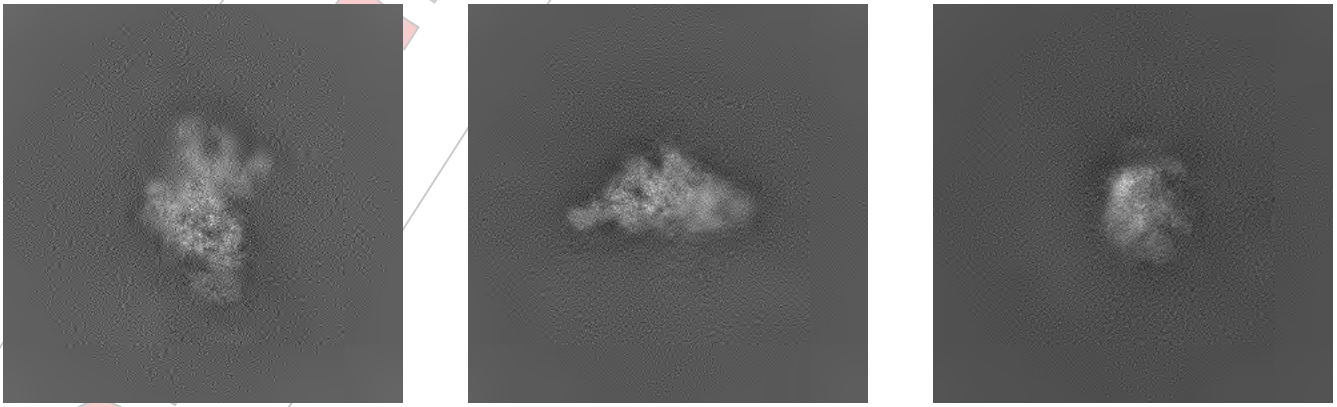
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

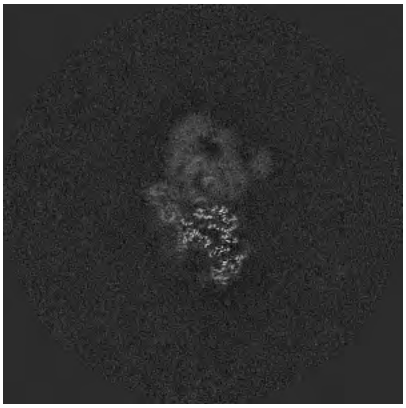


X Y Z

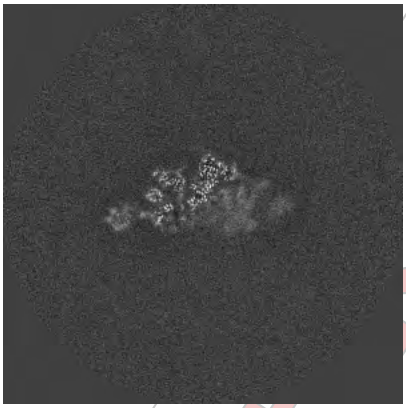
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

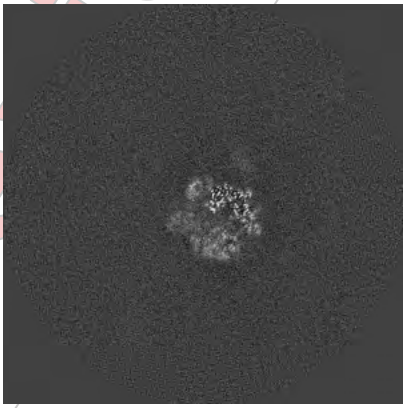
6.2.1 Primary map



X Index: 300

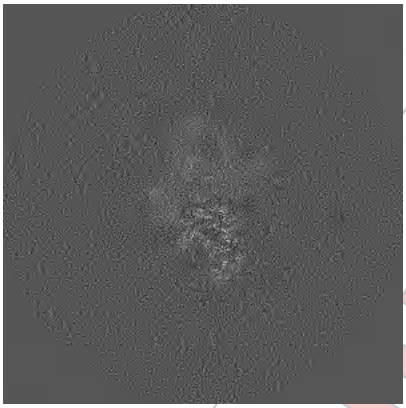


Y Index: 300

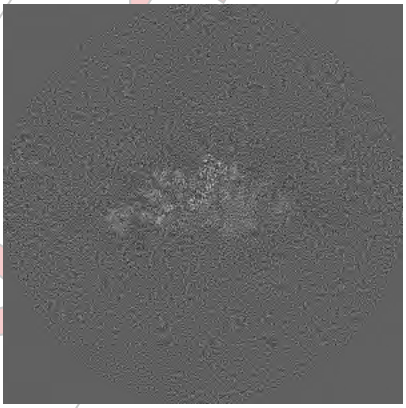


Z Index: 300

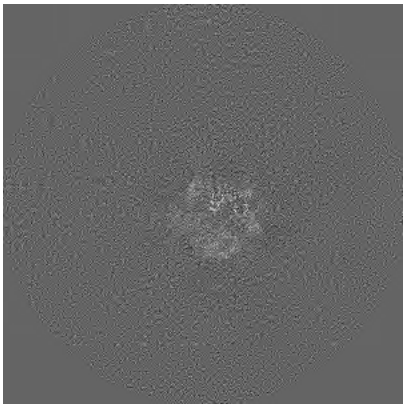
6.2.2 Raw map



X Index: 300



Y Index: 300

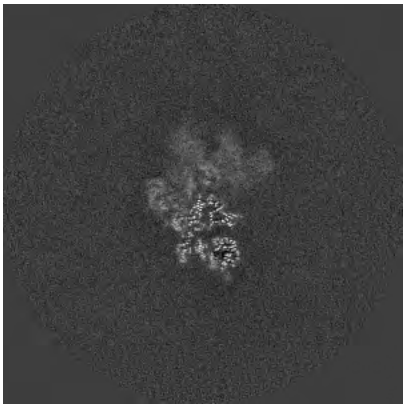


Z Index: 300

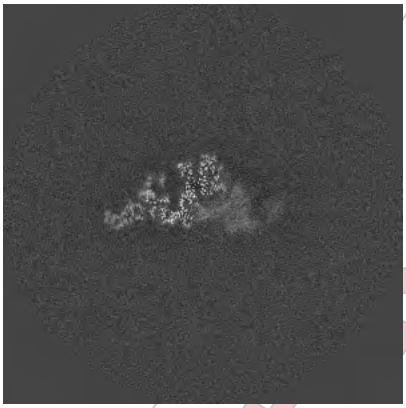
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



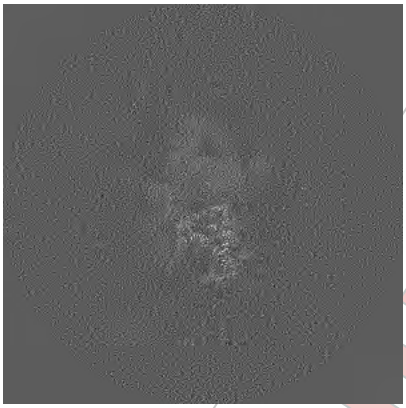
X Index: 314



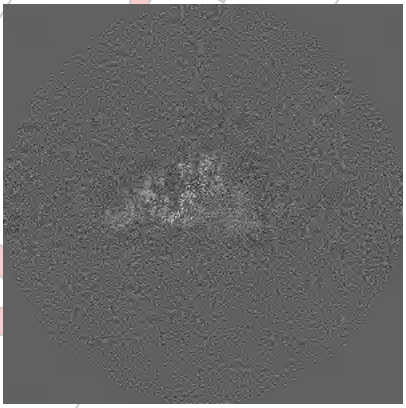
Y Index: 313

Z Index: 273

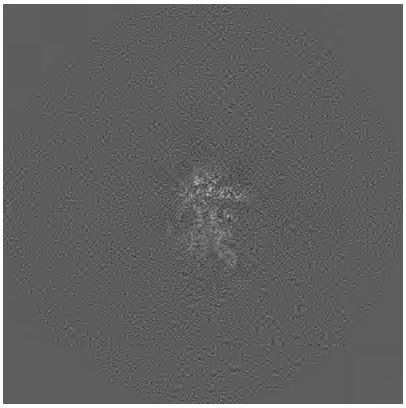
6.3.2 Raw map



X Index: 297



Y Index: 313

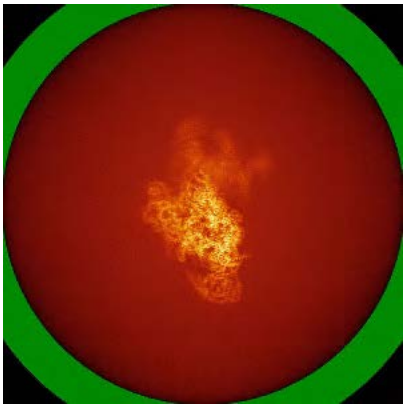


Z Index: 278

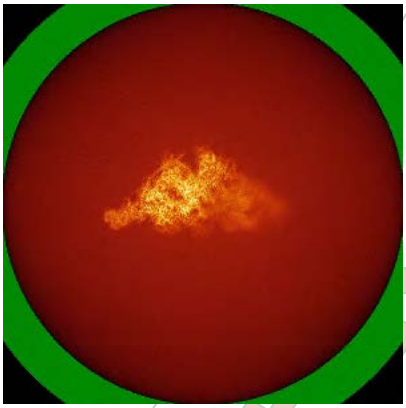
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

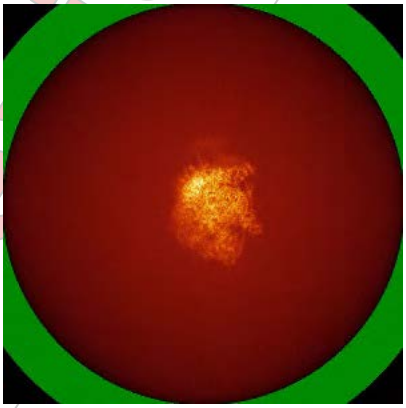
6.4.1 Primary map



X

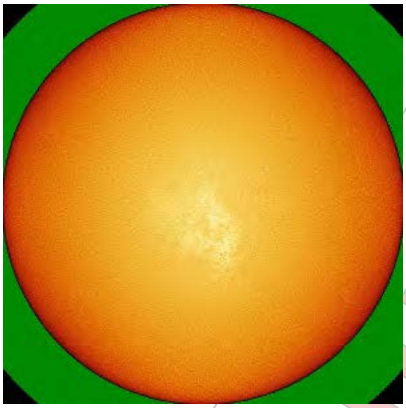


Y

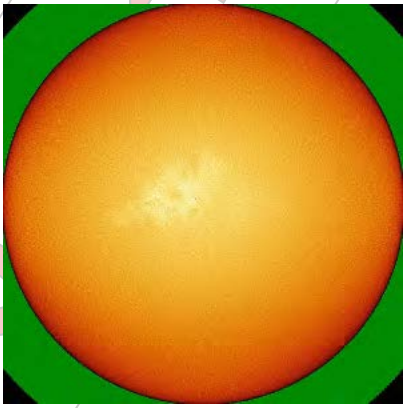


Z

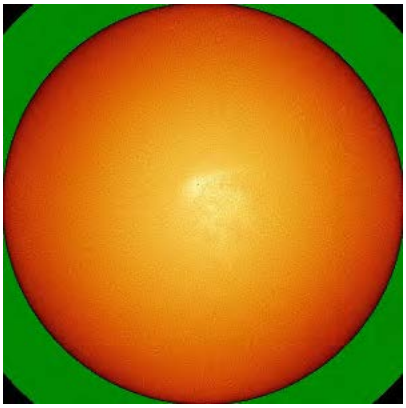
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

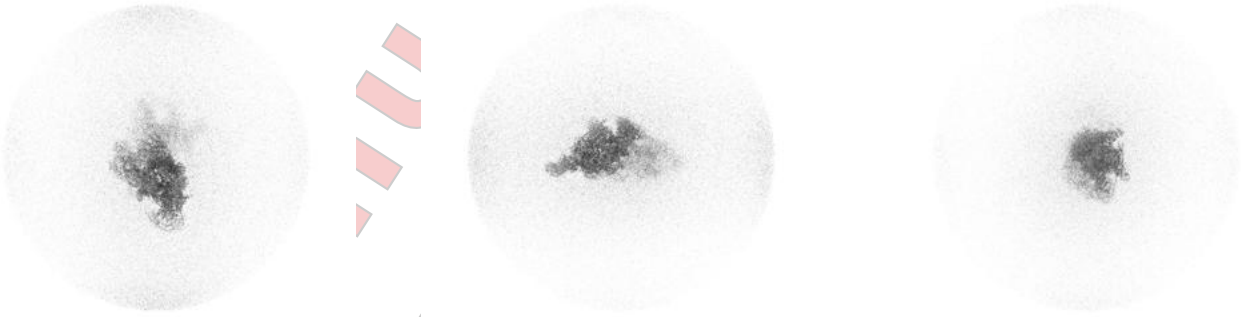
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0054. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

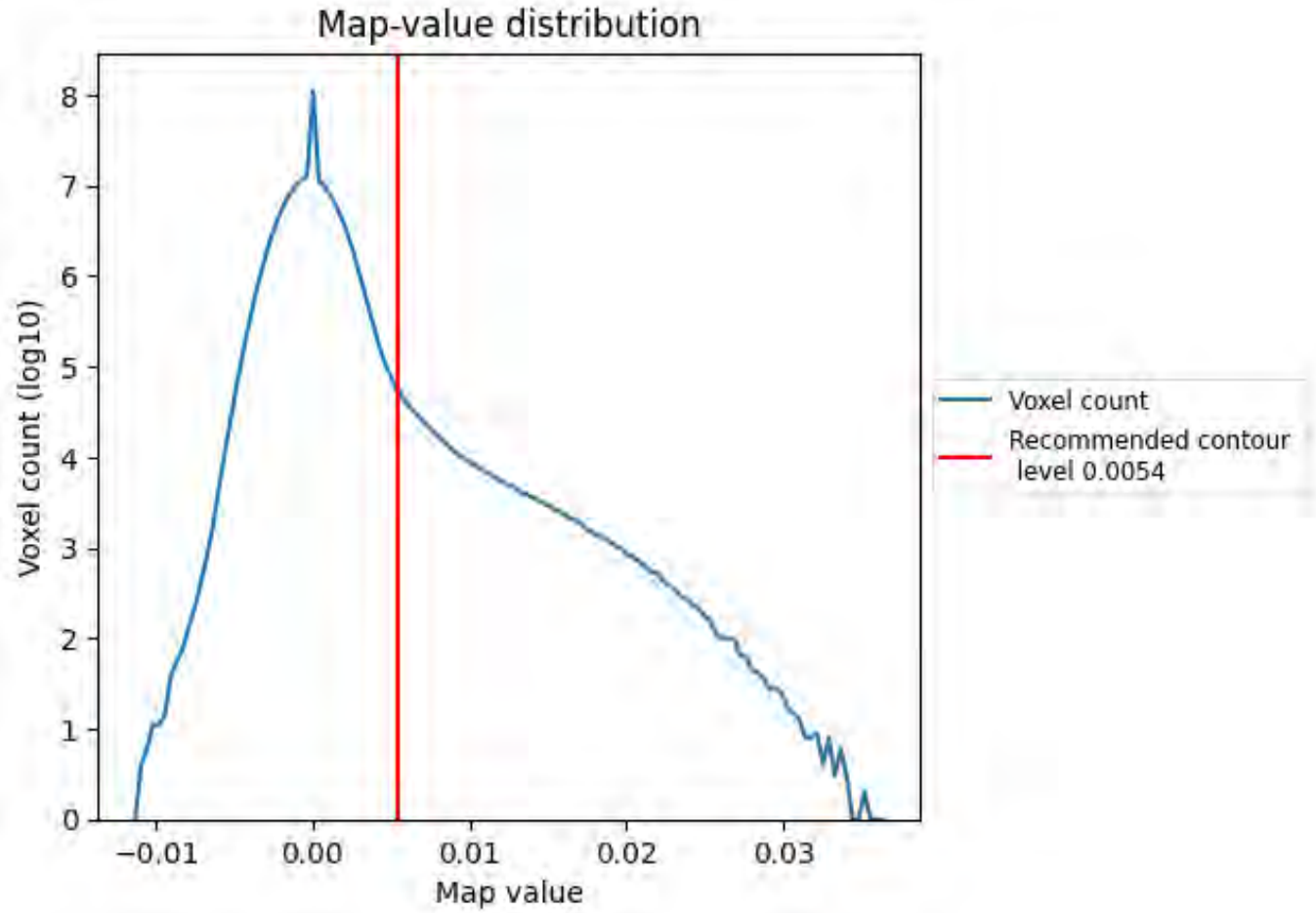
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

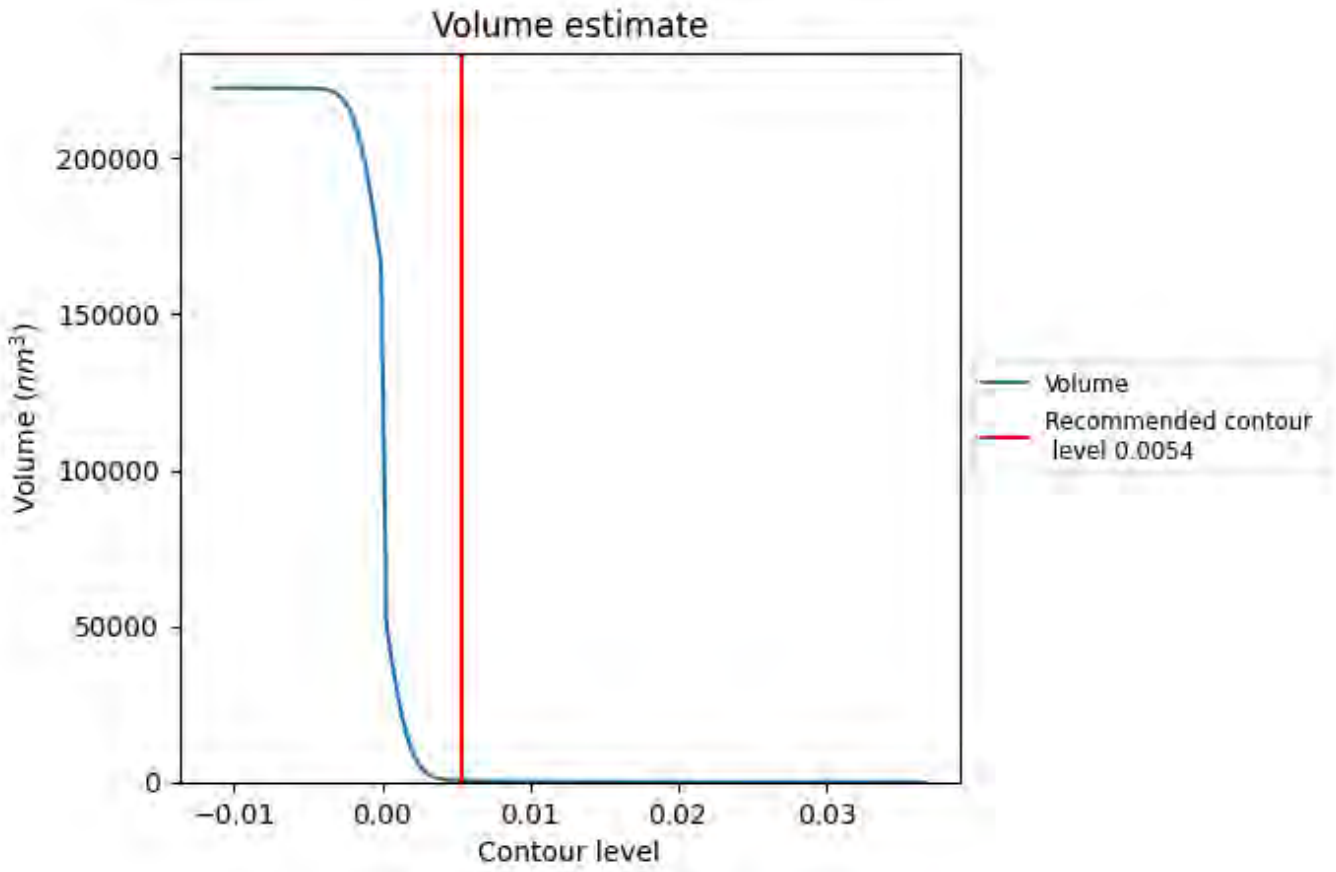
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

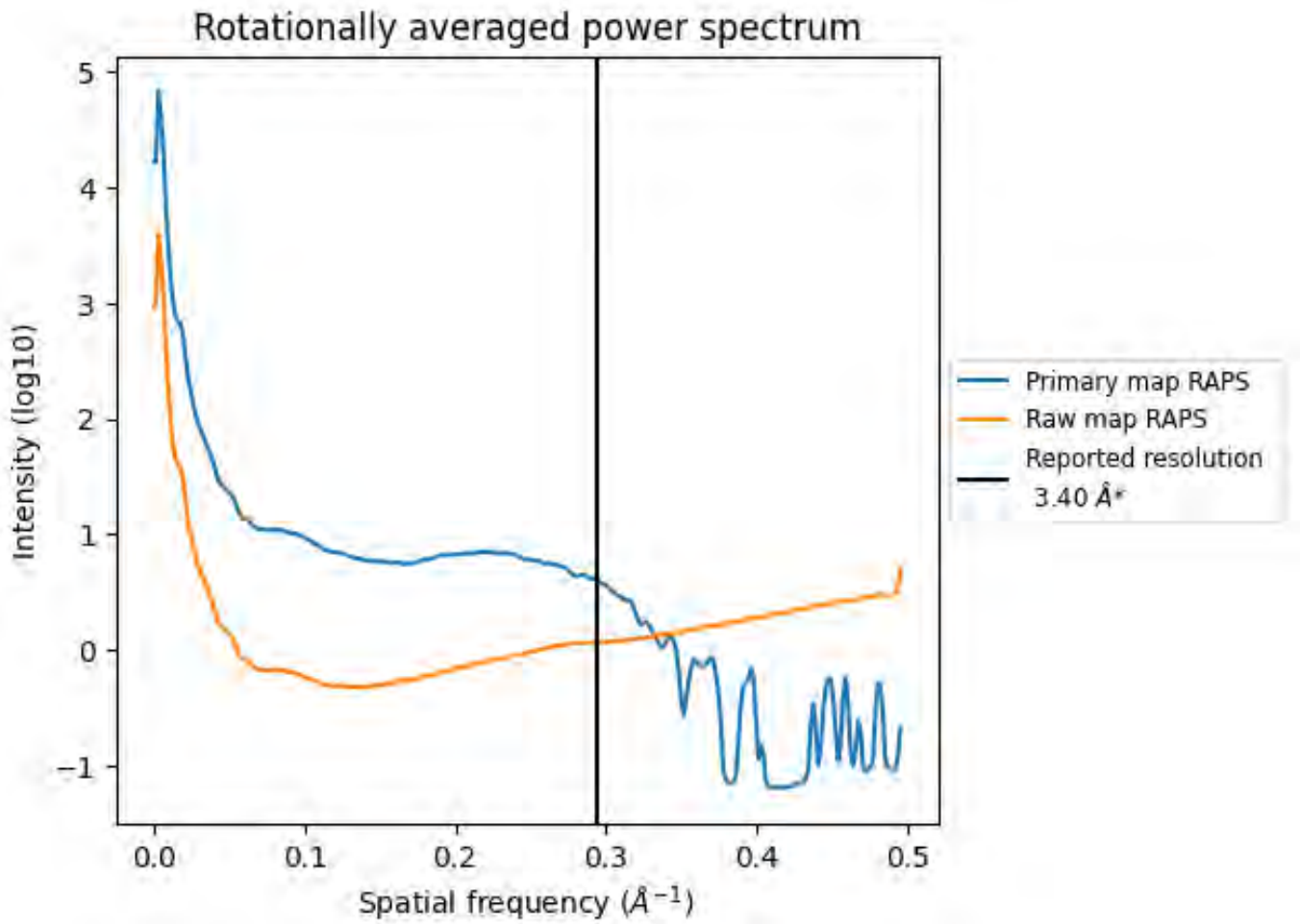
7.2 Volume estimate



The volume at the recommended contour level is 419 nm^3; this corresponds to an approximate mass of 379 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

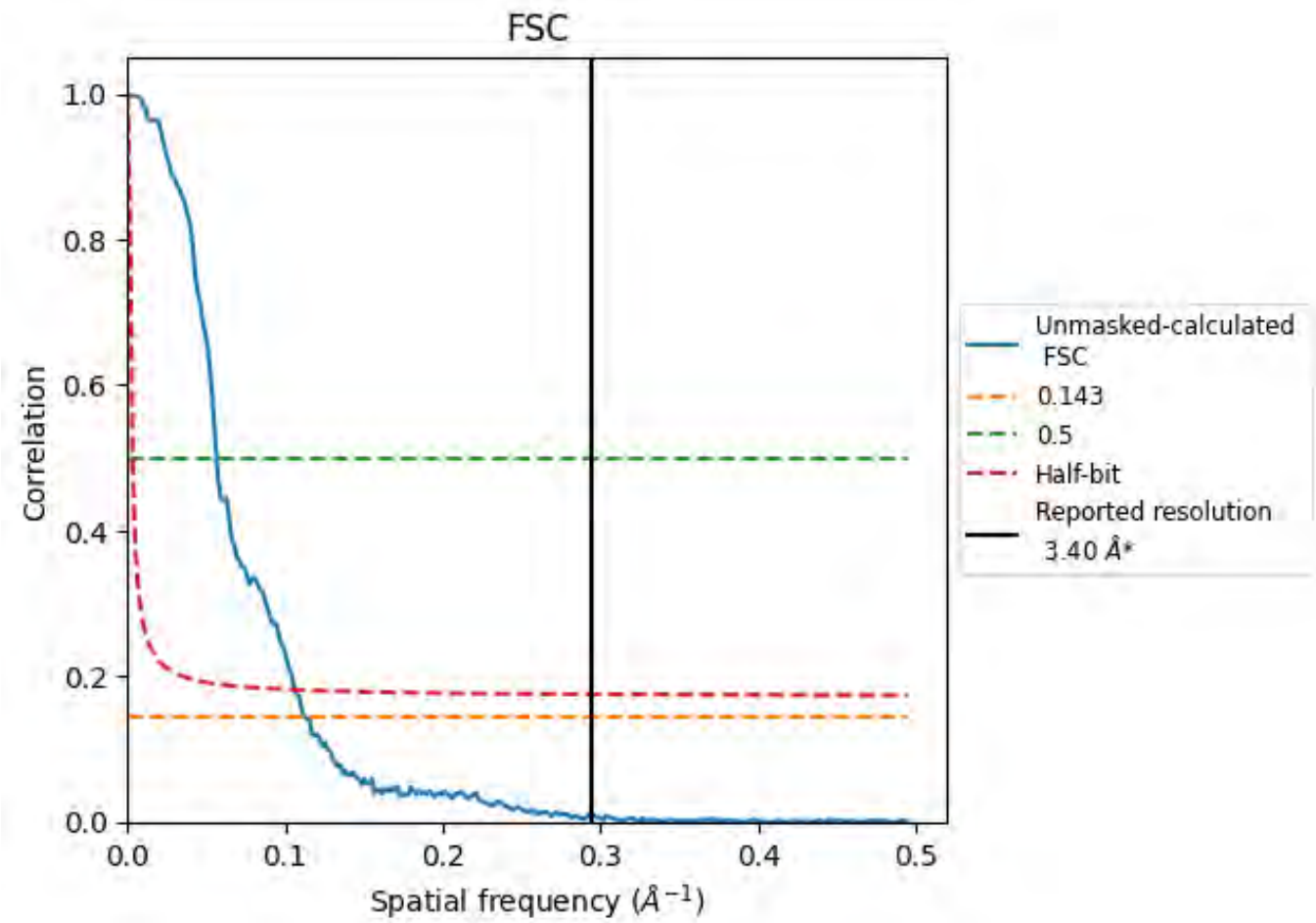


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8.2 Resolution estimates (i)

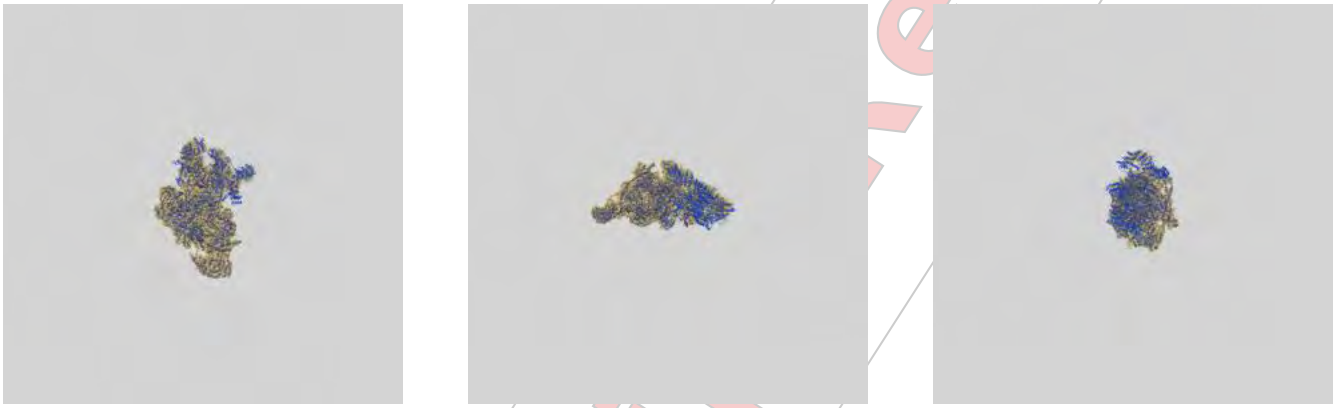
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.40	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.87	17.70	9.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 17.70 differs from the reported value 3.4 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51877 and PDB model 9H55. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay



X Y Z

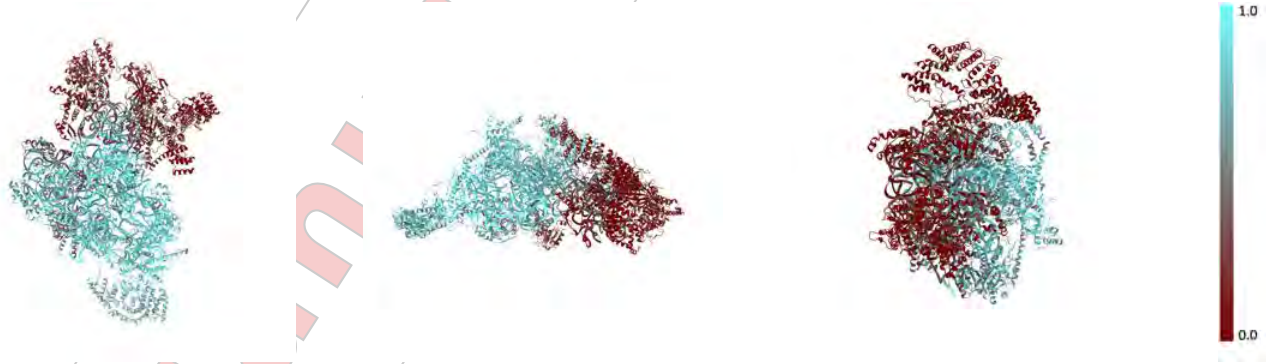
The images above show the 3D surface view of the map at the recommended contour level 0.0054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

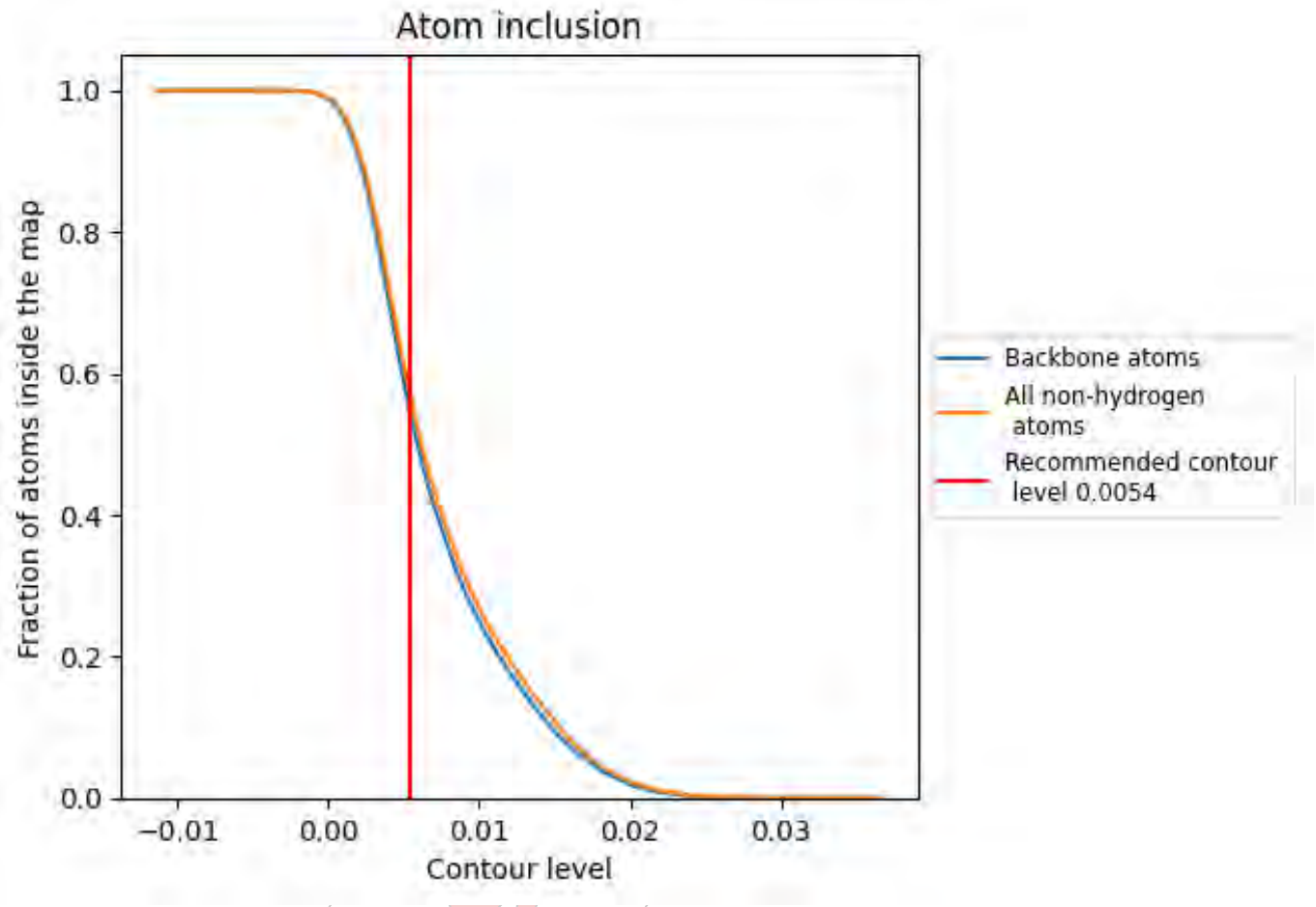
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0054).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5710	0.3030
0	0.8260	0.4810
1	0.1190	0.0360
4	0.0860	0.0430
5	0.2970	0.1760
9	0.4940	0.2860
A	0.7210	0.3670
B	0.8910	0.5310
C	0.2420	0.1160
D	0.6660	0.4240
E	0.7240	0.3530
F	0.1110	0.0300
G	0.4150	0.2050
H	0.2110	0.0980
I	0.4950	0.2520
J	0.7880	0.4850
K	0.2530	0.0780
L	0.7280	0.4230
M	0.9070	0.5610
N	0.8720	0.5330
O	0.9030	0.5410
P	0.7320	0.3830
Q	0.6240	0.3680
R	0.8700	0.5130
S	0.8200	0.4500
T	0.8650	0.5210
U	0.7710	0.4110
V	0.7030	0.3220
W	0.8050	0.4860
X	0.0910	0.0340
Y	0.0920	0.0630
Z	0.1700	0.0910
a	0.0950	0.1280

Full wwPDB EM Validation Report (i)

Oct 25, 2024 – 06:55 pm BST

PDB ID	:	9H51
EMDB ID	:	EMD-51873
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit in complex with PUS1, METTL15 and RBFA(IN conformation) (state A4)
Deposited on	:	2024-10-22
Resolution	:	3.10 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

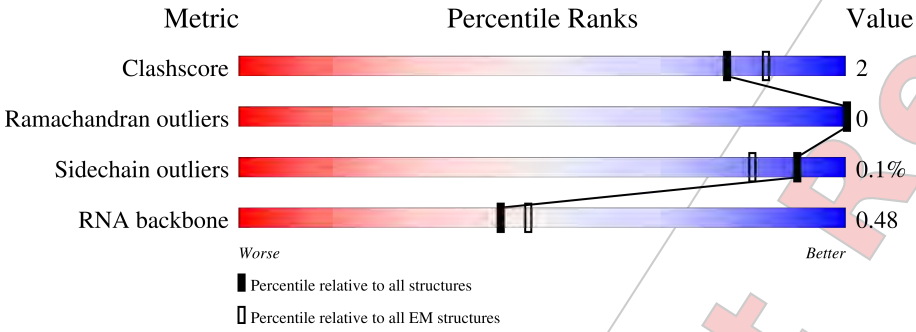
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	c	384	9% 81% 19%
2	A	959	11% 69% 23% 5%
3	B	296	71% 5% 24%
4	D	430	24% 76% 21%
5	E	125	88% 10%

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Mol	Chain	Length	Quality of chain
6	I	194	65% 5% 29%
7	J	138	75% 22%
8	L	257	64% 32%
9	M	137	83% 13%
10	N	130	82% 15%
11	O	258	72% 25%
12	P	142	68% 32%
13	Q	87	95% 5%
14	R	360	78% 18%
15	S	190	69% 29%
16	T	173	94%
17	U	205	82% 14%
18	V	414	26% 82% 5% 13%
19	W	187	53% 47%
20	0	215	7% 92% 7%
21	3	199	34% 65%
22	b	407	47% 74% 26%
23	a	343	15% 46% 54%
24	4	689	84% 80% 6% 15%
25	H	201	65% 65% 30%
26	1	323	81% 78% 7% 15%
27	Z	106	76% 80% 8% 12%
28	X	398	87% 78% 10% 12%
29	K	128	61% 70% 9% 21%
30	Y	395	37% 36% 62%

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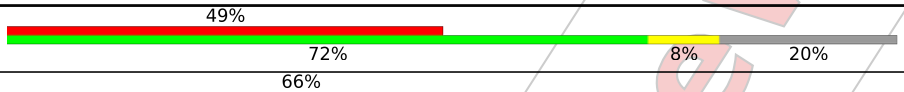
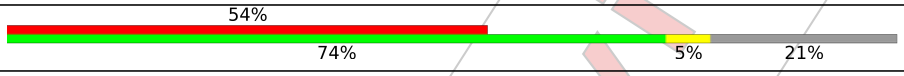
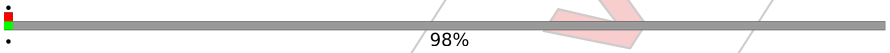
Mol	Chain	Length	Quality of chain
31	G	396	
32	F	242	
33	C	167	
34	9	698	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 134127 atoms, of which 62565 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pseudouridylate synthase 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	c	311	4988	1580	2493	448	451	16	0	0

- Molecule 2 is a RNA chain called RNA (969-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	A	925	29610	8812	9962	3535	6376	925	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1076	5MU	-	insertion	GB 1858621102
A	1485A	C	-	insertion	GB 1858621102
A	1583	MA6	-	insertion	GB 1858621102
A	1584	MA6	-	insertion	GB 1858621102

- Molecule 3 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	B	225	3653	1164	1825	331	323	10	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	341	5511	1704	2794	515	485	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	113	Total	C	H	N	O	S	0	0
			1806	563	914	162	163	4		

- Molecule 6 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	137	Total	C	H	N	O	S	0	0
			2085	642	1065	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 7 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	108	Total	C	H	N	O	S	0	0
			1730	521	891	169	143	6		

- Molecule 8 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	L	174	Total	C	H	N	O	S	0	0
			2997	925	1544	270	251	7		

- Molecule 9 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	M	119	Total	C	H	N	O	S	0	0
			1913	594	971	185	157	6		

- Molecule 10 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	N	110	Total	C	H	N	O	S	0	0
			1800	562	932	156	147	3		

- Molecule 11 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	O	194	Total	C	H	N	O	S	0	0
			3173	1019	1574	295	278	7		

- Molecule 12 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	P	97	Total	C	H	N	O	S	0	0
			1589	501	808	134	138	8		

- Molecule 13 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Q	87	Total	C	H	N	O	S	0	0
			1504	460	760	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 14 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	R	295	Total	C	H	N	O	S	0	0
			4844	1533	2435	413	455	8		

- Molecule 15 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	S	135	Total	C	H	N	O	S	0	0
			2227	716	1116	198	196	1		

- Molecule 16 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	T	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

- Molecule 17 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	U	176	Total	C	H	N	O	S	0	0
			2992	916	1504	301	267	4		

- Molecule 18 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	V	362	Total	C	H	N	O	S	0	0
			5939	1904	2970	495	558	12		

- Molecule 19 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	W	100	Total	C	H	N	O	S	0	0
			1594	498	805	141	146	4		

- Molecule 20 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	0	215	Total	C	H	N	O	S	0	0
			3588	1130	1801	339	313	5		

- Molecule 21 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	3	70	Total	C	H	N	O	S	0	0
			1326	401	701	134	89	1		

- Molecule 22 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	b	303	Total	C	H	N	O	S	0	0
			4796	1498	2433	421	431	13		

- Molecule 23 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	a	157	Total	C	H	N	O	S	0	0
			2503	788	1251	220	238	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	286	PRO	ARG	conflict	UNP Q8N0V3
a	319	THR	ASP	conflict	UNP Q8N0V3

- Molecule 24 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	4	588	9550	3053	4782	808	879	28	0	0

- Molecule 25 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	H	140	2342	745	1190	194	210	3	0	0

- Molecule 26 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	1	276	4512	1419	2274	381	427	11	0	0

- Molecule 27 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	Z	93	1593	504	805	141	139	4	0	0

- Molecule 28 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	X	352	5707	1822	2858	499	517	11	0	0

- Molecule 29 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	K	101	1750	537	888	179	141	5	0	0

- Molecule 30 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Y	149	Total	C	H	N	O	S	0	0
			2448	801	1202	207	234	4		

- Molecule 31 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	G	316	Total	C	H	N	O	S	0	0
			5202	1652	2599	463	474	14		

- Molecule 32 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	F	202	Total	C	H	N	O	S	0	0
			3397	1066	1726	303	291	11		

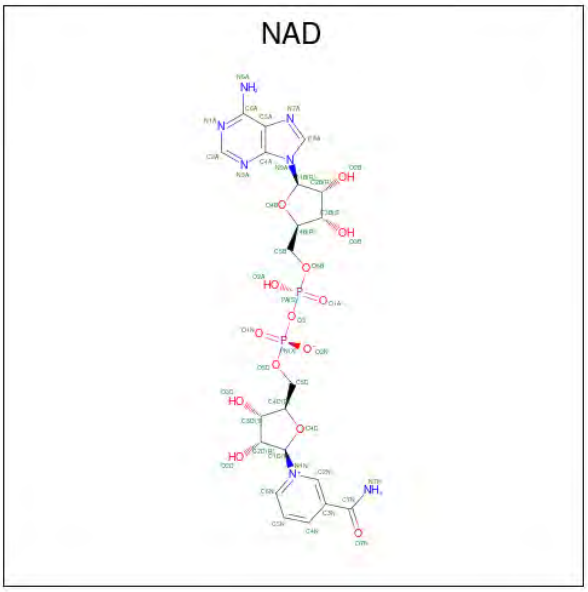
- Molecule 33 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	C	132	Total	C	H	N	O	S	0	0
			2178	699	1095	195	185	4		

- Molecule 34 is a protein called Nitric oxide-associated protein 1.

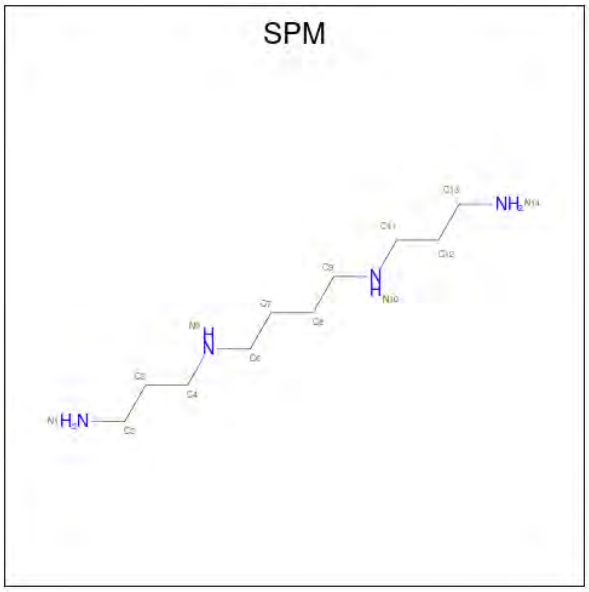
Mol	Chain	Residues	Atoms						AltConf	Trace
34	9	12	Total	C	H	N	O	S	0	0
			219	76	108	16	18	1		

- Molecule 35 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
35	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 36 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	H	N	0
			40	10	26	4	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
37	A	38	Total Mg 38 38	0
37	B	1	Total Mg 1 1	0
37	3	1	Total Mg 1 1	0

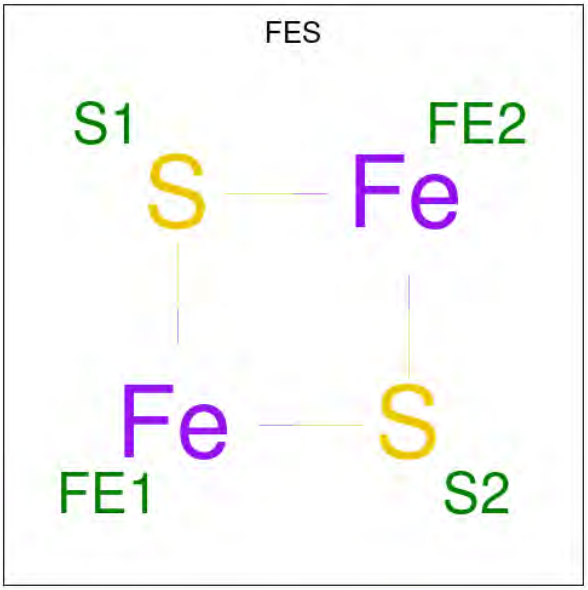
- Molecule 38 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
38	A	6	Total K 6 6	0

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

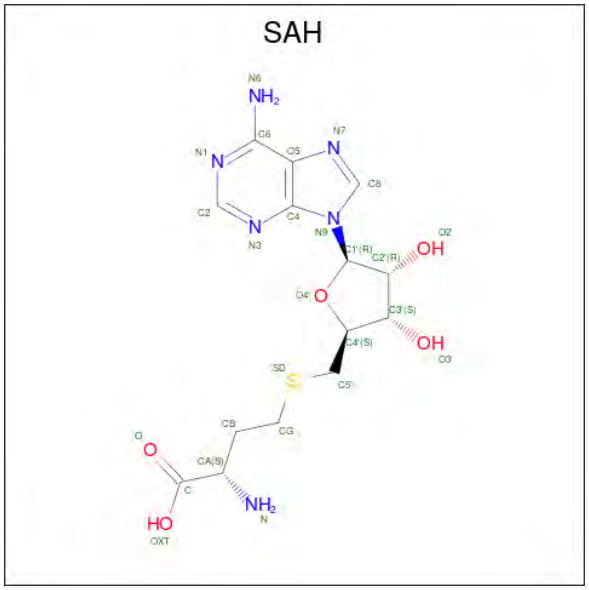
Mol	Chain	Residues	Atoms	AltConf
39	O	1	Total Zn 1 1	0

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



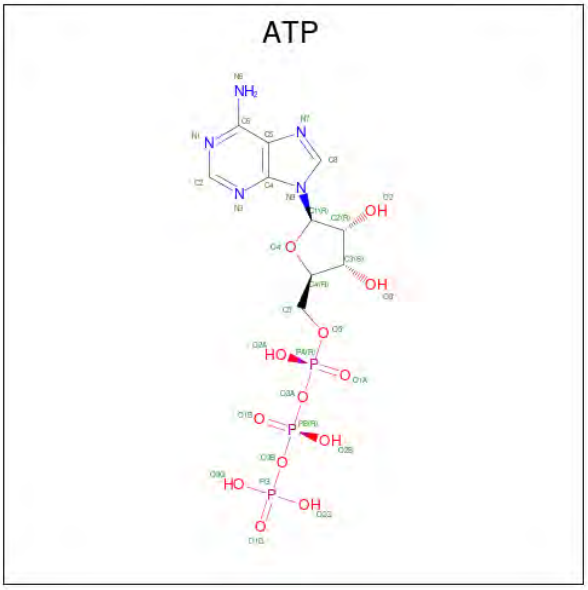
Mol	Chain	Residues	Atoms	AltConf
40	P	1	Total Fe S 4 2 2	0
40	T	1	Total Fe S 4 2 2	0

- Molecule 41 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



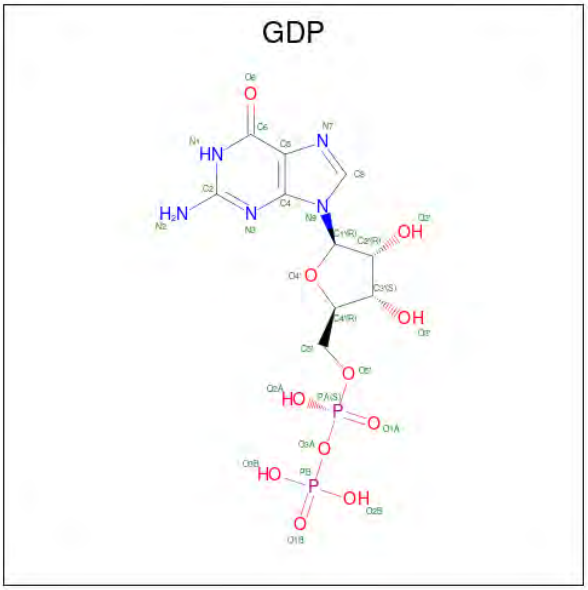
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
41	b	1	45	14	19	6	5	1	0

- Molecule 42 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
42	X	1	43	10	12	5	13	3	0

- Molecule 43 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
43	X	1	38	10	10	5	11	2	0

- Molecule 44 is water.

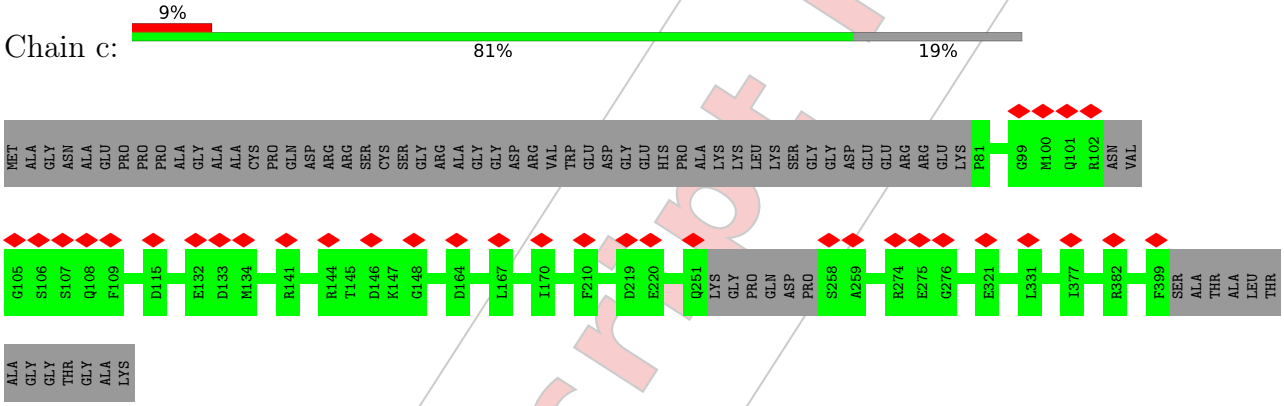
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
44	A	1	1	1	0
44	I	1	Total	O	0
			1	1	
44	0	1	Total	O	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

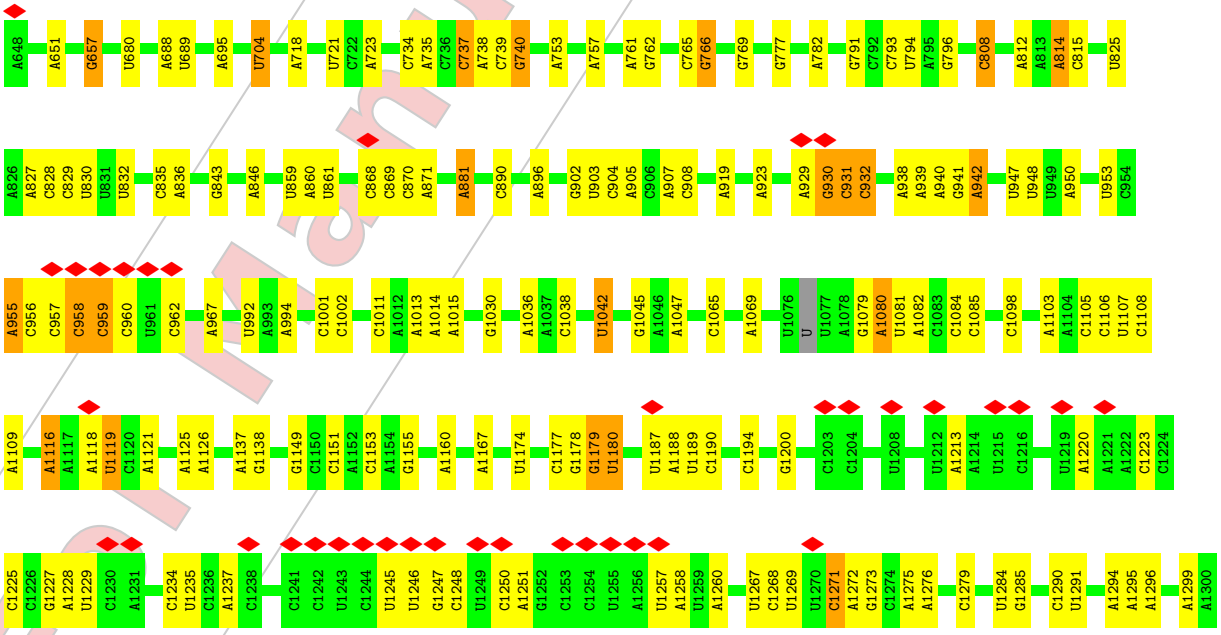
- Molecule 1: Pseudouridylate synthase 1 homolog

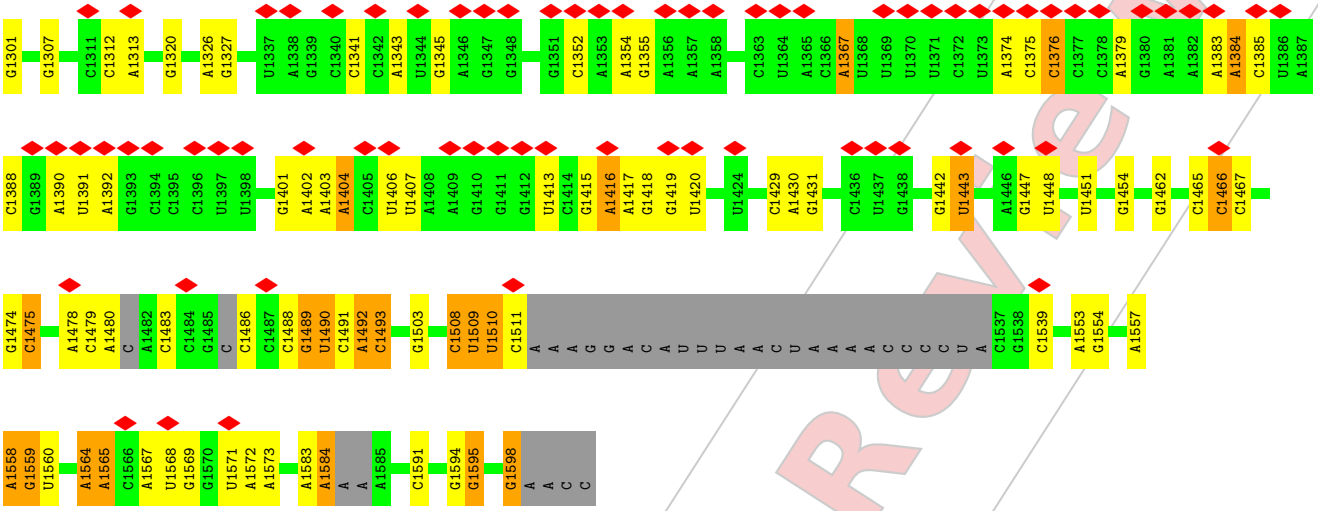
Chain c:



- Molecule 2: RNA (969-MER)

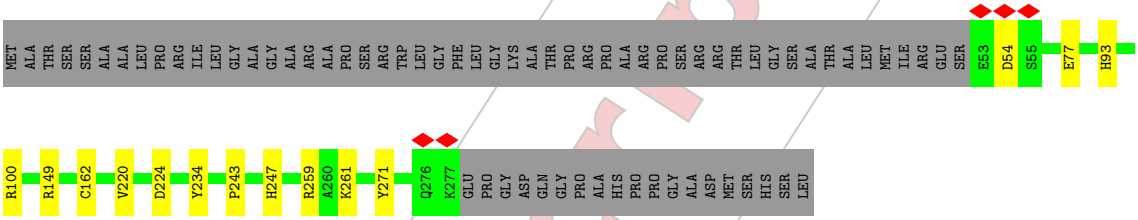
Chain A:





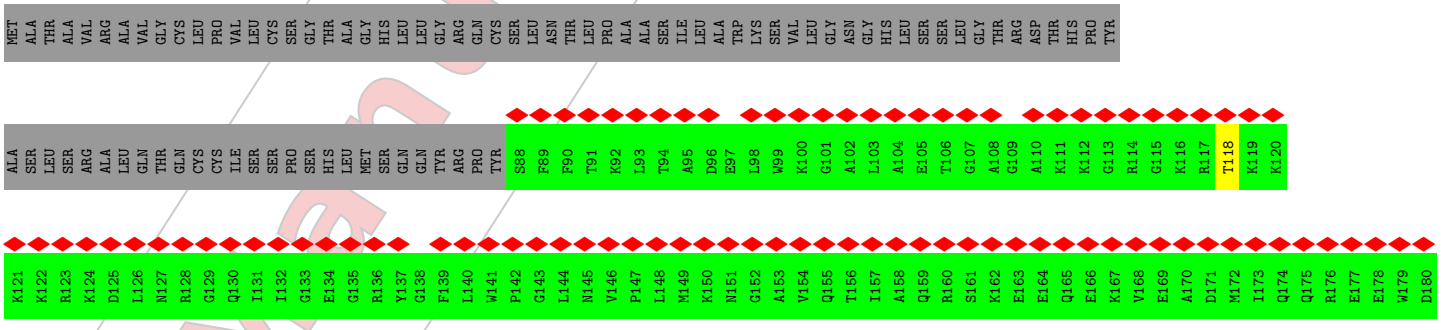
• Molecule 3: 28S ribosomal protein S2, mitochondrial

Chain B:



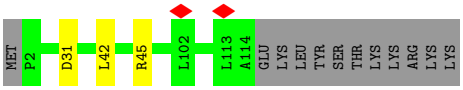
• Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain D:



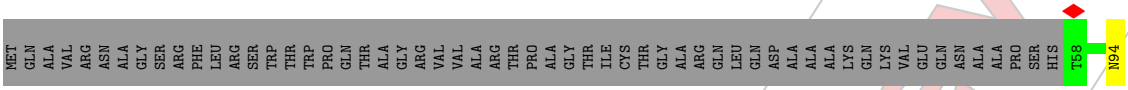
• Molecule 5: 28S ribosomal protein S6, mitochondrial

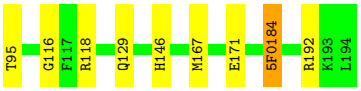
Chain E:



• Molecule 6: 28S ribosomal protein S11, mitochondrial

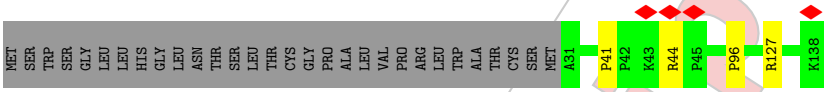
Chain I:





• Molecule 7: 28S ribosomal protein S12, mitochondrial

Chain J:

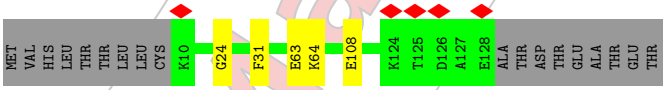


• Molecule 8: 28S ribosomal protein S15, mitochondrial

Chain L:

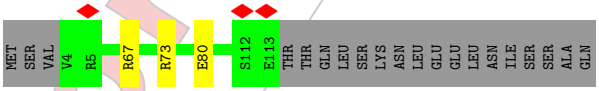
• Molecule 9: 28S ribosomal protein S16, mitochondrial

Chain M:



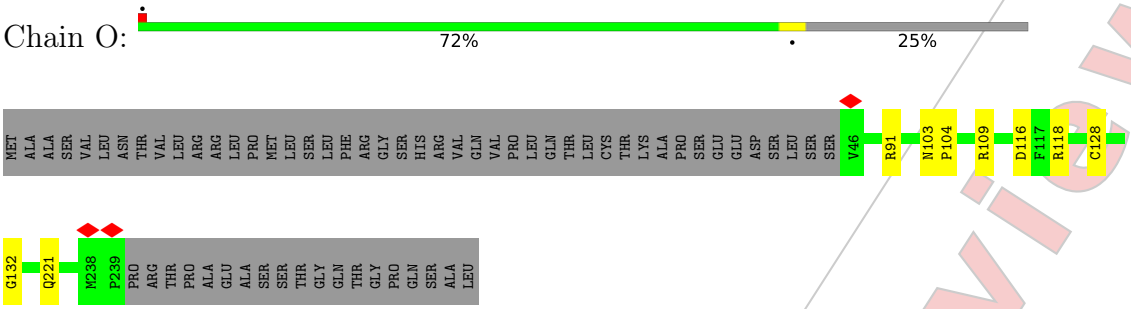
• Molecule 10: 28S ribosomal protein S17, mitochondrial

Chain N:



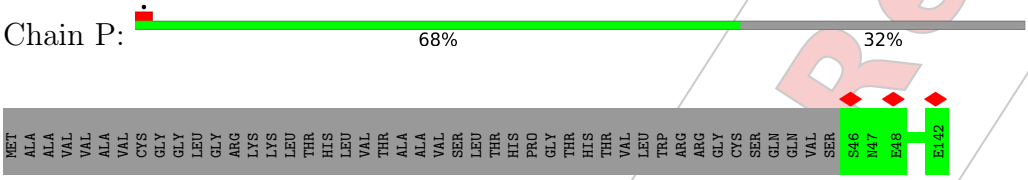
• Molecule 11: 28S ribosomal protein S18b, mitochondrial

Chain O:



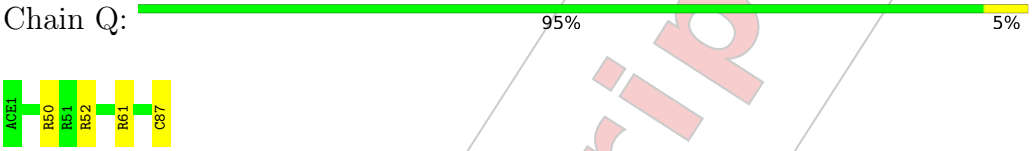
• Molecule 12: 28S ribosomal protein S18c, mitochondrial

Chain P:



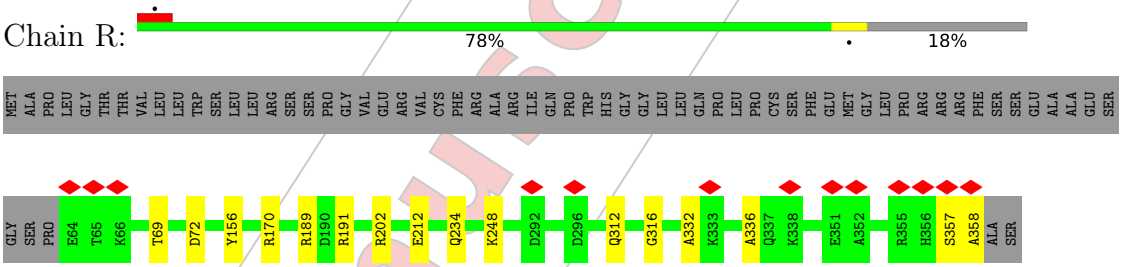
• Molecule 13: Small ribosomal subunit protein bS21m

Chain Q:



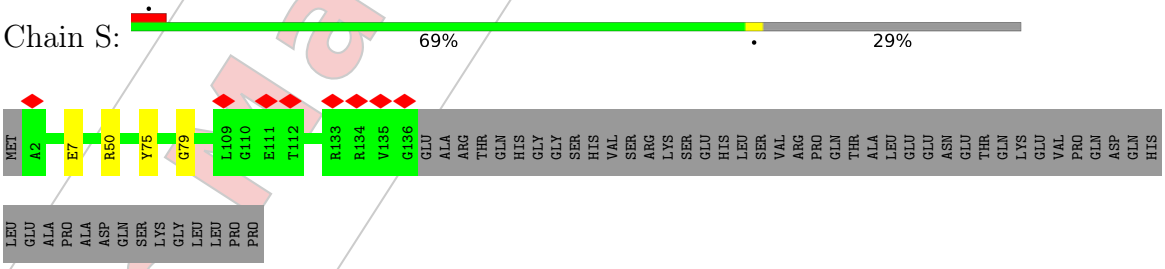
• Molecule 14: 28S ribosomal protein S22, mitochondrial

Chain R:



• Molecule 15: 28S ribosomal protein S23, mitochondrial

Chain S:

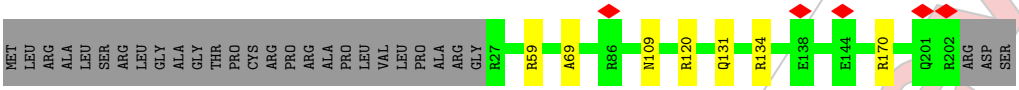


• Molecule 16: 28S ribosomal protein S25, mitochondrial

Chain T:

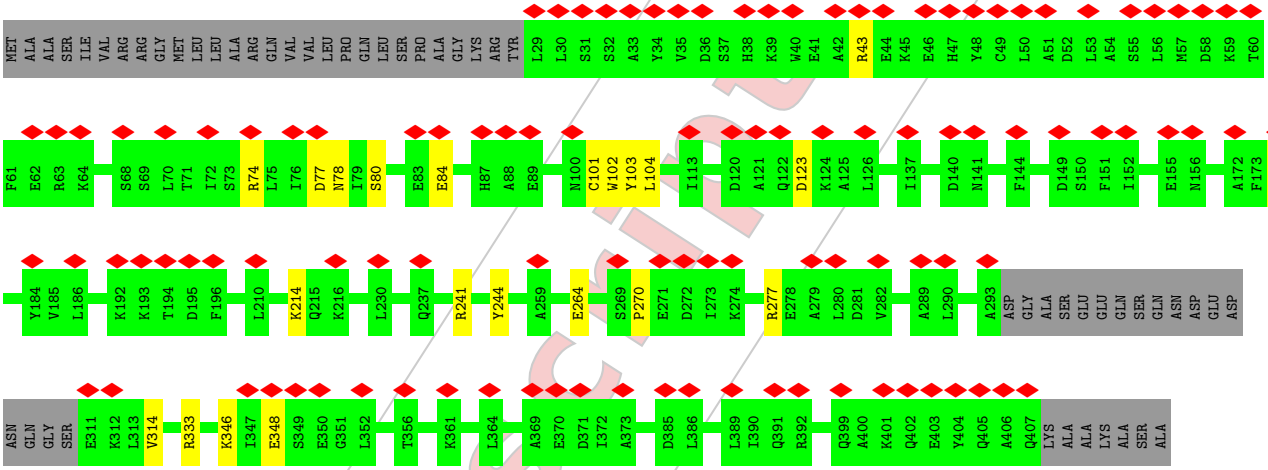
• Molecule 17: 28S ribosomal protein S26, mitochondrial

Chain U:



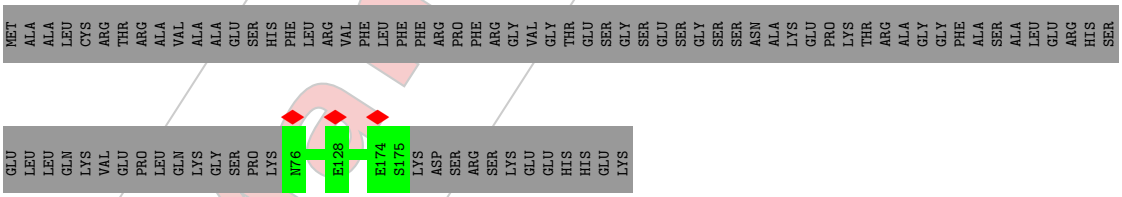
• Molecule 18: 28S ribosomal protein S27, mitochondrial

Chain V:



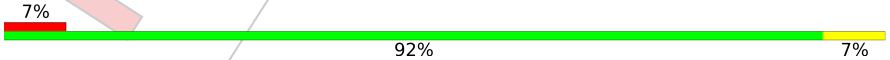
• Molecule 19: 28S ribosomal protein S28, mitochondrial

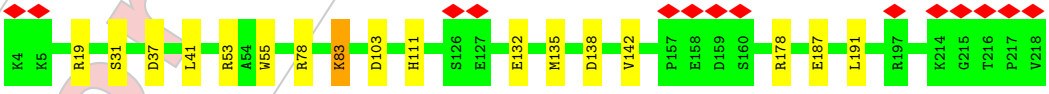
Chain W:



• Molecule 20: Small ribosomal subunit protein mS34

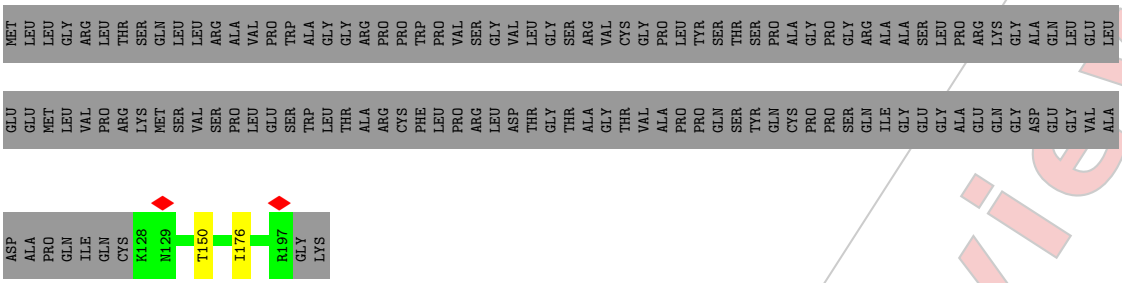
Chain 0:





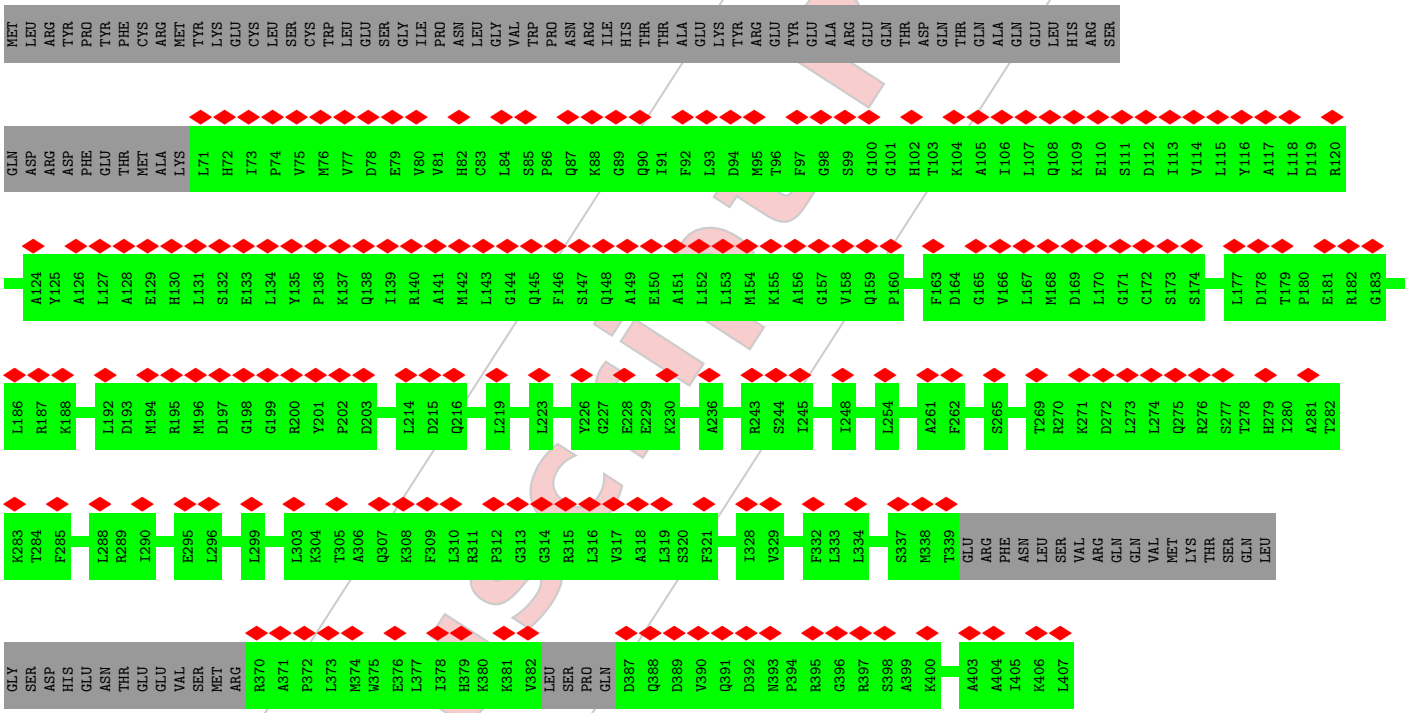
• Molecule 21: Aurora kinase A-interacting protein

Chain 3:



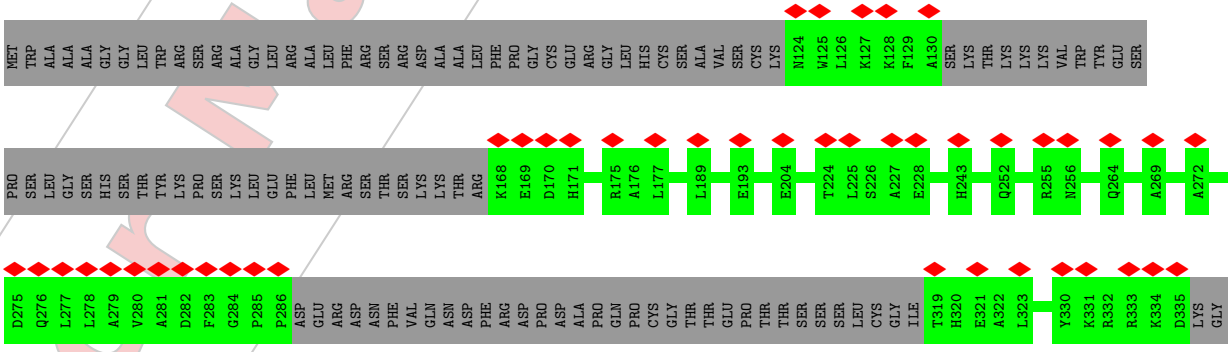
• Molecule 22: 12S rRNA N4-methylcytidine (m4C) methyltransferase

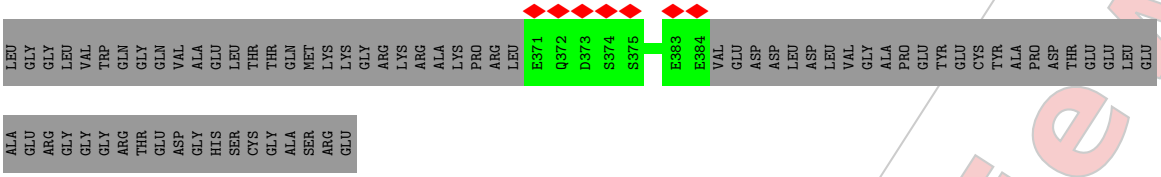
Chain b:



• Molecule 23: Putative ribosome-binding factor A, mitochondrial

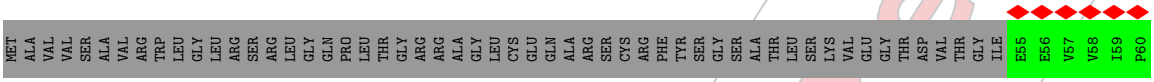
Chain a:

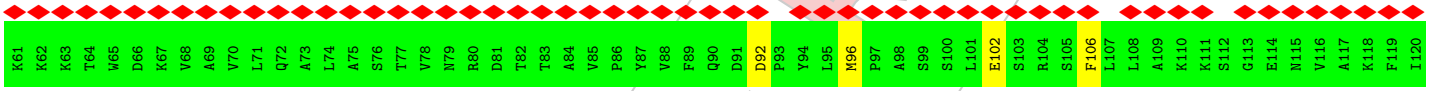


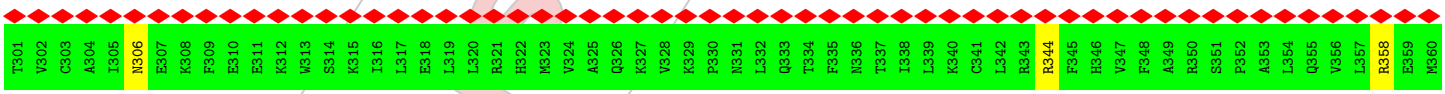


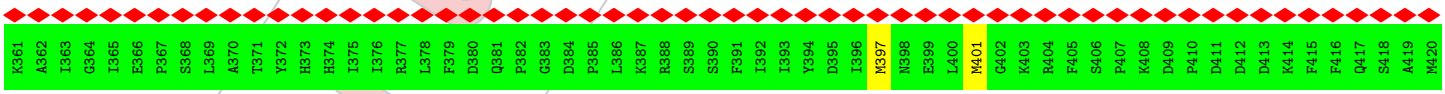
• Molecule 24: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

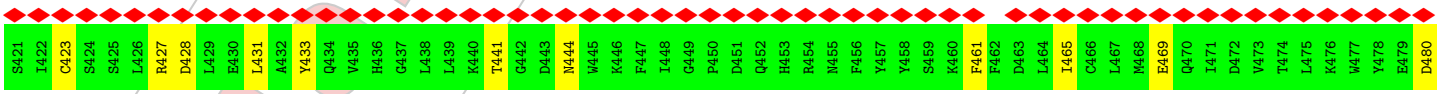
Chain 4:

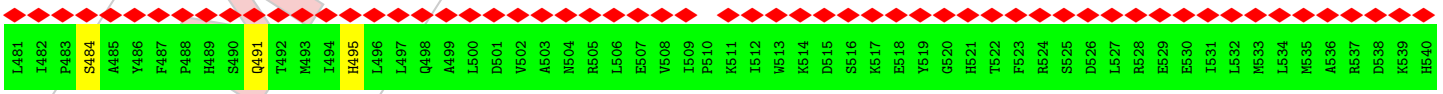


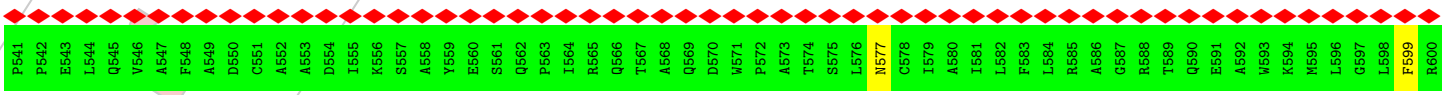


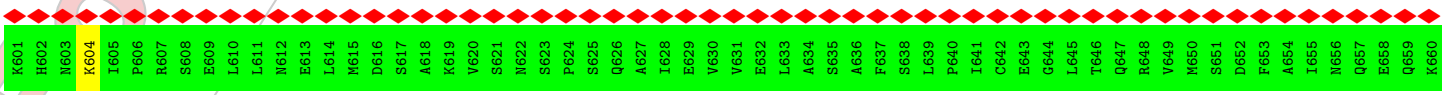






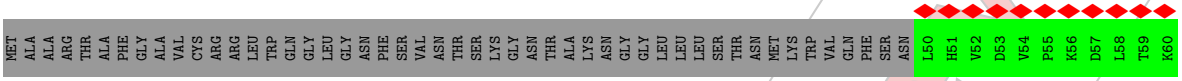


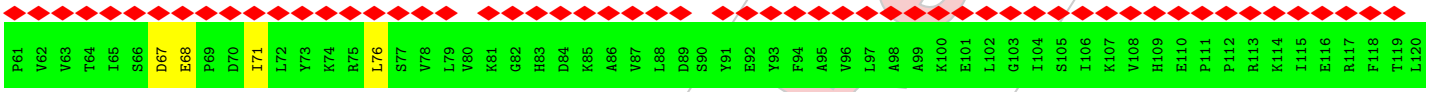


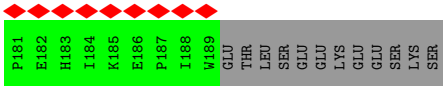


• Molecule 25: 28S ribosomal protein S10, mitochondrial

Chain H:

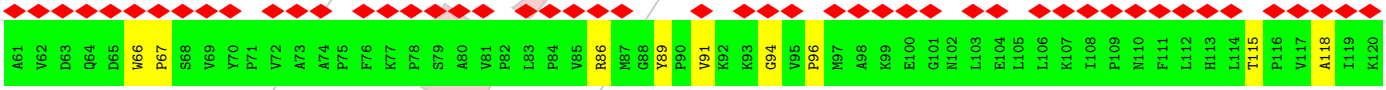


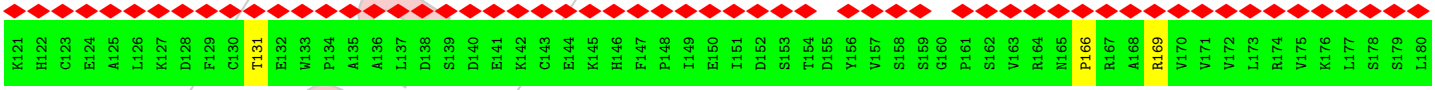


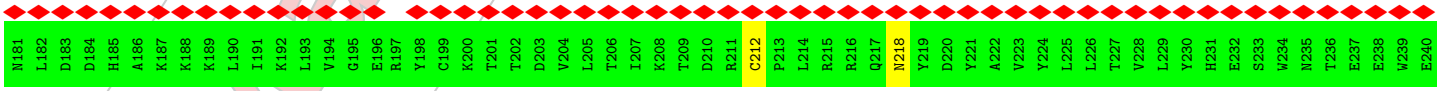


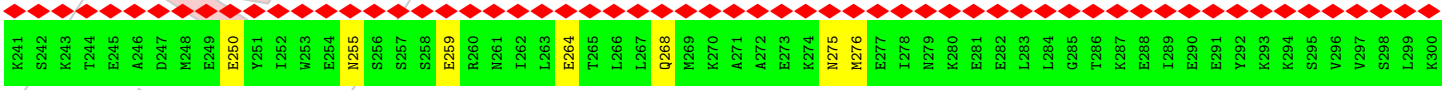
• Molecule 26: 28S ribosomal protein S35, mitochondrial

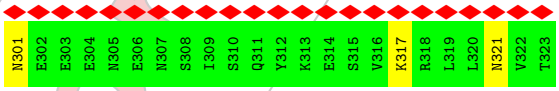
Chain 1:





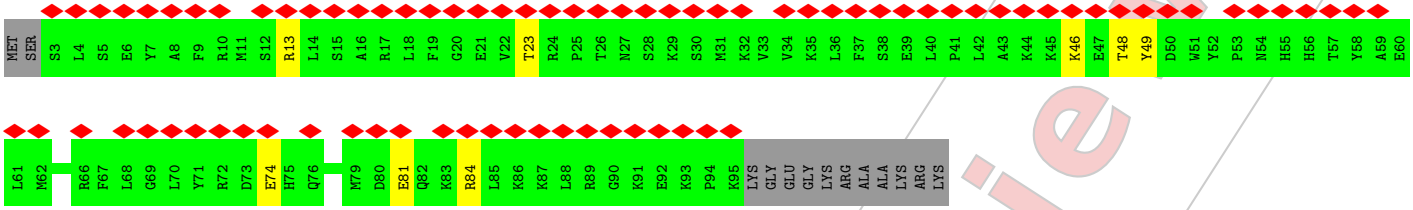




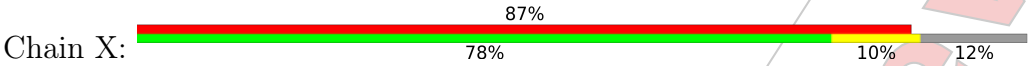


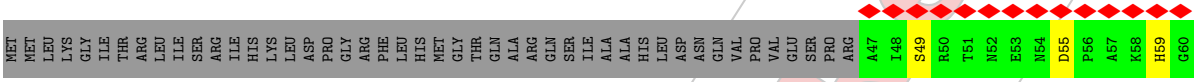
• Molecule 27: 28S ribosomal protein S33, mitochondrial

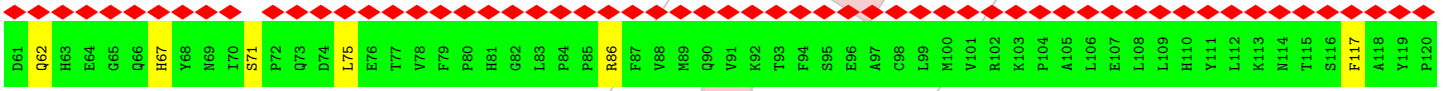
Chain Z:

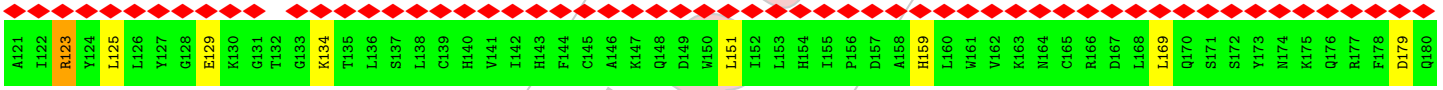


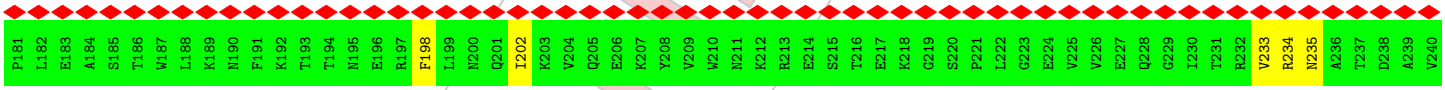
• Molecule 28: 28S ribosomal protein S29, mitochondrial

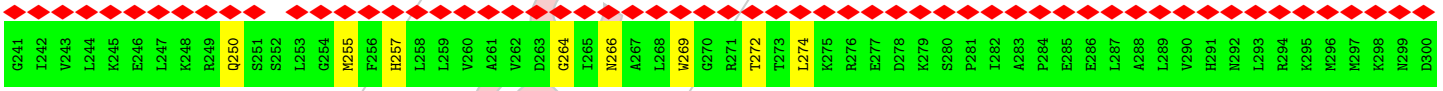


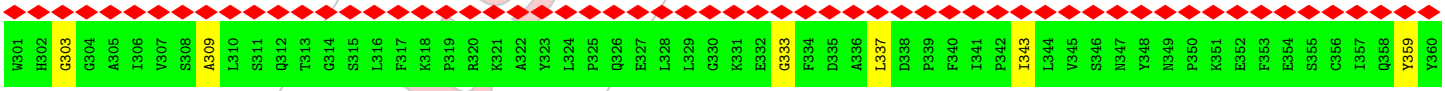


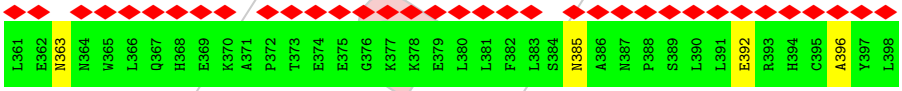




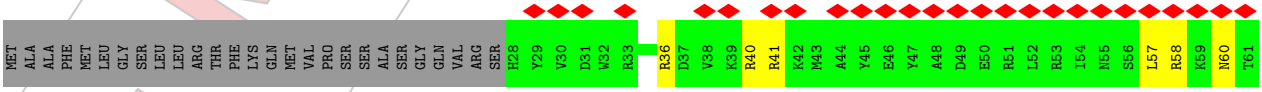


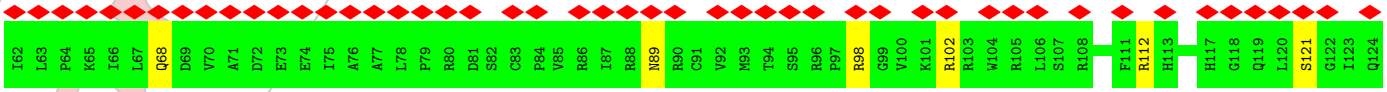






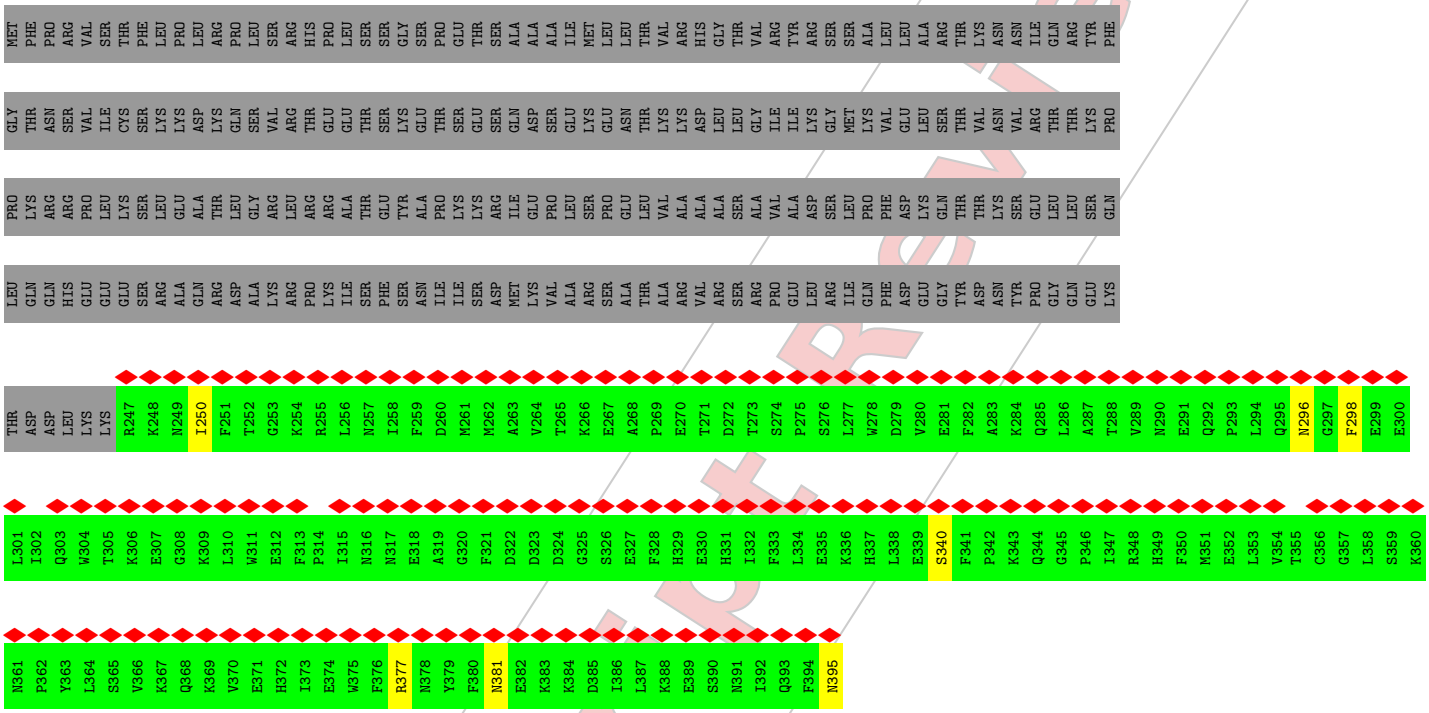
• Molecule 29: 28S ribosomal protein S14, mitochondrial





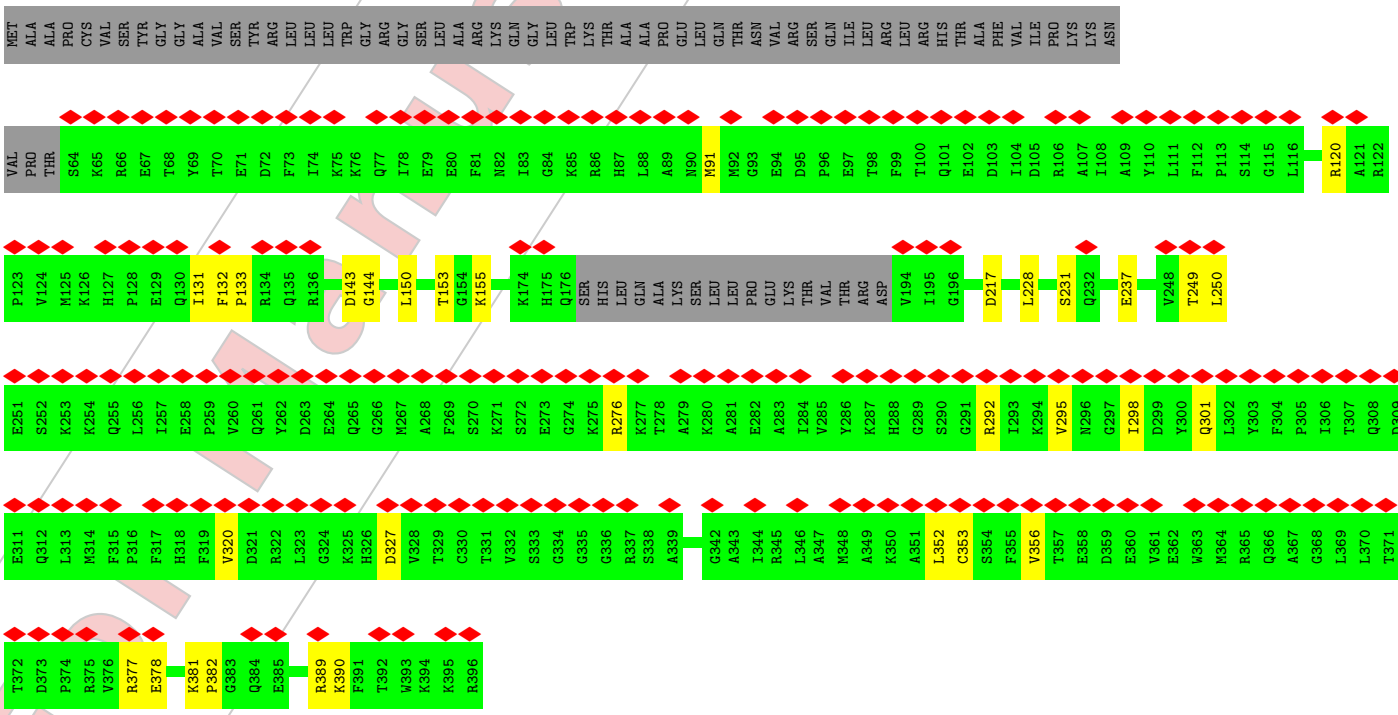
• Molecule 30: 28S ribosomal protein S31, mitochondrial

Chain Y:



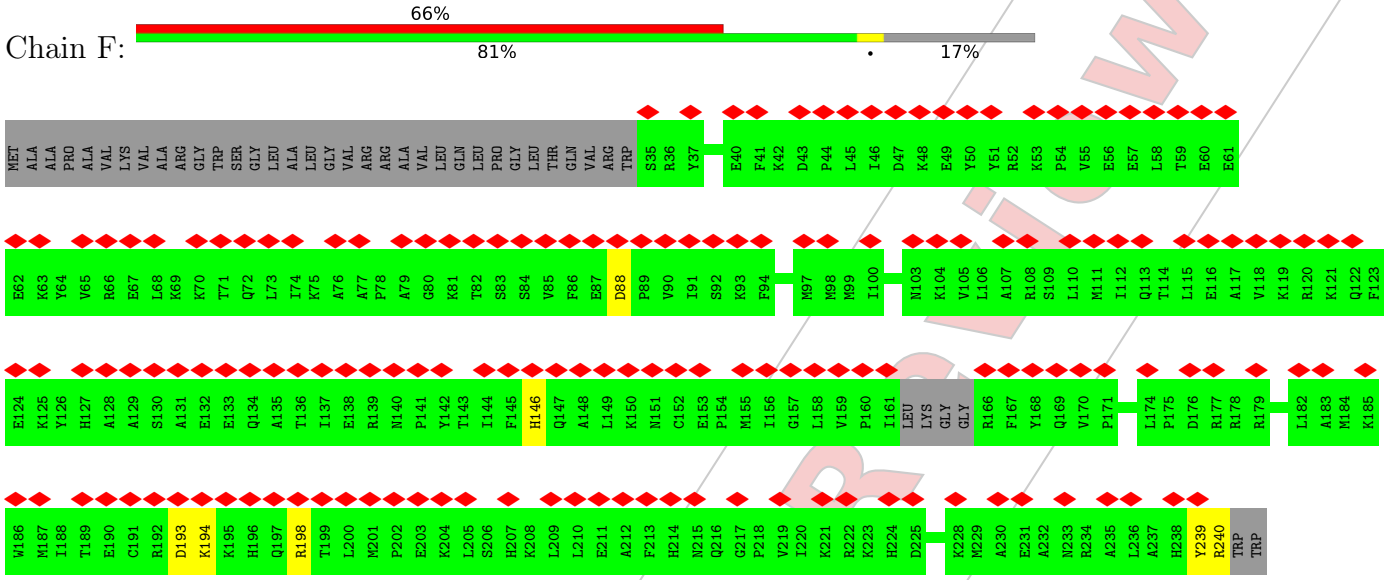
• Molecule 31: 28S ribosomal protein S9, mitochondrial

Chain G:



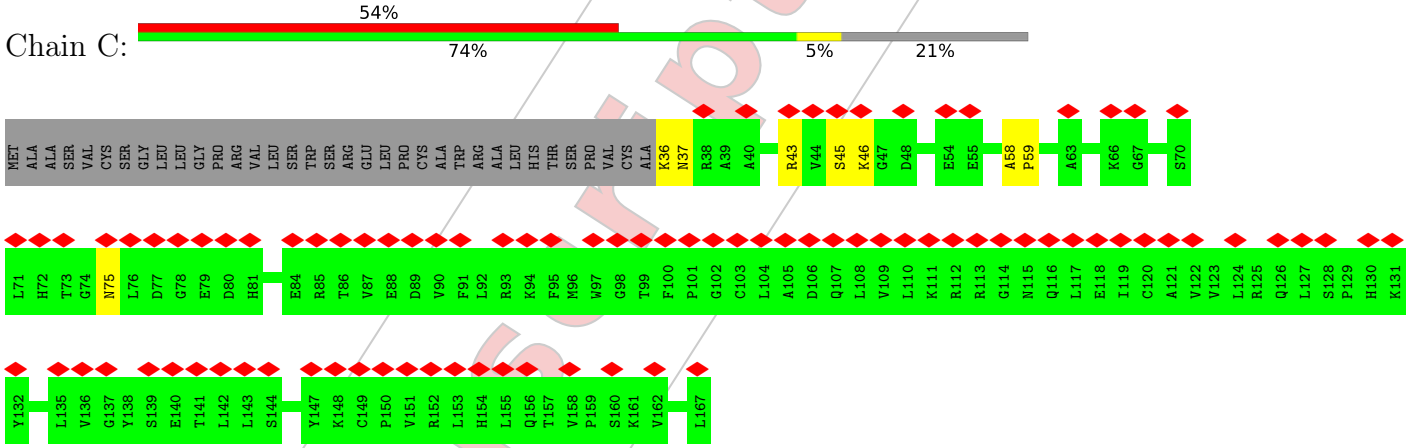
• Molecule 32: 28S ribosomal protein S7, mitochondrial

Chain F:



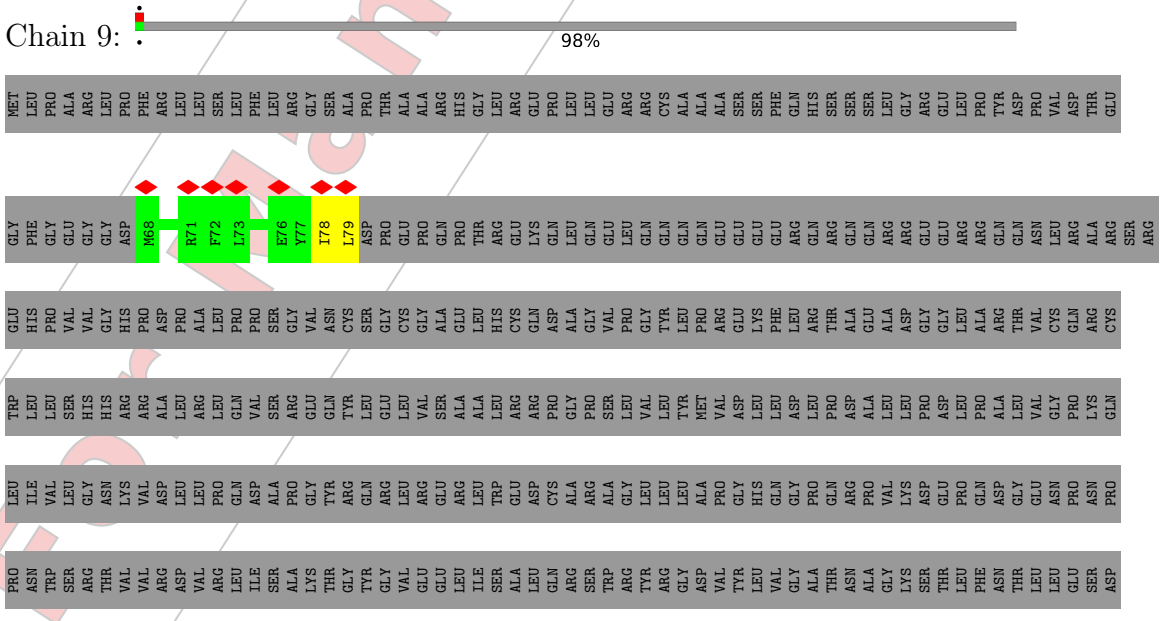
• Molecule 33: 28S ribosomal protein S24, mitochondrial

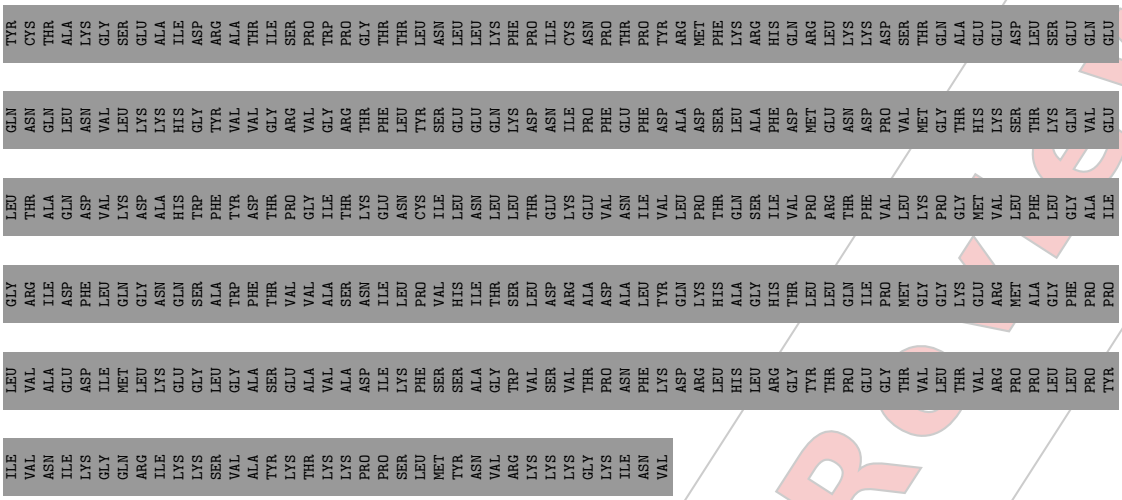
Chain C:



• Molecule 34: Nitric oxide-associated protein 1

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0065	Depositor
Map size (Å)	609.12, 609.12, 609.12	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0152, 1.0152, 1.0152	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SPM, 5MC, ZN, NAD, FES, MA6, GDP, MG, 5F0, SAH, K, B8T, ATP, ACE, 5MU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	c	0.27	0/2549	0.49	0/3431
2	A	0.38	0/21850	0.70	0/34012
3	B	0.29	0/1871	0.50	0/2531
4	D	0.28	0/2768	0.52	0/3703
5	E	0.27	0/908	0.53	0/1229
6	I	0.26	0/1030	0.50	0/1386
7	J	0.29	0/855	0.57	0/1148
8	L	0.28	0/1477	0.49	0/1974
9	M	0.29	0/963	0.54	0/1295
10	N	0.28	0/886	0.51	0/1199
11	O	0.29	0/1655	0.49	0/2254
12	P	0.28	0/798	0.45	0/1070
13	Q	0.28	0/754	0.58	0/1003
14	R	0.28	0/2456	0.46	0/3317
15	S	0.28	0/1138	0.51	0/1533
16	T	0.29	0/1402	0.47	0/1883
17	U	0.26	0/1510	0.54	0/2025
18	V	0.26	0/3030	0.42	0/4093
19	W	0.27	0/801	0.52	0/1079
20	0	0.27	0/1834	0.55	0/2484
21	3	0.26	0/636	0.58	0/839
22	b	0.24	0/2404	0.48	0/3241
23	a	0.25	0/1272	0.46	0/1715
24	4	0.24	0/4877	0.43	0/6598
25	H	0.25	0/1178	0.47	0/1598
26	1	0.25	0/2285	0.44	0/3090
27	Z	0.26	0/806	0.47	0/1076
28	X	0.25	0/2921	0.45	0/3954
29	K	0.24	0/880	0.57	0/1182
30	Y	0.24	0/1280	0.40	0/1725
31	G	0.27	0/2658	0.50	0/3560
32	F	0.24	0/1708	0.47	0/2292

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	C	0.26	0/1113	0.48	0/1505
34	9	0.26	0/114	0.47	0/152
All	All	0.30	0/74667	0.56	0/105176

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	I	184	5F0	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	c	2495	2493	2481	0	0
2	A	19648	9962	9976	83	0
3	B	1828	1825	1815	8	0
4	D	2717	2794	2785	10	0
5	E	892	914	910	2	0
6	I	1020	1065	1053	6	0
7	J	839	891	887	3	0
8	L	1453	1544	1540	8	0
9	M	942	971	965	4	0
10	N	868	932	928	2	0
11	O	1599	1574	1565	5	0
12	P	781	808	806	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	Q	744	760	758	4	0
14	R	2409	2435	2428	9	0
15	S	1111	1116	1115	3	0
16	T	1371	1396	1393	4	0
17	U	1488	1504	1499	6	0
18	V	2969	2970	2961	12	0
19	W	789	805	802	0	0
20	0	1787	1801	1796	13	0
21	3	625	701	699	2	0
22	b	2363	2433	2425	0	0
23	a	1252	1251	1248	0	0
24	4	4768	4782	4766	20	0
25	H	1152	1190	1183	6	0
26	1	2238	2274	2269	14	0
27	Z	788	805	802	5	0
28	X	2849	2858	2844	22	0
29	K	862	888	885	12	0
30	Y	1246	1202	1197	4	0
31	G	2603	2599	2591	22	0
32	F	1671	1726	1718	4	0
33	C	1083	1095	1088	6	0
34	9	111	108	108	1	0
35	A	44	26	26	0	0
36	A	14	26	26	0	0
37	3	1	0	0	0	0
37	A	38	0	0	0	0
37	B	1	0	0	0	0
38	A	6	0	0	0	0
39	O	1	0	0	0	0
40	P	4	0	0	0	0
40	T	4	0	0	0	0
41	b	26	19	19	0	0
42	X	31	12	12	0	0
43	X	28	10	12	0	0
44	0	1	0	0	1	0
44	A	1	0	0	0	0
44	I	1	0	0	0	0
All	All	71562	62565	62381	250	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:942:A:N6	2:A:1047:A:OP2	2.13	0.81
2:A:1085:C:OP1	6:I:192:ARG:NH1	2.18	0.76
17:U:69:ALA:CB	20:0:191:LEU:HD21	2.16	0.75
24:4:295:ASN:OD1	24:4:296:ALA:N	2.20	0.75
2:A:808:C:OP1	20:0:19:ARG:NH1	2.20	0.74
2:A:1598:G:O6	13:Q:61:ARG:NH1	2.21	0.73
24:4:397:MET:O	24:4:401:MET:N	2.22	0.73
33:C:37:ASN:O	33:C:43:ARG:NH2	2.22	0.71
2:A:1267:U:O4	33:C:36:LYS:N	2.25	0.70
2:A:1401:G:N1	2:A:1404:A:OP2	2.24	0.70
27:Z:48:THR:O	29:K:41:ARG:NH1	2.25	0.69
31:G:320:VAL:HG21	31:G:352:LEU:HD21	1.74	0.69
25:H:71:ILE:O	25:H:150:GLY:N	2.26	0.69
2:A:1235:U:OP1	29:K:36:ARG:NH1	2.27	0.68
6:I:129:GLN:NE2	6:I:167:MET:SD	2.67	0.68
2:A:1508:C:O2'	2:A:1509:U:OP1	2.12	0.67
2:A:1307:G:O2'	31:G:120:ARG:NH2	2.28	0.67
18:V:43:ARG:NH2	18:V:77:ASP:OD1	2.28	0.67
2:A:762:G:OP1	8:L:206:LYS:NZ	2.28	0.66
2:A:1488:5MC:H2'	2:A:1489:G:O4'	1.94	0.66
24:4:480:ASP:O	24:4:484:SER:OG	2.12	0.66
17:U:69:ALA:HB3	20:0:191:LEU:HD21	1.77	0.66
17:U:131:GLN:OE1	17:U:134:ARG:NH2	2.30	0.65
18:V:74:ARG:O	18:V:78:ASN:ND2	2.30	0.64
28:X:359:TYR:O	28:X:363:ASN:ND2	2.30	0.64
31:G:228:LEU:O	31:G:231:SER:OG	2.16	0.64
24:4:156:ALA:O	24:4:160:ARG:NH1	2.31	0.63
27:Z:74:GLU:OE1	27:Z:74:GLU:N	2.30	0.63
2:A:947:U:P	2:A:1045:G:O6	2.56	0.63
28:X:49:SER:O	28:X:67:HIS:N	2.32	0.62
2:A:1595:G:O6	13:Q:50:ARG:NH2	2.32	0.62
29:K:57:LEU:O	29:K:60:ASN:ND2	2.31	0.62
6:I:94:ASN:OD1	6:I:95:THR:N	2.33	0.62
20:0:78:ARG:NH2	20:0:142:VAL:O	2.33	0.61
5:E:42:LEU:O	5:E:45:ARG:NH2	2.33	0.61
27:Z:13:ARG:NH1	27:Z:23:THR:O	2.34	0.60
26:1:212:CYS:O	26:1:218:ASN:ND2	2.35	0.60
29:K:60:ASN:O	29:K:68:GLN:NE2	2.35	0.59
28:X:385:ASN:ND2	31:G:301:GLN:OE1	2.32	0.59
24:4:599:PHE:O	24:4:604:LYS:N	2.35	0.59
2:A:904:C:N3	4:D:118:THR:OG1	2.35	0.59
4:D:283:GLU:O	4:D:356:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:264:GLY:N	28:X:309:ALA:O	2.36	0.59
2:A:1454:G:OP2	31:G:377:ARG:NH1	2.34	0.58
3:B:93:HIS:CD2	3:B:224:ASP:OD2	2.56	0.58
31:G:249:THR:HA	31:G:250:LEU:HB3	1.84	0.58
29:K:121:SER:O	33:C:75:ASN:ND2	2.36	0.57
28:X:250:GLN:NE2	28:X:255:MET:SD	2.77	0.57
2:A:1320:G:OP2	33:C:37:ASN:ND2	2.38	0.57
9:M:63:GLU:OE2	14:R:191:ARG:NH2	2.35	0.57
14:R:69:THR:N	14:R:72:ASP:OD2	2.37	0.56
26:1:255:ASN:N	26:1:259:GLU:OE1	2.36	0.56
2:A:1367:A:OP2	2:A:1384:A:N6	2.35	0.56
2:A:843:G:N2	2:A:846:A:OP2	2.36	0.56
2:A:1275:A:O2'	2:A:1276:A:O4'	2.22	0.56
2:A:657:G:HO2'	4:D:237:ARG:HE	1.53	0.56
24:4:433:TYR:OH	24:4:469:GLU:OE1	2.24	0.56
11:O:221:GLN:NE2	18:V:314:VAL:O	2.39	0.55
2:A:1177:C:N4	2:A:1178:G:O6	2.40	0.55
28:X:159:HIS:NE2	28:X:266:ASN:OD1	2.40	0.55
11:O:91:ARG:NH1	11:O:103:ASN:O	2.37	0.55
28:X:86:ARG:NE	28:X:392:GLU:OE1	2.37	0.55
2:A:1036:A:O2'	8:L:142:HIS:ND1	2.33	0.54
31:G:150:LEU:O	31:G:153:THR:OG1	2.24	0.54
2:A:1558:A:O2'	2:A:1559:G:P	2.65	0.54
25:H:152:THR:OG1	26:1:131:THR:O	2.25	0.54
30:Y:340:SER:O	30:Y:395:ASN:ND2	2.39	0.54
2:A:1080:A:H1'	2:A:1081:U:C6	2.44	0.53
16:T:92:THR:O	16:T:92:THR:HG22	2.08	0.53
20:0:178:ARG:NH1	20:0:187:GLU:O	2.38	0.53
31:G:292:ARG:NH1	31:G:327:ASP:OD2	2.41	0.53
26:1:115:THR:OG1	31:G:91:MET:O	2.23	0.53
2:A:1229:U:O2'	2:A:1442:G:O4'	2.26	0.53
3:B:243:PRO:O	3:B:247:HIS:ND1	2.35	0.53
2:A:657:G:O3'	4:D:237:ARG:NH2	2.40	0.52
5:E:31:ASP:OD1	17:U:170:ARG:NH2	2.41	0.52
18:V:270:PRO:O	18:V:346:LYS:NZ	2.43	0.52
2:A:812:A:O2'	2:A:814:A:N1	2.41	0.51
18:V:264:GLU:OE2	18:V:333:ARG:NH2	2.42	0.51
2:A:825:U:O2'	2:A:827:A:N7	2.36	0.51
24:4:148:GLN:N	24:4:159:GLU:OE2	2.42	0.51
31:G:143:ASP:OD1	31:G:144:GLY:N	2.44	0.51
10:N:67:ARG:NH2	10:N:80:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:363:ALA:O	4:D:367:GLY:N	2.43	0.51
2:A:1272:A:N6	2:A:1320:G:O2'	2.35	0.51
2:A:1384:A:OP1	32:F:198:ARG:NH1	2.44	0.51
11:O:104:PRO:HB2	11:O:109:ARG:HB3	1.94	0.51
24:4:200:ASP:OD2	24:4:243:ASN:N	2.44	0.50
3:B:77:GLU:OE2	3:B:259:ARG:NH1	2.42	0.50
24:4:491:GLN:O	24:4:495:HIS:ND1	2.44	0.50
2:A:948:U:OP2	2:A:1045:G:N2	2.41	0.50
8:L:112:MET:O	8:L:116:VAL:HG12	2.11	0.50
2:A:1591:C:OP1	13:Q:52:ARG:NH2	2.44	0.50
3:B:162:CYS:O	3:B:261:LYS:NZ	2.39	0.50
4:D:219:ASP:OD1	4:D:220:THR:N	2.45	0.50
29:K:41:ARG:NH2	29:K:89:ASN:OD1	2.40	0.50
20:0:132:GLU:O	44:0:301:HOH:O	2.19	0.50
18:V:174:GLU:OE1	18:V:214:LYS:NZ	2.45	0.49
20:0:37:ASP:O	20:0:41:LEU:N	2.44	0.49
24:4:441:THR:OG1	24:4:444:ASN:ND2	2.45	0.49
28:X:151:LEU:N	28:X:257:HIS:O	2.44	0.49
24:4:237:THR:O	24:4:237:THR:HG22	2.13	0.49
28:X:55:ASP:O	28:X:59:HIS:ND1	2.45	0.48
28:X:129:GLU:O	28:X:134:LYS:NZ	2.40	0.48
24:4:428:ASP:OD1	24:4:431:LEU:N	2.33	0.48
28:X:123:ARG:NH2	28:X:337:LEU:O	2.47	0.48
24:4:239:ARG:O	24:4:242:ASN:ND2	2.47	0.48
6:I:146:HIS:NE2	6:I:171:GLU:OE1	2.47	0.48
33:C:45:SER:OG	33:C:46:LYS:N	2.46	0.48
16:T:89:ASP:OD2	17:U:120:ARG:NH2	2.38	0.48
2:A:1584:MA6:O5'	2:A:1584:MA6:H8	2.14	0.47
11:O:128:CYS:O	11:O:132:GLY:N	2.46	0.47
31:G:389:ARG:NH1	31:G:390:LYS:O	2.47	0.47
28:X:198:PHE:O	28:X:202:ILE:N	2.43	0.47
26:1:166:PRO:O	26:1:169:ARG:NH1	2.44	0.47
26:1:66:TRP:N	26:1:67:PRO:CD	2.78	0.47
28:X:233:VAL:HG12	28:X:233:VAL:O	2.15	0.47
31:G:131:ILE:HG23	31:G:132:PHE:N	2.29	0.47
2:A:738:A:H2'	2:A:739:C:O4'	2.15	0.47
14:R:202:ARG:NE	14:R:234:GLN:O	2.48	0.47
2:A:932:C:N3	16:T:11:ARG:NH2	2.61	0.47
18:V:277:ARG:N	18:V:348:GLU:O	2.43	0.46
24:4:102:GLU:O	24:4:106:PHE:N	2.42	0.46
2:A:1079:G:C6	2:A:1080:A:N7	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1234:C:O3'	29:K:40:ARG:NH2	2.49	0.46
2:A:1443:U:OP2	29:K:102:ARG:NH1	2.49	0.46
2:A:1491:C:H3'	2:A:1492:A:H5"	1.97	0.46
2:A:1492:A:H4'	2:A:1493:C:OP1	2.13	0.46
14:R:312:GLN:O	14:R:316:GLY:N	2.37	0.46
16:T:132:ARG:NH1	16:T:136:LEU:O	2.49	0.46
2:A:737:C:H2'	2:A:738:A:C8	2.51	0.46
32:F:88:ASP:OD2	32:F:146:HIS:NE2	2.49	0.46
2:A:1257:U:O2'	2:A:1260:A:OP2	2.28	0.45
20:0:41:LEU:HD13	20:0:55:TRP:CG	2.51	0.45
18:V:80:SER:N	18:V:84:GLU:OE1	2.49	0.45
3:B:54:ASP:OD1	3:B:271:TYR:OH	2.35	0.45
28:X:392:GLU:O	28:X:396:ALA:N	2.50	0.45
2:A:1431:G:O6	31:G:276:ARG:NH2	2.50	0.45
26:1:86:ARG:HG2	26:1:96:PRO:HB2	1.98	0.45
2:A:739:C:H2'	2:A:740:G:C1'	2.47	0.45
2:A:1237:A:OP1	29:K:36:ARG:NH2	2.50	0.45
20:0:103:ASP:N	20:0:111:HIS:O	2.39	0.45
28:X:117:PHE:O	28:X:303:GLY:N	2.50	0.45
2:A:734:C:H3'	2:A:735:A:C5'	2.47	0.44
26:1:250:GLU:OE2	26:1:301:ASN:ND2	2.49	0.44
4:D:372:GLU:N	4:D:382:ILE:O	2.49	0.44
18:V:101:CYS:SG	18:V:102:TRP:N	2.91	0.44
3:B:149:ARG:NE	13:Q:87:CYS:OXT	2.46	0.44
28:X:125:LEU:O	28:X:343:ILE:N	2.49	0.44
31:G:353:CYS:HA	31:G:356:VAL:HG22	2.00	0.44
2:A:1179:G:O5'	2:A:1180:U:OP1	2.35	0.44
8:L:65:ASP:OD1	8:L:65:ASP:N	2.50	0.44
9:M:24:GLY:N	9:M:31:PHE:O	2.46	0.44
24:4:306:ASN:OD1	24:4:344:ARG:NH2	2.51	0.44
25:H:76:LEU:N	25:H:145:LEU:O	2.51	0.44
28:X:62:GLN:OE1	28:X:62:GLN:N	2.48	0.44
2:A:1564:A:OP2	2:A:1564:A:H3'	2.17	0.44
26:1:264:GLU:OE2	26:1:268:GLN:NE2	2.51	0.44
2:A:1489:G:H3'	2:A:1490:U:O4'	2.17	0.44
31:G:155:LYS:NZ	31:G:217:ASP:OD2	2.50	0.44
24:4:358:ARG:NE	30:Y:250:ILE:O	2.51	0.43
25:H:67:ASP:OD1	25:H:68:GLU:N	2.51	0.43
28:X:71:SER:O	28:X:75:LEU:N	2.48	0.43
2:A:1079:G:H2'	2:A:1080:A:H5'	2.00	0.43
24:4:423:CYS:O	24:4:427:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:H:122:GLN:O	29:K:112:ARG:NH1	2.50	0.43
2:A:1415:G:H4'	2:A:1416:A:H5'	2.00	0.43
4:D:394:ASP:OD1	4:D:394:ASP:N	2.47	0.43
20:0:135:MET:SD	20:0:135:MET:N	2.86	0.43
26:1:115:THR:HG23	26:1:118:ALA:H	1.83	0.43
31:G:320:VAL:CG2	31:G:352:LEU:HD21	2.46	0.43
2:A:1108:C:C4	2:A:1125:A:C5	3.06	0.43
11:O:116:ASP:OD2	11:O:118:ARG:NH2	2.48	0.43
2:A:1475:C:H6	2:A:1475:C:O5'	2.01	0.43
24:4:461:PHE:O	24:4:465:ILE:HG13	2.19	0.43
25:H:166:GLU:OE1	25:H:166:GLU:N	2.48	0.43
31:G:378:GLU:OE2	31:G:381:LYS:NZ	2.52	0.43
2:A:1084:C:O3'	6:I:192:ARG:NH2	2.52	0.43
2:A:1375:C:H2'	2:A:1376:C:O4'	2.18	0.43
24:4:92:ASP:O	24:4:96:MET:N	2.51	0.43
31:G:295:VAL:N	31:G:298:ILE:O	2.50	0.43
2:A:1119:U:OP2	15:S:50:ARG:NH2	2.47	0.43
2:A:1492:A:H8	2:A:1492:A:OP1	2.02	0.43
30:Y:296:ASN:OD1	30:Y:298:PHE:N	2.51	0.43
32:F:193:ASP:OD1	32:F:194:LYS:N	2.51	0.43
2:A:1116:A:P	3:B:100:ARG:HH22	2.41	0.43
14:R:332:ALA:HA	14:R:336:ALA:HB3	2.00	0.43
2:A:765:C:H5'	2:A:766:G:OP2	2.19	0.42
2:A:955:A:O4'	2:A:1042:U:H1'	2.17	0.42
2:A:1491:C:C3'	2:A:1492:A:H5"	2.49	0.42
4:D:285:TYR:N	4:D:289:THR:O	2.48	0.42
9:M:108:GLU:OE2	17:U:59:ARG:NH2	2.44	0.42
2:A:931:C:C4	7:J:41:PRO:HA	2.54	0.42
15:S:7:GLU:OE1	15:S:7:GLU:N	2.42	0.42
15:S:75:TYR:O	15:S:79:GLY:N	2.53	0.42
26:1:275:ASN:OD1	26:1:276:MET:N	2.52	0.42
28:X:169:LEU:O	28:X:179:ASP:N	2.40	0.42
18:V:241:ARG:HA	18:V:244:TYR:CE2	2.54	0.42
8:L:206:LYS:HE3	21:3:176:ILE:HD11	2.00	0.42
18:V:123:ASP:OD1	18:V:123:ASP:N	2.49	0.42
21:3:150:THR:HG22	21:3:150:THR:O	2.19	0.42
32:F:239:TYR:O	32:F:240:ARG:C	2.57	0.42
2:A:1374:A:H2'	2:A:1375:C:O4'	2.20	0.42
2:A:1417:A:H2'	2:A:1418:G:H5'	2.02	0.42
6:I:116:GLY:O	6:I:118:ARG:NH1	2.52	0.42
7:J:96:PRO:O	7:J:127:ARG:NH2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:317:LYS:O	26:1:321:ASN:N	2.52	0.42
27:Z:46:LYS:HA	27:Z:49:TYR:CE2	2.55	0.42
2:A:1565:A:H5'	2:A:1573:A:H5"	2.02	0.41
9:M:64:LYS:HD2	14:R:156:TYR:CE1	2.55	0.41
2:A:704:U:OP1	20:0:53:ARG:NH1	2.48	0.41
2:A:1228:A:N7	29:K:98:ARG:NH1	2.68	0.41
28:X:269:TRP:CD2	28:X:333:GLY:HA2	2.54	0.41
2:A:1403:A:OP1	29:K:58:ARG:NH2	2.54	0.41
2:A:1451:U:OP1	31:G:382:PRO:O	2.38	0.41
8:L:221:LYS:HD3	8:L:221:LYS:HA	1.91	0.41
26:1:89:TYR:OH	31:G:120:ARG:NH1	2.53	0.41
14:R:212:GLU:OE1	14:R:248:LYS:NZ	2.45	0.41
28:X:234:ARG:NH1	28:X:235:ASN:OD1	2.54	0.41
26:1:91:VAL:O	26:1:94:GLY:N	2.54	0.41
28:X:272:THR:HG22	28:X:274:LEU:H	1.84	0.41
8:L:126:GLU:HG2	8:L:177:VAL:HG21	2.02	0.41
8:L:137:ARG:NH1	8:L:140:GLU:OE1	2.54	0.41
27:Z:81:GLU:OE2	27:Z:84:ARG:NH2	2.44	0.41
2:A:881:A:OP1	4:D:195:GLY:N	2.53	0.41
2:A:1419:G:H5"	2:A:1420:U:H5'	2.02	0.41
20:0:83:LYS:N	20:0:138:ASP:OD1	2.54	0.41
24:4:255:ASN:O	24:4:258:SER:OG	2.32	0.41
3:B:220:VAL:HG22	3:B:234:TYR:HB2	2.03	0.41
14:R:170:ARG:O	14:R:189:ARG:NH1	2.47	0.41
14:R:357:SER:O	14:R:358:ALA:C	2.58	0.41
30:Y:377:ARG:O	30:Y:381:ASN:ND2	2.54	0.41
31:G:132:PHE:HB2	31:G:133:PRO:HD3	2.03	0.41
2:A:1271:C:N4	2:A:1320:G:O2'	2.53	0.40
2:A:1466:C:H2'	2:A:1467:C:O4'	2.20	0.40
2:A:947:U:OP2	2:A:1045:G:O6	2.39	0.40
2:A:1415:G:H4'	2:A:1416:A:C5'	2.52	0.40
2:A:1509:U:C4	2:A:1510:U:C4	3.09	0.40
2:A:1510:U:N3	2:A:1511:C:N3	2.70	0.40
20:0:31:SER:OG	20:0:103:ASP:OD2	2.33	0.40
31:G:237:GLU:OE1	31:G:237:GLU:N	2.50	0.40
34:9:78:ILE:CG2	34:9:79:LEU:N	2.85	0.40
2:A:769:G:OP2	10:N:73:ARG:NH2	2.52	0.40
2:A:958:C:H4'	2:A:959:C:O4'	2.21	0.40
2:A:1388:C:O2	2:A:1419:G:N2	2.51	0.40
18:V:103:TYR:O	18:V:104:LEU:C	2.59	0.40
33:C:58:ALA:HB1	33:C:59:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:930:G:N7	7:J:44:ARG:CZ	2.85	0.40
2:A:1279:C:O2'	2:A:1296:A:N1	2.49	0.40
2:A:1553:A:H2'	2:A:1554:G:O4'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	305/384 (79%)	296 (97%)	9 (3%)	0	100	100
3	B	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
4	D	337/430 (78%)	335 (99%)	2 (1%)	0	100	100
5	E	111/125 (89%)	108 (97%)	3 (3%)	0	100	100
6	I	134/194 (69%)	132 (98%)	2 (2%)	0	100	100
7	J	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
8	L	172/257 (67%)	170 (99%)	2 (1%)	0	100	100
9	M	117/137 (85%)	114 (97%)	3 (3%)	0	100	100
10	N	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
11	O	192/258 (74%)	188 (98%)	4 (2%)	0	100	100
12	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
13	Q	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
14	R	293/360 (81%)	290 (99%)	3 (1%)	0	100	100
15	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
16	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
17	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
18	V	358/414 (86%)	355 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	W	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
20	0	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
21	3	68/199 (34%)	68 (100%)	0	0	100	100
22	b	297/407 (73%)	286 (96%)	11 (4%)	0	100	100
23	a	149/343 (43%)	146 (98%)	3 (2%)	0	100	100
24	4	584/689 (85%)	569 (97%)	15 (3%)	0	100	100
25	H	138/201 (69%)	134 (97%)	4 (3%)	0	100	100
26	1	274/323 (85%)	266 (97%)	8 (3%)	0	100	100
27	Z	91/106 (86%)	89 (98%)	2 (2%)	0	100	100
28	X	350/398 (88%)	343 (98%)	7 (2%)	0	100	100
29	K	99/128 (77%)	99 (100%)	0	0	100	100
30	Y	147/395 (37%)	146 (99%)	1 (1%)	0	100	100
31	G	312/396 (79%)	303 (97%)	9 (3%)	0	100	100
32	F	198/242 (82%)	195 (98%)	3 (2%)	0	100	100
33	C	130/167 (78%)	130 (100%)	0	0	100	100
34	9	10/698 (1%)	10 (100%)	0	0	100	100
All	All	6267/9014 (70%)	6149 (98%)	118 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	269/319 (84%)	269 (100%)	0	100	100
3	B	198/249 (80%)	198 (100%)	0	100	100
4	D	285/357 (80%)	285 (100%)	0	100	100
5	E	95/107 (89%)	95 (100%)	0	100	100
6	I	104/146 (71%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	J	93/118 (79%)	93 (100%)	0	100	100
8	L	158/226 (70%)	158 (100%)	0	100	100
9	M	97/113 (86%)	97 (100%)	0	100	100
10	N	96/115 (84%)	96 (100%)	0	100	100
11	O	175/230 (76%)	175 (100%)	0	100	100
12	P	88/123 (72%)	88 (100%)	0	100	100
13	Q	78/78 (100%)	78 (100%)	0	100	100
14	R	264/318 (83%)	264 (100%)	0	100	100
15	S	116/164 (71%)	116 (100%)	0	100	100
16	T	153/157 (98%)	153 (100%)	0	100	100
17	U	152/174 (87%)	151 (99%)	1 (1%)	81	90
18	V	325/364 (89%)	325 (100%)	0	100	100
19	W	87/158 (55%)	87 (100%)	0	100	100
20	0	188/188 (100%)	187 (100%)	1 (0%)	86	92
21	3	65/166 (39%)	65 (100%)	0	100	100
22	b	253/350 (72%)	253 (100%)	0	100	100
23	a	136/288 (47%)	136 (100%)	0	100	100
24	4	526/609 (86%)	525 (100%)	1 (0%)	92	96
25	H	130/180 (72%)	130 (100%)	0	100	100
26	1	254/291 (87%)	254 (100%)	0	100	100
27	Z	86/95 (90%)	86 (100%)	0	100	100
28	X	311/351 (89%)	310 (100%)	1 (0%)	91	95
29	K	91/113 (80%)	91 (100%)	0	100	100
30	Y	137/357 (38%)	137 (100%)	0	100	100
31	G	275/342 (80%)	275 (100%)	0	100	100
32	F	181/209 (87%)	181 (100%)	0	100	100
33	C	115/143 (80%)	115 (100%)	0	100	100
34	9	12/600 (2%)	12 (100%)	0	100	100
All	All	5593/7798 (72%)	5589 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	U	109	ASN
20	0	83	LYS
24	4	577	ASN
28	X	123	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	64	ASN
3	B	69	HIS
5	E	58	HIS
8	L	146	HIS
9	M	82	HIS
14	R	246	HIS
23	a	320	HIS
24	4	269	HIS
24	4	373	HIS
24	4	540	HIS
25	H	109	HIS
28	X	140	HIS
29	K	113	HIS
30	Y	349	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	919/959 (95%)	196 (21%)	2 (0%)

All (196) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	651	A
2	A	657	G
2	A	680	U
2	A	688	A
2	A	689	U
2	A	695	A
2	A	704	U
2	A	718	A
2	A	721	U
2	A	723	A

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Mol	Chain	Res	Type
2	A	737	C
2	A	740	G
2	A	753	A
2	A	757	A
2	A	761	A
2	A	766	G
2	A	777	G
2	A	782	A
2	A	791	G
2	A	793	C
2	A	794	U
2	A	796	G
2	A	808	C
2	A	814	A
2	A	815	C
2	A	828	C
2	A	829	C
2	A	830	U
2	A	832	U
2	A	835	C
2	A	836	A
2	A	859	U
2	A	860	A
2	A	861	U
2	A	868	C
2	A	869	C
2	A	870	C
2	A	871	A
2	A	881	A
2	A	890	C
2	A	896	A
2	A	902	G
2	A	903	U
2	A	905	A
2	A	907	A
2	A	908	C
2	A	919	A
2	A	923	A
2	A	929	A
2	A	930	G
2	A	931	C
2	A	932	C

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Mol	Chain	Res	Type
2	A	938	A
2	A	939	A
2	A	940	A
2	A	941	G
2	A	942	A
2	A	950	A
2	A	953	U
2	A	955	A
2	A	956	C
2	A	957	C
2	A	958	C
2	A	959	C
2	A	960	C
2	A	962	C
2	A	967	A
2	A	992	U
2	A	994	A
2	A	1001	C
2	A	1002	C
2	A	1011	C
2	A	1013	A
2	A	1014	A
2	A	1015	A
2	A	1030	G
2	A	1038	C
2	A	1042	U
2	A	1065	C
2	A	1069	A
2	A	1080	A
2	A	1082	A
2	A	1098	C
2	A	1103	A
2	A	1105	C
2	A	1106	C
2	A	1107	U
2	A	1109	A
2	A	1116	A
2	A	1118	A
2	A	1119	U
2	A	1121	A
2	A	1126	A
2	A	1137	A

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Mol	Chain	Res	Type
2	A	1138	G
2	A	1149	G
2	A	1151	C
2	A	1153	C
2	A	1155	G
2	A	1160	A
2	A	1167	A
2	A	1174	U
2	A	1179	G
2	A	1180	U
2	A	1187	U
2	A	1188	A
2	A	1189	U
2	A	1190	C
2	A	1194	C
2	A	1200	G
2	A	1213	A
2	A	1220	A
2	A	1223	C
2	A	1225	C
2	A	1227	G
2	A	1245	U
2	A	1246	U
2	A	1247	G
2	A	1248	C
2	A	1250	C
2	A	1251	A
2	A	1258	A
2	A	1268	C
2	A	1269	U
2	A	1271	C
2	A	1273	G
2	A	1284	U
2	A	1285	G
2	A	1290	C
2	A	1291	U
2	A	1294	A
2	A	1295	A
2	A	1299	A
2	A	1301	G
2	A	1312	C
2	A	1313	A

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Mol	Chain	Res	Type
2	A	1326	A
2	A	1327	G
2	A	1341	C
2	A	1343	A
2	A	1345	G
2	A	1352	C
2	A	1354	A
2	A	1355	G
2	A	1367	A
2	A	1376	C
2	A	1379	A
2	A	1383	A
2	A	1384	A
2	A	1385	C
2	A	1390	A
2	A	1391	U
2	A	1392	A
2	A	1402	A
2	A	1404	A
2	A	1406	U
2	A	1407	U
2	A	1413	U
2	A	1416	A
2	A	1429	C
2	A	1430	A
2	A	1443	U
2	A	1447	G
2	A	1448	U
2	A	1462	G
2	A	1465	C
2	A	1466	C
2	A	1474	G
2	A	1475	C
2	A	1478	A
2	A	1479	C
2	A	1480	A
2	A	1483	C
2	A	1489	G
2	A	1490	U
2	A	1492	A
2	A	1493	C
2	A	1503	G

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Mol	Chain	Res	Type
2	A	1508	C
2	A	1509	U
2	A	1510	U
2	A	1539	C
2	A	1557	A
2	A	1558	A
2	A	1559	G
2	A	1560	U
2	A	1564	A
2	A	1565	A
2	A	1567	A
2	A	1568	U
2	A	1569	G
2	A	1571	U
2	A	1572	A
2	A	1594	G
2	A	1595	G
2	A	1598	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	1492	A
2	A	1508	C

5.4 Non-standard residues in protein, DNA, RNA chains (i)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5MC	A	1488	2	18,22,23	0.54	0	26,32,35	0.60	0
6	5F0	I	184	6	8,8,9	0.56	0	7,9,11	1.22	1 (14%)
2	MA6	A	1584	2	18,26,27	1.00	2 (11%)	19,38,41	3.00	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	5MU	A	1076	2	19,22,23	0.31	0	28,32,35	0.33	0
2	MA6	A	1583	2	18,26,27	0.98	2 (11%)	19,38,41	3.16	2 (10%)
2	B8T	A	1486	2	19,22,23	3.66	8 (42%)	26,31,34	0.87	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	A	1488	2	-	2/7/25/26	0/2/2/2
6	5F0	I	184	6	-	0/9/9/10	-
2	MA6	A	1584	2	-	0/7/29/30	0/3/3/3
2	5MU	A	1076	2	-	0/7/25/26	0/2/2/2
2	MA6	A	1583	2	-	2/7/29/30	0/3/3/3
2	B8T	A	1486	2	-	0/7/27/28	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1486	B8T	C2-N3	7.48	1.51	1.36
2	A	1486	B8T	C4-N3	7.28	1.45	1.32
2	A	1486	B8T	C6-C5	6.86	1.51	1.35
2	A	1486	B8T	C4-N4	6.40	1.49	1.35
2	A	1486	B8T	C2-N1	4.73	1.50	1.40
2	A	1486	B8T	C5-C4	3.90	1.49	1.40
2	A	1486	B8T	C6-N1	3.26	1.45	1.38
2	A	1583	MA6	C5-C4	-2.77	1.33	1.40
2	A	1486	B8T	O2-C2	-2.74	1.18	1.23
2	A	1584	MA6	C5-C4	-2.67	1.33	1.40
2	A	1584	MA6	C2-N3	2.22	1.35	1.32
2	A	1583	MA6	C2-N3	2.10	1.35	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1583	MA6	N1-C6-N6	-12.47	103.94	117.06
2	A	1584	MA6	N1-C6-N6	-11.75	104.69	117.06
2	A	1583	MA6	N3-C2-N1	-5.43	120.19	128.68
2	A	1584	MA6	N3-C2-N1	-5.28	120.42	128.68
6	I	184	5F0	O-C-CB	-2.88	117.04	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1486	B8T	C6-C5-C4	2.73	120.31	116.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1583	MA6	O4'-C4'-C5'-O5'
2	A	1488	5MC	O4'-C4'-C5'-O5'
2	A	1488	5MC	C3'-C4'-C5'-O5'
2	A	1583	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1488	5MC	1	0
2	A	1584	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 47 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
40	FES	P	201	12,5	0,4,4	-	-	-		
43	GDP	X	502	-	24,30,30	0.89	2 (8%)	30,47,47	0.61	0
35	NAD	A	1701	37	42,48,48	0.60	0	50,73,73	0.62	1 (2%)
40	FES	T	201	16,9	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	SAH	b	501	-	24,28,28	1.22	3 (12%)	25,40,40	1.47	3 (12%)
42	ATP	X	501	-	26,33,33	0.74	0	31,52,52	0.68	0
36	SPM	A	1702	-	13,13,13	0.26	0	12,12,12	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	FES	P	201	12,5	-	-	0/1/1/1
43	GDP	X	502	-	-	3/12/32/32	0/3/3/3
35	NAD	A	1701	37	-	2/26/62/62	0/5/5/5
40	FES	T	201	16,9	-	-	0/1/1/1
41	SAH	b	501	-	-	1/11/31/31	0/3/3/3
42	ATP	X	501	-	-	5/18/38/38	0/3/3/3
36	SPM	A	1702	-	-	2/11/11/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	b	501	SAH	C2-N3	3.94	1.38	1.32
41	b	501	SAH	C2-N1	2.46	1.38	1.33
43	X	502	GDP	C5-C6	-2.22	1.42	1.47
41	b	501	SAH	OXT-C	-2.14	1.23	1.30
43	X	502	GDP	C8-N7	-2.03	1.31	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	b	501	SAH	N3-C2-N1	-5.50	120.09	128.68
41	b	501	SAH	OXT-C-O	-2.73	117.89	124.09
35	A	1701	NAD	C5A-C6A-N6A	2.33	123.90	120.35
41	b	501	SAH	OXT-C-CA	2.25	121.06	113.38

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	1702	SPM	C7-C8-C9-N10

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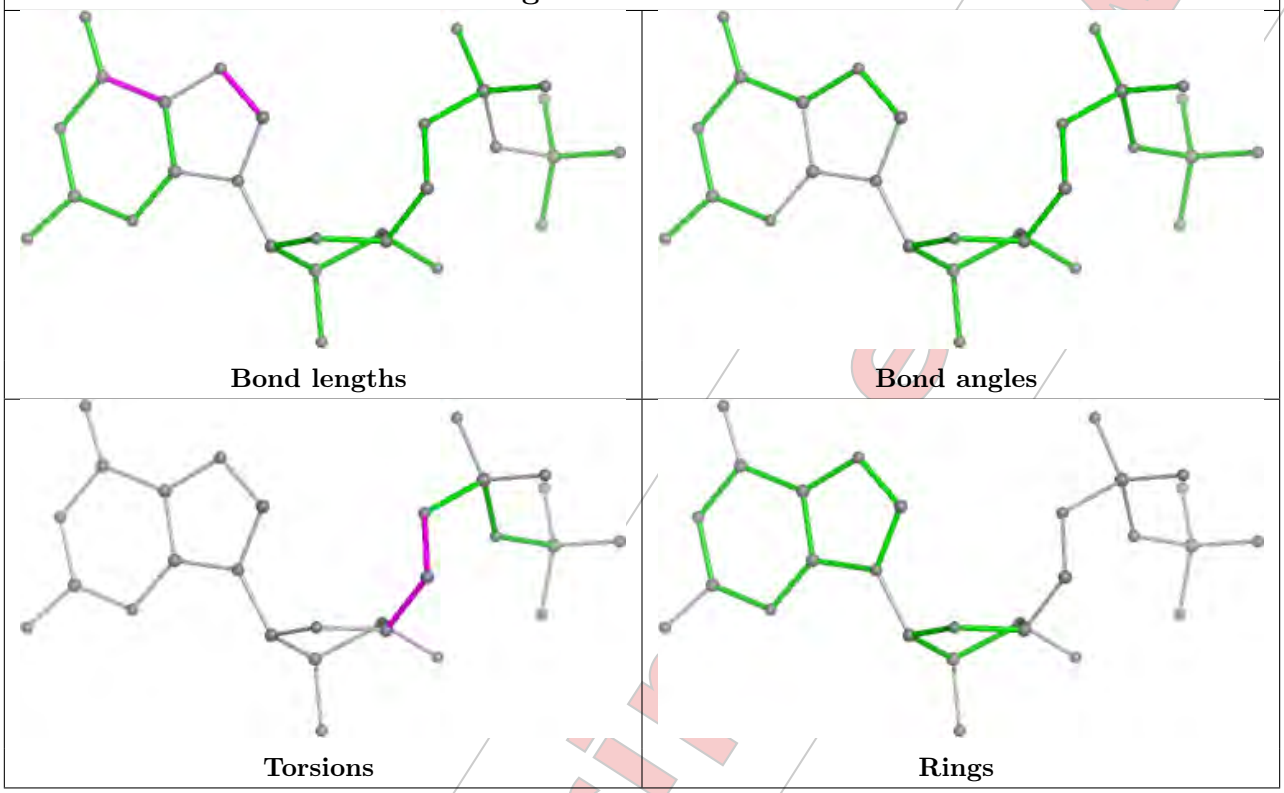
Mol	Chain	Res	Type	Atoms
42	X	501	ATP	O4'-C4'-C5'-O5'
42	X	501	ATP	PB-O3B-PG-O1G
43	X	502	GDP	C4'-C5'-O5'-PA
42	X	501	ATP	C3'-C4'-C5'-O5'
43	X	502	GDP	O4'-C4'-C5'-O5'
41	b	501	SAH	C4'-C5'-SD-CG
35	A	1701	NAD	PA-O3-PN-O2N
42	X	501	ATP	C4'-C5'-O5'-PA
36	A	1702	SPM	C6-C7-C8-C9
42	X	501	ATP	PB-O3A-PA-O1A
43	X	502	GDP	C3'-C4'-C5'-O5'
35	A	1701	NAD	PA-O3-PN-O1N

There are no ring outliers.

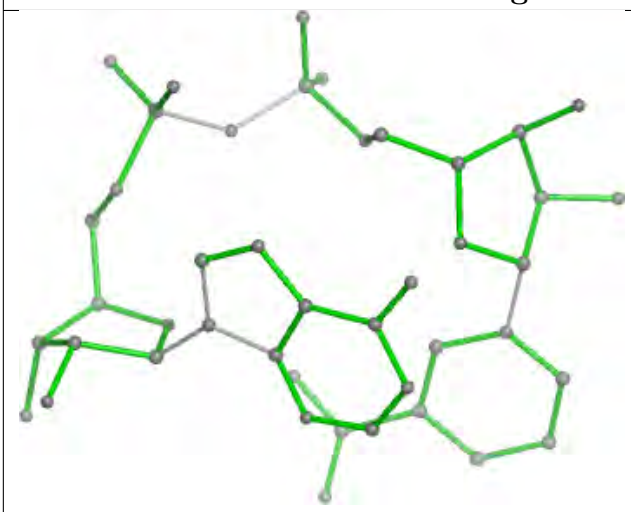
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

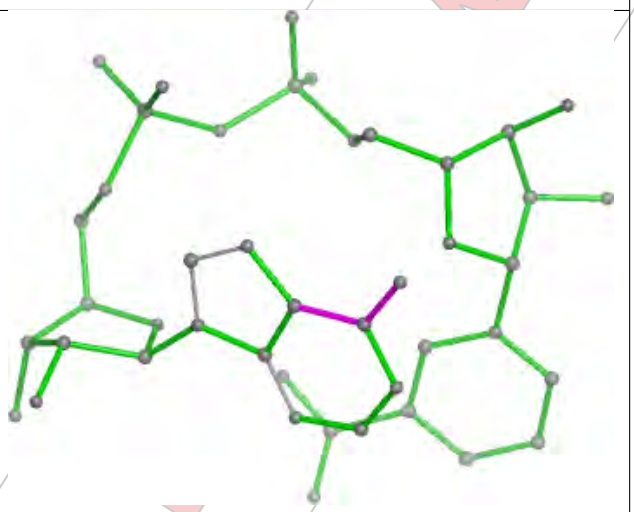
Ligand GDP X 502



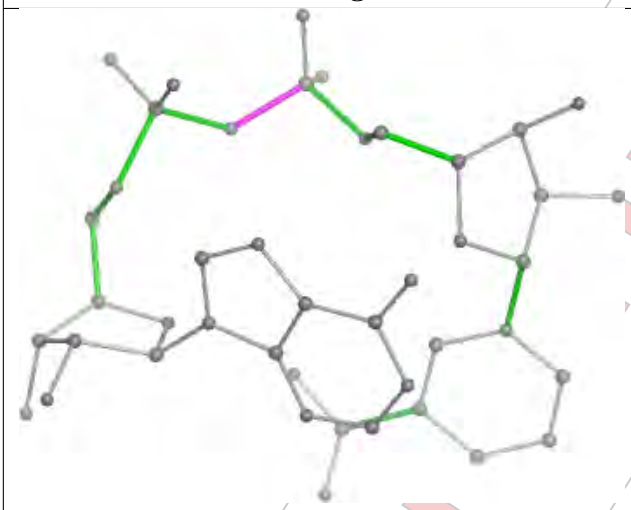
Ligand NAD A 1701



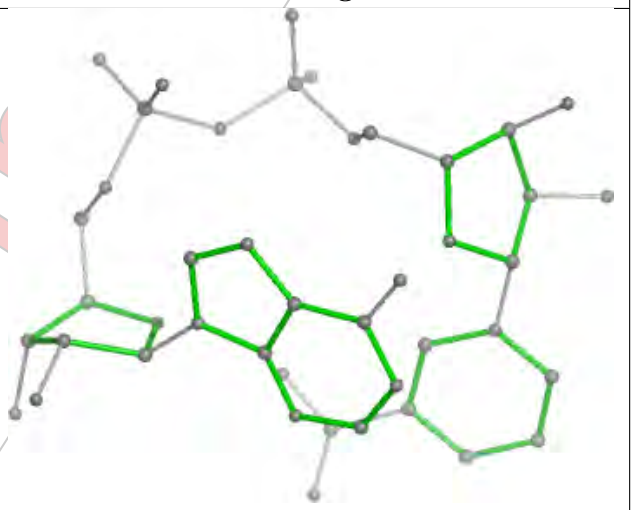
Bond lengths



Bond angles

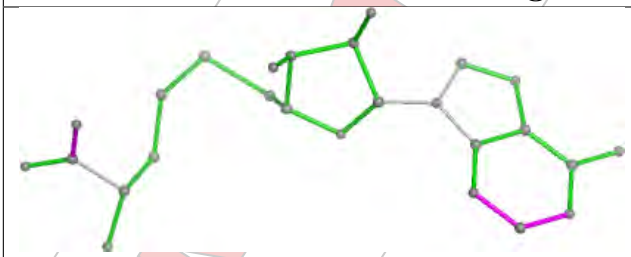


Torsions

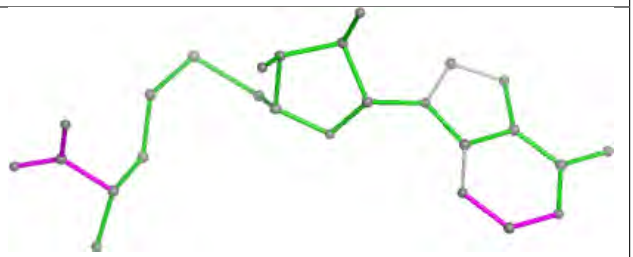


Rings

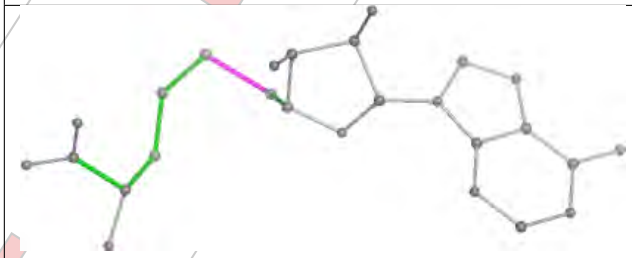
Ligand SAH b 501



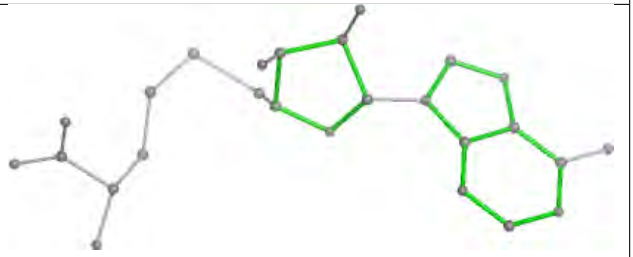
Bond lengths



Bond angles

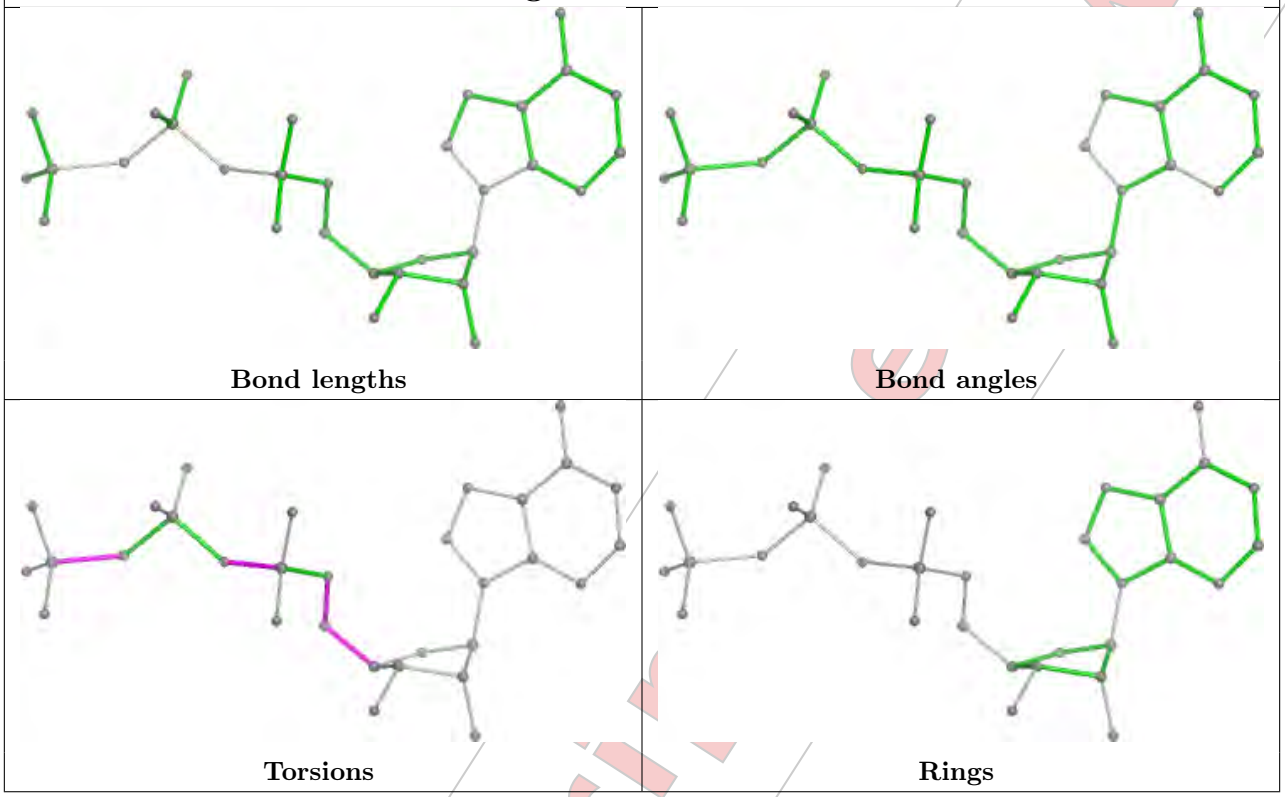


Torsions



Rings

Ligand ATP X 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

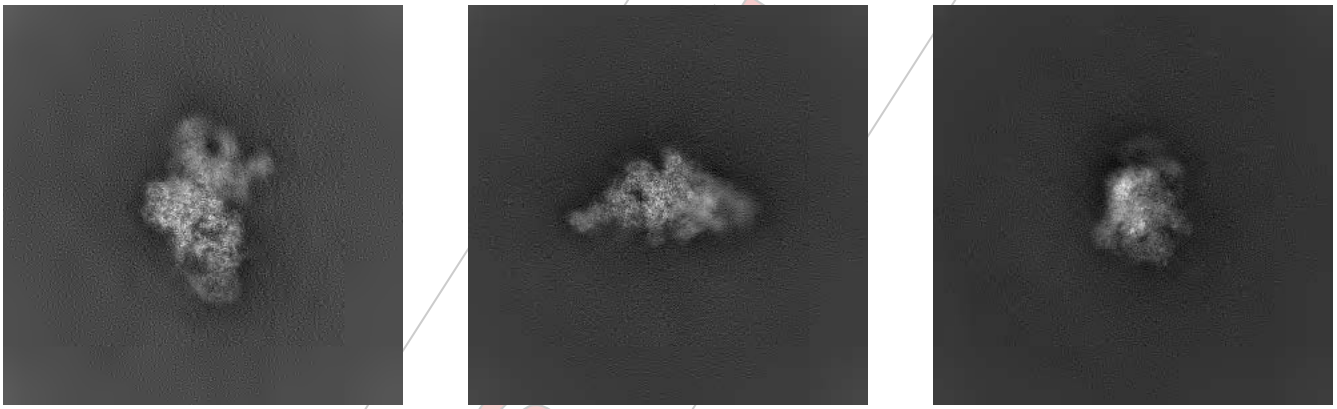
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51873. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

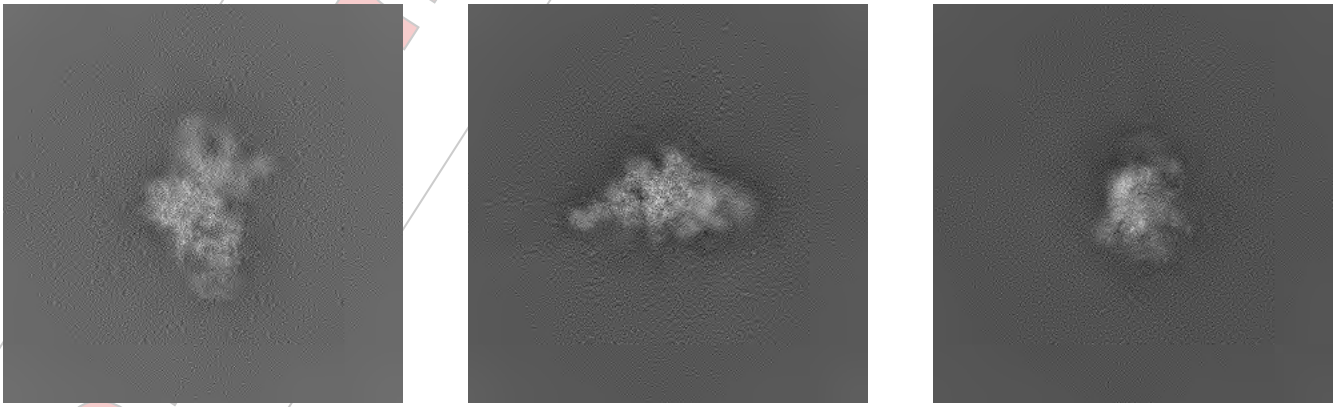
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



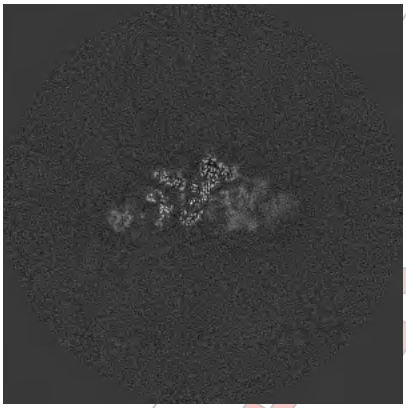
X Y Z

The images above show the map projected in three orthogonal directions.

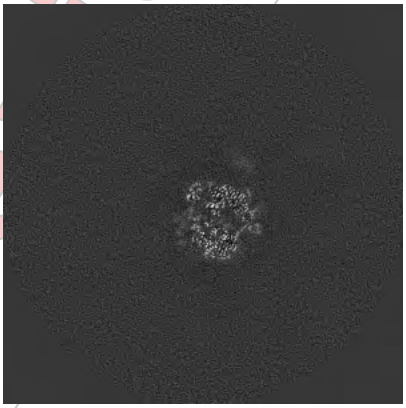
6.2 Central slices (i)

6.2.1 Primary map

X Index: 300

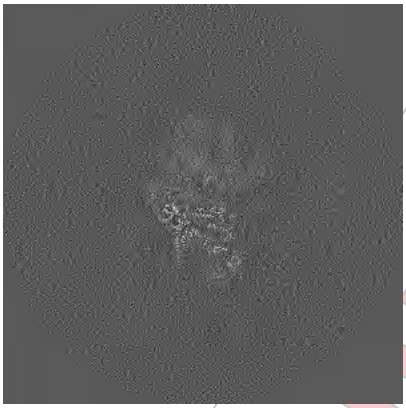


Y Index: 300

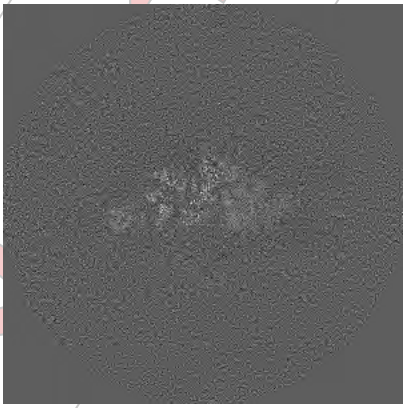


Z Index: 300

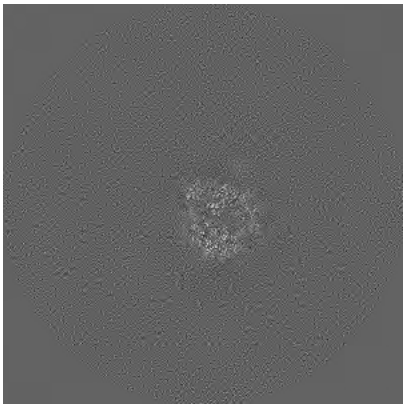
6.2.2 Raw map



X Index: 300



Y Index: 300



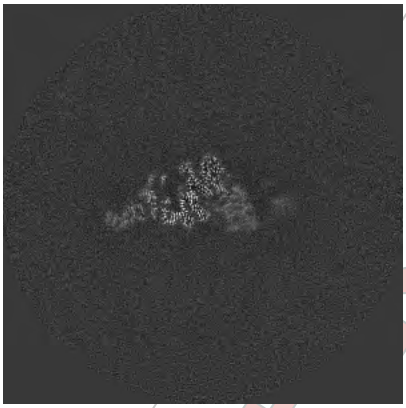
Z Index: 300

The images above show central slices of the map in three orthogonal directions.

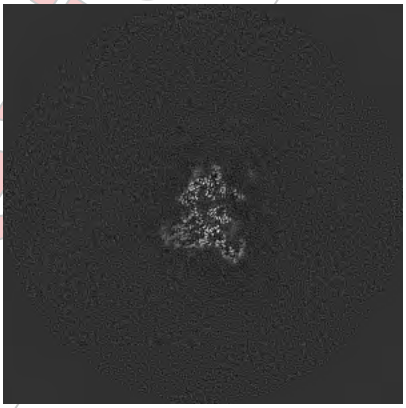
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 313

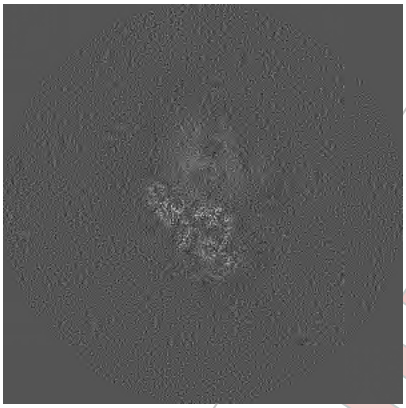


Y Index: 310

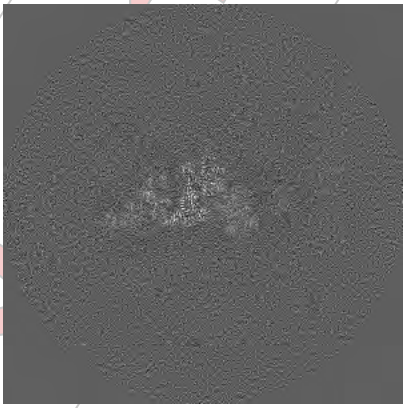


Z Index: 275

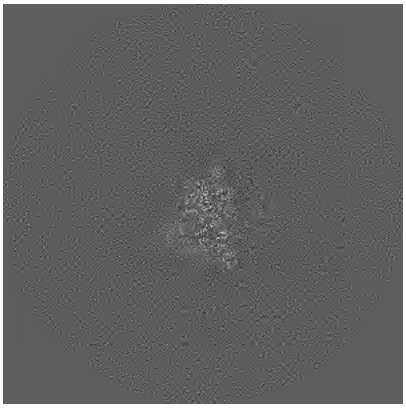
6.3.2 Raw map



X Index: 304



Y Index: 311

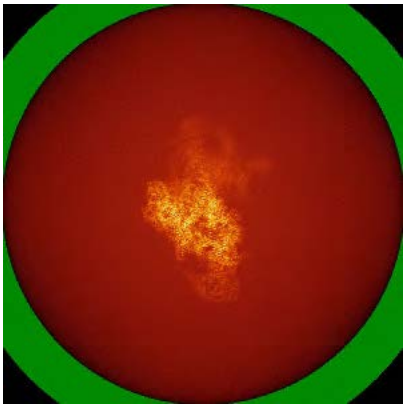


Z Index: 289

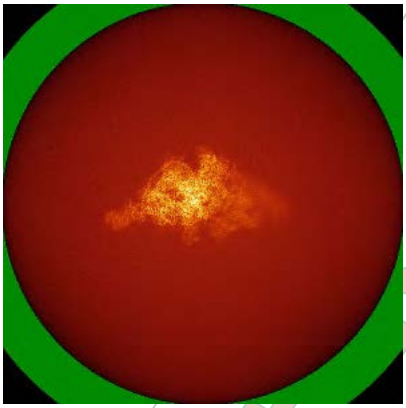
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

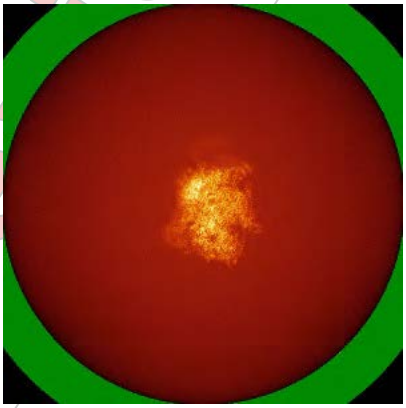
6.4.1 Primary map



X

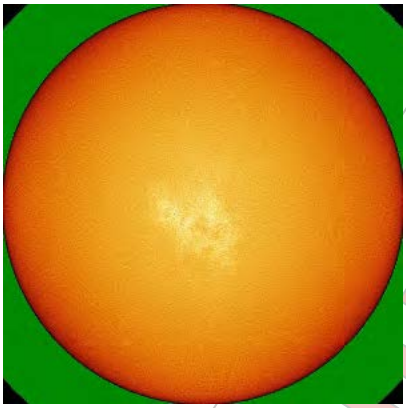


Y

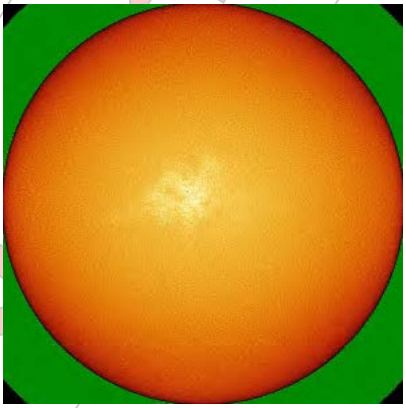


Z

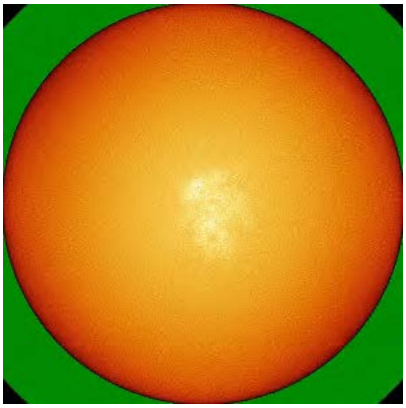
6.4.2 Raw map



X



Y

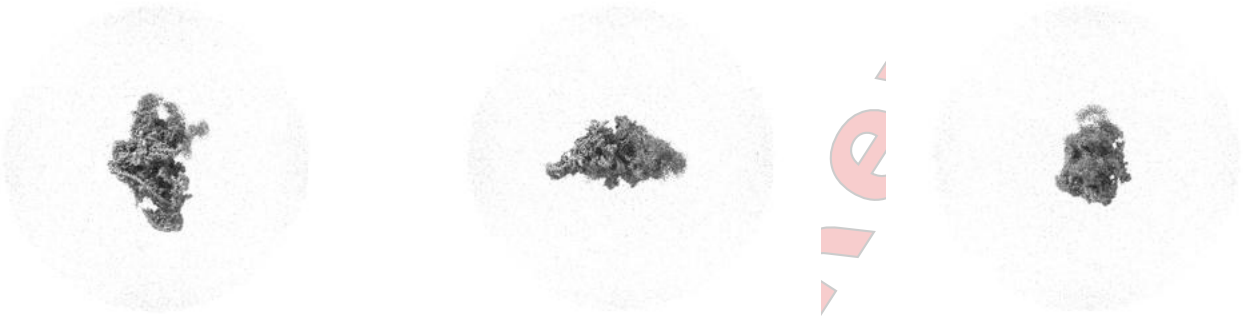


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

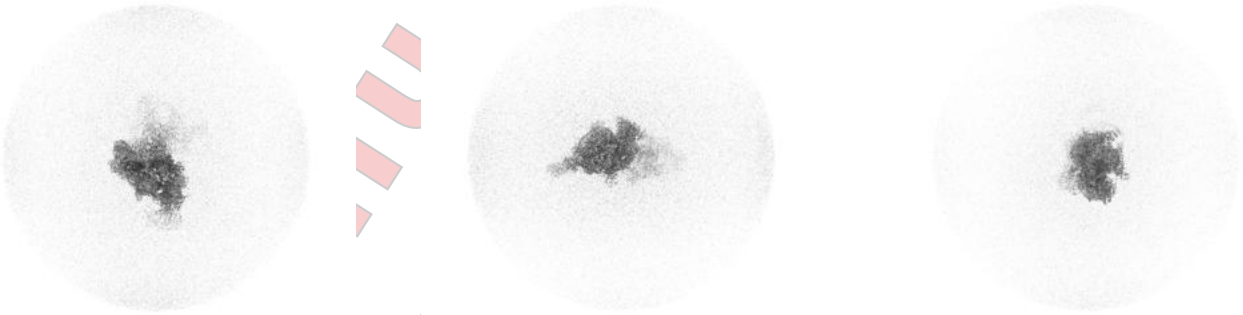
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

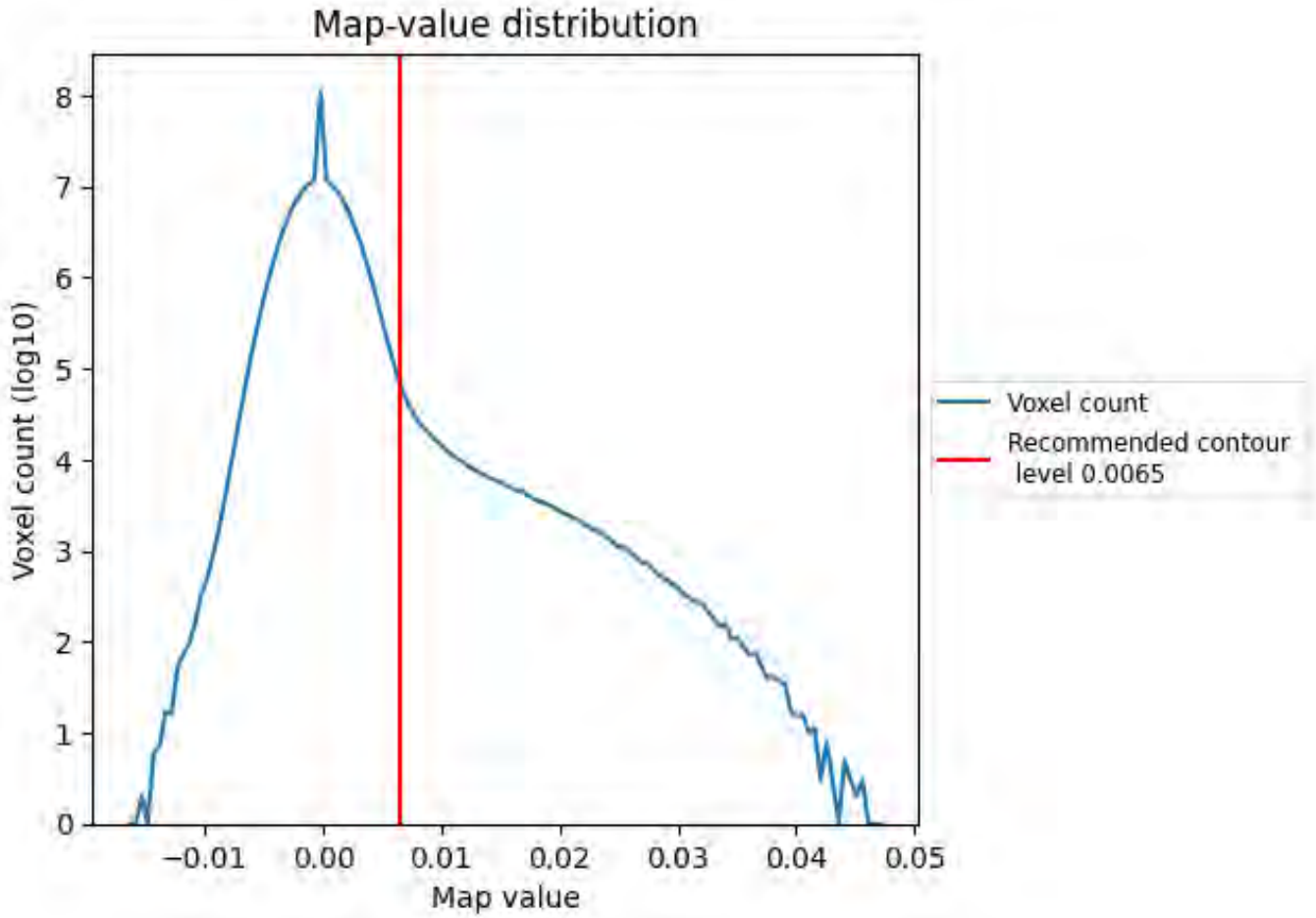
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

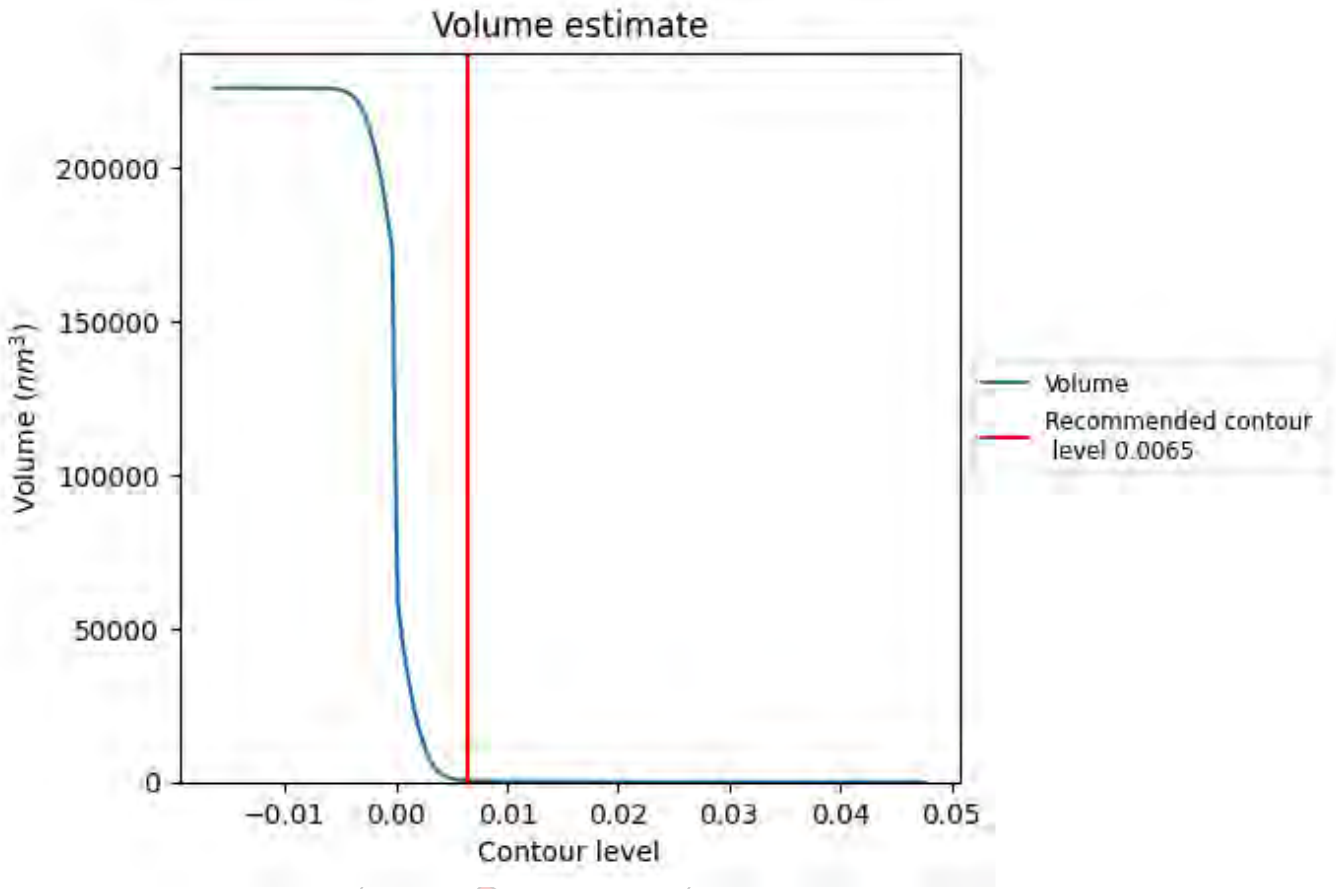
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

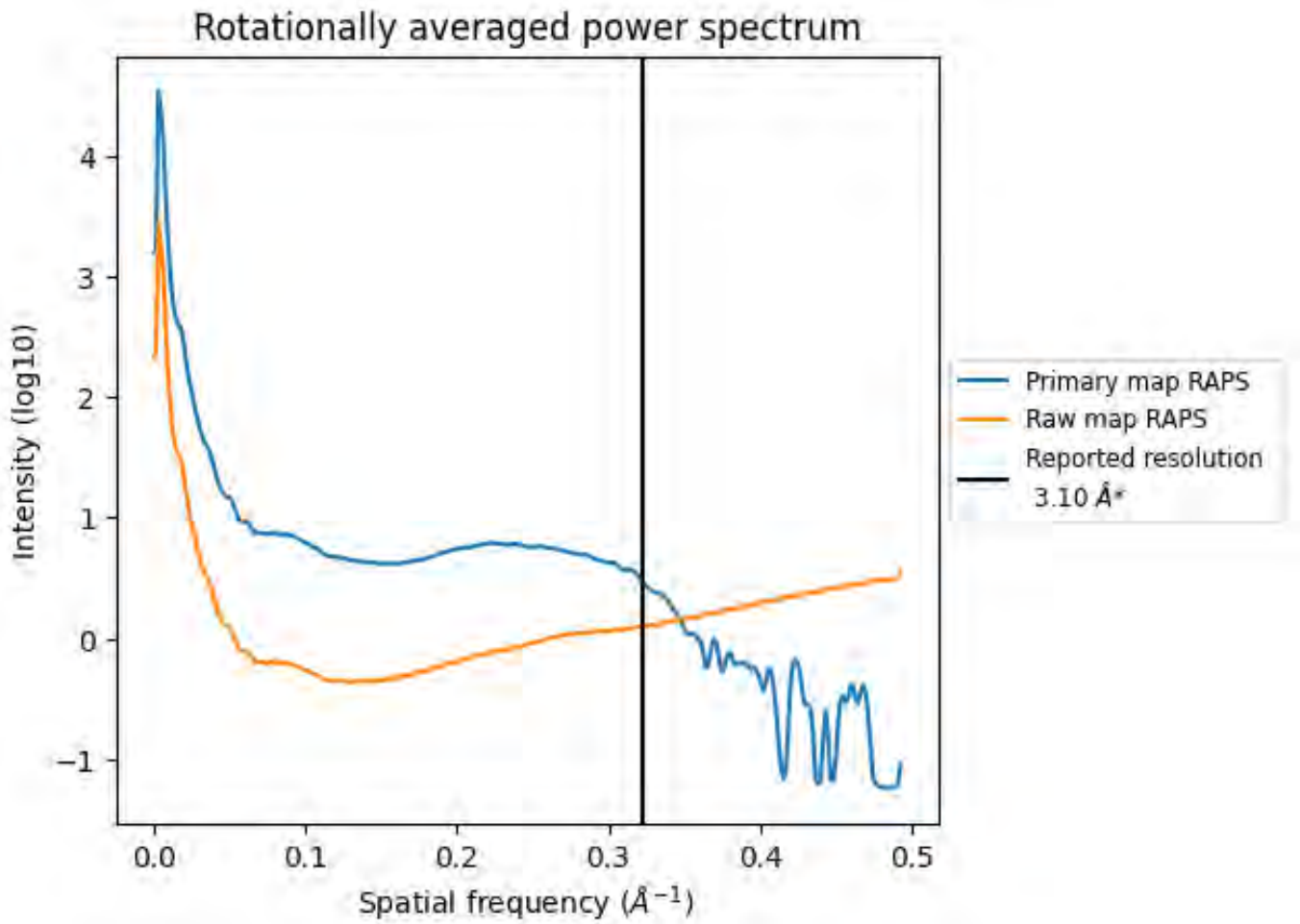
7.2 Volume estimate (i)



The volume at the recommended contour level is 419 nm^3; this corresponds to an approximate mass of 378 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

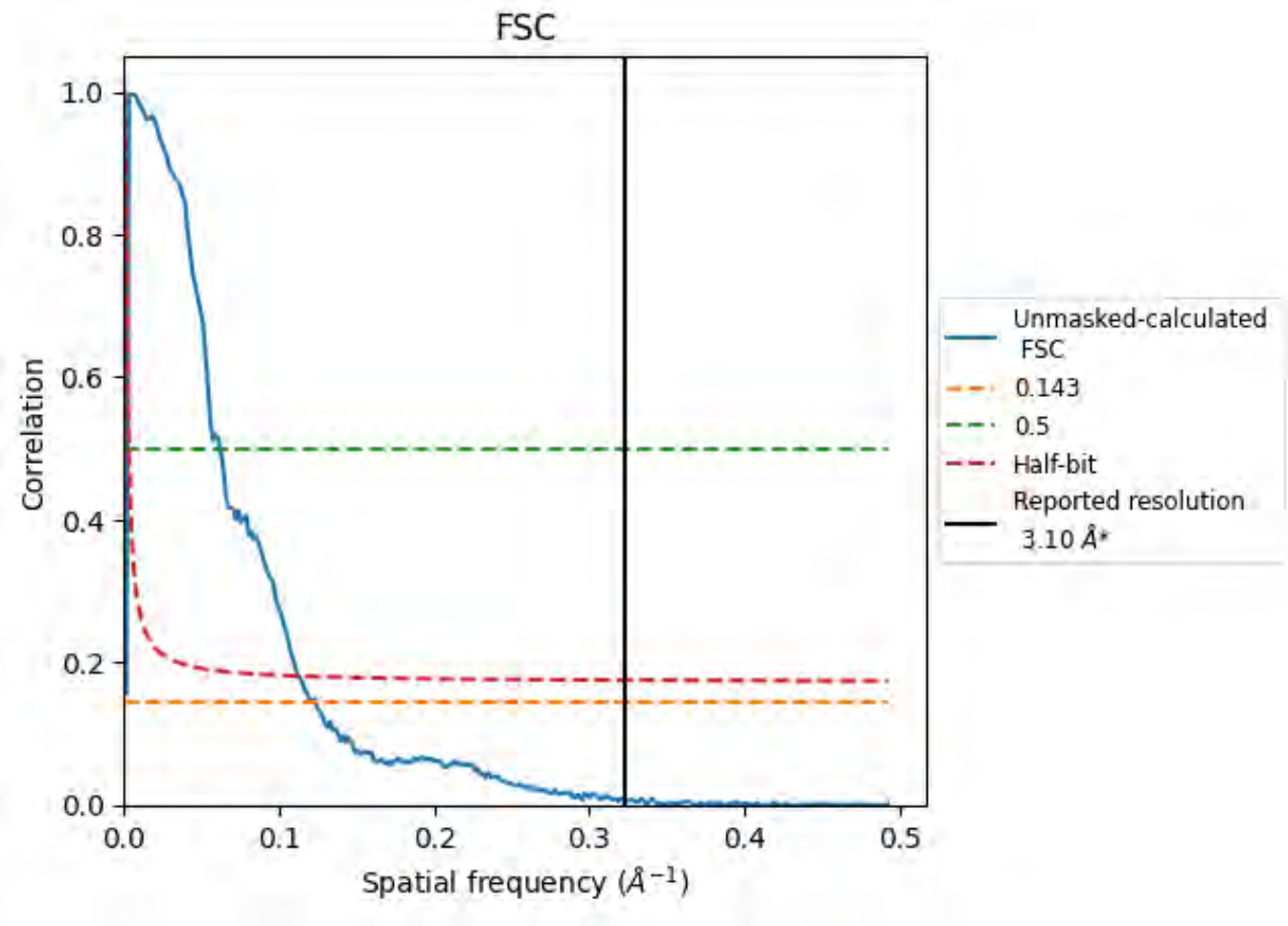


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

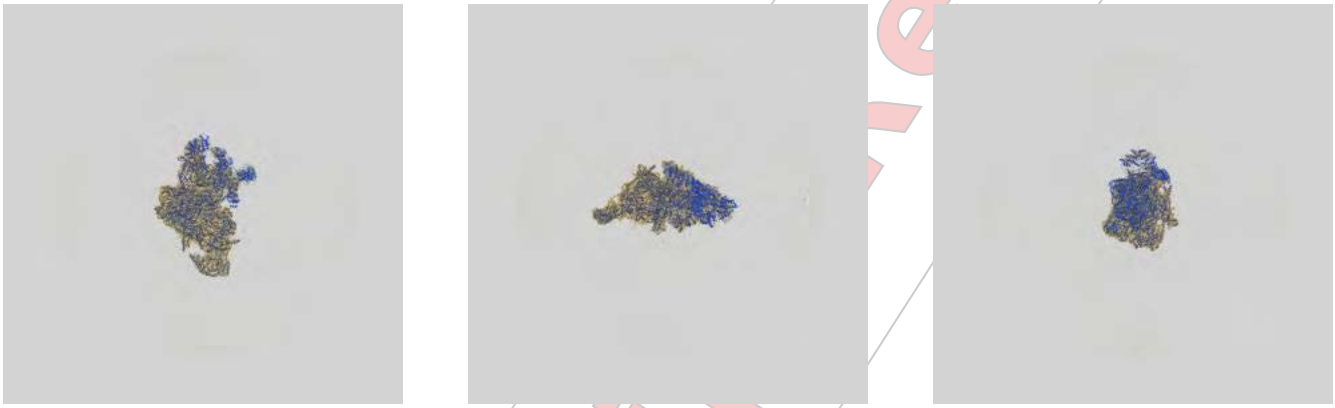
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.08	434.78	384.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.08 differs from the reported value 3.1 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51873 and PDB model 9H51. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay



X Y Z

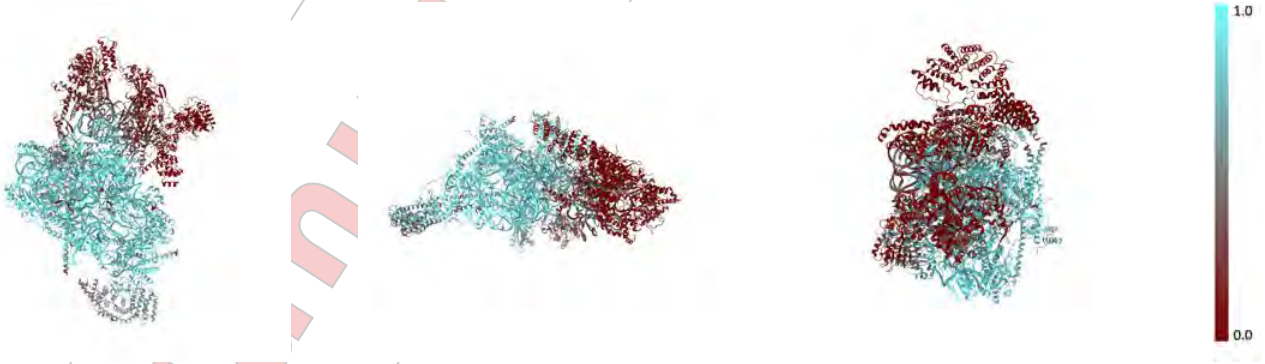
The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

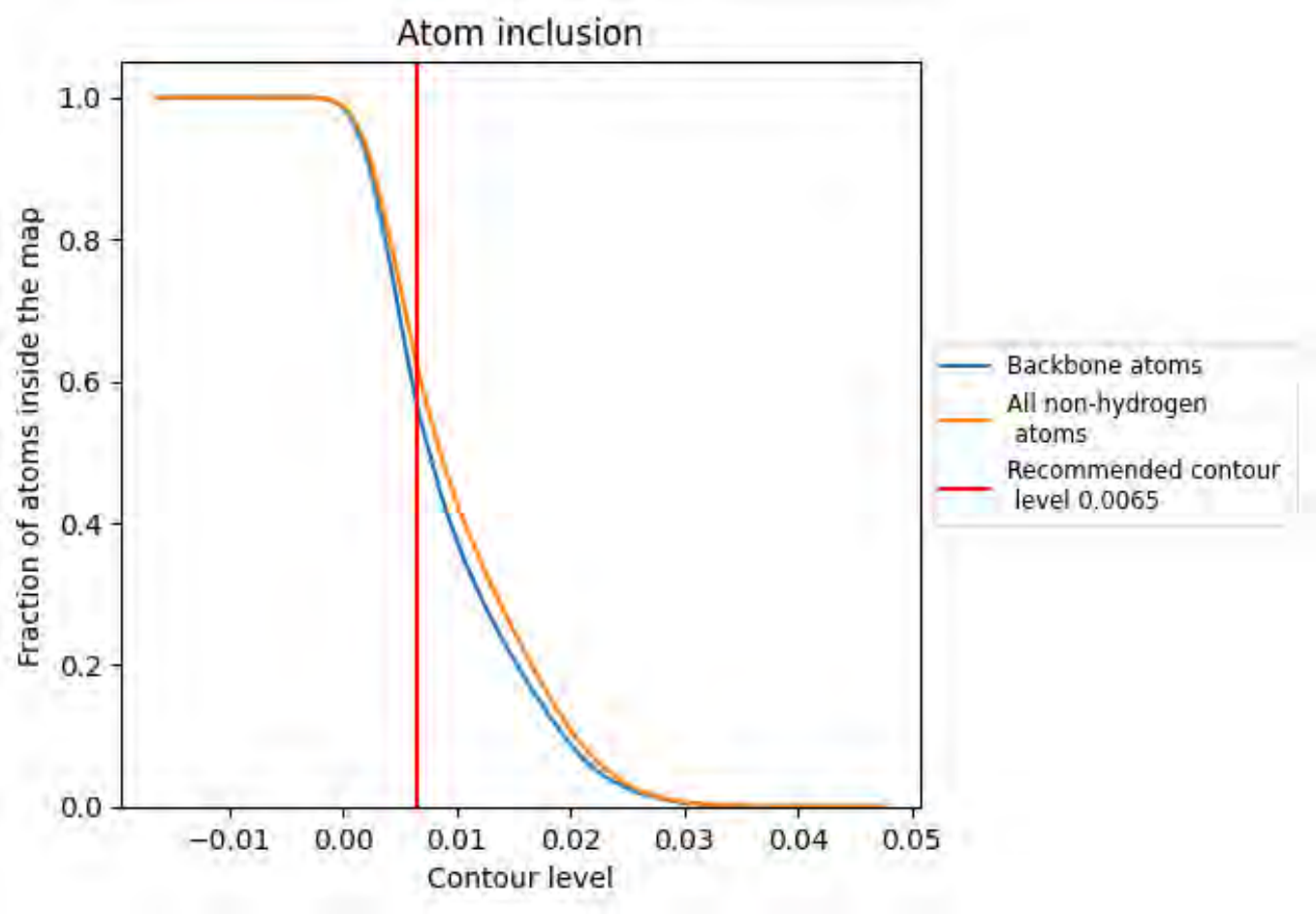
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0065).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6220	0.3670
0	0.7630	0.4860
1	0.0920	0.0790
3	0.8410	0.5570
4	0.0560	0.0470
9	0.3890	0.2340
A	0.8180	0.4640
B	0.8800	0.5600
C	0.3020	0.2190
D	0.6440	0.4540
E	0.8330	0.5550
F	0.2310	0.1340
G	0.3670	0.2140
H	0.1510	0.1060
I	0.8400	0.5390
J	0.8850	0.5750
K	0.2520	0.1450
L	0.8340	0.5340
M	0.8830	0.5730
N	0.8940	0.5900
O	0.8890	0.5680
P	0.8650	0.5590
Q	0.8710	0.5690
R	0.8130	0.5150
S	0.7820	0.4780
T	0.8650	0.5630
U	0.7950	0.4940
V	0.5200	0.2830
W	0.8120	0.5330
X	0.0760	0.0330
Y	0.0520	0.0720
Z	0.1880	0.1120
a	0.5010	0.3660
b	0.3320	0.1910
c	0.6670	0.4440

Full wwPDB EM Validation Report ⓘ

Oct 25, 2024 – 02:18 pm BST

PDB ID	:	9H53
EMDB ID	:	EMD-51875
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit bound to METTL15 and RBFA (inward conformation) (state A5)
Deposited on	:	2024-10-22
Resolution	:	4.10 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ①) were used in the production of this report:

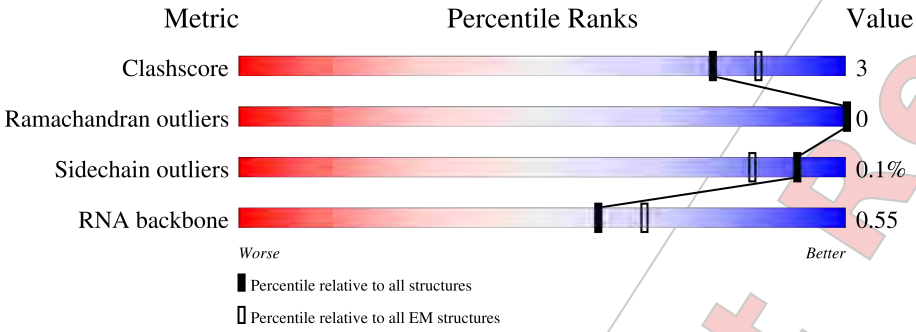
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	296	5% 73% · 24%
2	C	167	65% 74% 5% 21%
3	D	430	22% 70% 5% 25%
4	E	125	18% 86% 6% 8%
5	F	242	73% 76% 8% 15%

Continued on next page...

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Mol	Chain	Length	Quality of chain
6	G	396	51% 76% 21%
7	I	194	9% 63% 7% 29%
8	J	138	7% 71% 7% 22%
9	K	128	67% 76% 21%
10	L	257	9% 67% 32%
11	M	137	7% 82% 13%
12	N	130	5% 79% 5% 15%
13	O	258	5% 69% 7% 25%
14	P	142	6% 67% 32%
15	Q	87	14% 87% 13%
16	R	360	7% 79% 18%
17	S	190	16% 66% 5% 29%
18	T	173	5% 91% 6%
19	U	205	10% 82% 14%
20	V	414	40% 83% 5% 13%
21	W	187	6% 50% 47%
22	X	398	84% 83% 5% 12%
23	Y	395	30% 28% 69%
24	Z	106	69% 80% 17%
25	0	218	24% 91% 7%
26	1	323	80% 82% 15%
27	3	199	7% 32% 65%
28	4	689	84% 80% 5% 15%
29	b	407	51% 73% 27%
30	A	955	17% 68% 24% 5%

Continued on next page...

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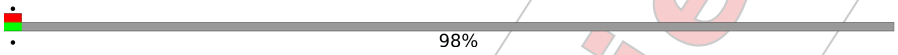
Mol	Chain	Length	Quality of chain
31	H	201	
32	9	698	
33	a	343	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 127284 atoms, of which 59147 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	B	225	3643	1164	1815	331	323	10	0	0

- Molecule 2 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C	132	2171	699	1088	195	185	4	0	0

- Molecule 3 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	321	5179	1614	2609	482	461	13	0	0

- Molecule 4 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	E	115	1840	574	930	165	167	4	0	0

- Molecule 5 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	205	3421	1076	1736	304	294	11	0	0

- Molecule 6 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	G	313	5136	1637	2560	456	469	14	0	0

- Molecule 7 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	I	137	2080	642	1060	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 8 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	J	108	1726	521	887	169	143	6	0	0

- Molecule 9 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	K	101	1747	537	885	179	141	5	0	0

- Molecule 10 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	L	174	2993	925	1540	270	251	7	0	0

- Molecule 11 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	M	119	1908	594	966	185	157	6	0	0

- Molecule 12 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	N	110	1796	562	928	156	147	3	0	0

- Molecule 13 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	194	Total	C	H	N	O	S	0	0
			3164	1019	1565	295	278	7		

- Molecule 14 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	97	Total	C	H	N	O	S	0	0
			1588	501	807	134	138	8		

- Molecule 15 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	87	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 16 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	295	Total	C	H	N	O	S	0	0
			4837	1533	2428	413	455	8		

- Molecule 17 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	135	Total	C	H	N	O	S	0	0
			2226	716	1115	198	196	1		

- Molecule 18 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

- Molecule 19 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	176	Total	C	H	N	O	S	0	0
			2987	916	1499	301	267	4		

- Molecule 20 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	362	Total	C	H	N	O	S	0	0
			5930	1904	2961	495	558	12		

- Molecule 21 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	W	100	Total	C	H	N	O	S	0	0
			1591	498	802	141	146	4		

- Molecule 22 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	X	352	Total	C	H	N	O	S	0	0
			5693	1822	2844	499	517	11		

- Molecule 23 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	121	Total	C	H	N	O	S	0	0
			1993	662	970	168	191	2		

- Molecule 24 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	88	Total	C	H	N	O	S	0	0
			1495	476	750	133	132	4		

- Molecule 25 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	0	215	Total	C	H	N	O	S	0	0
			3583	1130	1796	339	313	5		

- Molecule 26 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	276	Total	C	H	N	O	S	0	0
			4507	1419	2269	381	427	11		

- Molecule 27 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	3	70	Total	C	H	N	O	S	0	0
			1324	401	699	134	89	1		

- Molecule 28 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	4	588	Total	C	H	N	O	S	0	0
			9534	3053	4766	808	879	28		

- Molecule 29 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	b	296	Total	C	H	N	O	S	0	0
			4679	1464	2366	410	426	13		

- Molecule 30 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	A	905	Total	C	H	N	O	P	0	0
			28985	8621	9762	3460	6237	905		

- Molecule 31 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	H	139	Total	C	H	N	O	S	0	0
			2317	739	1173	193	209	3		

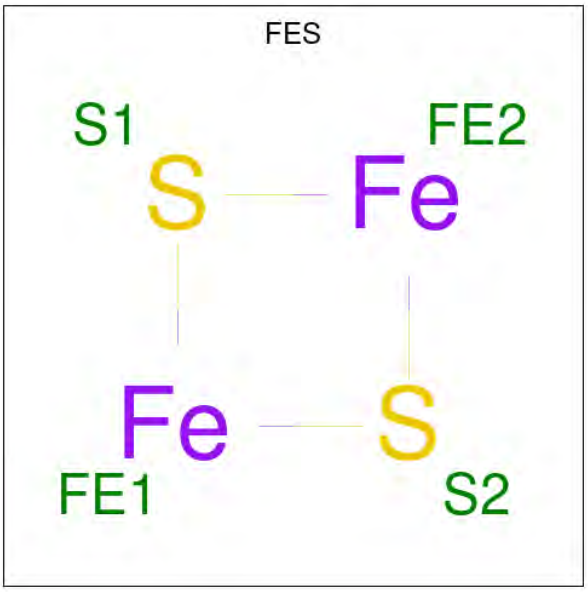
- Molecule 32 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	9	12	Total	C	H	N	O	S	0	0
			219	76	108	16	18	1		

- Molecule 33 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	a	158	Total	C	H	N	O	S	0	0
			2513	783	1261	221	241	7		

- Molecule 34 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

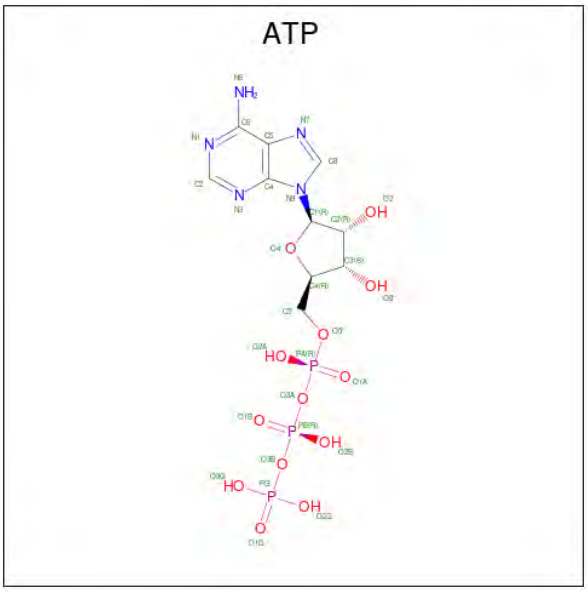


Mol	Chain	Residues	Atoms			AltConf
34	M	1	Total	Fe	S	0
			4	2	2	
34	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

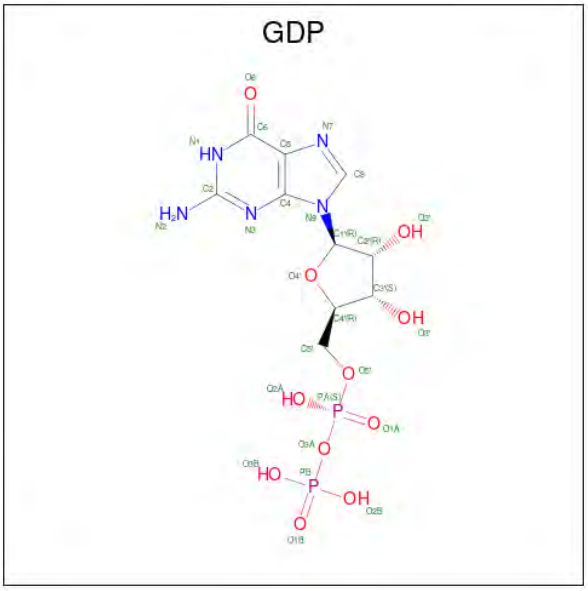
Mol	Chain	Residues	Atoms		AltConf
35	O	1	Total	Zn	0
			1	1	

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
36	X	1	43	10	12	5	13	3	0

- Molecule 37 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

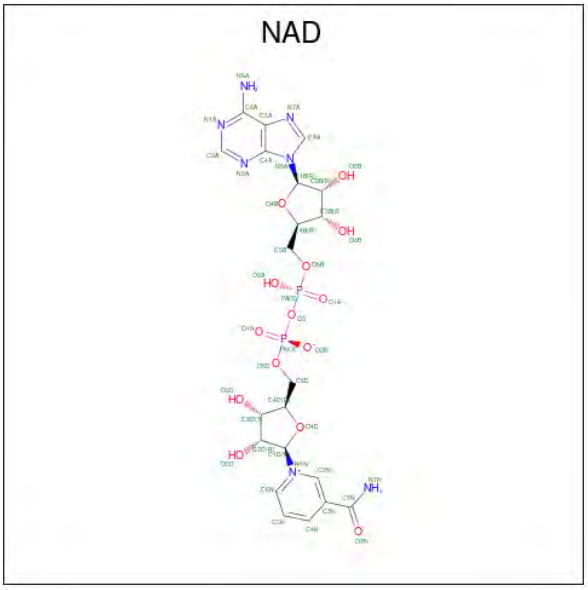


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
37	X	1	38	10	10	5	11	2	0

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

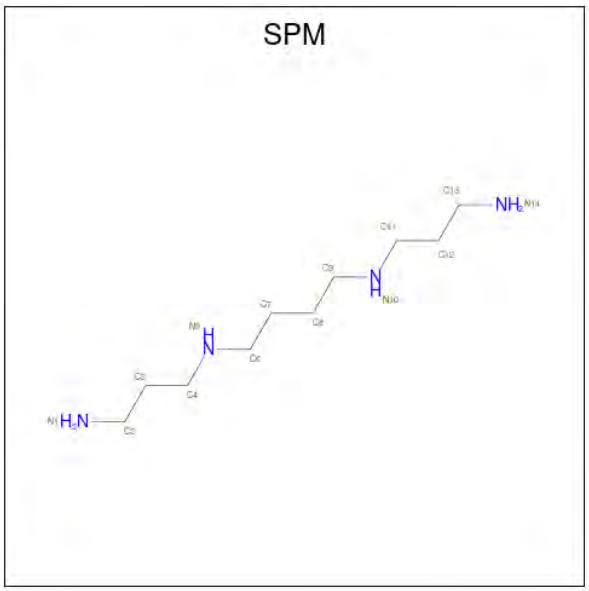
Mol	Chain	Residues	Atoms		AltConf
38	A	31	Total	Mg	0
			31	31	

- Molecule 39 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
39	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 40 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
40	A	1	Total 14	C 10	N 4	0

- Molecule 41 is water.

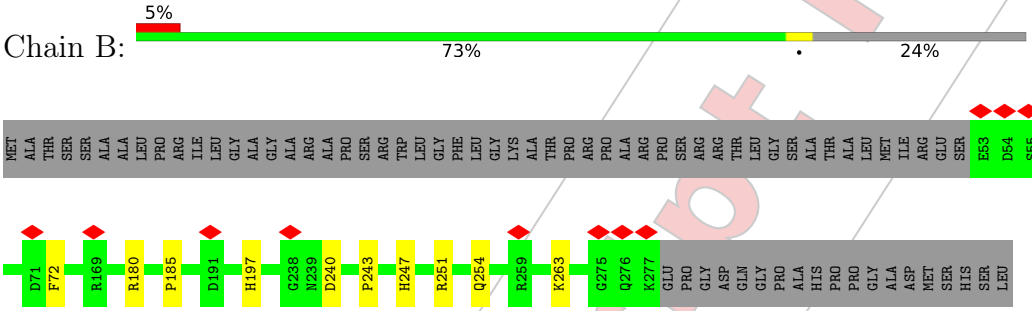
Mol	Chain	Residues	Atoms		AltConf
41	G	1	Total 1	O 1	0
41	T	1	Total 1	O 1	0
41	0	1	Total 1	O 1	0
41	b	1	Total 1	O 1	0
41	A	1	Total 1	O 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

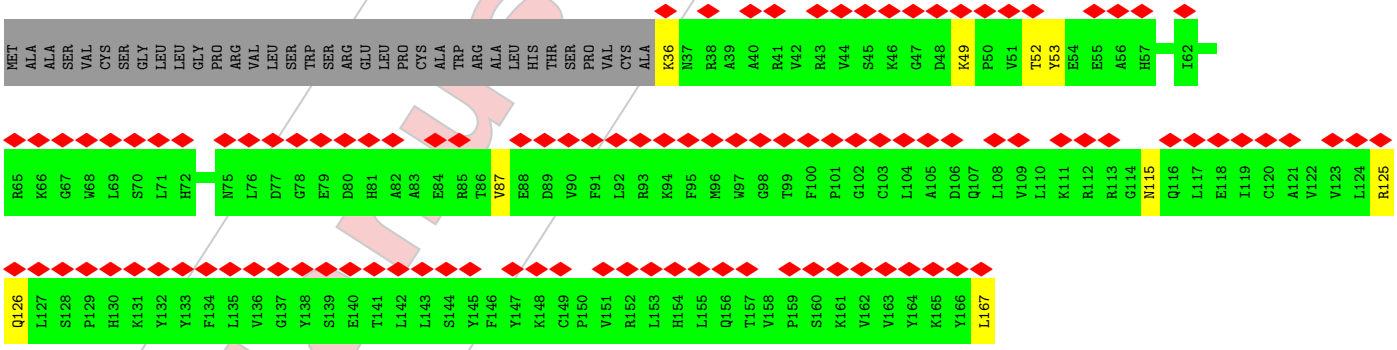
• Molecule 1: 28S ribosomal protein S2, mitochondrial

Chain B:



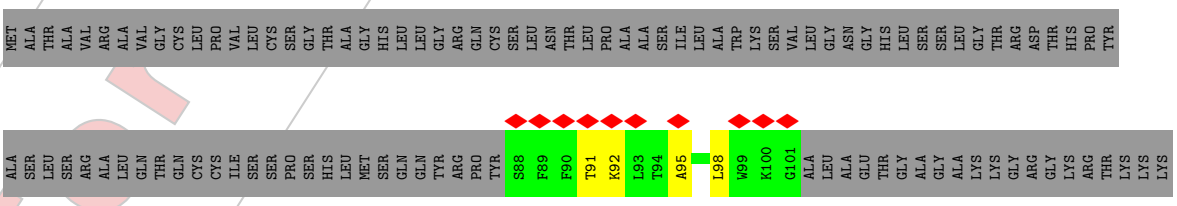
• Molecule 2: 28S ribosomal protein S24, mitochondrial

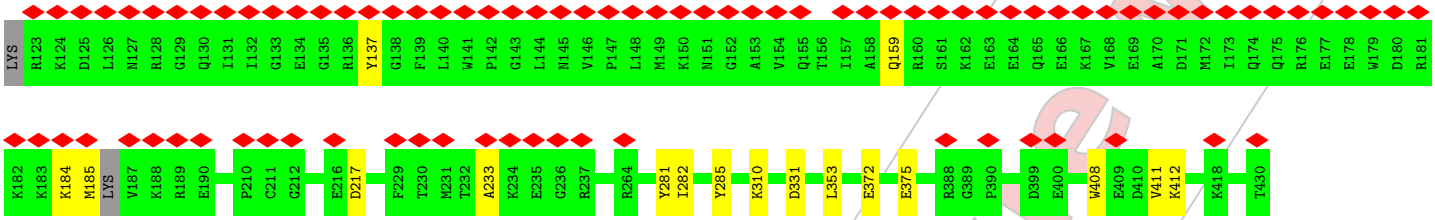
Chain C:



• Molecule 3: 28S ribosomal protein S5, mitochondrial

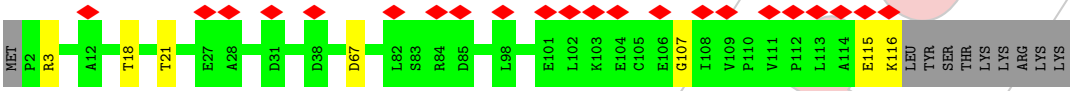
Chain D:





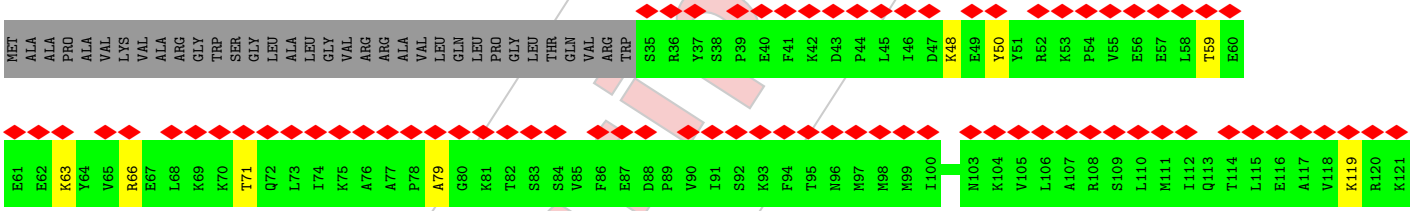
• Molecule 4: 28S ribosomal protein S6, mitochondrial

Chain E:



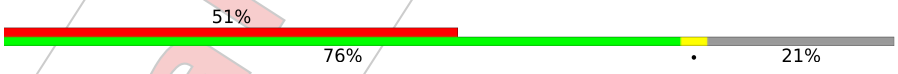
• Molecule 5: 28S ribosomal protein S7, mitochondrial

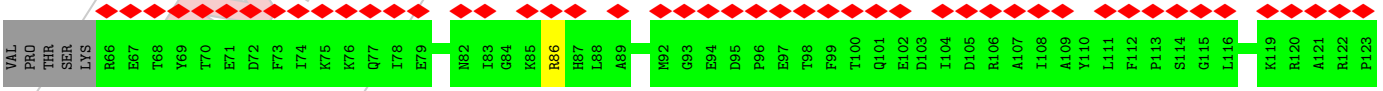
Chain F:

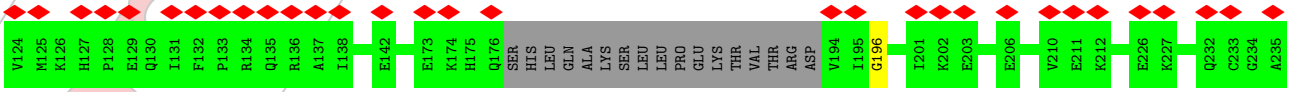


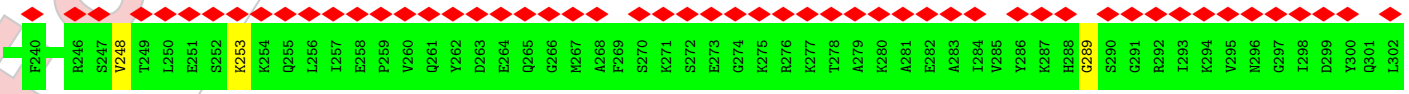
• Molecule 6: 28S ribosomal protein S9, mitochondrial

Chain G:

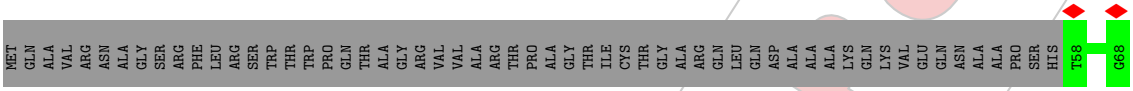


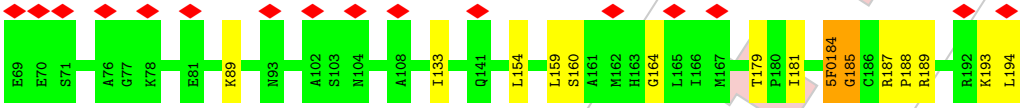




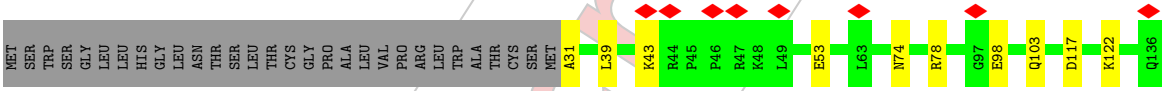


• Molecule 7: 28S ribosomal protein S11, mitochondrial

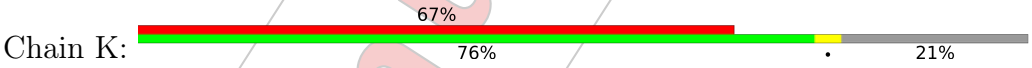


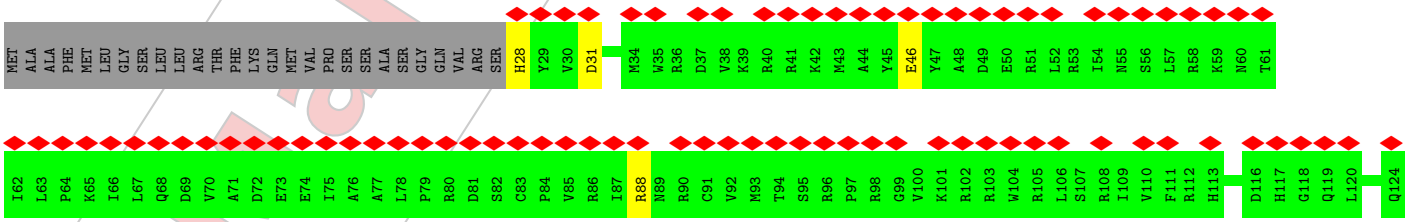


• Molecule 8: 28S ribosomal protein S12, mitochondrial

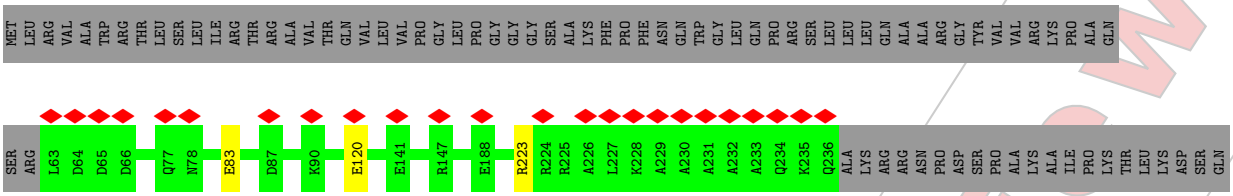


• Molecule 9: 28S ribosomal protein S14, mitochondrial



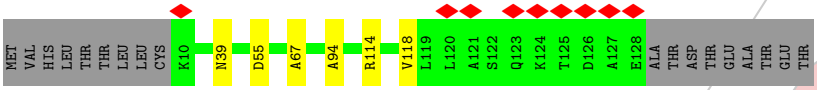


• Molecule 10: 28S ribosomal protein S15, mitochondrial



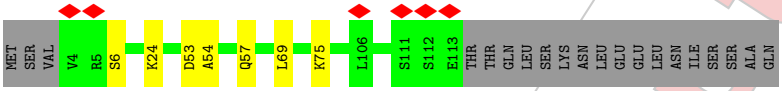
• Molecule 11: 28S ribosomal protein S16, mitochondrial

Chain M:



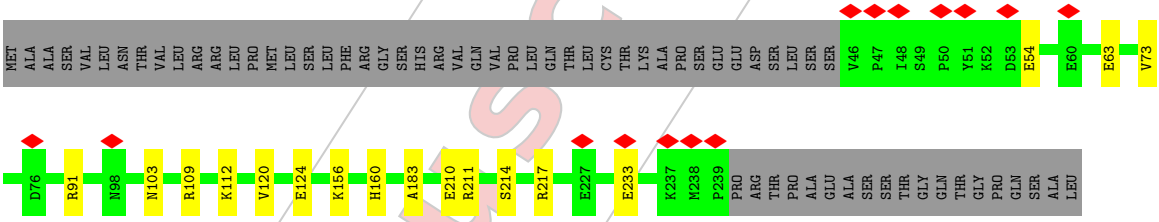
• Molecule 12: 28S ribosomal protein S17, mitochondrial

Chain N:



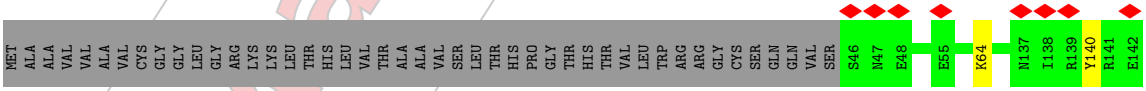
• Molecule 13: 28S ribosomal protein S18b, mitochondrial

Chain O:



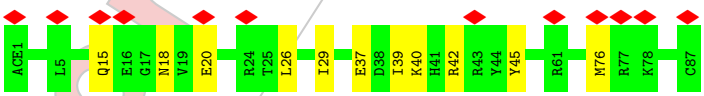
• Molecule 14: 28S ribosomal protein S18c, mitochondrial

Chain P:



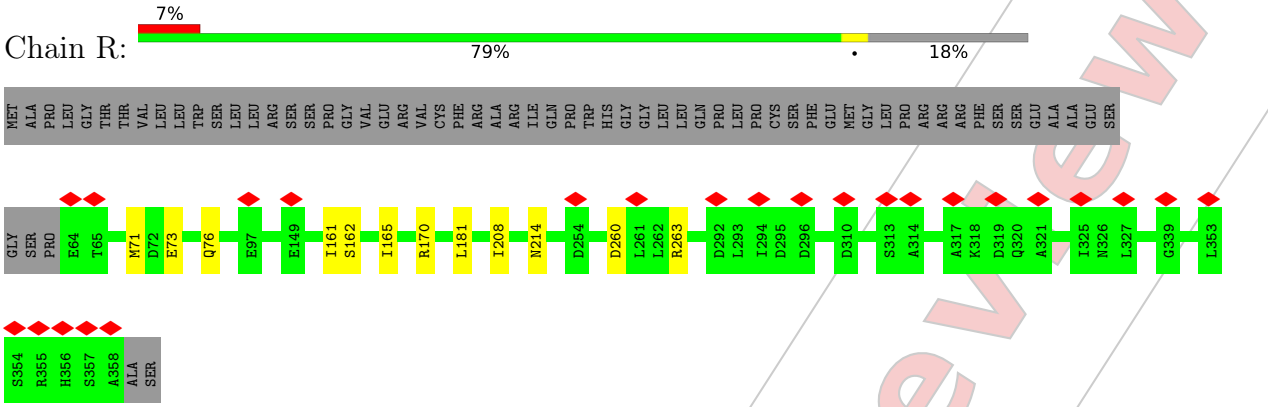
• Molecule 15: Small ribosomal subunit protein bS21m

Chain Q:



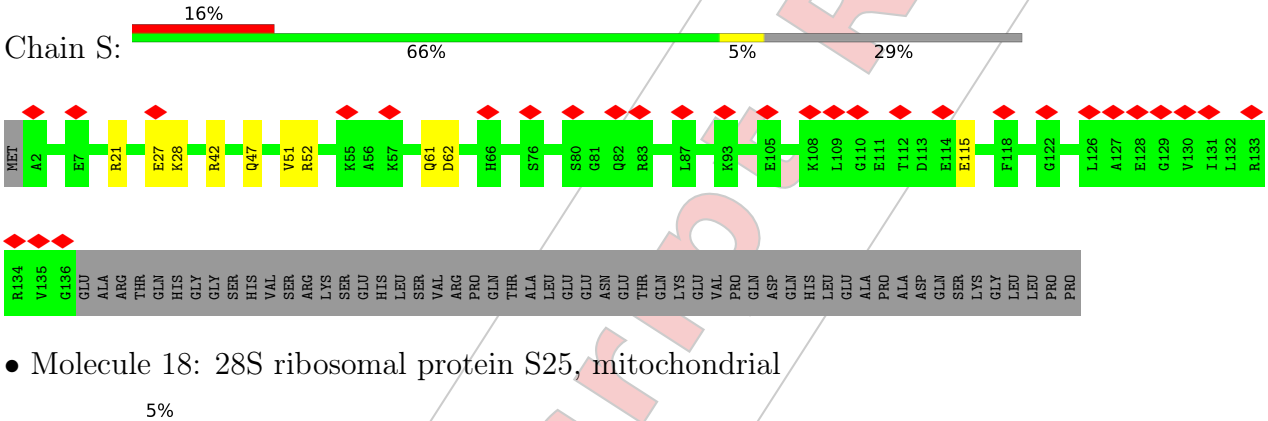
• Molecule 16: 28S ribosomal protein S22, mitochondrial

Chain R:



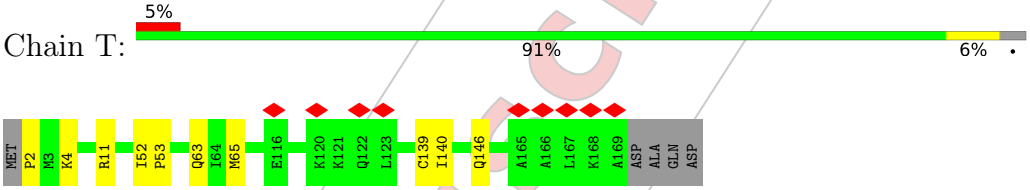
• Molecule 17: 28S ribosomal protein S23, mitochondrial

Chain S:



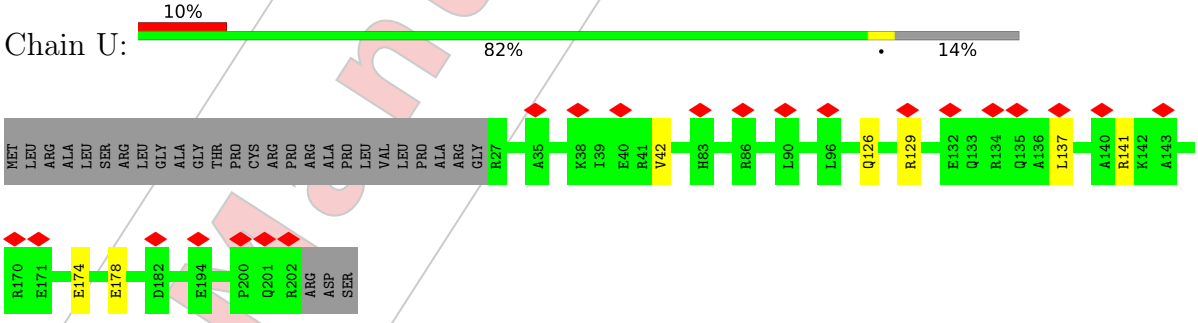
• Molecule 18: 28S ribosomal protein S25, mitochondrial

Chain T:



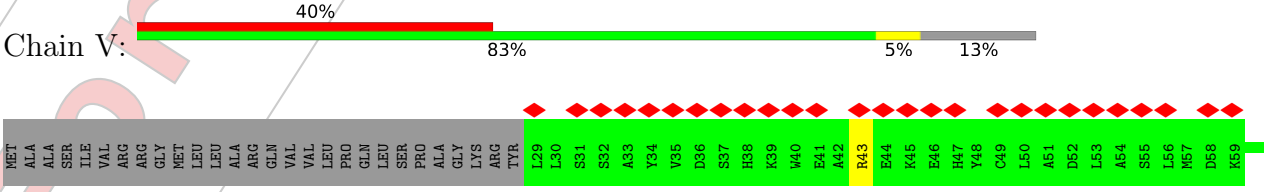
• Molecule 19: 28S ribosomal protein S26, mitochondrial

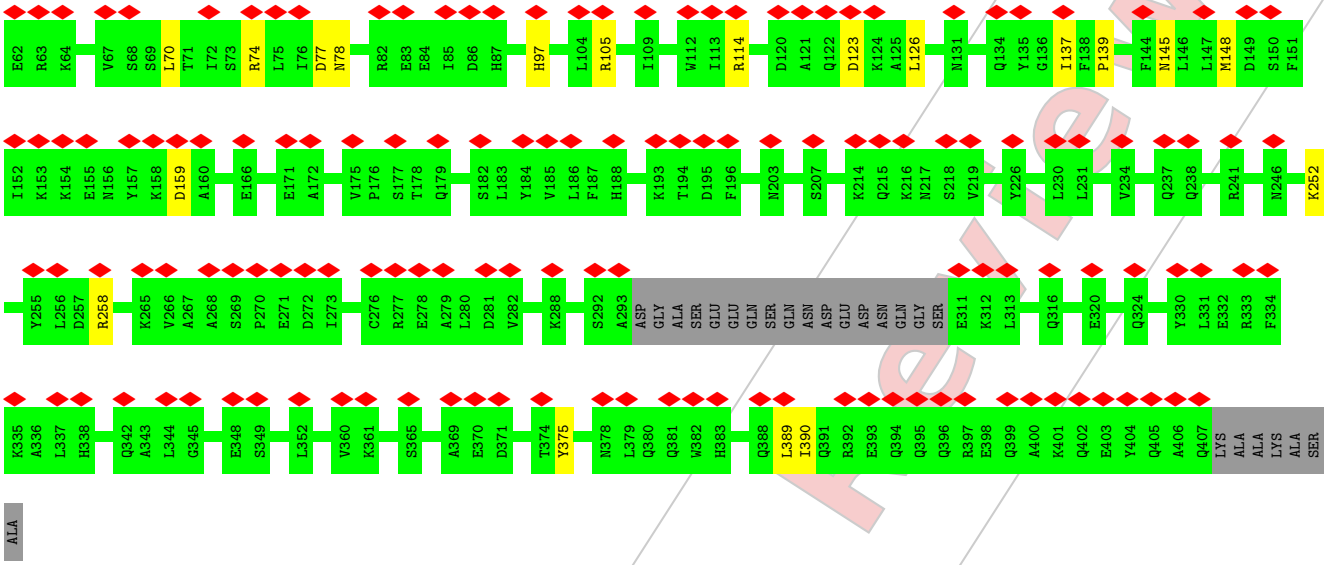
Chain U:



• Molecule 20: 28S ribosomal protein S27, mitochondrial

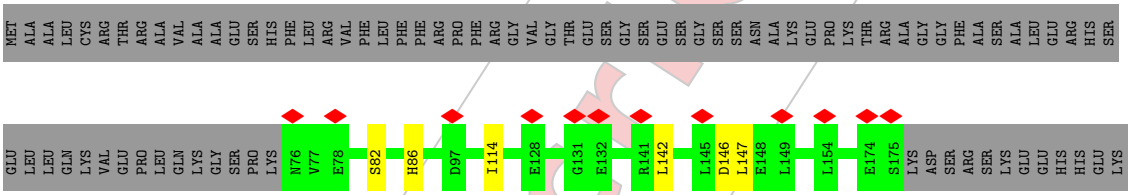
Chain V:





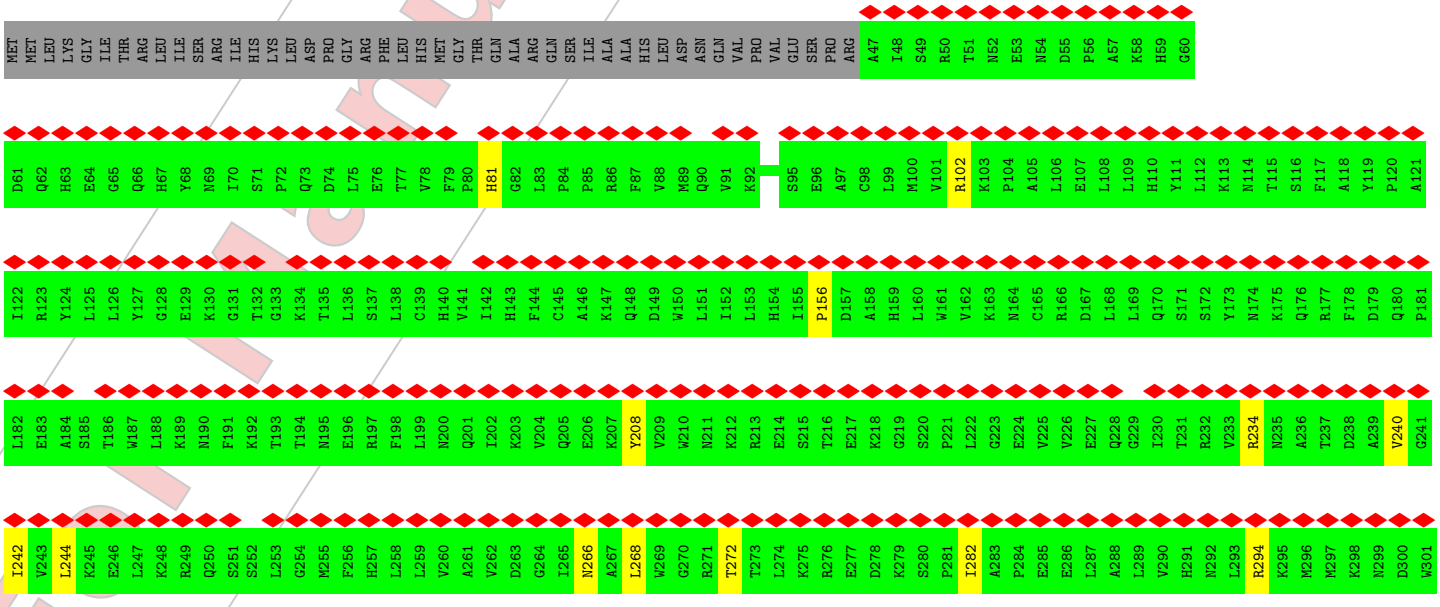
• Molecule 21: 28S ribosomal protein S28, mitochondrial

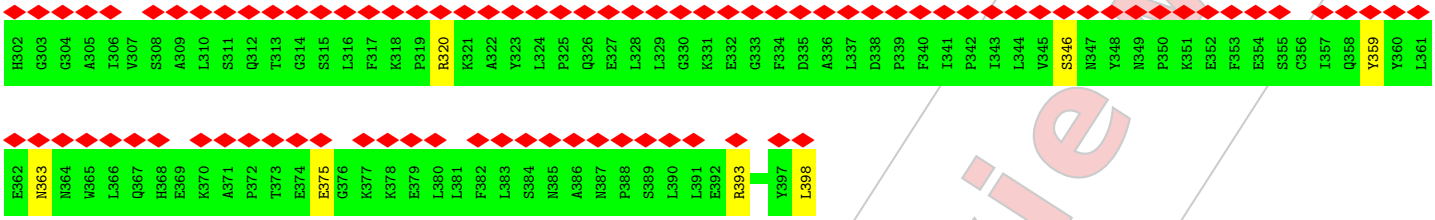
Chain W:



• Molecule 22: 28S ribosomal protein S29, mitochondrial

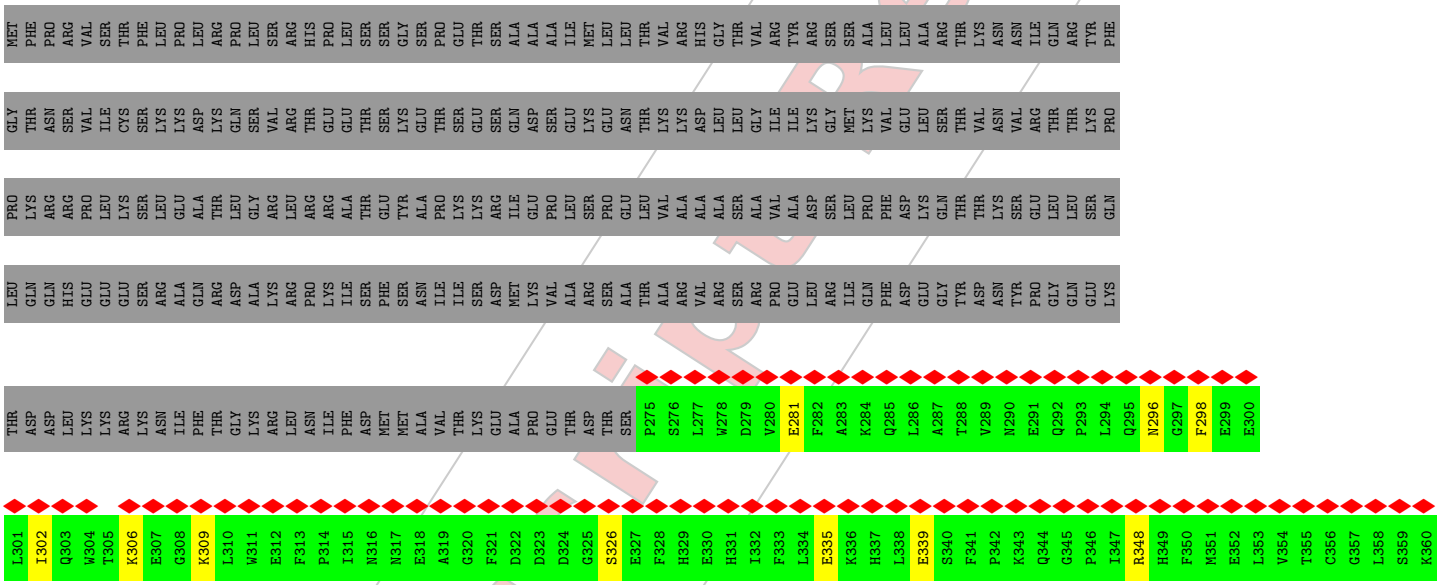
Chain X:





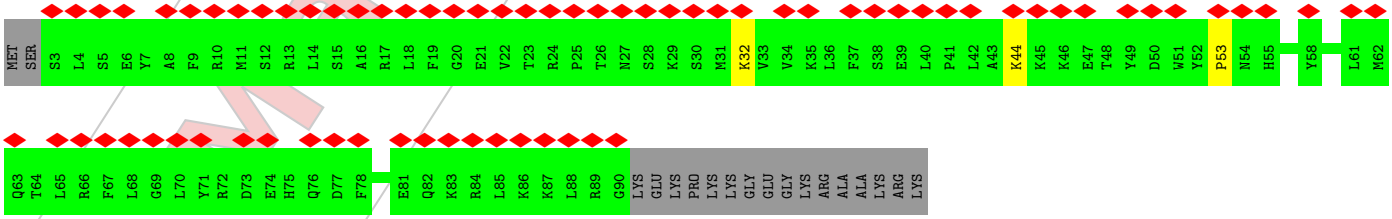
• Molecule 23: 28S ribosomal protein S31, mitochondrial

Chain Y:



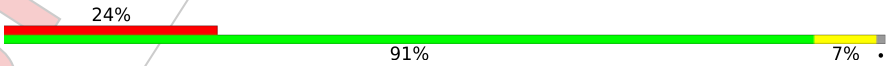
• Molecule 24: 28S ribosomal protein S33, mitochondrial

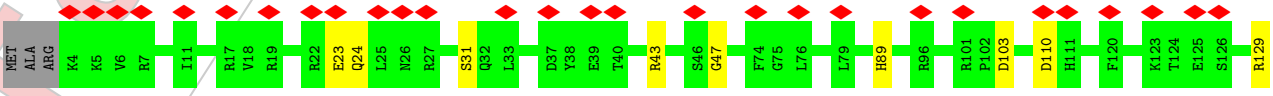
Chain Z:

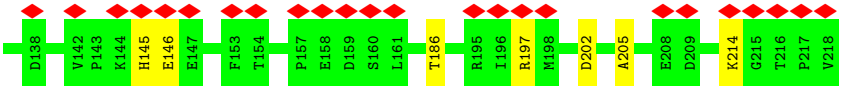


• Molecule 25: 28S ribosomal protein S34, mitochondrial

Chain 0:

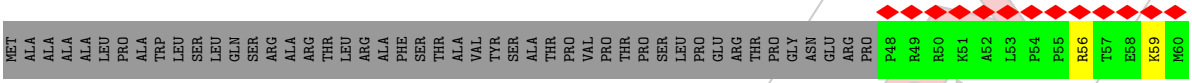


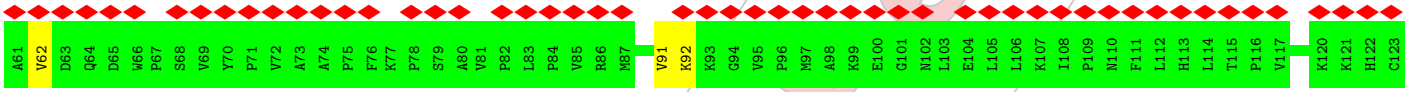


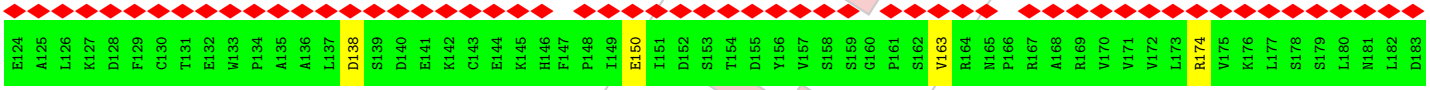


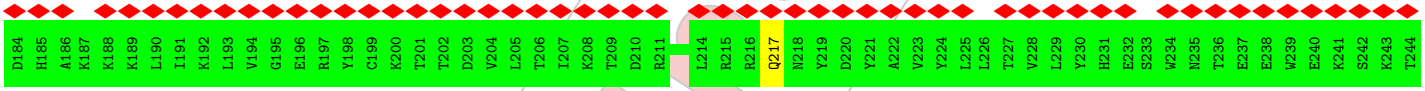
• Molecule 26: 28S ribosomal protein S35, mitochondrial

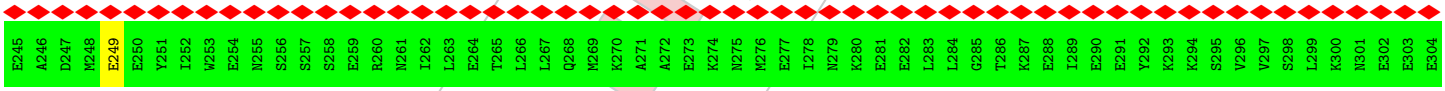
Chain 1:

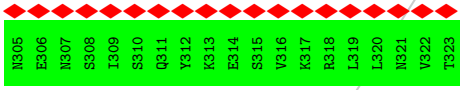






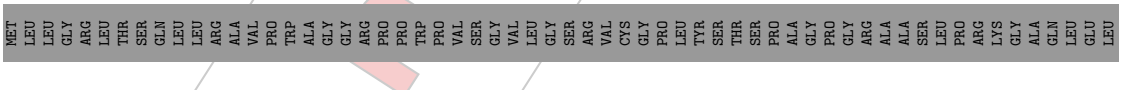


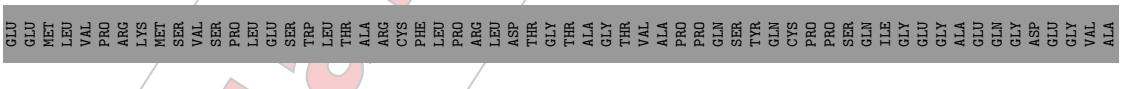


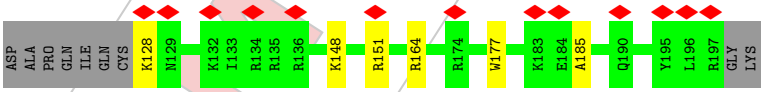


• Molecule 27: Aurora kinase A-interacting protein

Chain 3:

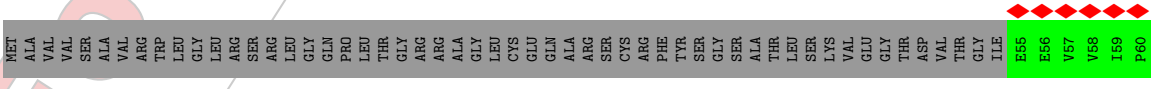


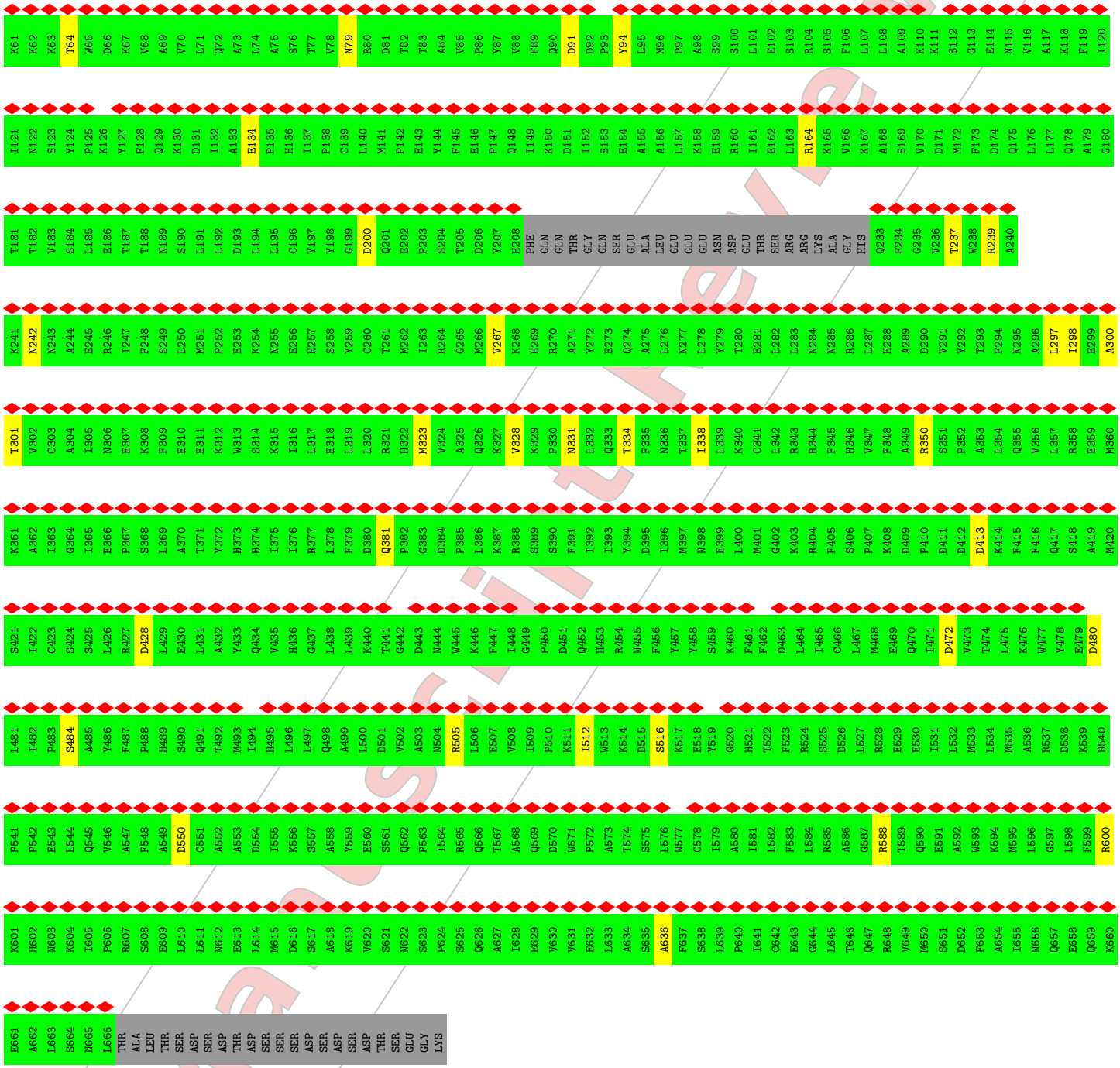




• Molecule 28: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

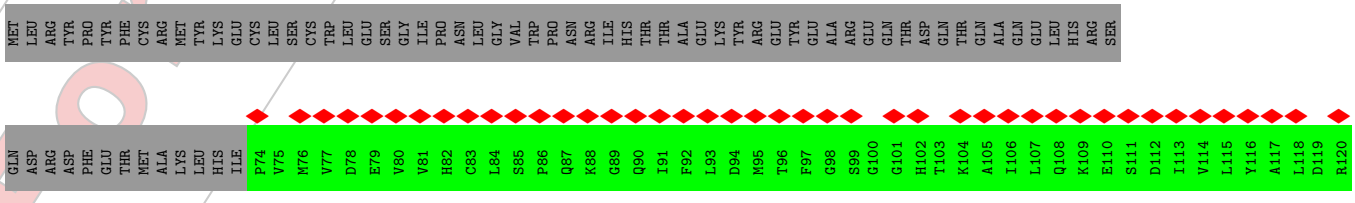
Chain 4:





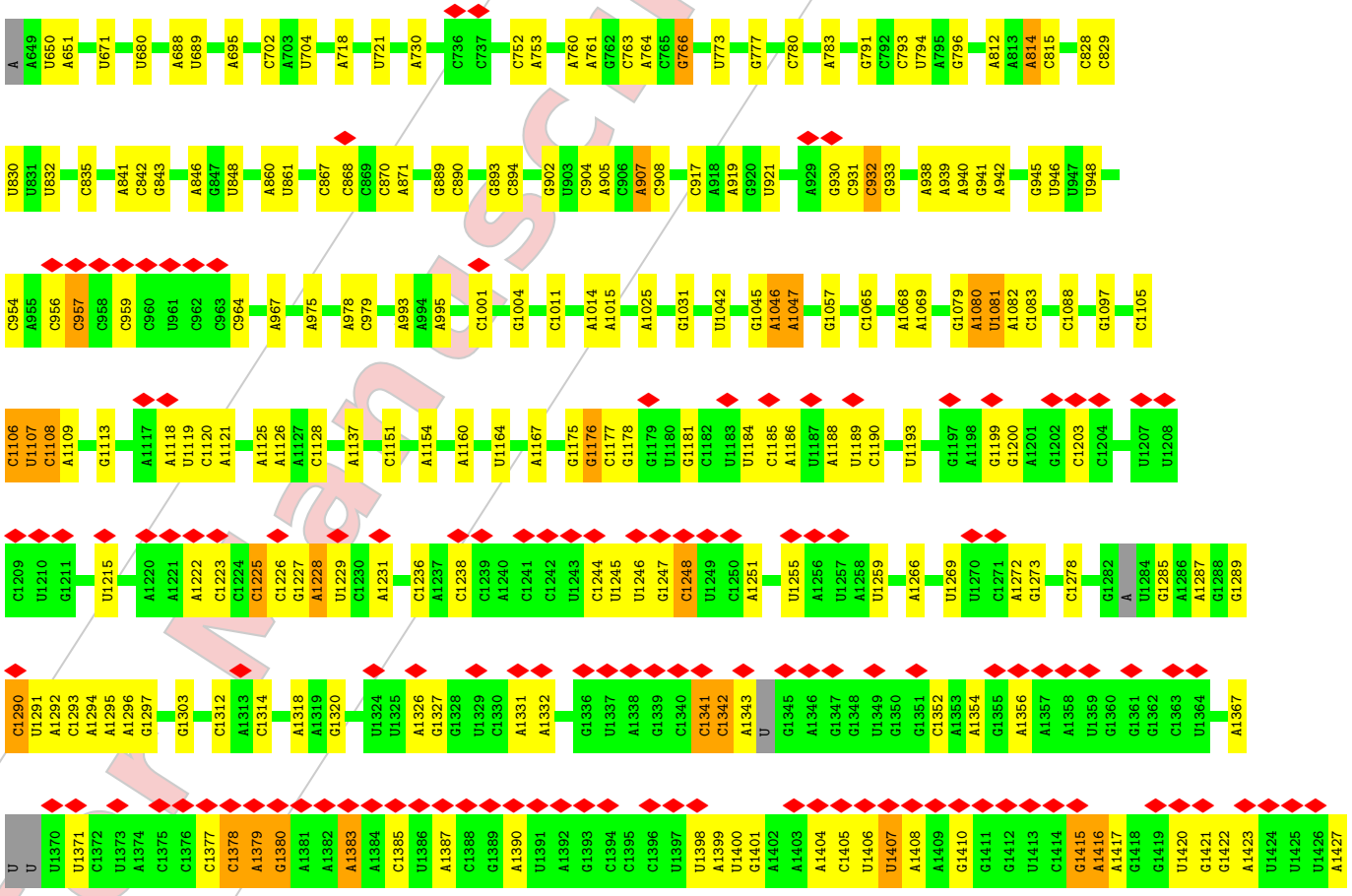
• Molecule 29: 12S rRNA N4-methylcytidine (m4C) methyltransferase

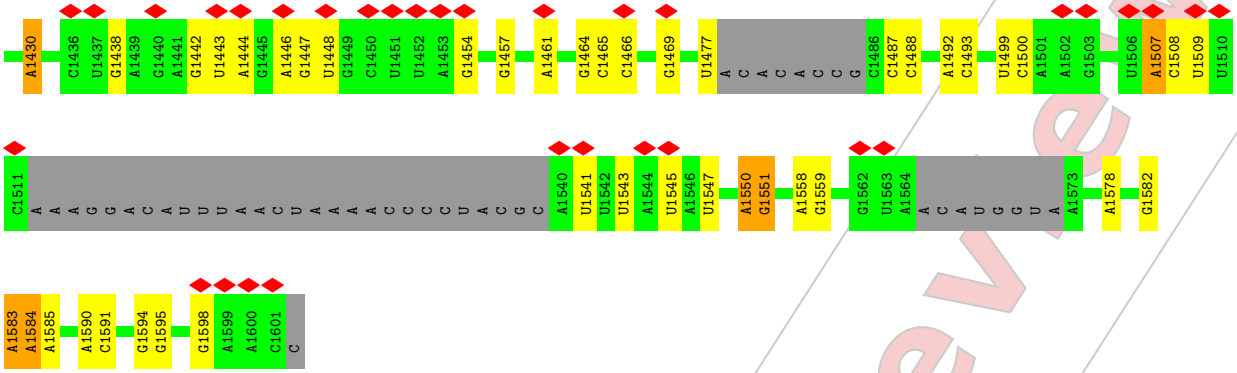
Chain b:



• Molecule 30: 12S mitochondrial rRNA

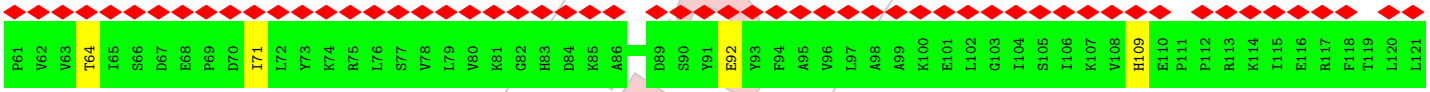
Chain A:

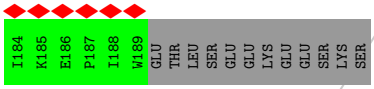




• Molecule 31: 28S ribosomal protein S10, mitochondrial

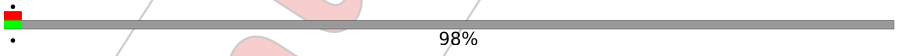
Chain H:

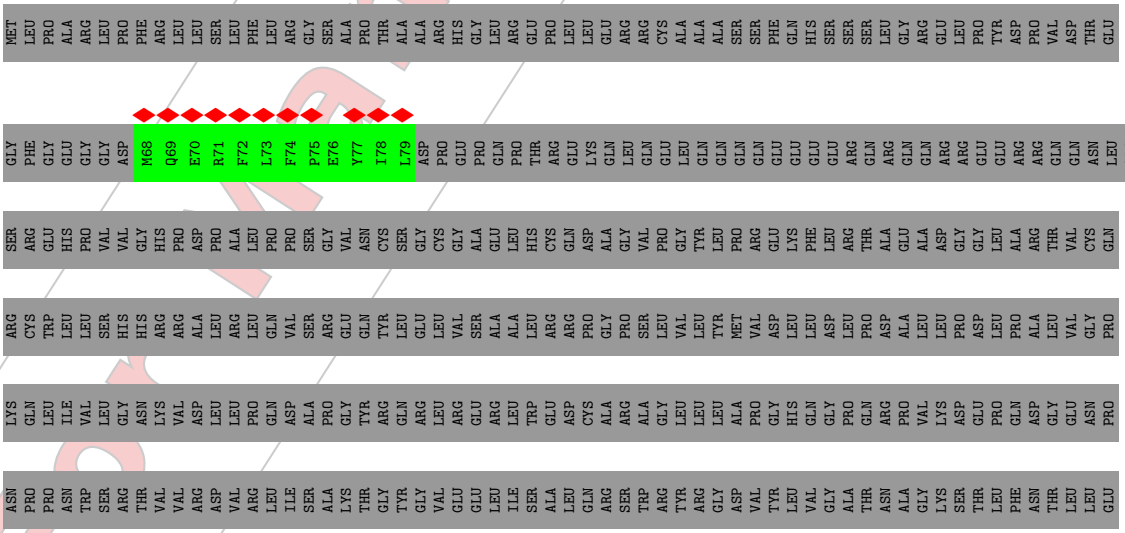


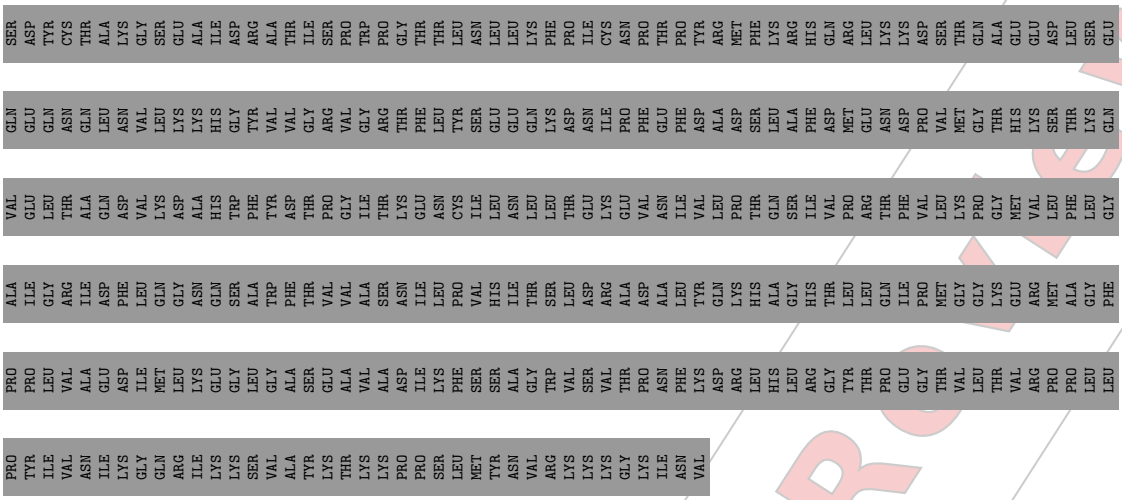


• Molecule 32: Nitric oxide-associated protein 1

Chain 9:







• Molecule 33: Putative ribosome-binding factor A, mitochondrial

Chain a:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10555	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.011	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SPM, MA6, 5MC, ACE, ATP, FES, GDP, 5F0, NAD, 5MU, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.25	0/1871	0.49	0/2531
2	C	0.24	0/1113	0.47	0/1505
3	D	0.25	0/2620	0.52	0/3511
4	E	0.33	0/926	0.58	0/1252
5	F	0.24	0/1723	0.46	0/2313
6	G	0.25	0/2631	0.49	0/3527
7	I	0.28	0/1030	0.53	1/1386 (0.1%)
8	J	0.26	0/855	0.55	0/1148
9	K	0.22	0/880	0.58	0/1182
10	L	0.24	0/1477	0.48	0/1974
11	M	0.27	0/963	0.56	0/1295
12	N	0.25	0/886	0.49	0/1199
13	O	0.25	0/1655	0.49	0/2254
14	P	0.25	0/798	0.45	0/1070
15	Q	0.31	0/754	0.59	0/1003
16	R	0.27	0/2456	0.47	0/3317
17	S	0.25	0/1138	0.52	0/1533
18	T	0.26	0/1402	0.47	0/1883
19	U	0.23	0/1510	0.55	0/2025
20	V	0.24	0/3030	0.43	0/4093
21	W	0.25	0/801	0.52	0/1079
22	X	0.24	0/2921	0.44	0/3954
23	Y	0.25	0/1054	0.39	0/1421
24	Z	0.32	0/762	0.53	0/1019
25	0	0.23	0/1834	0.54	0/2484
26	1	0.27	0/2285	0.46	0/3090
27	3	0.23	0/636	0.58	0/839
28	4	0.24	0/4877	0.44	0/6598
29	b	0.25	0/2353	0.49	0/3171
30	A	0.19	0/21395	0.67	0/33296
31	H	0.23	0/1170	0.47	0/1587
32	9	0.27	0/114	0.52	0/152

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	a	0.39	0/1267	0.57	0/1705
All	All	0.24	0/71187	0.56	1/100396 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	I	0	5
15	Q	0	1
33	a	0	2
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	185	GLY	O-C-N	-6.10	112.95	122.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	I	184	5F0	Peptide,Mainchain
7	I	185	GLY	Mainchain
7	I	187	ARG	Sidechain
7	I	189	ARG	Sidechain
15	Q	42	ARG	Sidechain
33	a	137	ARG	Sidechain
33	a	174	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1828	1815	1815	5	0
2	C	1083	1088	1088	7	0
3	D	2570	2609	2609	13	0
4	E	910	930	929	4	0
5	F	1685	1736	1736	17	0
6	G	2576	2560	2560	9	0
7	I	1020	1060	1053	7	0
8	J	839	887	887	9	0
9	K	862	885	885	4	0
10	L	1453	1540	1540	3	0
11	M	942	966	966	6	0
12	N	868	928	928	4	0
13	O	1599	1565	1565	10	0
14	P	781	807	808	2	0
15	Q	744	758	758	9	0
16	R	2409	2428	2428	9	0
17	S	1111	1115	1115	7	0
18	T	1371	1396	1396	8	0
19	U	1488	1499	1499	4	0
20	V	2969	2961	2961	14	0
21	W	789	802	802	3	0
22	X	2849	2844	2844	13	0
23	Y	1023	970	970	7	0
24	Z	745	750	750	3	0
25	0	1787	1796	1796	10	0
26	1	2238	2269	2269	10	0
27	3	625	699	699	4	0
28	4	4768	4766	4766	26	0
29	b	2313	2366	2366	0	0
30	A	19223	9762	9779	65	0
31	H	1144	1173	1172	9	0
32	9	111	108	108	0	0
33	a	1252	1261	1261	0	0
34	M	4	0	0	0	0
34	P	4	0	0	0	0
35	O	1	0	0	0	0
36	X	31	12	12	0	0
37	X	28	10	12	0	0
38	A	31	0	0	0	0
39	A	44	26	26	0	0
40	A	14	0	26	3	0
41	0	1	0	0	0	0
41	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	G	1	0	0	0	0
41	T	1	0	0	0	0
41	b	1	0	0	0	0
All	All	68137	59147	59184	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:156:ILE:HD12	5:F:230:ALA:HB3	1.57	0.83
5:F:156:ILE:HD12	5:F:230:ALA:CB	2.16	0.75
6:G:382:PRO:O	31:H:131:ARG:NH1	2.20	0.75
5:F:156:ILE:CD1	5:F:230:ALA:HB3	2.17	0.74
8:J:31:ALA:O	18:T:4:LYS:NZ	2.19	0.73
20:V:43:ARG:NH2	20:V:77:ASP:OD2	2.24	0.71
17:S:42:ARG:NH2	17:S:47:GLN:OE1	2.25	0.69
12:N:24:LYS:NZ	12:N:54:ALA:O	2.25	0.68
6:G:196:GLY:O	6:G:248:VAL:N	2.27	0.68
30:A:1415:G:O2'	30:A:1416:A:OP2	2.08	0.68
31:H:71:ILE:O	31:H:150:GLY:N	2.28	0.67
10:L:83:GLU:N	10:L:83:GLU:OE1	2.29	0.65
6:G:318:HIS:NE2	22:X:375:GLU:OE2	2.31	0.64
13:O:73:VAL:O	13:O:109:ARG:NH2	2.31	0.63
1:B:197:HIS:NE2	1:B:240:ASP:O	2.31	0.63
30:A:1550:A:O2'	30:A:1551:G:OP1	2.15	0.63
12:N:75:LYS:NZ	30:A:766:G:OP2	2.32	0.62
9:K:46:GLU:N	9:K:46:GLU:OE1	2.33	0.62
7:I:89:LYS:NZ	30:A:1004:G:OP1	2.32	0.62
19:U:126:GLN:OE1	19:U:129:ARG:NH2	2.32	0.62
20:V:97:HIS:O	20:V:97:HIS:ND1	2.33	0.62
8:J:98:GLU:N	8:J:98:GLU:OE1	2.33	0.61
30:A:1401:G:N1	30:A:1404:A:OP2	2.33	0.61
30:A:945:G:N7	40:A:1733:SPM:H62	2.16	0.60
28:4:64:THR:HG1	31:H:64:THR:HG1	1.49	0.60
28:4:331:ASN:OD1	28:4:334:THR:OG1	2.09	0.60
1:B:243:PRO:O	1:B:247:HIS:ND1	2.34	0.60
30:A:1225:C:N4	30:A:1448:U:O2'	2.34	0.59
5:F:119:LYS:NZ	22:X:398:LEU:OXT	2.35	0.59
30:A:1407:U:HO2'	30:A:1446:A:HO2'	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:117:ASP:OD2	30:A:894:C:N4	2.36	0.57
28:4:237:THR:O	28:4:237:THR:HG22	2.04	0.57
3:D:95:ALA:HB1	3:D:98:LEU:HD13	1.86	0.57
10:L:120:GLU:OE1	10:L:120:GLU:N	2.33	0.56
28:4:239:ARG:O	28:4:242:ASN:ND2	2.38	0.56
13:O:211:ARG:O	13:O:214:SER:OG	2.18	0.56
23:Y:281:GLU:OE2	28:4:164:ARG:NH2	2.39	0.56
9:K:88:ARG:NH2	30:A:1231:A:OP1	2.38	0.56
7:I:188:PRO:HB2	15:Q:45:TYR:N	2.22	0.55
3:D:137:TYR:O	3:D:159:GLN:NE2	2.36	0.55
30:A:942:A:N6	30:A:1047:A:OP2	2.34	0.55
26:1:249:GLU:OE1	26:1:249:GLU:N	2.32	0.55
28:4:297:LEU:O	28:4:301:THR:OG1	2.19	0.55
30:A:1487:C:C5	30:A:1488:5MC:HM52	2.42	0.55
30:A:843:G:N2	30:A:846:A:OP2	2.38	0.55
3:D:285:TYR:OH	3:D:372:GLU:OE2	2.21	0.54
30:A:1080:A:H2'	30:A:1081:U:H5'	1.89	0.54
8:J:39:LEU:O	8:J:43:LYS:NZ	2.40	0.54
28:4:267:VAL:HG22	28:4:300:ALA:HB2	1.90	0.54
28:4:550:ASP:OD1	28:4:588:ARG:NH2	2.39	0.54
5:F:79:ALA:O	6:G:312:GLN:NE2	2.41	0.54
28:4:200:ASP:O	28:4:239:ARG:NH2	2.40	0.54
4:E:107:GLY:HA2	14:P:64:LYS:HG2	1.90	0.54
22:X:393:ARG:NE	30:A:1378:C:O2	2.41	0.54
2:C:126:GLN:OE1	2:C:126:GLN:N	2.39	0.53
24:Z:32:LYS:NZ	30:A:1400:U:OP1	2.35	0.53
30:A:1379:A:O2'	30:A:1380:G:OP1	2.18	0.53
20:V:70:LEU:HD22	20:V:389:LEU:HB3	1.90	0.53
25:0:31:SER:OG	25:0:103:ASP:OD2	2.24	0.53
8:J:78:ARG:NH2	8:J:117:ASP:OD2	2.42	0.53
17:S:27:GLU:OE1	17:S:28:LYS:N	2.42	0.53
22:X:359:TYR:O	22:X:363:ASN:ND2	2.42	0.53
12:N:53:ASP:OD2	12:N:57:GLN:N	2.42	0.52
13:O:210:GLU:OE2	13:O:217:ARG:NH2	2.42	0.52
22:X:268:LEU:O	22:X:294:ARG:NH2	2.38	0.52
19:U:42:VAL:HG13	19:U:42:VAL:O	2.11	0.51
28:4:297:LEU:O	28:4:301:THR:N	2.43	0.51
30:A:905:A:O2'	30:A:907:A:OP1	2.28	0.51
5:F:48:LYS:NZ	22:X:375:GLU:OE2	2.43	0.51
5:F:168:TYR:O	5:F:170:VAL:HG13	2.09	0.51
30:A:1379:A:HO2'	30:A:1380:G:P	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:114:ARG:O	11:M:118:VAL:HG23	2.11	0.51
6:G:388:ARG:NH1	30:A:1430:A:OP1	2.41	0.51
20:V:105:ARG:NH1	20:V:389:LEU:HD11	2.26	0.51
8:J:74:ASN:ND2	8:J:117:ASP:OD1	2.42	0.50
25:0:89:HIS:NE2	25:0:202:ASP:OD2	2.42	0.50
3:D:91:THR:HG23	3:D:92:LYS:N	2.26	0.50
5:F:156:ILE:HD11	5:F:227:HIS:HA	1.94	0.50
5:F:198:ARG:NH2	30:A:1383:A:N7	2.59	0.50
13:O:183:ALA:HB1	16:R:170:ARG:O	2.12	0.50
17:S:61:GLN:N	17:S:61:GLN:OE1	2.44	0.49
3:D:281:TYR:OH	17:S:21:ARG:NH1	2.45	0.49
30:A:1106:C:O2'	30:A:1108:C:OP2	2.31	0.49
30:A:1464:G:H21	30:A:1466:C:H41	1.58	0.49
30:A:1583:MA6:H93	30:A:1584:MA6:C2	2.43	0.49
11:M:67:ALA:HB1	16:R:161:ILE:HD13	1.95	0.49
30:A:1272:A:N6	30:A:1320:G:O2'	2.46	0.49
1:B:251:ARG:NH2	1:B:254:GLN:OE1	2.39	0.49
18:T:139:CYS:SG	18:T:140:ILE:N	2.86	0.48
30:A:1415:G:HO2'	30:A:1416:A:P	2.32	0.48
13:O:233:GLU:N	13:O:233:GLU:OE1	2.46	0.48
30:A:1415:G:O2'	30:A:1416:A:P	2.71	0.48
7:I:154:LEU:HD12	15:Q:39:ILE:HG21	1.94	0.48
23:Y:339:GLU:OE1	23:Y:339:GLU:N	2.38	0.48
5:F:50:TYR:O	5:F:66:ARG:NH2	2.46	0.48
26:1:150:GLU:OE1	26:1:174:ARG:NH2	2.46	0.48
30:A:917:C:O2'	30:A:921:U:OP1	2.32	0.48
30:A:1289:G:H5'	30:A:1290:C:OP1	2.14	0.48
28:4:472:ASP:OD1	28:4:505:ARG:NH1	2.46	0.48
30:A:1582:G:H3'	30:A:1583:MA6:H8	1.94	0.48
11:M:67:ALA:HB1	16:R:161:ILE:HG21	1.96	0.48
2:C:36:LYS:N	30:A:1266:A:OP2	2.47	0.47
9:K:28:HIS:N	30:A:1248:C:O2	2.47	0.47
3:D:375:GLU:OE1	3:D:375:GLU:N	2.40	0.47
28:4:267:VAL:HG22	28:4:300:ALA:CB	2.43	0.47
2:C:49:LYS:N	2:C:167:LEU:OXT	2.42	0.47
31:H:109:HIS:NE2	31:H:144:GLU:OE2	2.47	0.47
18:T:11:ARG:NH2	30:A:932:C:N3	2.61	0.47
23:Y:296:ASN:OD1	23:Y:298:PHE:N	2.46	0.47
4:E:115:GLU:O	4:E:116:LYS:C	2.52	0.47
22:X:272:THR:OG1	22:X:282:ILE:O	2.31	0.47
23:Y:326:SER:O	26:1:217:GLN:NE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:74:ARG:O	20:V:78:ASN:ND2	2.48	0.46
28:4:600:ARG:NH2	28:4:636:ALA:O	2.48	0.46
30:A:702:C:O2'	30:A:842:C:O2	2.31	0.46
22:X:208:TYR:CE2	22:X:242:ILE:HG23	2.50	0.46
30:A:946:U:OP2	40:A:1733:SPM:N10	2.49	0.46
30:A:1379:A:O2'	30:A:1380:G:P	2.73	0.46
25:0:129:ARG:NH1	25:0:205:ALA:O	2.47	0.46
15:Q:76:MET:O	15:Q:76:MET:SD	2.73	0.46
16:R:71:MET:SD	16:R:76:GLN:NE2	2.89	0.46
30:A:1550:A:O2'	30:A:1551:G:P	2.74	0.46
8:J:122:LYS:NZ	30:A:1164:U:OP1	2.43	0.46
25:0:186:THR:O	25:0:186:THR:HG22	2.15	0.46
20:V:70:LEU:HD21	20:V:390:ILE:HG13	1.98	0.45
25:0:23:GLU:OE1	25:0:24:GLN:NE2	2.48	0.45
25:0:43:ARG:O	25:0:47:GLY:N	2.37	0.45
30:A:760:A:N1	30:A:780:C:O2'	2.46	0.45
30:A:867:C:O2	30:A:870:C:N4	2.43	0.45
4:E:3:ARG:NH2	4:E:67:ASP:OD2	2.46	0.45
13:O:63:GLU:OE1	13:O:112:LYS:NZ	2.49	0.45
12:N:6:SER:OG	12:N:69:LEU:O	2.32	0.45
28:4:428:ASP:OD1	28:4:428:ASP:N	2.49	0.45
30:A:948:U:OP2	30:A:1045:G:N1	2.42	0.45
5:F:170:VAL:O	5:F:170:VAL:HG23	2.17	0.45
15:Q:37:GLU:HA	15:Q:40:LYS:HE2	1.99	0.45
11:M:55:ASP:OD2	18:T:146:GLN:NE2	2.49	0.45
30:A:1550:A:HO2'	30:A:1551:G:P	2.37	0.45
18:T:52:ILE:HG12	18:T:53:PRO:HD3	1.99	0.45
20:V:114:ARG:NH2	20:V:375:TYR:OH	2.47	0.45
11:M:39:ASN:ND2	30:A:841:A:OP1	2.38	0.45
7:I:179:THR:O	7:I:181:ILE:HD12	2.17	0.45
20:V:137:ILE:HG22	20:V:139:PRO:HD3	1.97	0.45
28:4:79:ASN:HB2	31:H:54:VAL:HG11	1.98	0.45
30:A:1487:C:C4	30:A:1488:5MC:HM52	2.51	0.45
22:X:320:ARG:NE	30:A:1377:C:OP1	2.49	0.45
19:U:137:LEU:O	19:U:141:ARG:N	2.42	0.44
28:4:350:ARG:NH2	28:4:381:GLN:OE1	2.41	0.44
3:D:184:LYS:O	3:D:185:MET:C	2.56	0.44
7:I:133:ILE:HD13	7:I:164:GLY:O	2.18	0.44
15:Q:15:GLN:N	15:Q:18:ASN:OD1	2.49	0.44
30:A:702:C:OP1	30:A:848:U:O2'	2.34	0.44
2:C:52:THR:HG22	2:C:53:TYR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:123:ASP:OD1	20:V:123:ASP:N	2.50	0.44
26:1:138:ASP:OD1	26:1:138:ASP:N	2.46	0.44
1:B:180:ARG:NH1	1:B:185:PRO:O	2.51	0.44
30:A:1014:A:O2'	30:A:1031:G:O4'	2.35	0.44
7:I:159:LEU:HD12	7:I:160:SER:N	2.32	0.44
8:J:103:GLN:N	8:J:103:GLN:OE1	2.51	0.44
13:O:54:GLU:O	13:O:54:GLU:HG3	2.17	0.44
11:M:94:ALA:O	16:R:181:LEU:HD21	2.18	0.44
30:A:1499:U:H2'	30:A:1500:C:O4'	2.18	0.44
16:R:162:SER:HB3	16:R:165:ILE:HD12	1.99	0.43
20:V:97:HIS:O	20:V:97:HIS:CG	2.71	0.43
30:A:752:C:O2'	30:A:793:C:N4	2.50	0.43
13:O:91:ARG:NH1	13:O:103:ASN:O	2.51	0.43
24:Z:44:LYS:O	24:Z:44:LYS:HG2	2.18	0.43
26:1:163:VAL:HG22	26:1:163:VAL:O	2.18	0.43
20:V:126:LEU:HD22	20:V:159:ASP:OD1	2.18	0.43
28:4:512:ILE:O	28:4:516:SER:N	2.47	0.43
16:R:260:ASP:OD1	16:R:263:ARG:NH2	2.50	0.43
19:U:174:GLU:O	19:U:178:GLU:OE1	2.36	0.43
20:V:70:LEU:HD22	20:V:389:LEU:CB	2.47	0.43
20:V:145:ASN:O	20:V:148:MET:HG3	2.19	0.43
30:A:1079:G:H2'	30:A:1080:A:O4'	2.17	0.43
27:3:148:LYS:O	27:3:151:ARG:NH1	2.51	0.43
23:Y:302:ILE:HG22	23:Y:306:LYS:NZ	2.33	0.43
17:S:62:ASP:N	17:S:62:ASP:OD1	2.49	0.43
31:H:54:VAL:HG13	31:H:55:PRO:HD2	2.01	0.43
3:D:233:ALA:HB2	30:A:1176:G:P	2.58	0.43
10:L:223:ARG:NE	10:L:223:ARG:HA	2.33	0.43
15:Q:26:LEU:O	15:Q:29:ILE:HG22	2.18	0.42
27:3:164:ARG:NH1	30:A:1543:U:OP1	2.52	0.42
26:1:56:ARG:NH2	28:4:91:ASP:OD2	2.52	0.42
27:3:128:LYS:NZ	30:A:1107:U:O4	2.40	0.42
3:D:310:LYS:HA	3:D:331:ASP:OD2	2.19	0.42
15:Q:20:GLU:OE1	15:Q:20:GLU:N	2.52	0.42
16:R:73:GLU:OE1	16:R:73:GLU:N	2.47	0.42
30:A:1227:G:O5'	30:A:1228:A:H2'	2.19	0.42
4:E:18:THR:O	4:E:21:THR:OG1	2.37	0.42
25:0:110:ASP:OD1	25:0:110:ASP:N	2.44	0.42
9:K:31:ASP:N	9:K:31:ASP:OD1	2.50	0.42
18:T:140:ILE:HG12	18:T:140:ILE:O	2.19	0.42
30:A:1046:A:H3'	40:A:1733:SPM:H22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:59:THR:O	5:F:63:LYS:N	2.53	0.42
26:1:163:VAL:HG12	28:4:134:GLU:O	2.20	0.42
31:H:92:GLU:OE1	31:H:141:ARG:NH1	2.45	0.42
6:G:86:ARG:HB2	26:1:62:VAL:HG11	2.01	0.42
17:S:115:GLU:OE1	17:S:115:GLU:N	2.46	0.42
30:A:956:C:H3'	30:A:957:C:H5"	2.02	0.42
6:G:289:GLY:N	6:G:325:LYS:O	2.48	0.42
7:I:194:LEU:HB2	30:A:1083:C:O2'	2.20	0.42
25:0:197:ARG:NE	25:0:197:ARG:HA	2.35	0.42
25:0:214:LYS:H	25:0:214:LYS:HD2	1.84	0.42
3:D:411:VAL:HG21	18:T:2:PRO:HG2	2.02	0.42
5:F:163:LYS:HG2	5:F:164:GLY:H	1.85	0.41
16:R:208:ILE:O	16:R:214:ASN:ND2	2.52	0.41
22:X:81:HIS:CD2	22:X:156:PRO:HB3	2.55	0.41
1:B:72:PHE:O	1:B:263:LYS:NZ	2.54	0.41
22:X:240:VAL:O	22:X:244:LEU:HG	2.20	0.41
26:1:56:ARG:HB2	26:1:59:LYS:HD3	2.01	0.41
31:H:52:VAL:HG12	31:H:52:VAL:O	2.20	0.41
5:F:136:THR:HG22	5:F:136:THR:O	2.20	0.41
3:D:217:ASP:OD1	3:D:217:ASP:N	2.53	0.41
21:W:114:ILE:CG2	21:W:142:LEU:HD11	2.51	0.41
22:X:266:ASN:OD1	22:X:266:ASN:N	2.53	0.41
26:1:91:VAL:HG12	26:1:92:LYS:N	2.36	0.41
28:4:323:MET:HB2	28:4:328:VAL:HB	2.03	0.41
30:A:1199:G:O2'	30:A:1423:A:N6	2.54	0.41
3:D:282:ILE:HG23	3:D:353:LEU:HB3	2.01	0.41
30:A:1057:G:H4'	30:A:1578:A:H4'	2.02	0.41
30:A:1106:C:O2'	30:A:1125:A:N6	2.53	0.41
21:W:82:SER:O	21:W:86:HIS:ND1	2.53	0.41
30:A:1341:C:H5"	30:A:1342:C:H2'	2.03	0.41
28:4:298:ILE:HG21	28:4:338:ILE:HG12	2.03	0.41
28:4:480:ASP:O	28:4:484:SER:OG	2.38	0.41
30:A:1584:MA6:H8	30:A:1584:MA6:OP2	2.21	0.41
2:C:115:ASN:ND2	23:Y:309:LYS:O	2.54	0.41
2:C:125:ARG:HD2	28:4:94:TYR:CD1	2.56	0.41
18:T:63:GLN:NE2	18:T:65:MET:SD	2.94	0.41
23:Y:335:GLU:OE2	23:Y:348:ARG:NH2	2.54	0.41
28:4:200:ASP:OD2	28:4:242:ASN:ND2	2.53	0.41
13:O:120:VAL:O	13:O:124:GLU:OE1	2.39	0.41
14:P:140:TYR:CD1	15:Q:29:ILE:HD12	2.56	0.41
3:D:408:TRP:NE1	3:D:412:LYS:HE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:37:GLU:HG3	15:Q:40:LYS:HE2	2.03	0.41
30:A:1507:A:H2'	30:A:1508:C:C6	2.56	0.41
5:F:71:THR:O	6:G:253:LYS:NZ	2.54	0.40
5:F:234:ARG:O	5:F:235:ALA:HB3	2.21	0.40
13:O:156:LYS:O	13:O:160:HIS:ND1	2.48	0.40
20:V:252:LYS:O	20:V:258:ARG:NH2	2.55	0.40
27:3:177:TRP:CZ2	27:3:185:ALA:HB2	2.56	0.40
28:4:237:THR:O	28:4:237:THR:CG2	2.69	0.40
28:4:413:ASP:OD1	28:4:413:ASP:N	2.53	0.40
31:H:172:VAL:O	31:H:172:VAL:HG13	2.22	0.40
2:C:87:VAL:HG21	24:Z:53:PRO:CG	2.50	0.40
21:W:146:ASP:OD1	21:W:147:LEU:N	2.53	0.40
25:0:145:HIS:CE1	25:0:146:GLU:HG2	2.57	0.40
5:F:125:LYS:O	5:F:125:LYS:HG2	2.22	0.40
6:G:377:ARG:NE	30:A:1454:G:N7	2.70	0.40
8:J:53:GLU:HA	8:J:53:GLU:OE1	2.20	0.40
17:S:51:VAL:HG12	17:S:52:ARG:N	2.37	0.40
30:A:812:A:O2'	30:A:814:A:N1	2.50	0.40
22:X:102:ARG:NH2	22:X:346:SER:O	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	223/296 (75%)	216 (97%)	7 (3%)	0	100	100
2	C	130/167 (78%)	123 (95%)	7 (5%)	0	100	100
3	D	315/430 (73%)	303 (96%)	12 (4%)	0	100	100
4	E	113/125 (90%)	111 (98%)	2 (2%)	0	100	100
5	F	203/242 (84%)	198 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	309/396 (78%)	296 (96%)	13 (4%)	0	100	100
7	I	134/194 (69%)	130 (97%)	4 (3%)	0	100	100
8	J	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
9	K	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
10	L	172/257 (67%)	167 (97%)	5 (3%)	0	100	100
11	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
12	N	108/130 (83%)	103 (95%)	5 (5%)	0	100	100
13	O	192/258 (74%)	187 (97%)	5 (3%)	0	100	100
14	P	95/142 (67%)	92 (97%)	3 (3%)	0	100	100
15	Q	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
16	R	293/360 (81%)	284 (97%)	9 (3%)	0	100	100
17	S	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
18	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
19	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
20	V	358/414 (86%)	349 (98%)	9 (2%)	0	100	100
21	W	98/187 (52%)	93 (95%)	5 (5%)	0	100	100
22	X	350/398 (88%)	344 (98%)	6 (2%)	0	100	100
23	Y	119/395 (30%)	118 (99%)	1 (1%)	0	100	100
24	Z	86/106 (81%)	86 (100%)	0	0	100	100
25	0	213/218 (98%)	208 (98%)	5 (2%)	0	100	100
26	1	274/323 (85%)	262 (96%)	12 (4%)	0	100	100
27	3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
28	4	584/689 (85%)	573 (98%)	11 (2%)	0	100	100
29	b	290/407 (71%)	266 (92%)	24 (8%)	0	100	100
31	H	137/201 (68%)	134 (98%)	3 (2%)	0	100	100
32	9	10/698 (1%)	9 (90%)	1 (10%)	0	100	100
33	a	150/343 (44%)	142 (95%)	8 (5%)	0	100	100
All	All	5904/8633 (68%)	5724 (97%)	180 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	198/249 (80%)	198 (100%)	0	100	100
2	C	115/143 (80%)	115 (100%)	0	100	100
3	D	272/357 (76%)	272 (100%)	0	100	100
4	E	97/107 (91%)	97 (100%)	0	100	100
5	F	182/209 (87%)	182 (100%)	0	100	100
6	G	272/342 (80%)	272 (100%)	0	100	100
7	I	104/146 (71%)	103 (99%)	1 (1%)	73	81
8	J	93/118 (79%)	93 (100%)	0	100	100
9	K	91/113 (80%)	91 (100%)	0	100	100
10	L	158/226 (70%)	158 (100%)	0	100	100
11	M	97/113 (86%)	97 (100%)	0	100	100
12	N	96/115 (84%)	96 (100%)	0	100	100
13	O	175/230 (76%)	175 (100%)	0	100	100
14	P	88/123 (72%)	88 (100%)	0	100	100
15	Q	78/78 (100%)	78 (100%)	0	100	100
16	R	264/318 (83%)	264 (100%)	0	100	100
17	S	116/164 (71%)	116 (100%)	0	100	100
18	T	153/157 (98%)	153 (100%)	0	100	100
19	U	152/174 (87%)	152 (100%)	0	100	100
20	V	325/364 (89%)	325 (100%)	0	100	100
21	W	87/158 (55%)	87 (100%)	0	100	100
22	X	311/351 (89%)	310 (100%)	1 (0%)	91	92
23	Y	112/357 (31%)	112 (100%)	0	100	100
24	Z	81/95 (85%)	81 (100%)	0	100	100
25	0	188/190 (99%)	188 (100%)	0	100	100
26	1	254/291 (87%)	254 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	3	65/166 (39%)	65 (100%)	0	100	100
28	4	526/609 (86%)	526 (100%)	0	100	100
29	b	249/350 (71%)	249 (100%)	0	100	100
31	H	129/180 (72%)	129 (100%)	0	100	100
32	9	12/600 (2%)	12 (100%)	0	100	100
33	a	138/288 (48%)	137 (99%)	1 (1%)	81	86
All	All	5278/7481 (71%)	5275 (100%)	3 (0%)	92	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	I	193	LYS
22	X	234	ARG
33	a	137	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	107	GLN
15	Q	15	GLN
20	V	38	HIS
21	W	106	HIS
22	X	190	ASN
26	1	64	GLN
29	b	138	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	A	896/955 (93%)	195 (21%)	8 (0%)

All (195) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	A	650	U
30	A	651	A
30	A	671	U

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Mol	Chain	Res	Type
30	A	680	U
30	A	688	A
30	A	689	U
30	A	695	A
30	A	704	U
30	A	718	A
30	A	721	U
30	A	730	A
30	A	753	A
30	A	761	A
30	A	763	C
30	A	764	A
30	A	766	G
30	A	773	U
30	A	777	G
30	A	783	A
30	A	791	G
30	A	794	U
30	A	796	G
30	A	814	A
30	A	815	C
30	A	828	C
30	A	829	C
30	A	830	U
30	A	832	U
30	A	835	C
30	A	860	A
30	A	861	U
30	A	868	C
30	A	871	A
30	A	889	G
30	A	890	C
30	A	893	G
30	A	902	G
30	A	904	C
30	A	907	A
30	A	908	C
30	A	919	A
30	A	930	G
30	A	931	C
30	A	932	C
30	A	933	G

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Mol	Chain	Res	Type
30	A	938	A
30	A	939	A
30	A	940	A
30	A	941	G
30	A	954	C
30	A	957	C
30	A	959	C
30	A	964	C
30	A	967	A
30	A	975	A
30	A	978	A
30	A	979	C
30	A	993	A
30	A	995	A
30	A	1001	C
30	A	1011	C
30	A	1015	A
30	A	1025	A
30	A	1042	U
30	A	1047	A
30	A	1065	C
30	A	1068	A
30	A	1069	A
30	A	1080	A
30	A	1081	U
30	A	1082	A
30	A	1088	C
30	A	1097	G
30	A	1105	C
30	A	1106	C
30	A	1107	U
30	A	1108	C
30	A	1109	A
30	A	1113	G
30	A	1118	A
30	A	1119	U
30	A	1120	C
30	A	1121	A
30	A	1126	A
30	A	1128	C
30	A	1137	A
30	A	1151	C

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Mol	Chain	Res	Type
30	A	1154	A
30	A	1160	A
30	A	1167	A
30	A	1175	G
30	A	1176	G
30	A	1177	C
30	A	1178	G
30	A	1181	G
30	A	1184	U
30	A	1185	C
30	A	1186	A
30	A	1188	A
30	A	1189	U
30	A	1190	C
30	A	1193	U
30	A	1200	G
30	A	1203	C
30	A	1215	U
30	A	1222	A
30	A	1223	C
30	A	1225	C
30	A	1226	C
30	A	1229	U
30	A	1236	C
30	A	1238	C
30	A	1244	C
30	A	1245	U
30	A	1246	U
30	A	1247	G
30	A	1248	C
30	A	1251	A
30	A	1255	U
30	A	1259	U
30	A	1269	U
30	A	1273	G
30	A	1278	C
30	A	1285	G
30	A	1287	A
30	A	1290	C
30	A	1291	U
30	A	1292	A
30	A	1293	C

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Mol	Chain	Res	Type
30	A	1294	A
30	A	1295	A
30	A	1296	A
30	A	1297	G
30	A	1303	G
30	A	1312	C
30	A	1314	C
30	A	1318	A
30	A	1326	A
30	A	1327	G
30	A	1331	A
30	A	1332	A
30	A	1341	C
30	A	1342	C
30	A	1343	A
30	A	1352	C
30	A	1354	A
30	A	1356	A
30	A	1367	A
30	A	1371	U
30	A	1378	C
30	A	1380	G
30	A	1383	A
30	A	1385	C
30	A	1387	A
30	A	1390	A
30	A	1398	U
30	A	1399	A
30	A	1405	C
30	A	1406	U
30	A	1407	U
30	A	1408	A
30	A	1410	G
30	A	1416	A
30	A	1417	A
30	A	1420	U
30	A	1421	G
30	A	1422	G
30	A	1427	A
30	A	1430	A
30	A	1438	G
30	A	1442	G

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Mol	Chain	Res	Type
30	A	1443	U
30	A	1444	A
30	A	1447	G
30	A	1457	G
30	A	1461	A
30	A	1465	C
30	A	1469	G
30	A	1477	U
30	A	1492	A
30	A	1493	C
30	A	1507	A
30	A	1509	U
30	A	1541	U
30	A	1545	U
30	A	1547	U
30	A	1551	G
30	A	1558	A
30	A	1559	G
30	A	1585	A
30	A	1590	A
30	A	1591	C
30	A	1594	G
30	A	1595	G
30	A	1598	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	A	930	G
30	A	1046	A
30	A	1228	A
30	A	1293	C
30	A	1379	A
30	A	1415	G
30	A	1550	A
30	A	1590	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	5F0	I	184	7	8,8,9	0.58	0	7,9,11	1.16	1 (14%)
30	5MU	A	1076	30	19,22,23	0.40	0	28,32,35	0.50	0
30	MA6	A	1583	30	18,26,27	0.99	2 (11%)	19,38,41	3.27	2 (10%)
30	5MC	A	1488	30	18,22,23	0.52	0	26,32,35	0.53	0
30	MA6	A	1584	30	18,26,27	0.99	2 (11%)	19,38,41	3.30	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	5F0	I	184	7	-	0/9/9/10	-
30	5MU	A	1076	30	-	0/7/25/26	0/2/2/2
30	MA6	A	1583	30	-	3/7/29/30	0/3/3/3
30	5MC	A	1488	30	-	0/7/25/26	0/2/2/2
30	MA6	A	1584	30	-	3/7/29/30	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	1584	MA6	C5-C4	-2.57	1.34	1.40
30	A	1583	MA6	C5-C4	-2.52	1.34	1.40
30	A	1584	MA6	C2-N3	2.40	1.36	1.32
30	A	1583	MA6	C2-N3	2.39	1.35	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	1584	MA6	N1-C6-N6	-13.06	103.31	117.06
30	A	1583	MA6	N1-C6-N6	-12.92	103.46	117.06
30	A	1583	MA6	N3-C2-N1	-5.49	120.10	128.68
30	A	1584	MA6	N3-C2-N1	-5.49	120.10	128.68
7	I	184	5F0	O-C-CB	-2.78	117.33	125.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	1583	MA6	O4'-C4'-C5'-O5'
30	A	1584	MA6	O4'-C4'-C5'-O5'
30	A	1583	MA6	C3'-C4'-C5'-O5'
30	A	1584	MA6	C3'-C4'-C5'-O5'
30	A	1583	MA6	C4'-C5'-O5'-P
30	A	1584	MA6	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	1583	MA6	2	0
30	A	1488	5MC	2	0
30	A	1584	MA6	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 32 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	FES	P	201	4,14	0,4,4	-	-	-		
37	GDP	X	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.20	3 (10%)
39	NAD	A	1732	38	42,48,48	0.90	2 (4%)	50,73,73	0.83	1 (2%)
40	SPM	A	1733	-	13,13,13	0.35	0	12,12,12	0.98	0
34	FES	M	201	-	0,4,4	-	-	-		
36	ATP	X	501	-	26,33,33	0.60	0	31,52,52	0.92	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	FES	P	201	4,14	-	-	0/1/1/1
37	GDP	X	502	-	-	2/12/32/32	0/3/3/3
39	NAD	A	1732	38	-	5/26/62/62	0/5/5/5
40	SPM	A	1733	-	-	0/11/11/11	-
34	FES	M	201	-	-	-	0/1/1/1
36	ATP	X	501	-	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	A	1732	NAD	C8A-N7A	-2.61	1.30	1.34
39	A	1732	NAD	O4D-C1D	-2.51	1.37	1.41
37	X	502	GDP	C6-N1	-2.38	1.34	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	502	GDP	PA-O3A-PB	-3.69	120.15	132.83
37	X	502	GDP	C8-N7-C5	2.56	107.87	102.99
37	X	502	GDP	C5-C6-N1	2.41	118.20	113.95
36	X	501	ATP	C5-C6-N6	2.30	123.85	120.35
39	A	1732	NAD	O2A-PA-O1A	2.19	123.05	112.24
36	X	501	ATP	PB-O3B-PG	2.04	139.82	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	A	1732	NAD	C5B-O5B-PA-O1A
39	A	1732	NAD	O4B-C4B-C5B-O5B
39	A	1732	NAD	C3B-C4B-C5B-O5B
36	X	501	ATP	C4'-C5'-O5'-PA
36	X	501	ATP	C3'-C4'-C5'-O5'
36	X	501	ATP	O4'-C4'-C5'-O5'
39	A	1732	NAD	PA-O3-PN-O2N
37	X	502	GDP	O4'-C4'-C5'-O5'
39	A	1732	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
37	X	502	GDP	C3'-C4'-C5'-O5'

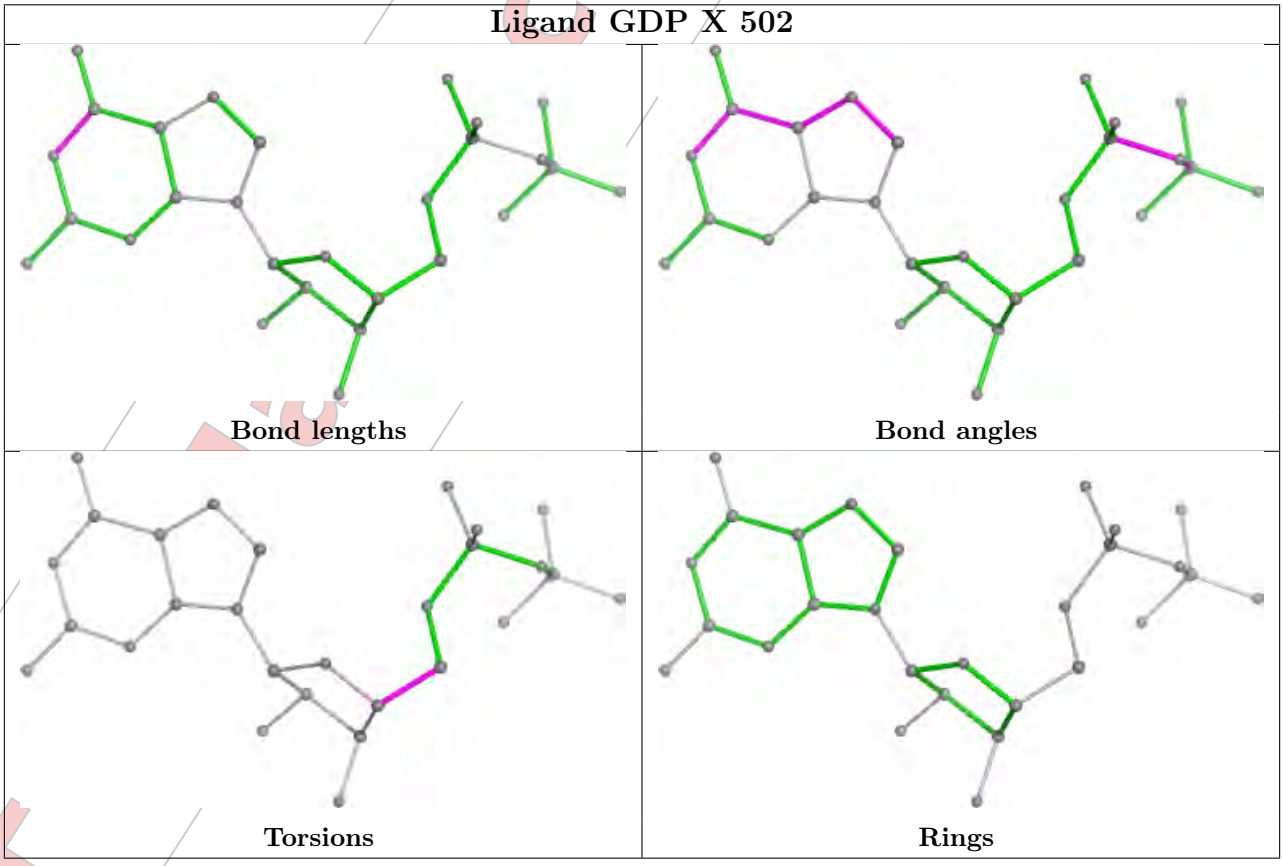
There are no ring outliers.

1 monomer is involved in 3 short contacts:

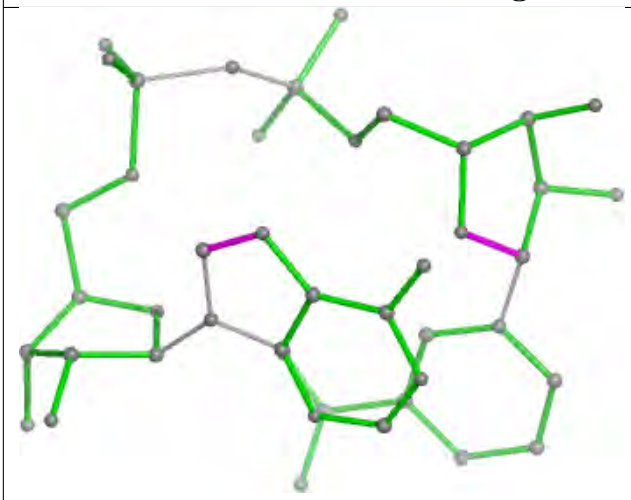
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	A	1733	SPM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

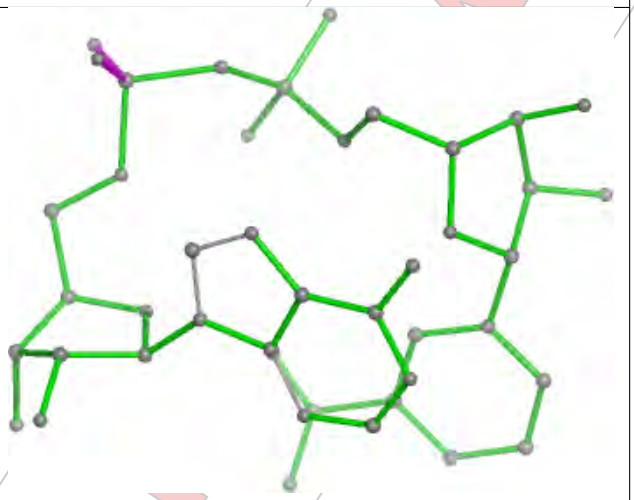
Ligand GDP X 502



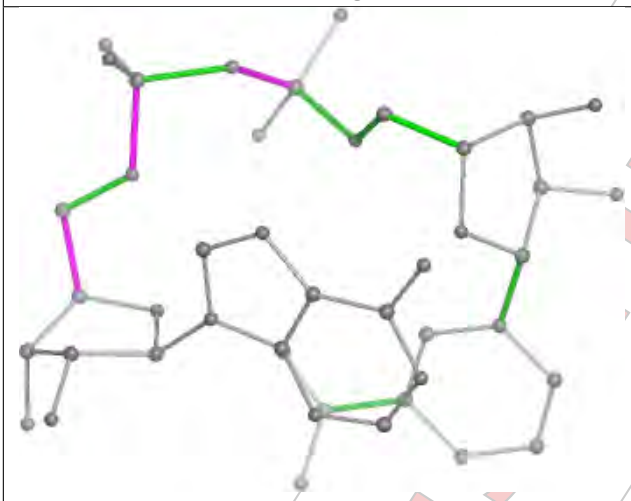
Ligand NAD A 1732



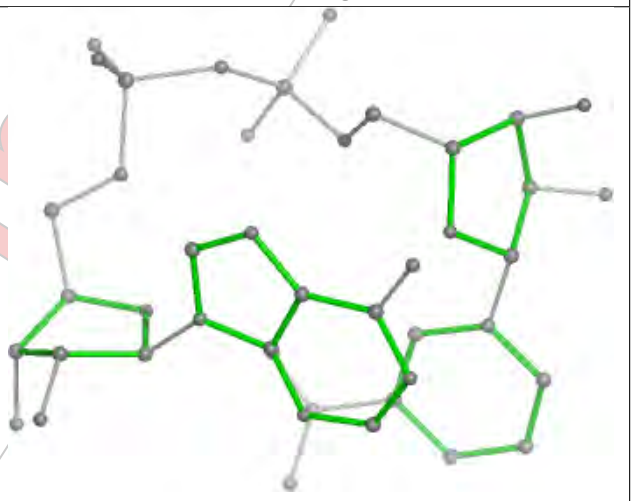
Bond lengths



Bond angles

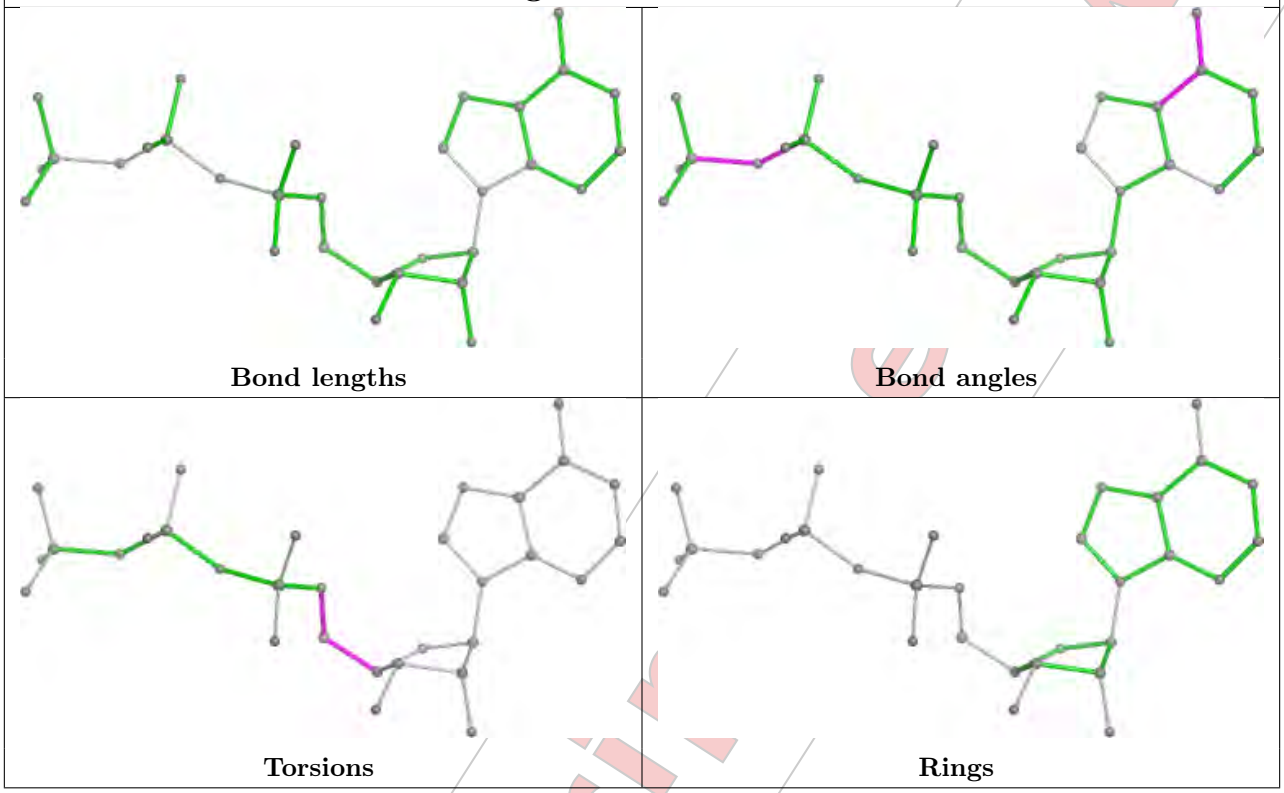


Torsions



Rings

Ligand ATP X 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

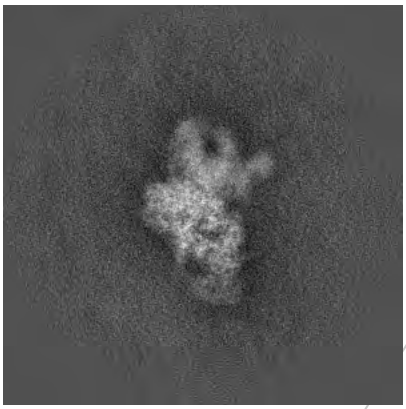
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51875. These allow visual inspection of the internal detail of the map and identification of artifacts.

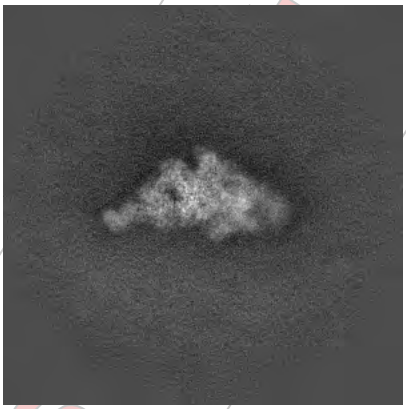
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

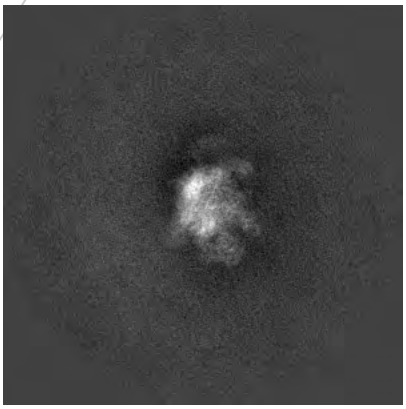
6.1.1 Primary map



X

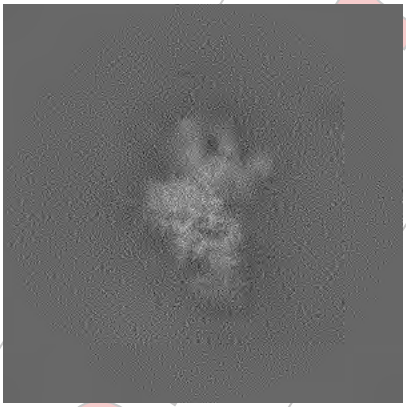


Y

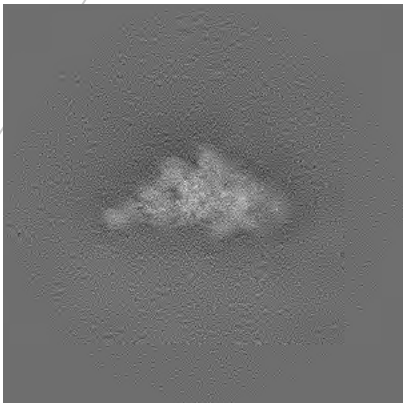


Z

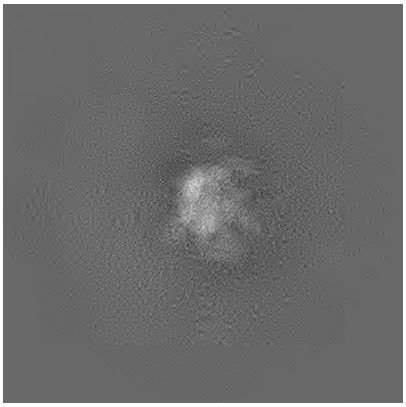
6.1.2 Raw map



X



Y

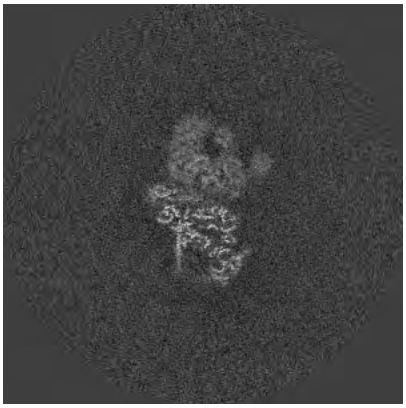


Z

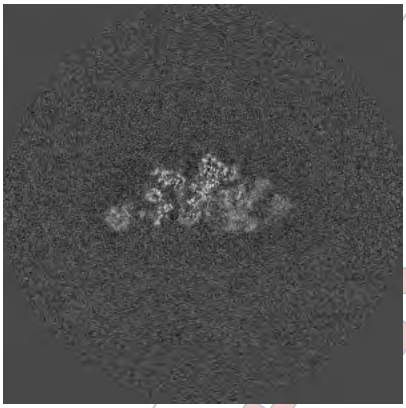
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

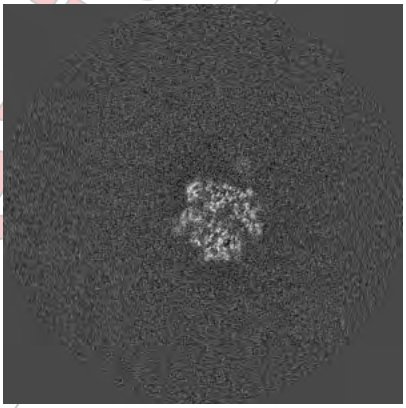
6.2.1 Primary map



X Index: 300

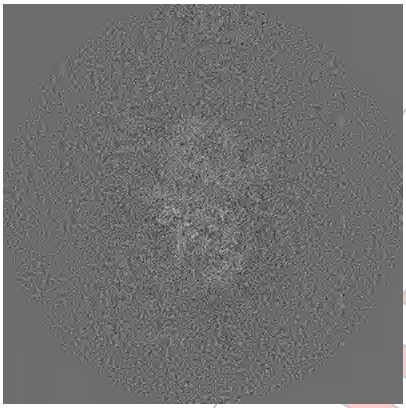


Y Index: 300

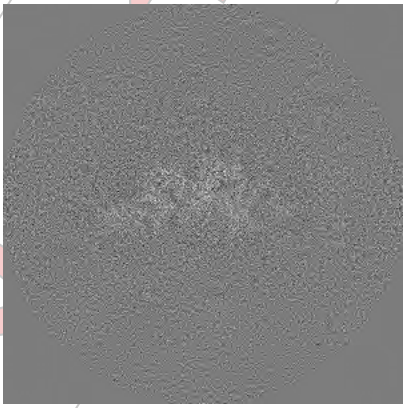


Z Index: 300

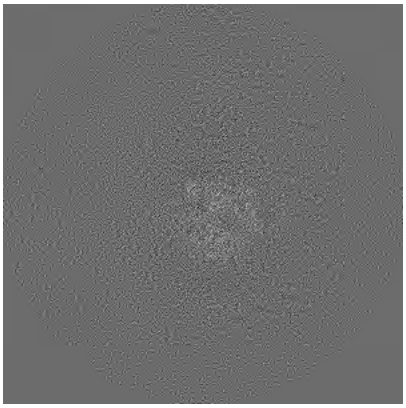
6.2.2 Raw map



X Index: 300



Y Index: 300

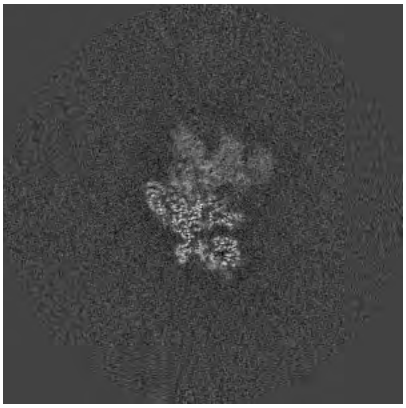


Z Index: 300

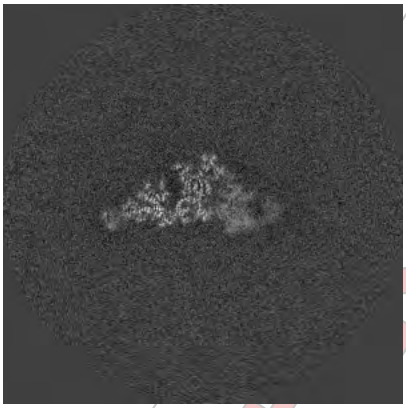
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

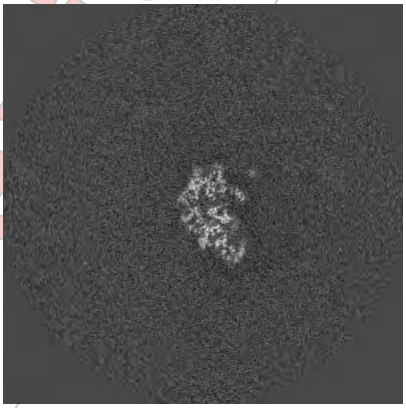
6.3.1 Primary map



X Index: 314

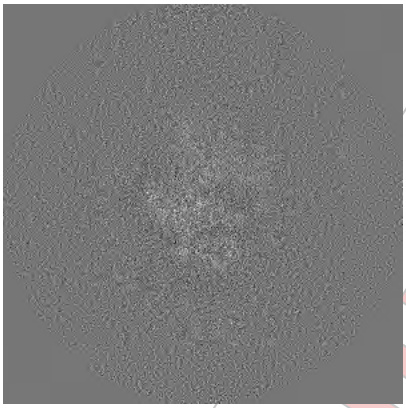


Y Index: 318

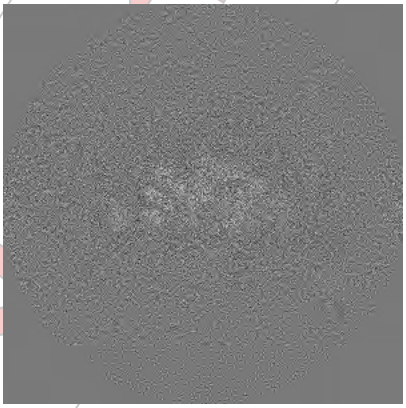


Z Index: 273

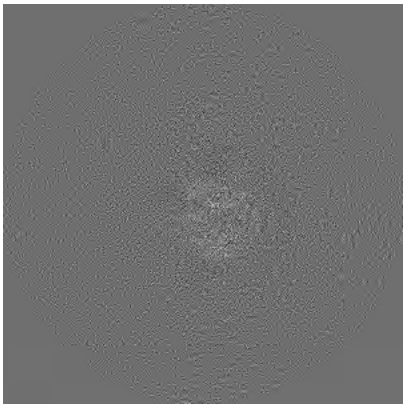
6.3.2 Raw map



X Index: 313



Y Index: 297

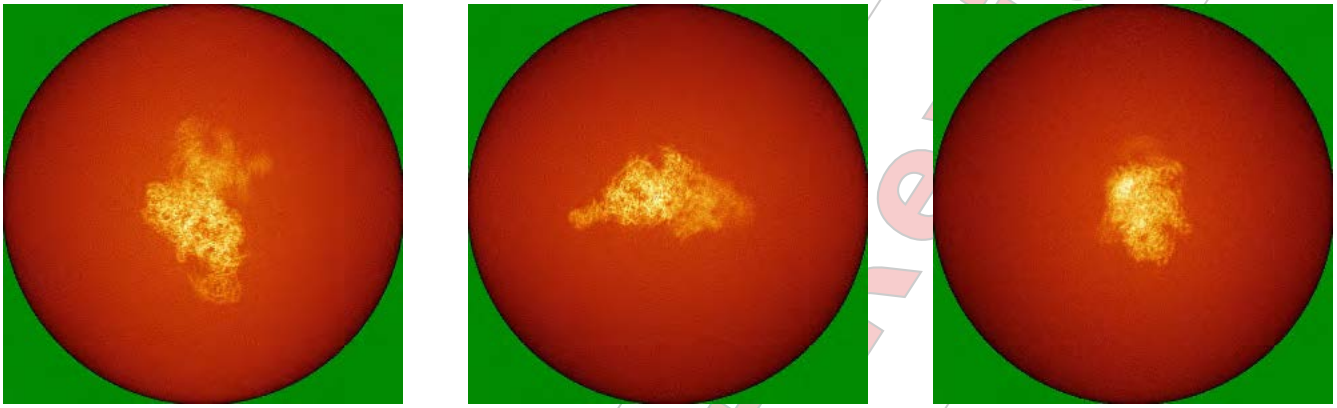


Z Index: 299

The images above show the largest variance slices of the map in three orthogonal directions.

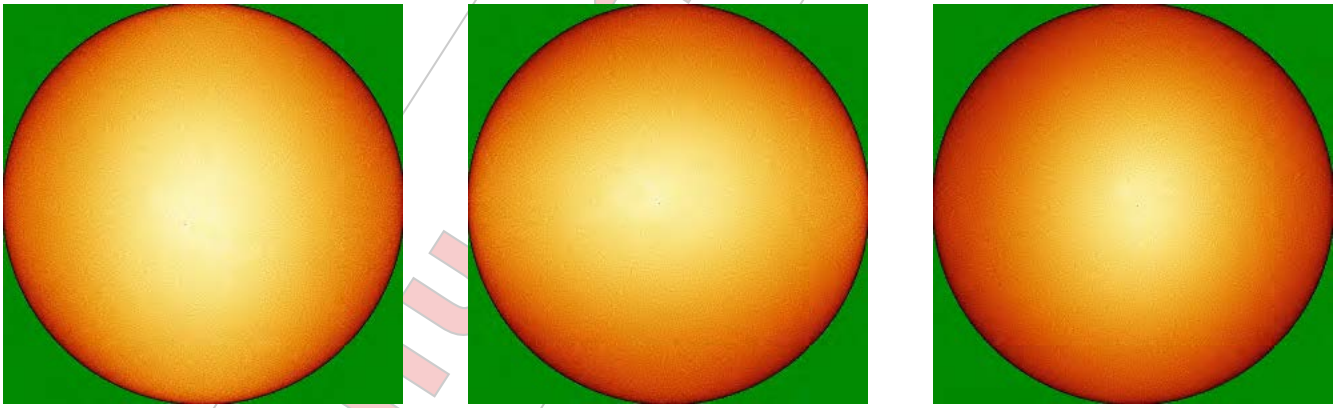
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

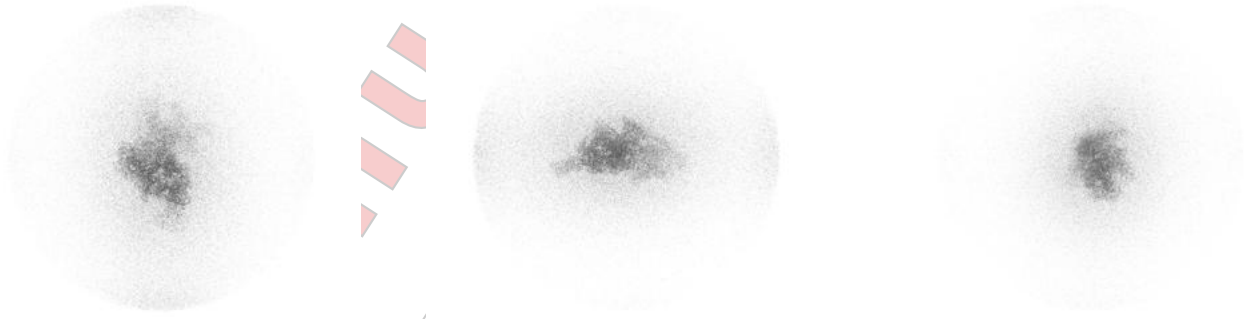
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

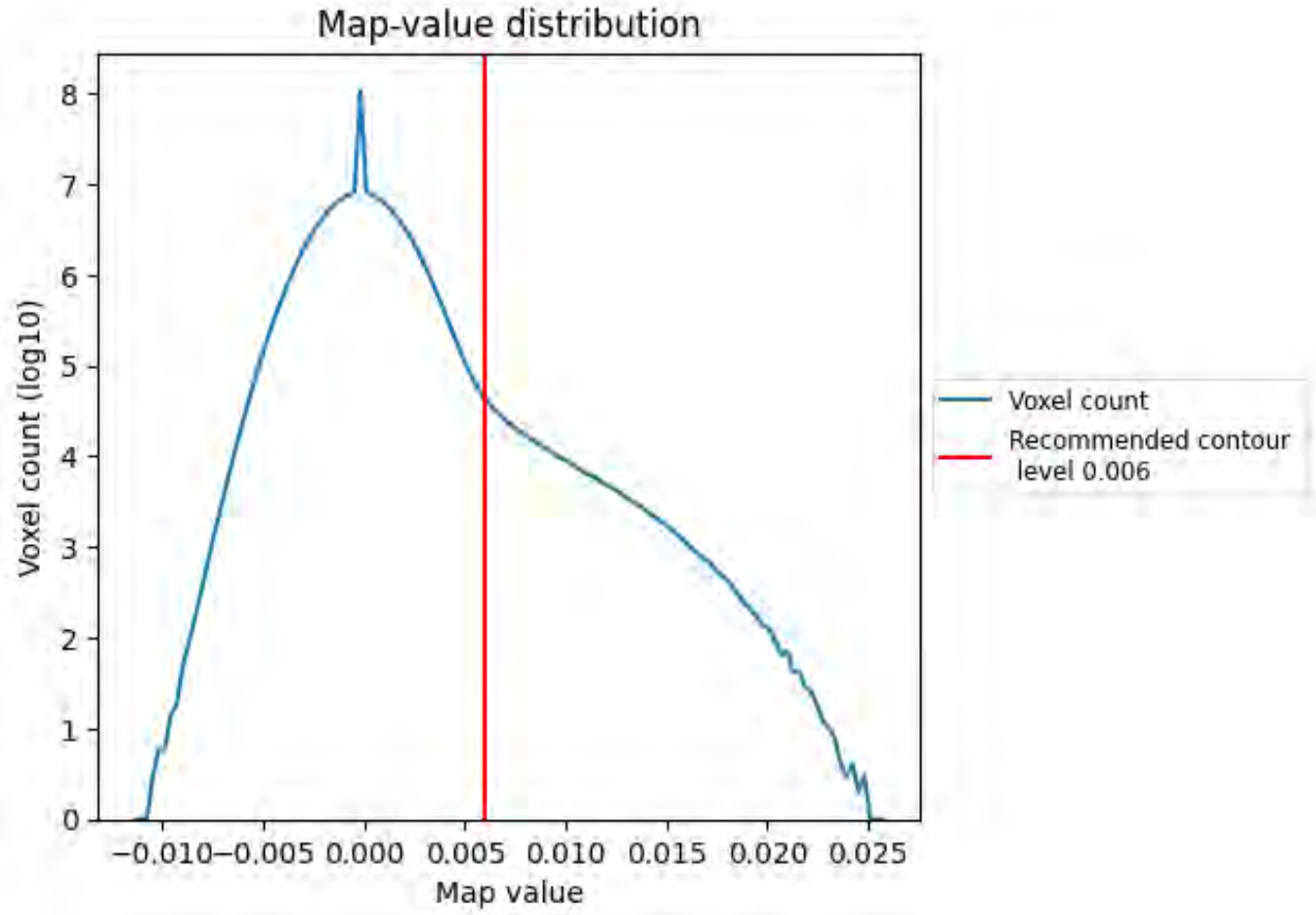
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

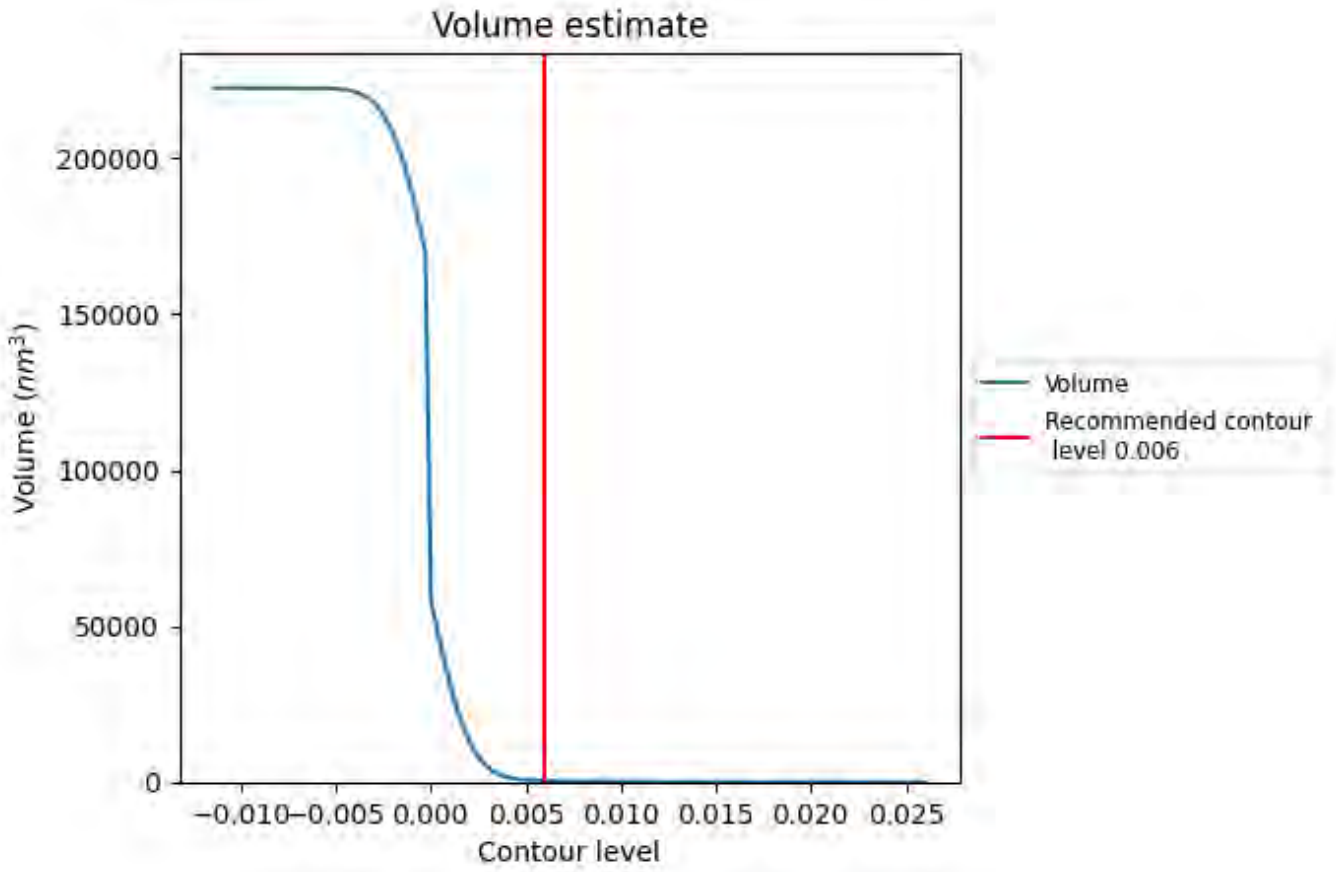
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

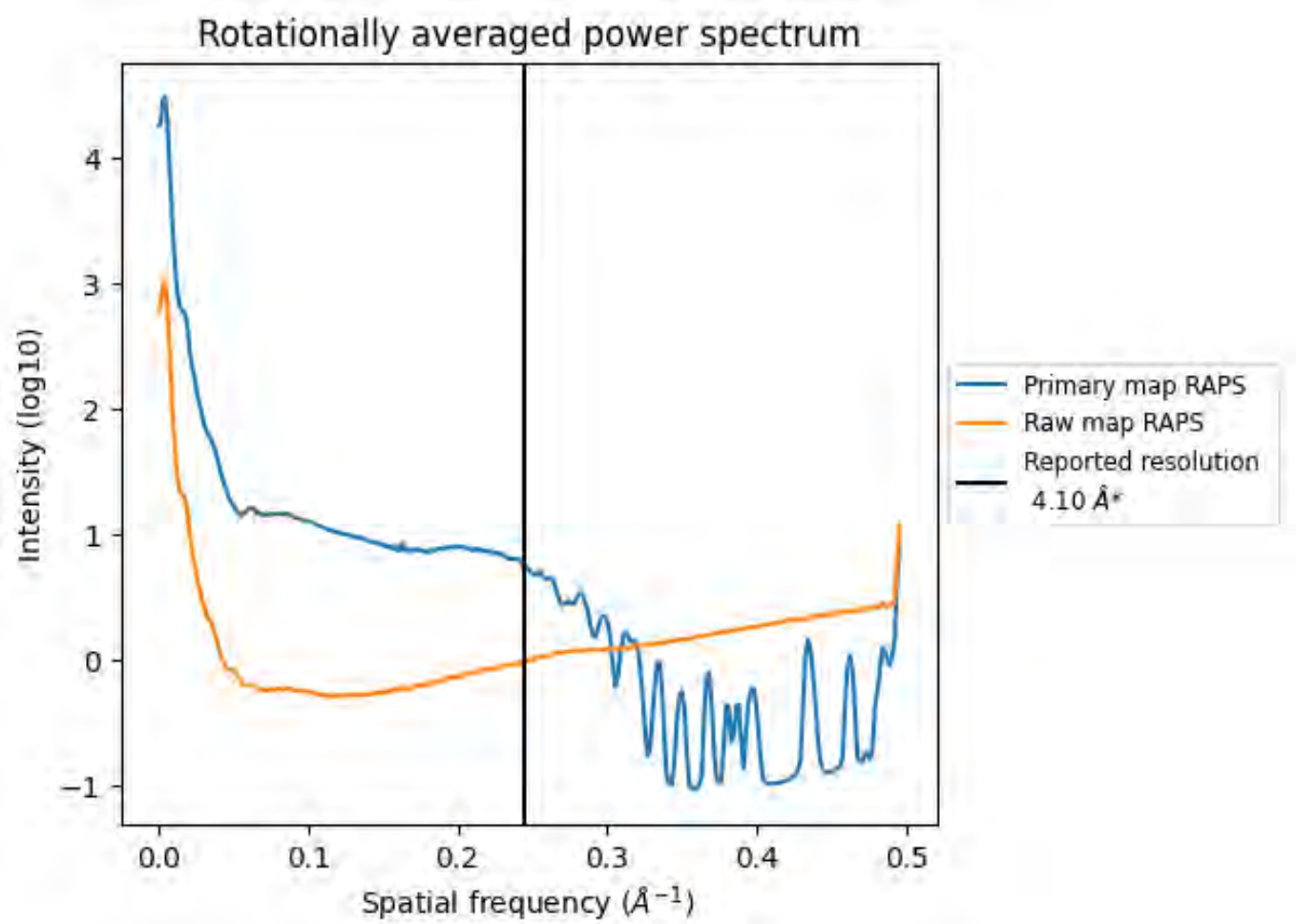
7.2 Volume estimate (i)



The volume at the recommended contour level is 392 nm^3; this corresponds to an approximate mass of 354 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

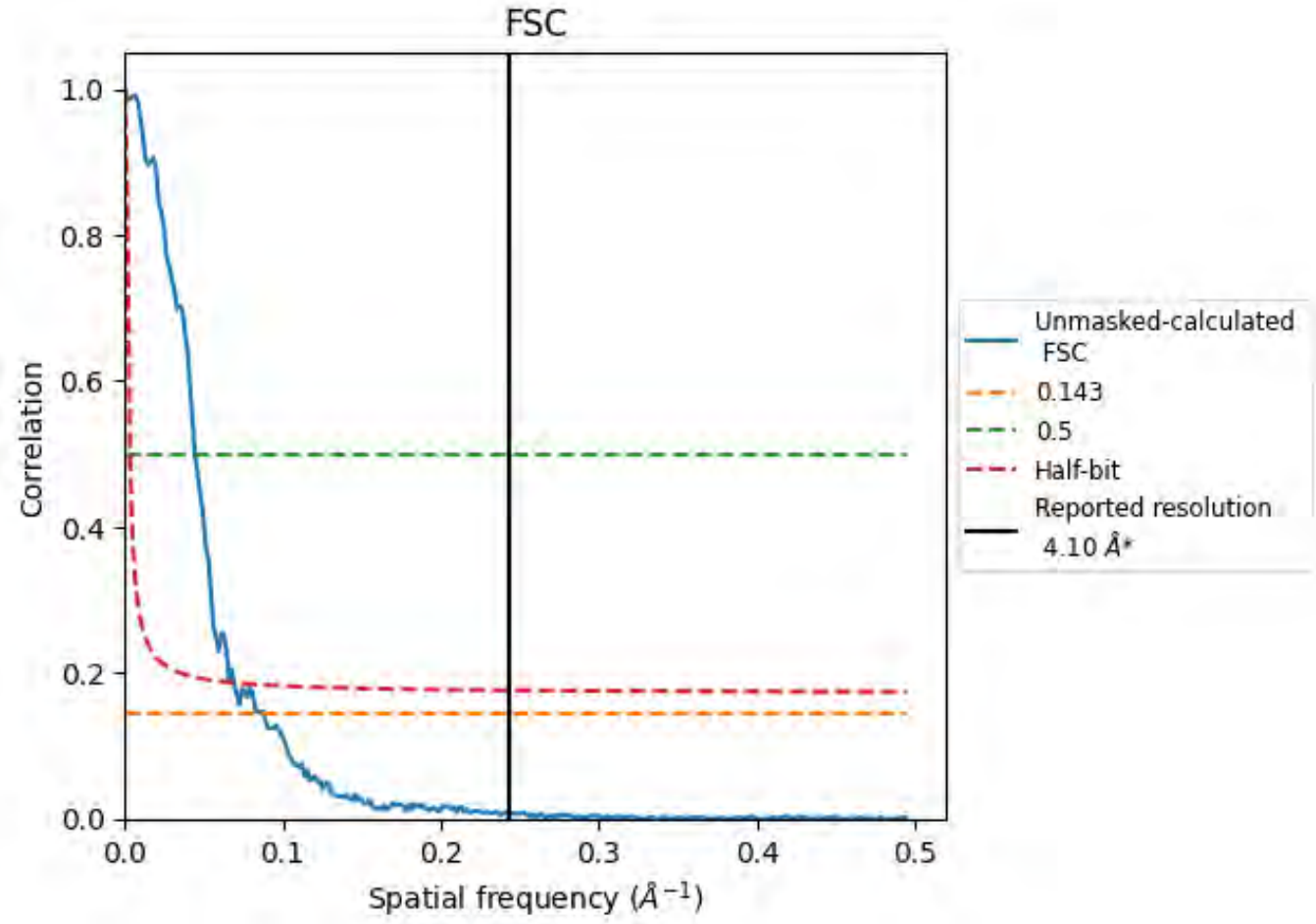


*Reported resolution corresponds to spatial frequency of 0.244 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8.2 Resolution estimates (i)

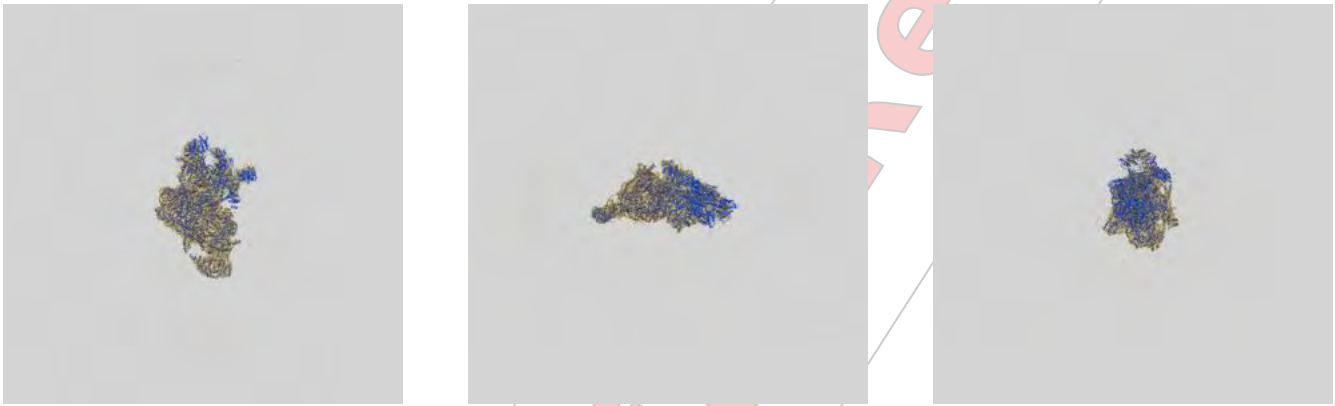
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.38	22.52	14.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 11.38 differs from the reported value 4.1 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51875 and PDB model 9H53. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay



X Y Z

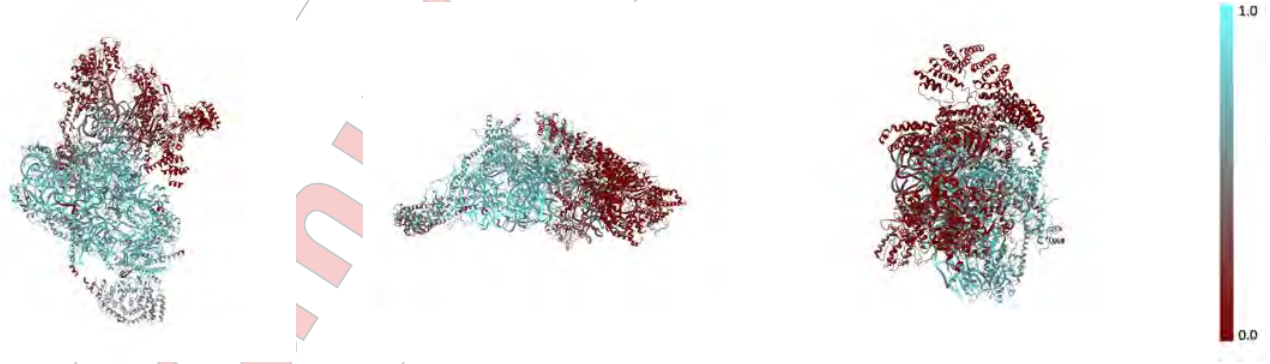
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

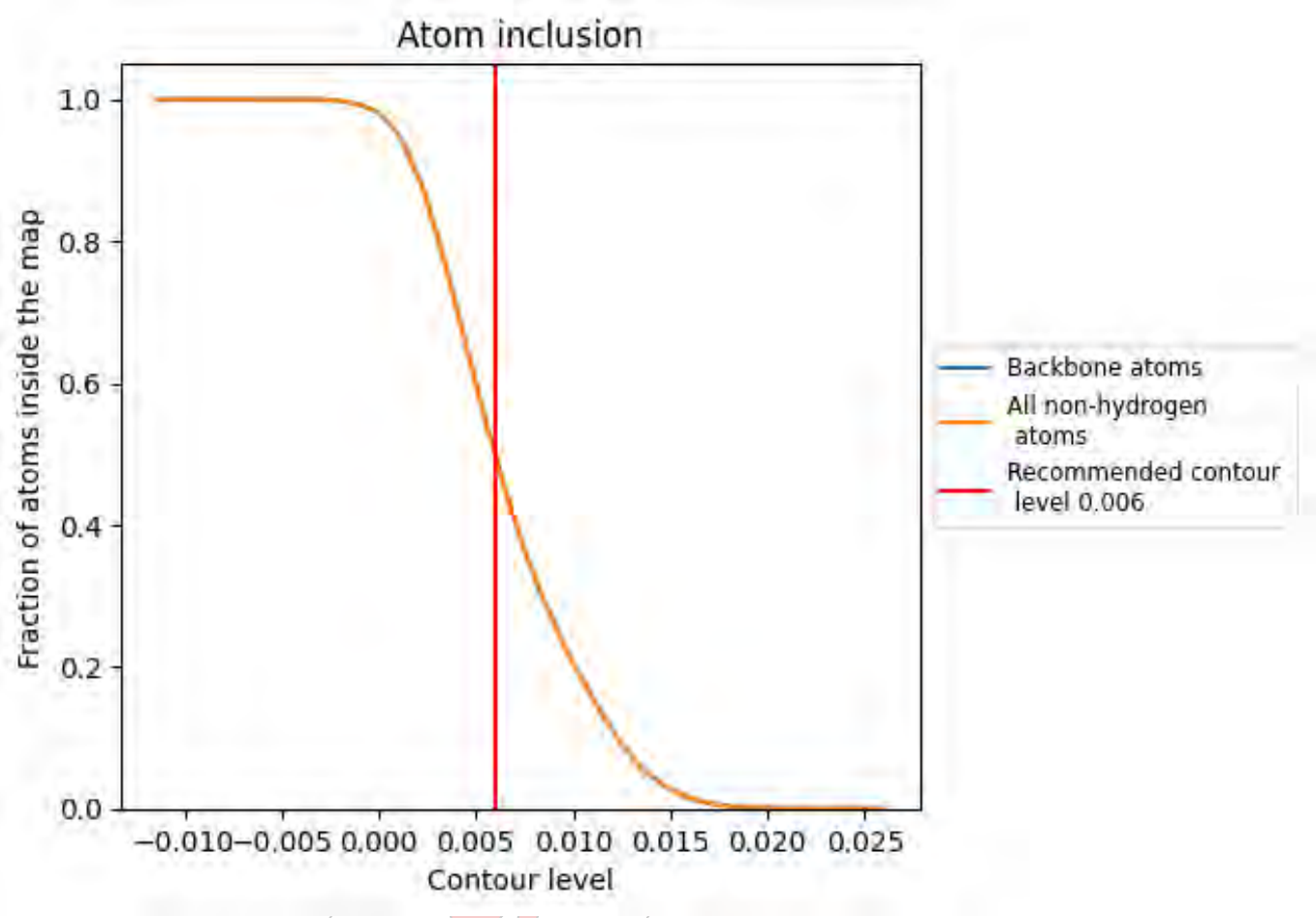
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4970	0.2560
0	0.5890	0.3230
1	0.0920	0.0660
3	0.5780	0.3250
4	0.0650	0.0380
9	0.1850	0.0290
A	0.7350	0.3350
B	0.6970	0.3720
C	0.2330	0.1490
D	0.5370	0.3380
E	0.6220	0.3480
F	0.1670	0.0810
G	0.3110	0.1410
H	0.1180	0.0550
I	0.6500	0.3480
J	0.6700	0.4070
K	0.2140	0.0900
L	0.6570	0.3790
M	0.7390	0.4270
N	0.7210	0.4470
O	0.7270	0.4030
P	0.6950	0.3950
Q	0.6560	0.3690
R	0.6840	0.3860
S	0.6010	0.3150
T	0.7210	0.4300
U	0.6550	0.3360
V	0.4230	0.1710
W	0.6210	0.3650
X	0.0900	0.0410
Y	0.0450	0.0320
Z	0.1840	0.0970
a	0.2830	0.1860
b	0.2770	0.1330

Full wwPDB EM Validation Report ⓘ

Apr 17, 2025 – 08:24 pm BST

PDB ID	:	9H56 / pdb_00009h56
EMDB ID	:	EMD-51878
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit bound to METTL15,RBFA and mtIF2 (state A5.1)
Deposited on	:	2024-10-22
Resolution	:	4.20 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

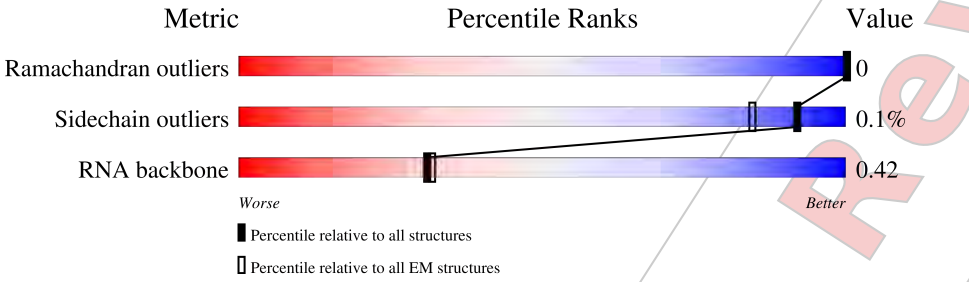
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	296	6% 76% 24%
2	C	167	67% 72% 28%
3	D	430	26% 76% 24%
4	E	125	21% 92% 8%
5	F	242	79% 81% • 18%
6	G	396	58% 76% • 23%
7	H	201	68% 70% 30%

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Mol	Chain	Length	Quality of chain
8	I	194	23% 70% 29%
9	J	138	7% 75% 25%
10	K	128	75% 79% 21%
11	L	257	11% 68% 32%
12	M	137	7% 87% 13%
13	N	130	6% 85% 15%
14	O	258	5% 75% 25%
15	P	142	7% 68% 32%
16	c	87	23% 98%
17	R	360	6% 82% 18%
18	S	190	16% 71% 29%
19	T	173	6% 97%
20	U	205	16% 86% 14%
21	V	414	43% 86% 14%
22	W	187	6% 53% 47%
23	X	398	87% 88% 12%
24	Y	395	30% 31% 69%
25	Z	106	87% 89% 11%
26	0	218	17% 98%
27	1	323	84% 85% 15%
28	3	199	7% 35% 65%
29	4	689	80% 81% 19%
30	b	407	68% 73% 25%
31	A	955	24% 65% 30% 5%
32	7	727	45% 63% 37%

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Mol	Chain	Length	Quality of chain
33	t	198	36% 36% 64%
34	9	698	98%
35	a	343	16% 18% 82%

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 133071 atoms, of which 62068 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	B	225	3643	1164	1815	331	323	10	0	0

- Molecule 2 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C	121	1979	646	985	172	172	4	0	0

- Molecule 3 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	327	5270	1641	2657	489	470	13	0	0

- Molecule 4 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	E	115	1839	574	929	165	167	4	0	0

- Molecule 5 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	199	3319	1043	1685	293	287	11	0	0

- Molecule 6 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	G	304	4991	1592	2483	445	457	14	0	0

- Molecule 7 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	H	140	2335	745	1183	194	210	3	0	0

- Molecule 8 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	I	137	2080	642	1060	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 9 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	J	103	1629	493	835	157	138	6	0	0

- Molecule 10 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	K	101	1747	537	885	179	141	5	0	0

- Molecule 11 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	L	174	2993	925	1540	270	251	7	0	0

- Molecule 12 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	M	119	1908	594	966	185	157	6	0	0

- Molecule 13 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	110	Total	C	H	N	O	S	0	0
			1796	562	928	156	147	3		

- Molecule 14 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	O	194	Total	C	H	N	O	S	0	0
			3165	1019	1566	295	278	7		

- Molecule 15 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	97	Total	C	H	N	O	S	0	0
			1589	501	808	134	138	8		

- Molecule 16 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	c	87	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	1	ACE	-	acetylation	UNP P82921
c	50	ARG	CYS	conflict	UNP P82921

- Molecule 17 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	295	Total	C	H	N	O	S	0	0
			4837	1533	2428	413	455	8		

- Molecule 18 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	135	Total	C	H	N	O	S	0	0
			2226	716	1115	198	196	1		

- Molecule 19 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	168	Total	C	H	N	O	S	0	0
			2765	877	1394	239	244	11		

- Molecule 20 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	U	176	Total	C	H	N	O	S	0	0
			2987	916	1499	301	267	4		

- Molecule 21 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	355	Total	C	H	N	O	S	0	0
			5805	1866	2898	485	544	12		

- Molecule 22 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	W	100	Total	C	H	N	O	S	0	0
			1590	498	801	141	146	4		

- Molecule 23 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	X	352	Total	C	H	N	O	S	0	0
			5689	1822	2840	499	517	11		

- Molecule 24 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Y	121	Total	C	H	N	O	S	0	0
			1993	662	970	168	191	2		

- Molecule 25 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	94	Total	C	H	N	O	S	0	0
			1612	510	815	143	140	4		

- Molecule 26 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	0	214	Total	C	H	N	O	S	0	0
			3562	1124	1784	337	312	5		

- Molecule 27 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	1	275	Total	C	H	N	O	S	0	0
			4489	1415	2259	380	424	11		

- Molecule 28 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	3	69	Total	C	H	N	O	S	0	0
			1302	395	686	132	88	1		

- Molecule 29 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	559	Total	C	H	N	O	S	0	0
			9083	2915	4539	770	833	26		

- Molecule 30 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	b	305	Total	C	H	N	O	S	0	0
			4815	1503	2436	425	438	13		

- Molecule 31 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	A	903	Total	C	H	N	O	P	0	0
			28917	8602	9735	3455	6222	903		

- Molecule 32 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	7	455	Total	C	H	N	O	S	0	0
			7049	2202	3548	612	675	12		

- Molecule 33 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	t	71	Total	C	H	N	O	0	0
			1146	352	599	93	102		

- Molecule 34 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	9	12	Total	C	H	N	O	S	0	0
			219	76	108	16	18	1		

- Molecule 35 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	a	62	Total	C	H	N	O	S	0	0
			955	300	473	81	99	2		

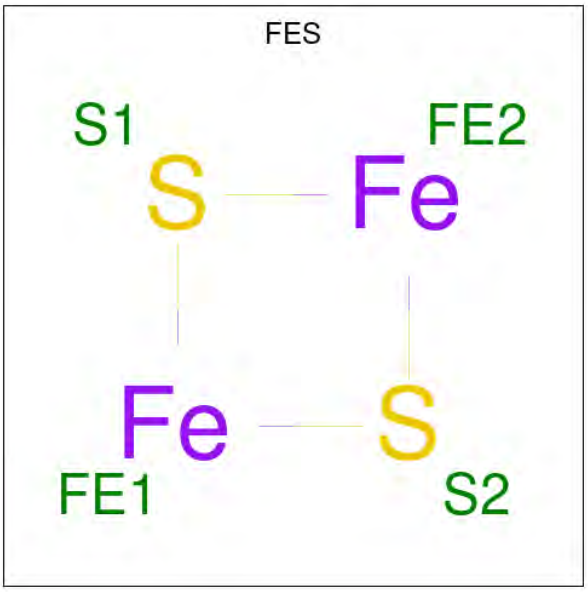
- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	B	1	Total	Mg	0
			1	1	
36	A	23	Total	Mg	0
			23	23	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

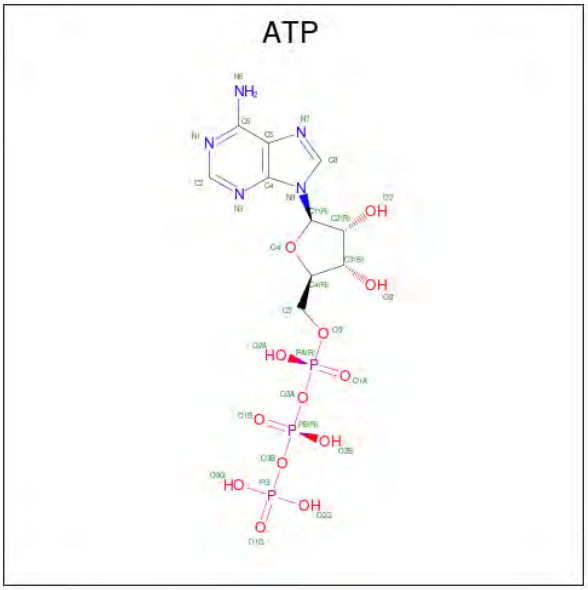
Mol	Chain	Residues	Atoms		AltConf
37	O	1	Total	Zn	0
			1	1	

- Molecule 38 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



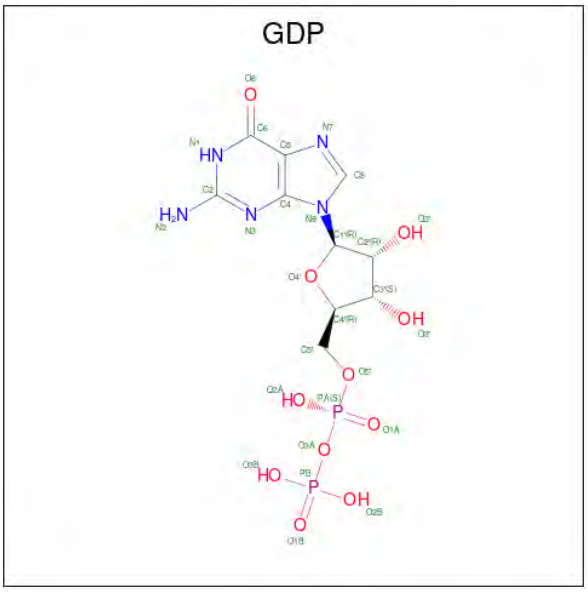
Mol	Chain	Residues	Atoms			AltConf
38	P	1	Total	Fe	S	0
			4	2	2	
38	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 39 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



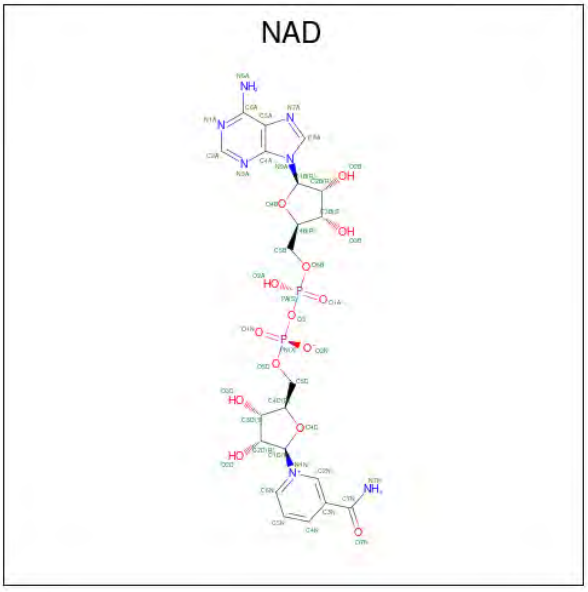
Mol	Chain	Residues	Atoms						AltConf
39	X	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 40 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



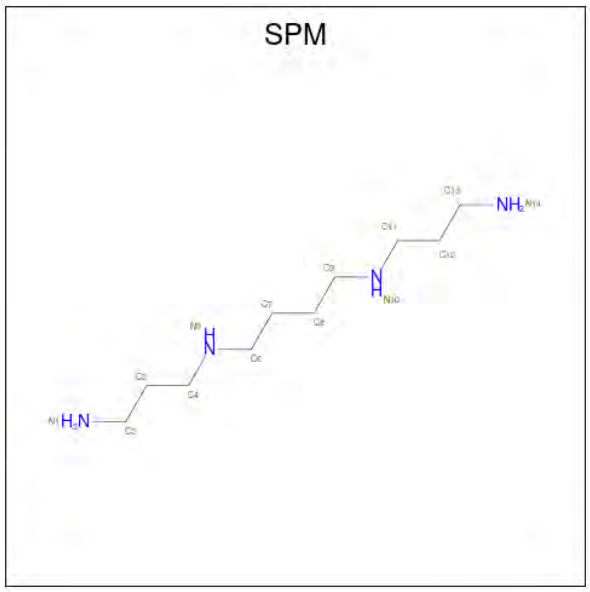
Mol	Chain	Residues	Atoms						AltConf
40	X	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	
40	7	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

- Molecule 41 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
41	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 42 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
42	A	1	Total C N 14 10 4	0

- Molecule 43 is water.

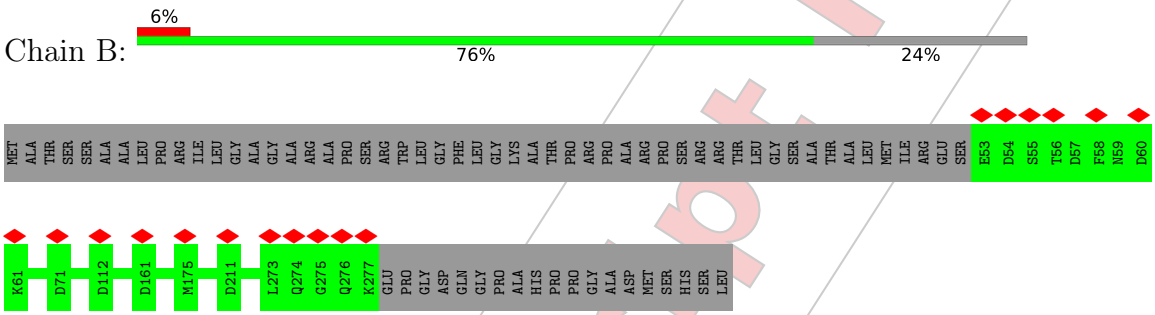
Mol	Chain	Residues	Atoms	AltConf
43	C	1	Total O 1 1	0
43	G	1	Total O 1 1	0
43	I	2	Total O 2 2	0
43	K	1	Total O 1 1	0
43	T	1	Total O 1 1	0
43	0	1	Total O 1 1	0
43	1	1	Total O 1 1	0
43	b	1	Total O 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

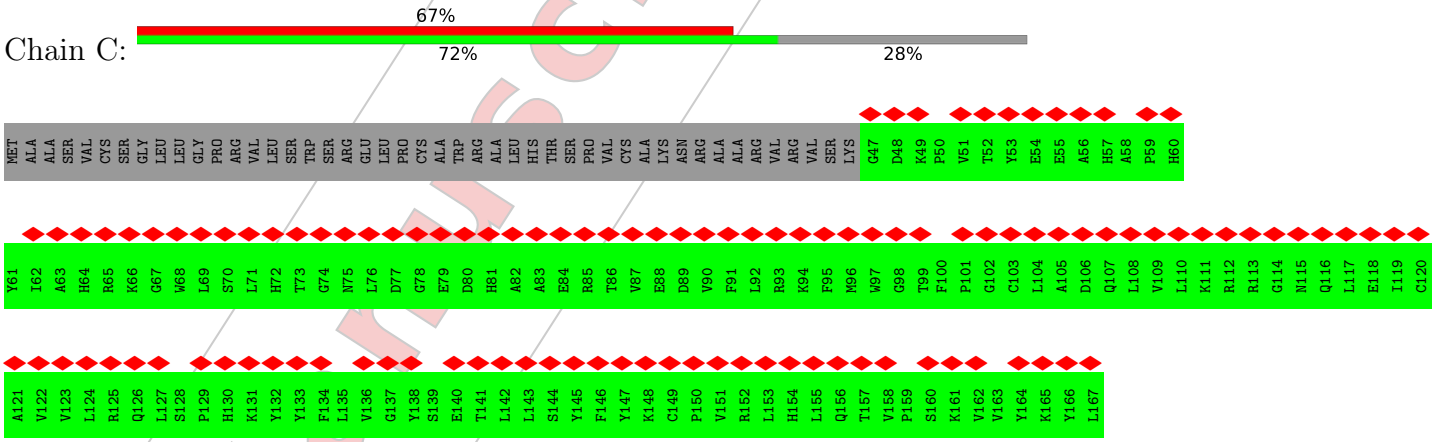
• Molecule 1: 28S ribosomal protein S2, mitochondrial

Chain B:



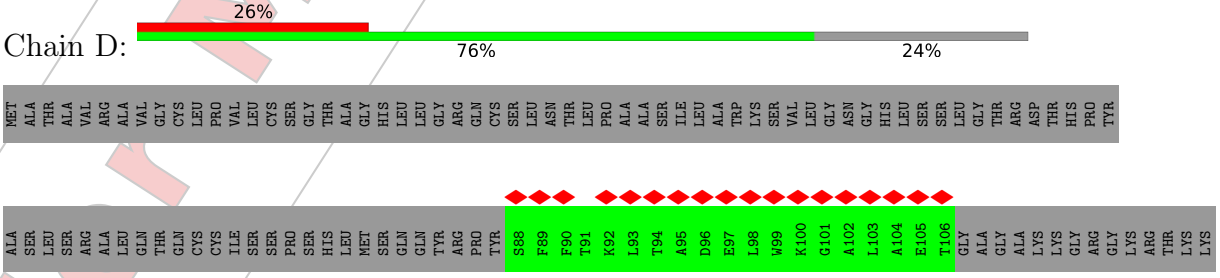
• Molecule 2: 28S ribosomal protein S24, mitochondrial

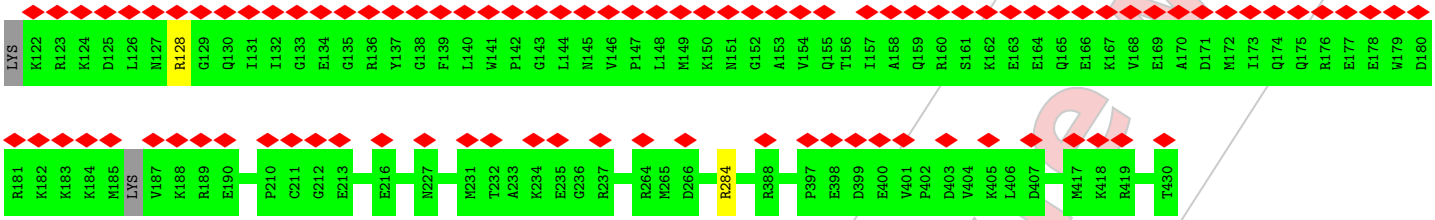
Chain C:



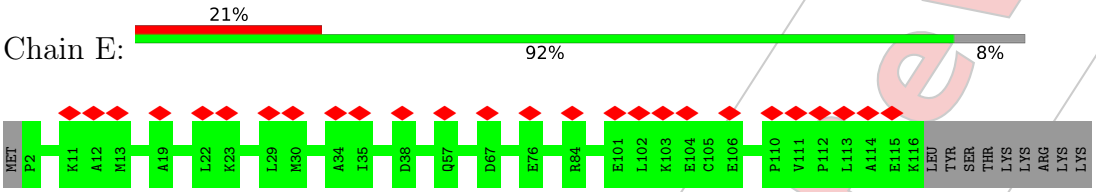
• Molecule 3: 28S ribosomal protein S5, mitochondrial

Chain D:

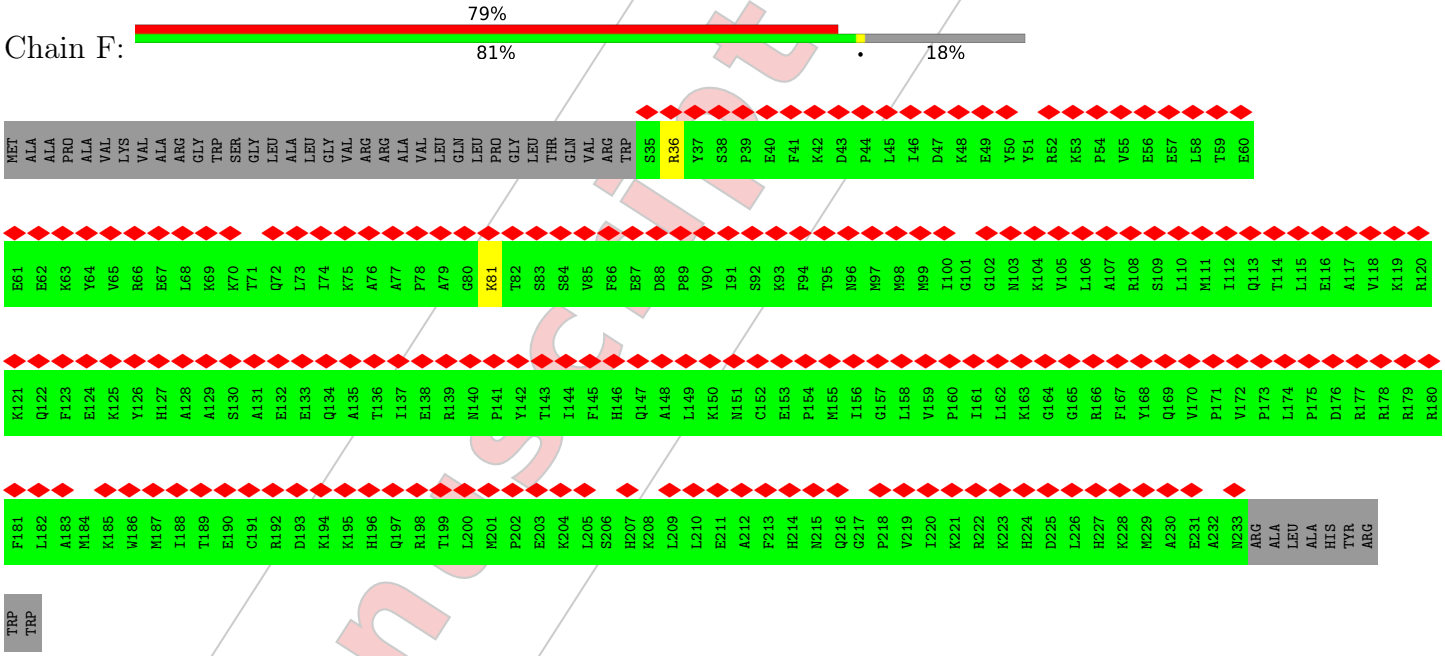




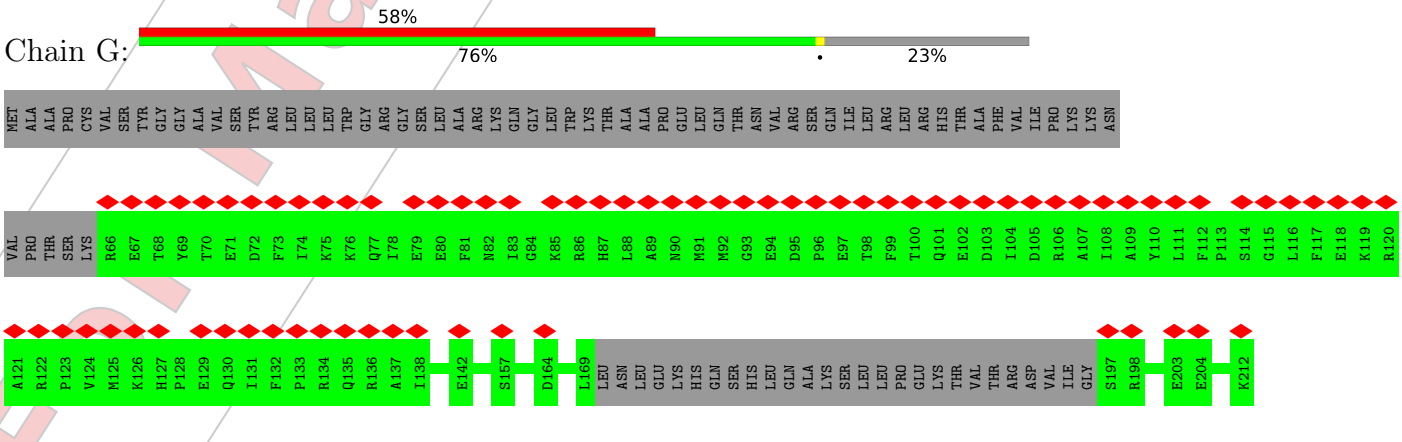
• Molecule 4: 28S ribosomal protein S6, mitochondrial

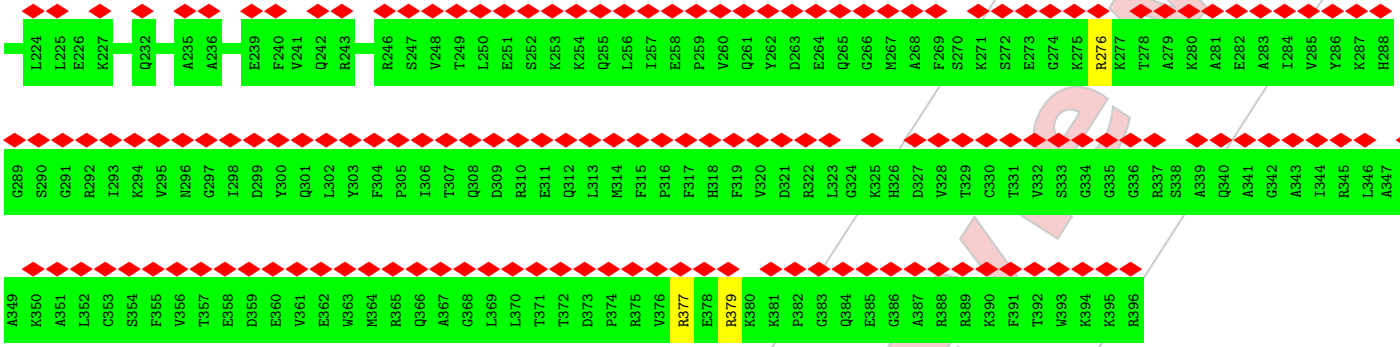


• Molecule 5: 28S ribosomal protein S7, mitochondrial



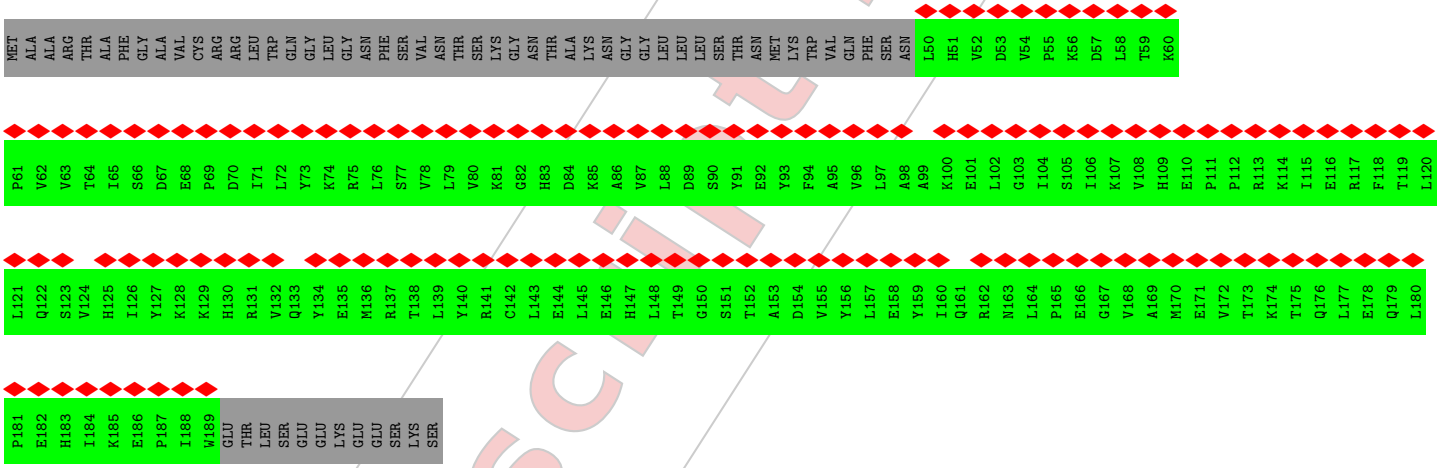
• Molecule 6: 28S ribosomal protein S9, mitochondrial





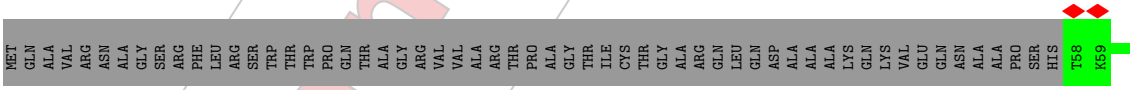
• Molecule 7: 28S ribosomal protein S10, mitochondrial

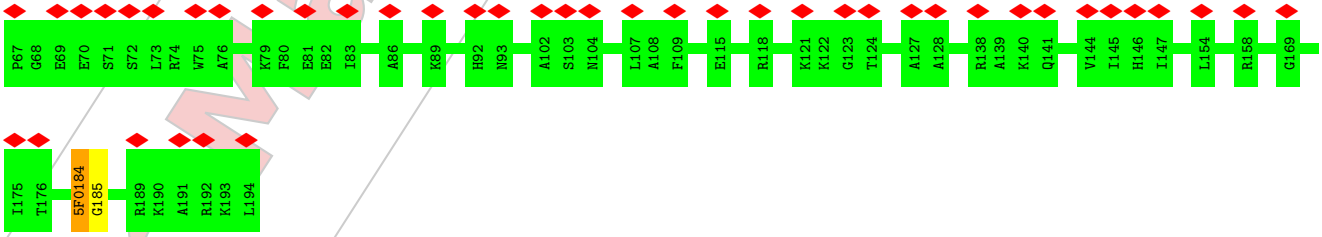
Chain H:



• Molecule 8: 28S ribosomal protein S11, mitochondrial

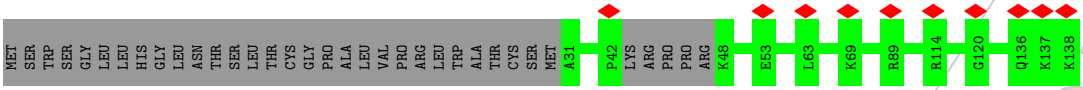
Chain I:





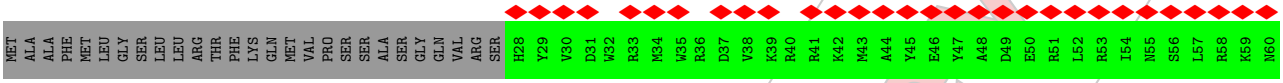
• Molecule 9: 28S ribosomal protein S12, mitochondrial

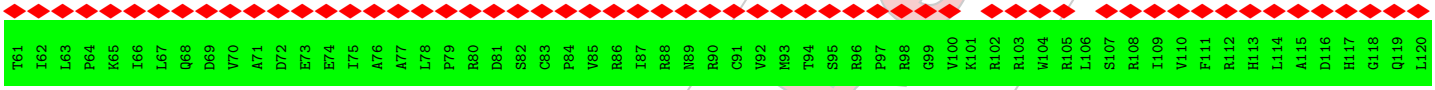
Chain J:

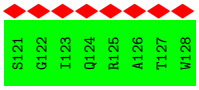


• Molecule 10: 28S ribosomal protein S14, mitochondrial

Chain K:







• Molecule 11: 28S ribosomal protein S15, mitochondrial

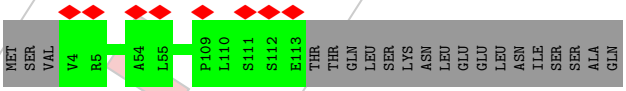
Chain L:

• Molecule 12: 28S ribosomal protein S16, mitochondrial

Chain M:

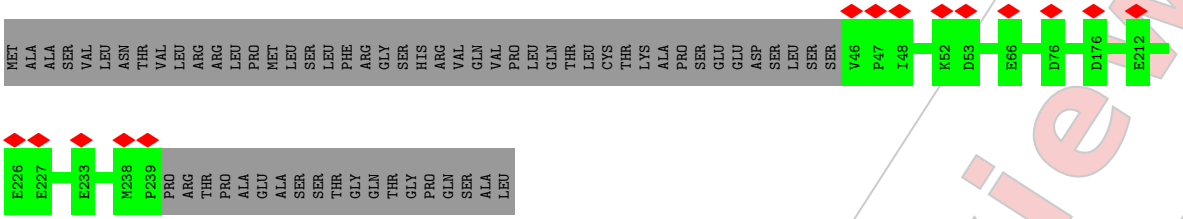
• Molecule 13: 28S ribosomal protein S17, mitochondrial

Chain N:

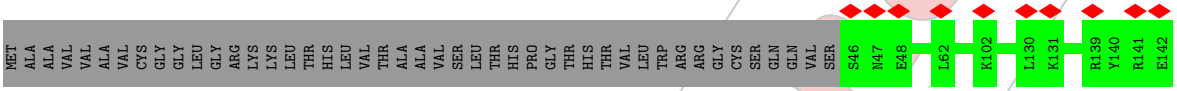


• Molecule 14: 28S ribosomal protein S18b, mitochondrial

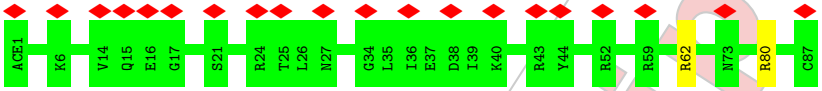
Chain O:



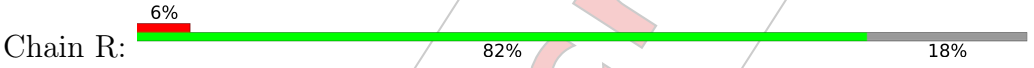
• Molecule 15: 28S ribosomal protein S18c, mitochondrial

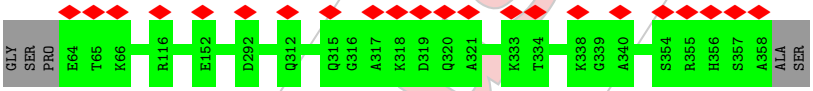


• Molecule 16: Small ribosomal subunit protein bS21m

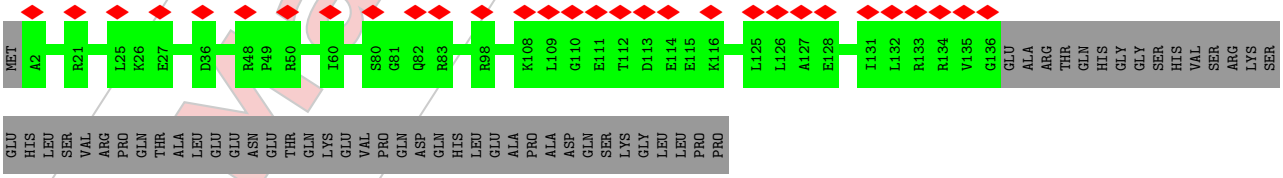


• Molecule 17: 28S ribosomal protein S22, mitochondrial

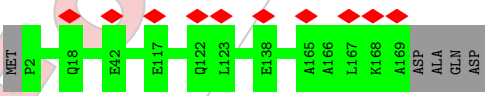




• Molecule 18: 28S ribosomal protein S23, mitochondrial

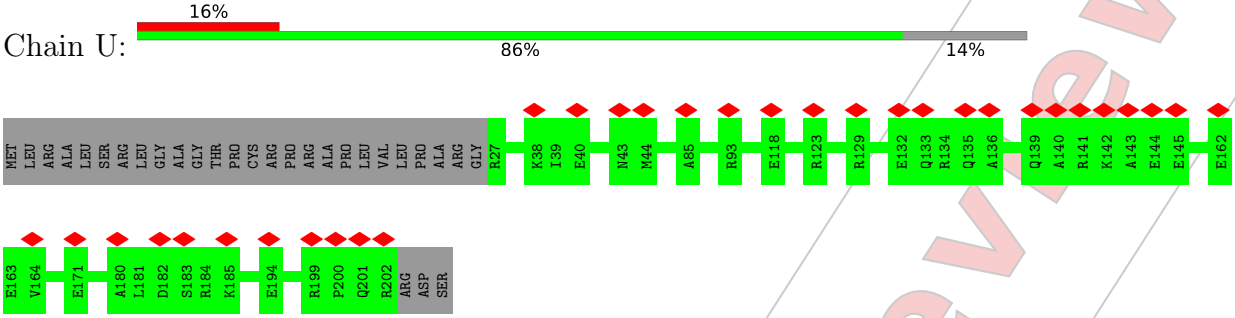


• Molecule 19: 28S ribosomal protein S25, mitochondrial



• Molecule 20: 28S ribosomal protein S26, mitochondrial

Chain U:

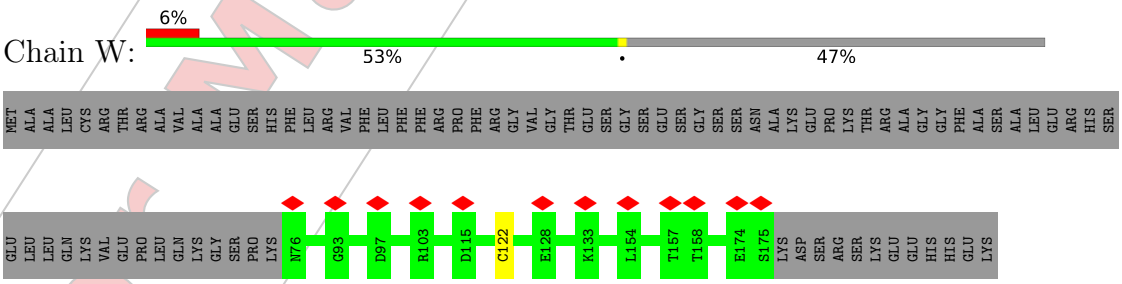


• Molecule 21: 28S ribosomal protein S27, mitochondrial

Chain V:

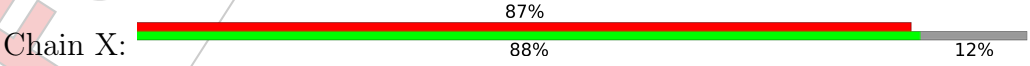
• Molecule 22: 28S ribosomal protein S28, mitochondrial

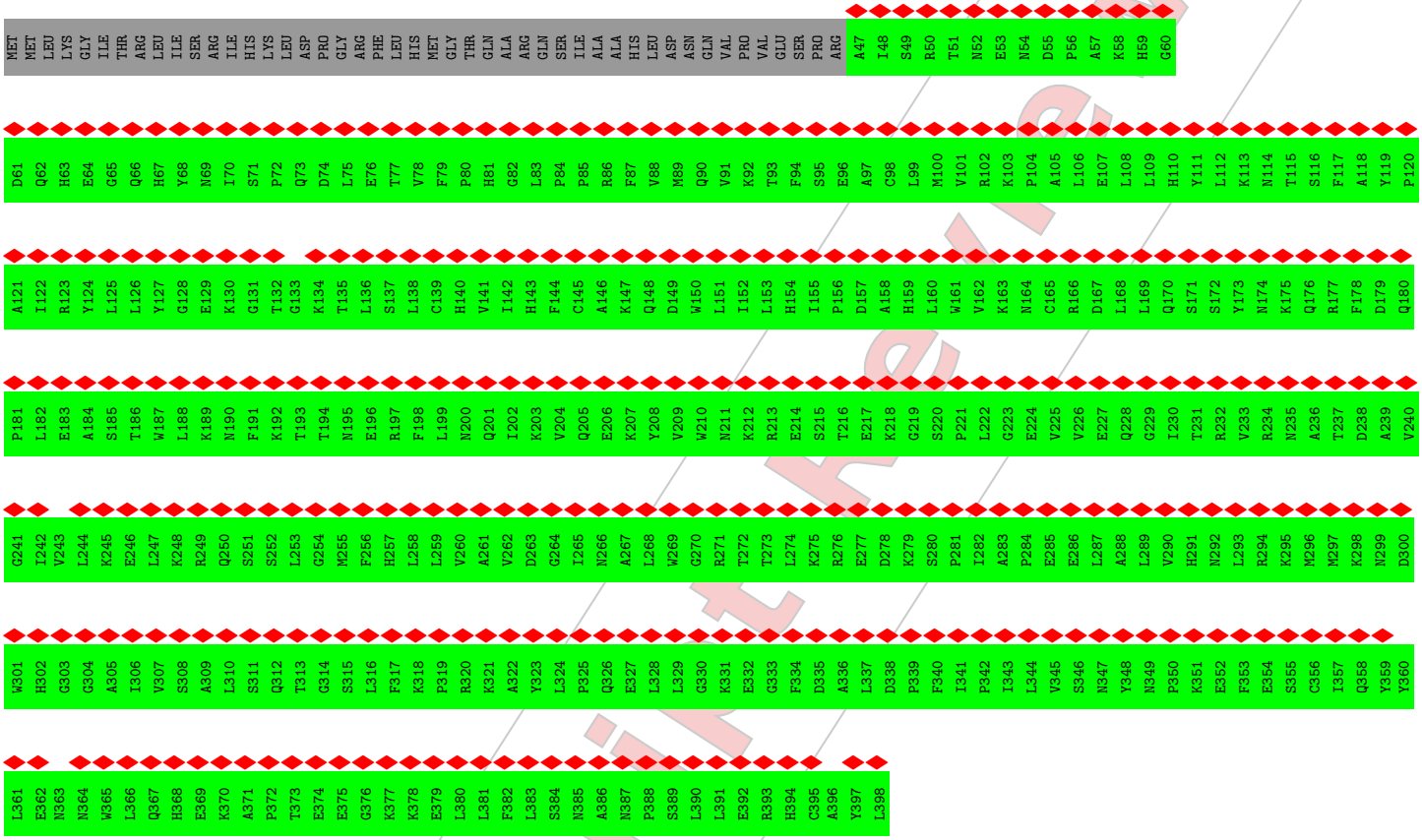
Chain W:



• Molecule 23: 28S ribosomal protein S29, mitochondrial

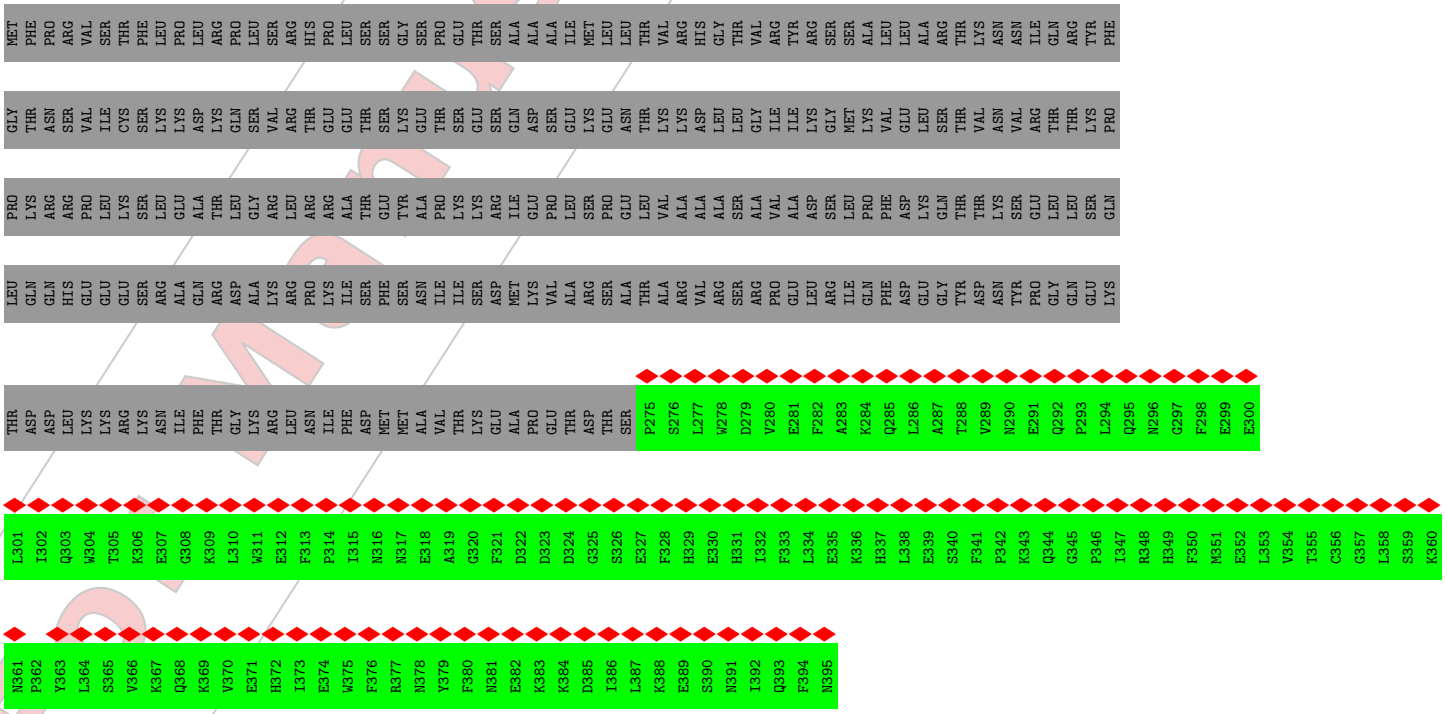
Chain X:





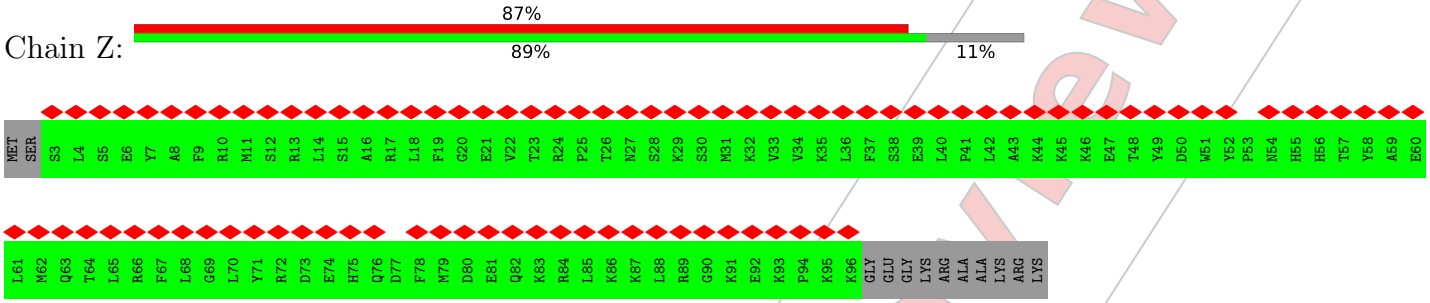
• Molecule 24: 28S ribosomal protein S31, mitochondrial

Chain Y:



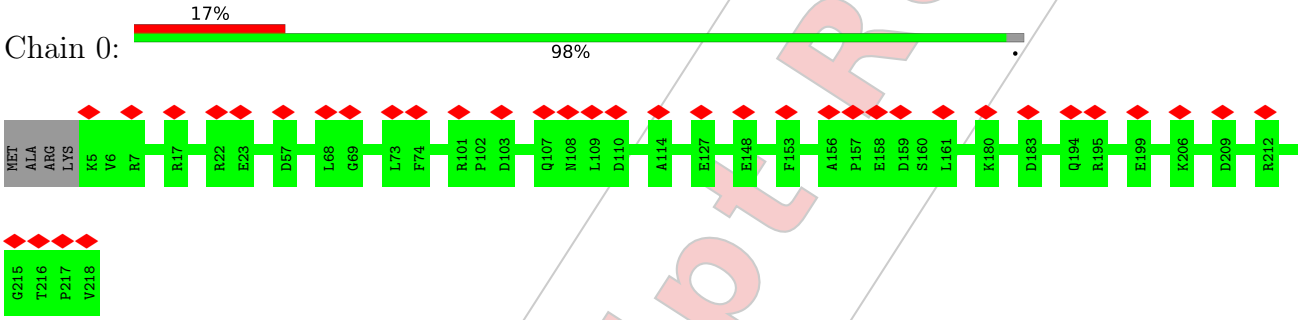
• Molecule 25: 28S ribosomal protein S33, mitochondrial

Chain Z:



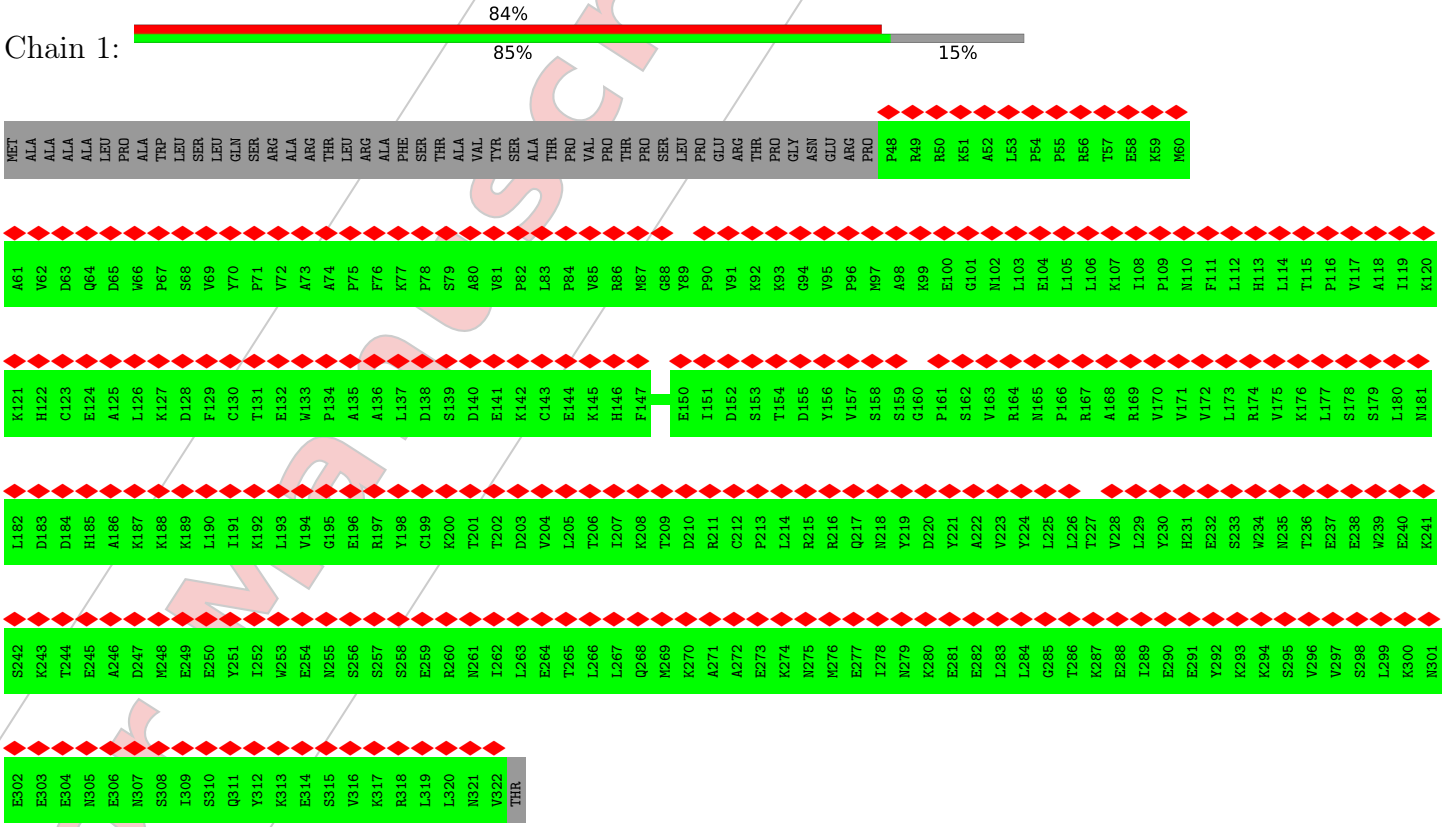
• Molecule 26: 28S ribosomal protein S34, mitochondrial

Chain 0:



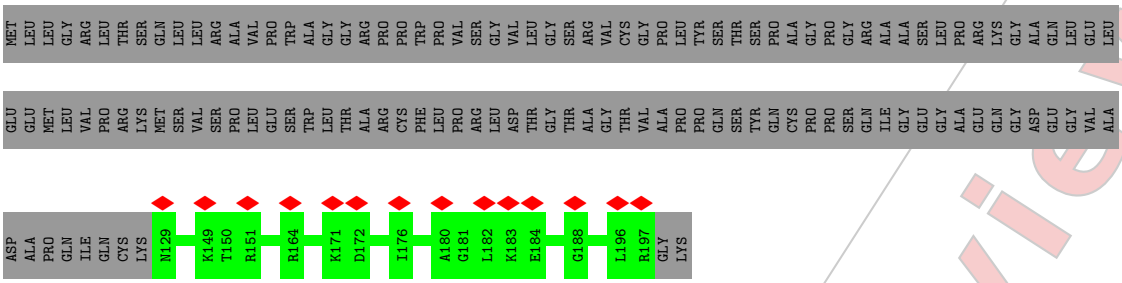
• Molecule 27: 28S ribosomal protein S35, mitochondrial

Chain 1:



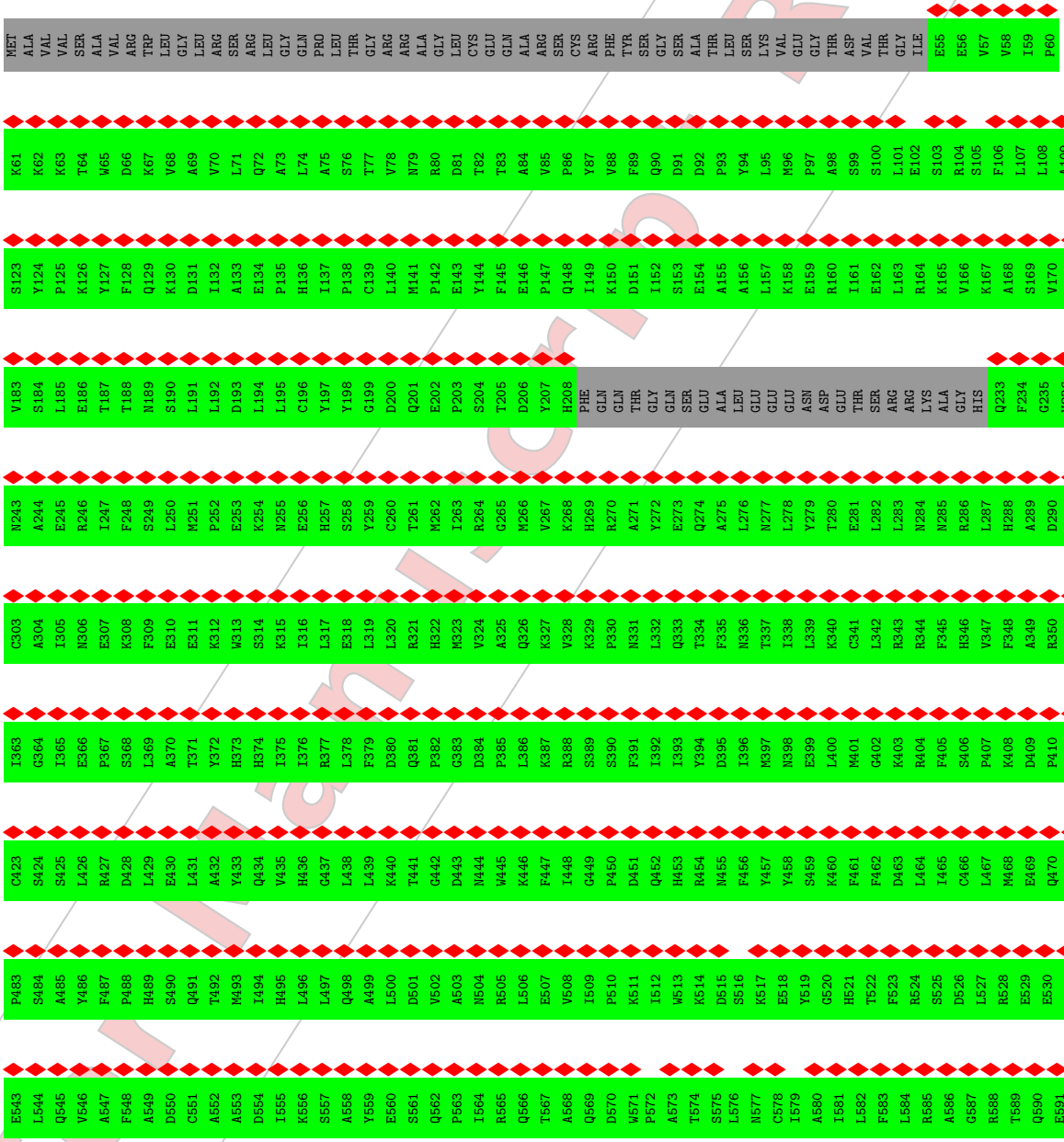
• Molecule 28: Aurora kinase A-interacting protein

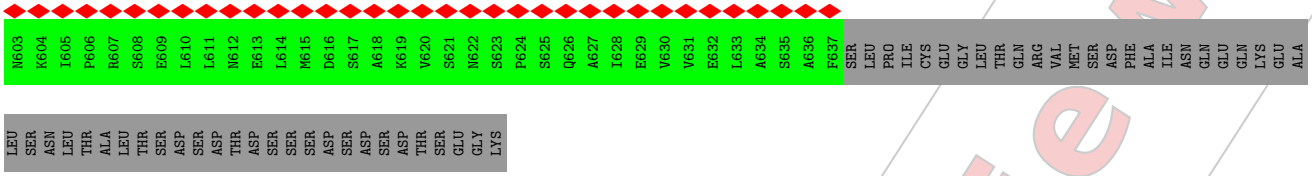
Chain 3:



• Molecule 29: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

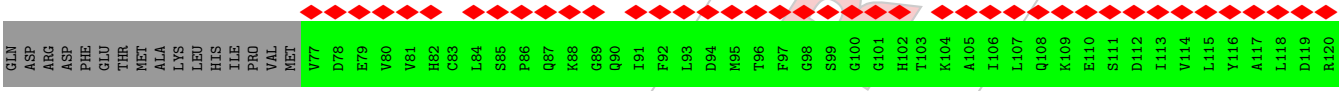
Chain 4:

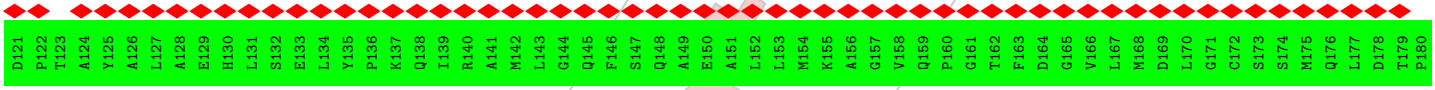


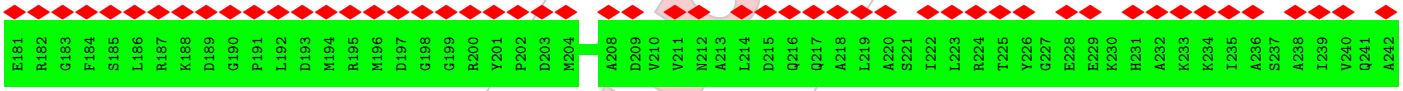


• Molecule 30: 12S rRNA N4-methylcytidine (m4C) methyltransferase

Chain b:

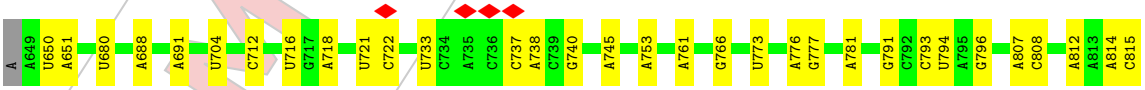


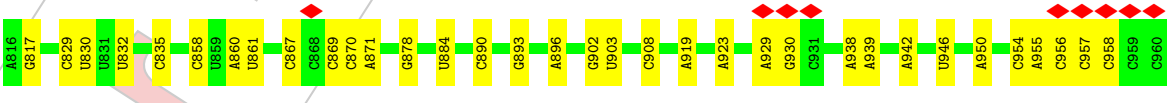


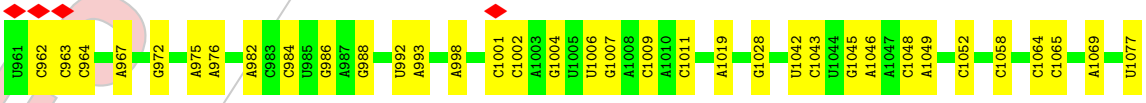


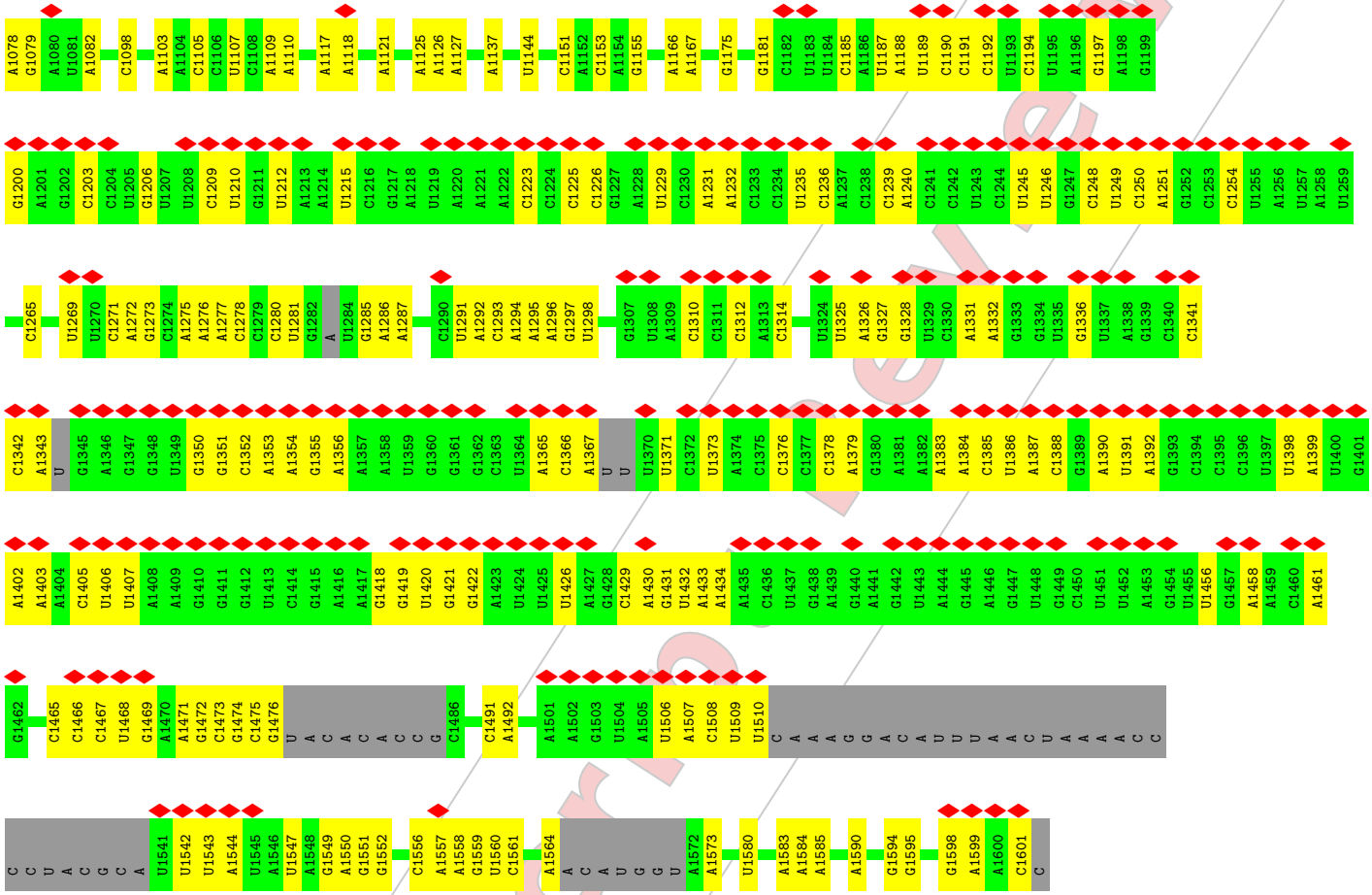
• Molecule 31: 12S mitochondrial rRNA

Chain A:



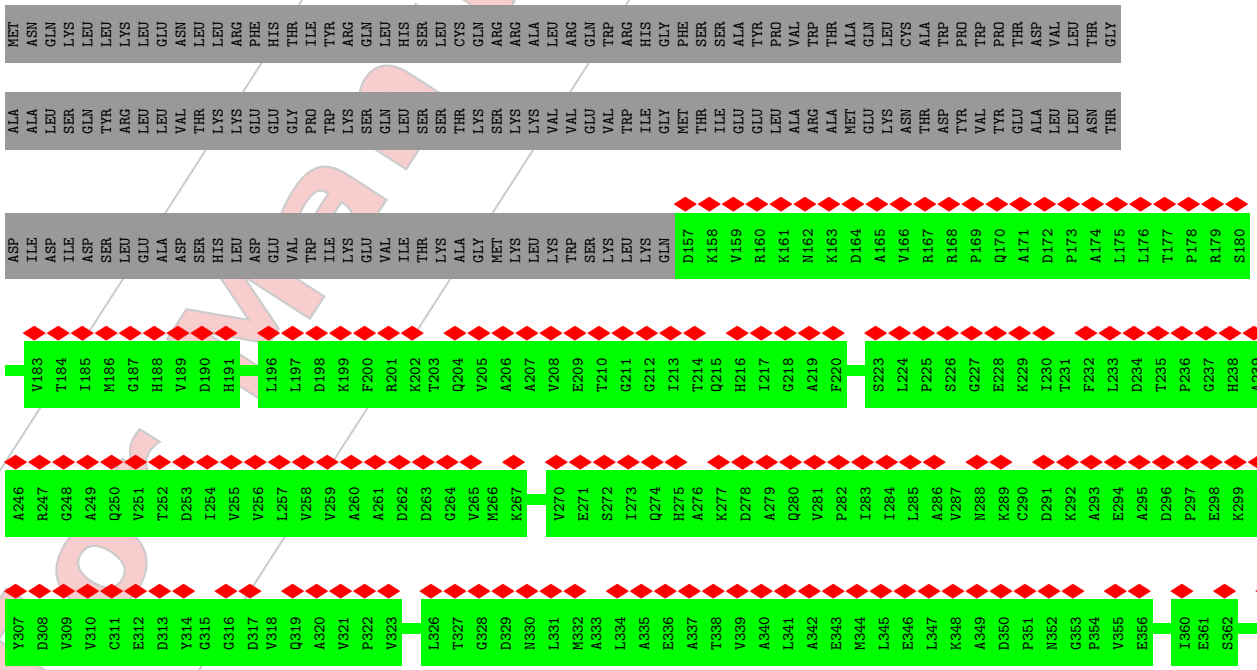




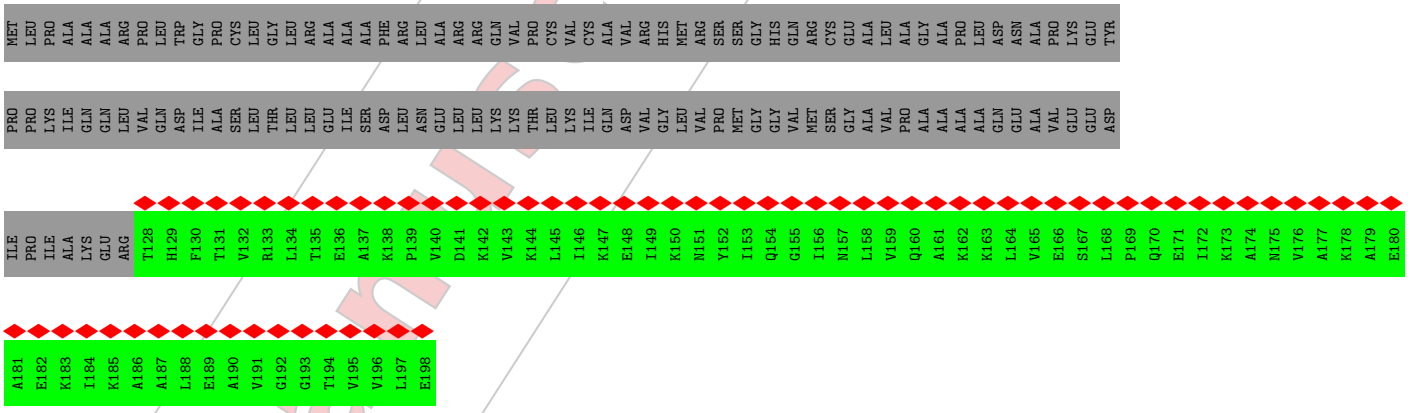


• Molecule 32: Translation initiation factor IF-2, mitochondrial

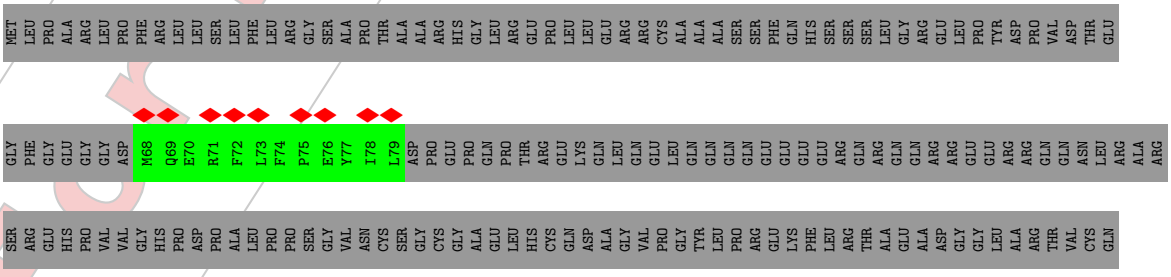
Chain 7:

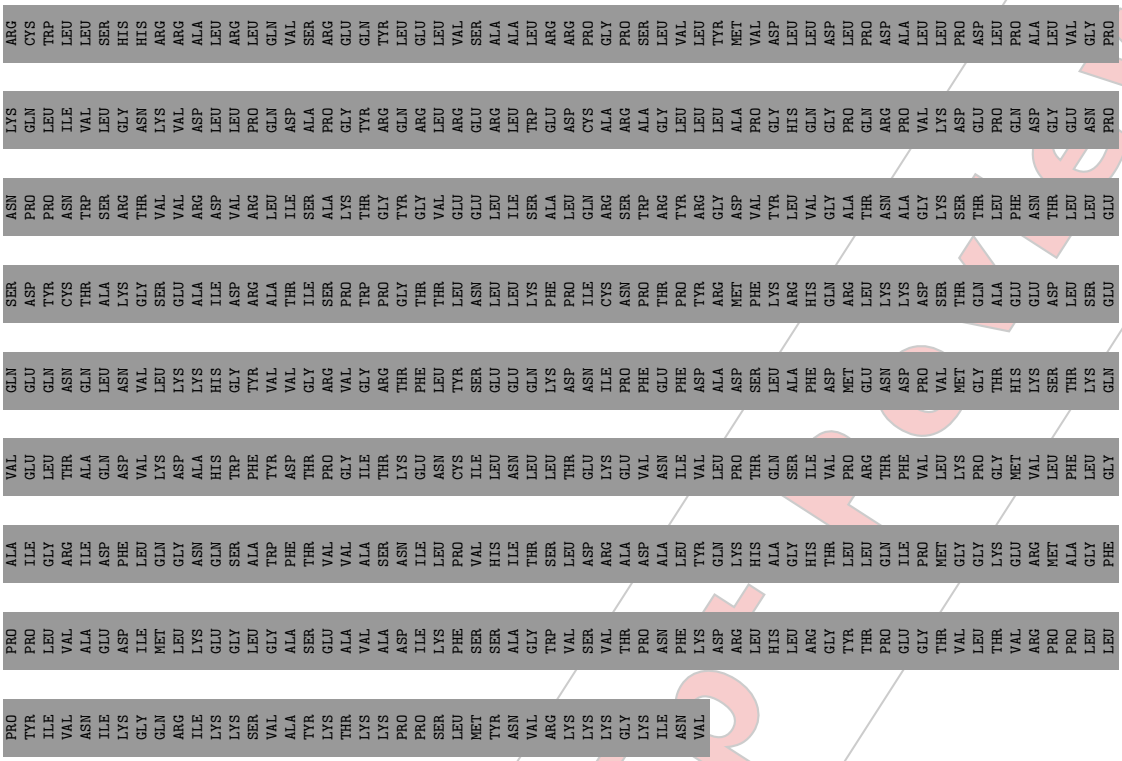


• Molecule 33: 39S ribosomal protein L12, mitochondrial

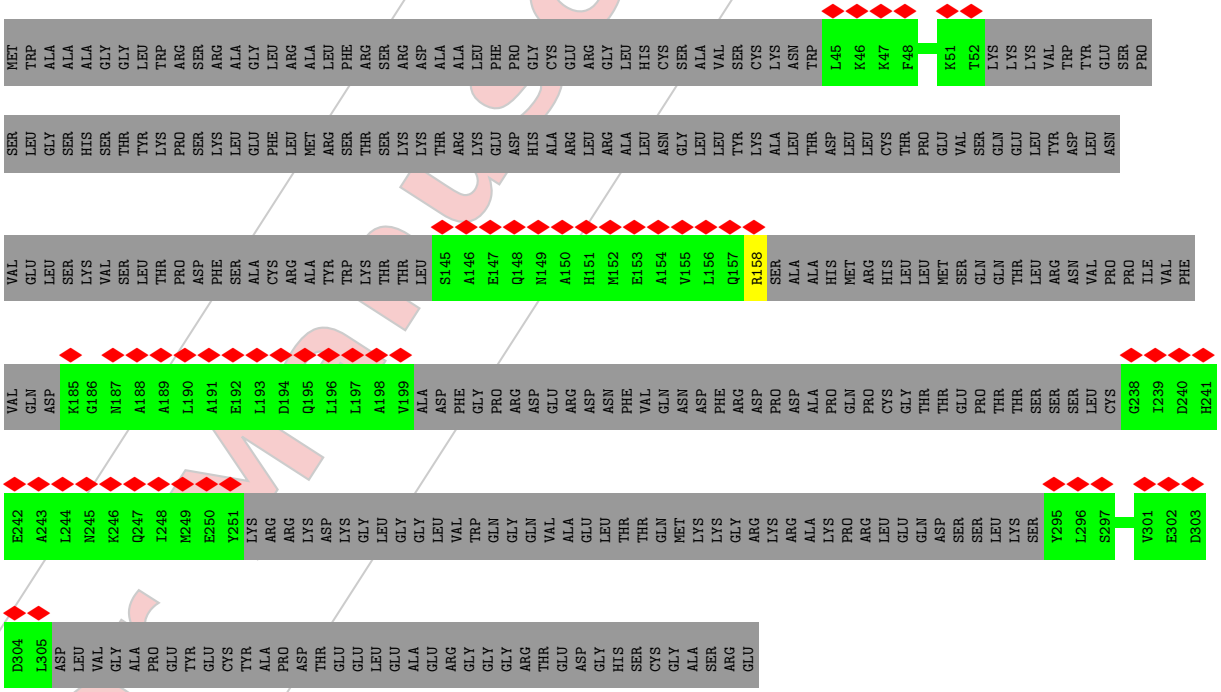


• Molecule 34: Nitric oxide-associated protein 1





• Molecule 35: Putative ribosome-binding factor A, mitochondrial



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4074	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0065	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5F0, ACE, FES, NAD, ATP, SPM, 5MC, MA6, ZN, MG, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.24	0/1871	0.49	0/2531
2	C	0.24	0/1024	0.46	0/1388
3	D	0.28	0/2663	0.52	0/3569
4	E	0.24	0/926	0.51	0/1252
5	F	0.25	0/1670	0.46	0/2241
6	G	0.28	0/2562	0.51	0/3432
7	H	0.23	0/1178	0.47	0/1598
8	I	0.28	0/1030	0.57	1/1386 (0.1%)
9	J	0.25	0/807	0.55	0/1082
10	K	0.25	0/880	0.58	0/1182
11	L	0.24	0/1477	0.47	0/1974
12	M	0.24	0/963	0.53	0/1295
13	N	0.24	0/886	0.49	0/1199
14	O	0.24	0/1655	0.49	0/2254
15	P	0.25	0/798	0.43	0/1070
16	c	0.36	0/754	0.62	0/1003
17	R	0.24	0/2456	0.45	0/3317
18	S	0.25	0/1138	0.51	0/1533
19	T	0.25	0/1402	0.46	0/1883
20	U	0.23	0/1510	0.53	0/2025
21	V	0.24	0/2967	0.42	0/4009
22	W	0.35	0/801	0.60	0/1079
23	X	0.24	0/2921	0.44	0/3954
24	Y	0.24	0/1054	0.37	0/1421
25	Z	0.32	0/815	0.52	0/1087
26	0	0.23	0/1825	0.54	0/2473
27	1	0.24	0/2277	0.44	0/3080
28	3	0.25	0/627	0.65	0/828
29	4	0.24	0/4651	0.43	0/6293
30	b	0.34	0/2420	0.51	0/3262
31	A	0.22	0/21373	0.71	1/33262 (0.0%)
32	7	0.25	0/3554	0.46	0/4805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	t	0.23	0/551	0.42	0/740
34	9	0.30	0/114	0.50	0/152
35	a	0.45	0/482	0.55	0/640
All	All	0.25	0/74082	0.57	2/104299 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	2
5	F	0	1
6	G	0	3
8	I	0	1
16	c	0	2
30	b	0	4
35	a	0	1
All	All	0	14

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	976	A	O4'-C1'-N9	11.26	117.21	108.20
8	I	185	GLY	O-C-N	-7.36	110.92	122.70

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	128	ARG	Sidechain
3	D	284	ARG	Sidechain
5	F	36	ARG	Sidechain
6	G	276	ARG	Sidechain
6	G	377	ARG	Sidechain
6	G	379	ARG	Sidechain
8	I	184	5F0	Peptide
35	a	158	ARG	Sidechain
30	b	327	ARG	Sidechain
30	b	331	ARG	Sidechain

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Mol	Chain	Res	Type	Group
30	b	369	ARG	Sidechain
30	b	370	ARG	Sidechain
16	c	62	ARG	Sidechain
16	c	80	ARG	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	223/296 (75%)	217 (97%)	6 (3%)	0	100	100
2	C	119/167 (71%)	116 (98%)	3 (2%)	0	100	100
3	D	321/430 (75%)	301 (94%)	20 (6%)	0	100	100
4	E	113/125 (90%)	109 (96%)	4 (4%)	0	100	100
5	F	197/242 (81%)	193 (98%)	4 (2%)	0	100	100
6	G	300/396 (76%)	284 (95%)	16 (5%)	0	100	100
7	H	138/201 (69%)	133 (96%)	5 (4%)	0	100	100
8	I	134/194 (69%)	123 (92%)	11 (8%)	0	100	100
9	J	99/138 (72%)	92 (93%)	7 (7%)	0	100	100
10	K	99/128 (77%)	99 (100%)	0	0	100	100
11	L	172/257 (67%)	167 (97%)	5 (3%)	0	100	100
12	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
13	N	108/130 (83%)	102 (94%)	6 (6%)	0	100	100
14	O	192/258 (74%)	184 (96%)	8 (4%)	0	100	100
15	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	c	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
17	R	293/360 (81%)	286 (98%)	7 (2%)	0	100	100
18	S	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
19	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
20	U	174/205 (85%)	171 (98%)	3 (2%)	0	100	100
21	V	351/414 (85%)	344 (98%)	7 (2%)	0	100	100
22	W	98/187 (52%)	93 (95%)	5 (5%)	0	100	100
23	X	350/398 (88%)	337 (96%)	13 (4%)	0	100	100
24	Y	119/395 (30%)	118 (99%)	1 (1%)	0	100	100
25	Z	92/106 (87%)	91 (99%)	1 (1%)	0	100	100
26	0	212/218 (97%)	205 (97%)	7 (3%)	0	100	100
27	1	273/323 (84%)	260 (95%)	13 (5%)	0	100	100
28	3	67/199 (34%)	65 (97%)	2 (3%)	0	100	100
29	4	555/689 (81%)	540 (97%)	15 (3%)	0	100	100
30	b	301/407 (74%)	285 (95%)	16 (5%)	0	100	100
32	7	449/727 (62%)	410 (91%)	39 (9%)	0	100	100
33	t	69/198 (35%)	68 (99%)	1 (1%)	0	100	100
34	9	10/698 (1%)	10 (100%)	0	0	100	100
35	a	52/343 (15%)	42 (81%)	10 (19%)	0	100	100
All	All	6276/9558 (66%)	6031 (96%)	245 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	198/249 (80%)	198 (100%)	0	100	100
2	C	106/143 (74%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	276/357 (77%)	276 (100%)	0	100	100
4	E	97/107 (91%)	97 (100%)	0	100	100
5	F	178/209 (85%)	177 (99%)	1 (1%)	84	88
6	G	264/342 (77%)	264 (100%)	0	100	100
7	H	130/180 (72%)	130 (100%)	0	100	100
8	I	104/146 (71%)	104 (100%)	0	100	100
9	J	88/118 (75%)	88 (100%)	0	100	100
10	K	91/113 (80%)	91 (100%)	0	100	100
11	L	158/226 (70%)	158 (100%)	0	100	100
12	M	97/113 (86%)	97 (100%)	0	100	100
13	N	96/115 (84%)	96 (100%)	0	100	100
14	O	175/230 (76%)	175 (100%)	0	100	100
15	P	88/123 (72%)	88 (100%)	0	100	100
16	c	78/78 (100%)	78 (100%)	0	100	100
17	R	264/318 (83%)	264 (100%)	0	100	100
18	S	116/164 (71%)	116 (100%)	0	100	100
19	T	153/157 (98%)	153 (100%)	0	100	100
20	U	152/174 (87%)	152 (100%)	0	100	100
21	V	319/364 (88%)	319 (100%)	0	100	100
22	W	87/158 (55%)	86 (99%)	1 (1%)	70	79
23	X	311/351 (89%)	311 (100%)	0	100	100
24	Y	112/357 (31%)	112 (100%)	0	100	100
25	Z	87/95 (92%)	87 (100%)	0	100	100
26	0	187/190 (98%)	187 (100%)	0	100	100
27	1	253/291 (87%)	253 (100%)	0	100	100
28	3	64/166 (39%)	64 (100%)	0	100	100
29	4	500/609 (82%)	500 (100%)	0	100	100
30	b	255/350 (73%)	252 (99%)	3 (1%)	67	78
32	7	377/621 (61%)	377 (100%)	0	100	100
33	t	59/158 (37%)	59 (100%)	0	100	100
34	9	12/600 (2%)	12 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	a	50/288 (17%)	50 (100%)	0	100	100
All	All	5582/8260 (68%)	5577 (100%)	5 (0%)	92	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	81	LYS
22	W	122	CYS
30	b	323	SER
30	b	334	LEU
30	b	381	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	280	HIS
3	D	341	ASN
8	I	183	HIS
11	L	162	GLN
16	c	85	GLN
23	X	174	ASN
24	Y	290	ASN
26	0	145	HIS
29	4	285	ASN
29	4	295	ASN
29	4	577	ASN
30	b	241	GLN
32	7	215	GLN
32	7	453	GLN
34	9	69	GLN
35	a	241	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	A	894/955 (93%)	275 (30%)	12 (1%)

All (275) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	A	650	U
31	A	651	A
31	A	680	U
31	A	688	A
31	A	691	A
31	A	704	U
31	A	712	C
31	A	716	U
31	A	718	A
31	A	721	U
31	A	722	C
31	A	733	U
31	A	737	C
31	A	738	A
31	A	740	G
31	A	745	A
31	A	753	A
31	A	761	A
31	A	766	G
31	A	773	U
31	A	776	A
31	A	777	G
31	A	781	A
31	A	791	G
31	A	793	C
31	A	794	U
31	A	796	G
31	A	807	A
31	A	808	C
31	A	812	A
31	A	814	A
31	A	815	C
31	A	817	G
31	A	829	C
31	A	830	U
31	A	832	U
31	A	835	C
31	A	858	C
31	A	860	A
31	A	861	U
31	A	867	C
31	A	869	C
31	A	870	C

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Mol	Chain	Res	Type
31	A	871	A
31	A	878	G
31	A	884	U
31	A	890	C
31	A	893	G
31	A	896	A
31	A	902	G
31	A	903	U
31	A	908	C
31	A	919	A
31	A	923	A
31	A	929	A
31	A	930	G
31	A	938	A
31	A	939	A
31	A	942	A
31	A	946	U
31	A	950	A
31	A	954	C
31	A	955	A
31	A	956	C
31	A	957	C
31	A	958	C
31	A	962	C
31	A	963	C
31	A	964	C
31	A	967	A
31	A	972	G
31	A	975	A
31	A	982	A
31	A	984	C
31	A	986	G
31	A	988	G
31	A	992	U
31	A	993	A
31	A	998	A
31	A	1001	C
31	A	1002	C
31	A	1004	G
31	A	1006	U
31	A	1007	G
31	A	1009	C

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Mol	Chain	Res	Type
31	A	1011	C
31	A	1019	A
31	A	1028	G
31	A	1042	U
31	A	1043	C
31	A	1045	G
31	A	1046	A
31	A	1048	C
31	A	1049	A
31	A	1052	C
31	A	1058	C
31	A	1064	C
31	A	1065	C
31	A	1069	A
31	A	1077	U
31	A	1078	A
31	A	1079	G
31	A	1082	A
31	A	1098	C
31	A	1103	A
31	A	1105	C
31	A	1107	U
31	A	1109	A
31	A	1110	A
31	A	1117	A
31	A	1118	A
31	A	1121	A
31	A	1126	A
31	A	1127	A
31	A	1137	A
31	A	1144	U
31	A	1151	C
31	A	1153	C
31	A	1155	G
31	A	1166	A
31	A	1167	A
31	A	1175	G
31	A	1181	G
31	A	1185	C
31	A	1187	U
31	A	1188	A
31	A	1189	U

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Mol	Chain	Res	Type
31	A	1190	C
31	A	1191	C
31	A	1192	C
31	A	1194	C
31	A	1197	G
31	A	1200	G
31	A	1203	C
31	A	1206	G
31	A	1209	C
31	A	1210	U
31	A	1212	U
31	A	1215	U
31	A	1223	C
31	A	1225	C
31	A	1226	C
31	A	1229	U
31	A	1231	A
31	A	1232	A
31	A	1235	U
31	A	1236	C
31	A	1239	C
31	A	1240	A
31	A	1245	U
31	A	1246	U
31	A	1248	C
31	A	1249	U
31	A	1250	C
31	A	1251	A
31	A	1254	C
31	A	1265	C
31	A	1269	U
31	A	1271	C
31	A	1272	A
31	A	1273	G
31	A	1275	A
31	A	1276	A
31	A	1277	A
31	A	1278	C
31	A	1280	C
31	A	1281	U
31	A	1285	G
31	A	1286	A

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Mol	Chain	Res	Type
31	A	1287	A
31	A	1291	U
31	A	1292	A
31	A	1294	A
31	A	1295	A
31	A	1296	A
31	A	1297	G
31	A	1298	U
31	A	1310	C
31	A	1312	C
31	A	1314	C
31	A	1325	U
31	A	1326	A
31	A	1327	G
31	A	1328	G
31	A	1331	A
31	A	1332	A
31	A	1336	G
31	A	1342	C
31	A	1343	A
31	A	1350	G
31	A	1351	G
31	A	1352	C
31	A	1353	A
31	A	1354	A
31	A	1355	G
31	A	1356	A
31	A	1365	A
31	A	1366	C
31	A	1367	A
31	A	1371	U
31	A	1373	U
31	A	1376	C
31	A	1378	C
31	A	1379	A
31	A	1383	A
31	A	1384	A
31	A	1385	C
31	A	1386	U
31	A	1387	A
31	A	1388	C
31	A	1390	A

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Mol	Chain	Res	Type
31	A	1391	U
31	A	1392	A
31	A	1398	U
31	A	1399	A
31	A	1402	A
31	A	1403	A
31	A	1405	C
31	A	1406	U
31	A	1407	U
31	A	1418	G
31	A	1419	G
31	A	1420	U
31	A	1421	G
31	A	1422	G
31	A	1426	U
31	A	1429	C
31	A	1430	A
31	A	1431	G
31	A	1432	U
31	A	1433	A
31	A	1434	A
31	A	1456	U
31	A	1458	A
31	A	1461	A
31	A	1465	C
31	A	1466	C
31	A	1467	C
31	A	1468	U
31	A	1469	G
31	A	1471	A
31	A	1472	G
31	A	1473	C
31	A	1474	G
31	A	1475	C
31	A	1476	G
31	A	1491	C
31	A	1492	A
31	A	1506	U
31	A	1507	A
31	A	1508	C
31	A	1509	U
31	A	1510	U

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Mol	Chain	Res	Type
31	A	1543	U
31	A	1544	A
31	A	1547	U
31	A	1549	G
31	A	1551	G
31	A	1552	G
31	A	1556	C
31	A	1557	A
31	A	1558	A
31	A	1559	G
31	A	1560	U
31	A	1561	C
31	A	1564	A
31	A	1573	A
31	A	1580	U
31	A	1585	A
31	A	1590	A
31	A	1594	G
31	A	1595	G
31	A	1598	G
31	A	1599	A
31	A	1601	C

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	A	1125	A
31	A	1293	C
31	A	1326	A
31	A	1341	C
31	A	1353	A
31	A	1386	U
31	A	1429	C
31	A	1432	U
31	A	1472	G
31	A	1542	U
31	A	1550	A
31	A	1598	G

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	MA6	A	1584	31	18,26,27	1.00	2 (11%)	19,38,41	3.25	2 (10%)
31	5MC	A	1488	31	18,22,23	0.53	0	26,32,35	0.55	0
8	5F0	I	184	8	8,8,9	0.58	0	7,9,11	1.19	1 (14%)
31	MA6	A	1583	31	18,26,27	1.00	2 (11%)	19,38,41	3.25	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	MA6	A	1584	31	-	3/7/29/30	0/3/3/3
31	5MC	A	1488	31	-	0/7/25/26	0/2/2/2
8	5F0	I	184	8	-	1/9/9/10	-
31	MA6	A	1583	31	-	4/7/29/30	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	1584	MA6	C5-C4	-2.53	1.34	1.40
31	A	1583	MA6	C2-N3	2.50	1.36	1.32
31	A	1583	MA6	C5-C4	-2.48	1.34	1.40
31	A	1584	MA6	C2-N3	2.46	1.36	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	1584	MA6	N1-C6-N6	-12.80	103.59	117.06
31	A	1583	MA6	N1-C6-N6	-12.56	103.84	117.06
31	A	1584	MA6	N3-C2-N1	-5.50	120.08	128.68
31	A	1583	MA6	N3-C2-N1	-5.43	120.19	128.68
8	I	184	5F0	O-C-CB	-2.76	117.39	125.43
31	A	1583	MA6	C3'-C2'-C1'	2.13	104.19	100.98

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	A	1583	MA6	C5-C6-N6-C9
31	A	1583	MA6	C5-C6-N6-C10
31	A	1584	MA6	C5-C6-N6-C9
31	A	1584	MA6	C5-C6-N6-C10
31	A	1583	MA6	N1-C6-N6-C9
31	A	1584	MA6	N1-C6-N6-C9
31	A	1583	MA6	C4'-C5'-O5'-P
8	I	184	5F0	O-C-CB-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 25 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	ATP	X	501	-	26,33,33	0.61	0	31,52,52	0.94	1 (3%)
38	FES	T	201	19	0,4,4	-	-	-		
41	NAD	A	1701	36	42,48,48	0.89	2 (4%)	50,73,73	0.84	1 (2%)
40	GDP	X	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
38	FES	P	201	4,15	0,4,4	-	-	-		
40	GDP	7	801	-	24,30,30	0.93	1 (4%)	30,47,47	1.27	4 (13%)
42	SPM	A	1702	-	13,13,13	0.36	0	12,12,12	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	ATP	X	501	-	-	0/18/38/38	0/3/3/3
38	FES	T	201	19	-	-	0/1/1/1
41	NAD	A	1701	36	-	0/26/62/62	0/5/5/5
40	GDP	X	502	-	-	3/12/32/32	0/3/3/3
38	FES	P	201	4,15	-	-	0/1/1/1
40	GDP	7	801	-	-	0/12/32/32	0/3/3/3
42	SPM	A	1702	-	-	1/11/11/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	A	1701	NAD	O4D-C1D	-2.60	1.37	1.41
41	A	1701	NAD	C8A-N7A	-2.56	1.30	1.34
40	7	801	GDP	C6-N1	-2.32	1.34	1.37
40	X	502	GDP	C6-N1	-2.31	1.34	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	X	502	GDP	PA-O3A-PB	-3.61	120.43	132.83
40	7	801	GDP	PA-O3A-PB	-3.36	121.29	132.83
40	X	502	GDP	C3'-C2'-C1'	2.89	105.33	100.98
40	X	502	GDP	C8-N7-C5	2.54	107.83	102.99
40	7	801	GDP	C8-N7-C5	2.50	107.74	102.99
40	X	502	GDP	C5-C6-N1	2.41	118.21	113.95
40	7	801	GDP	C5-C6-N1	2.40	118.20	113.95
40	7	801	GDP	O4'-C1'-C2'	-2.36	103.47	106.93
39	X	501	ATP	C5-C6-N6	2.34	123.90	120.35
41	A	1701	NAD	O2A-PA-O1A	2.03	122.28	112.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

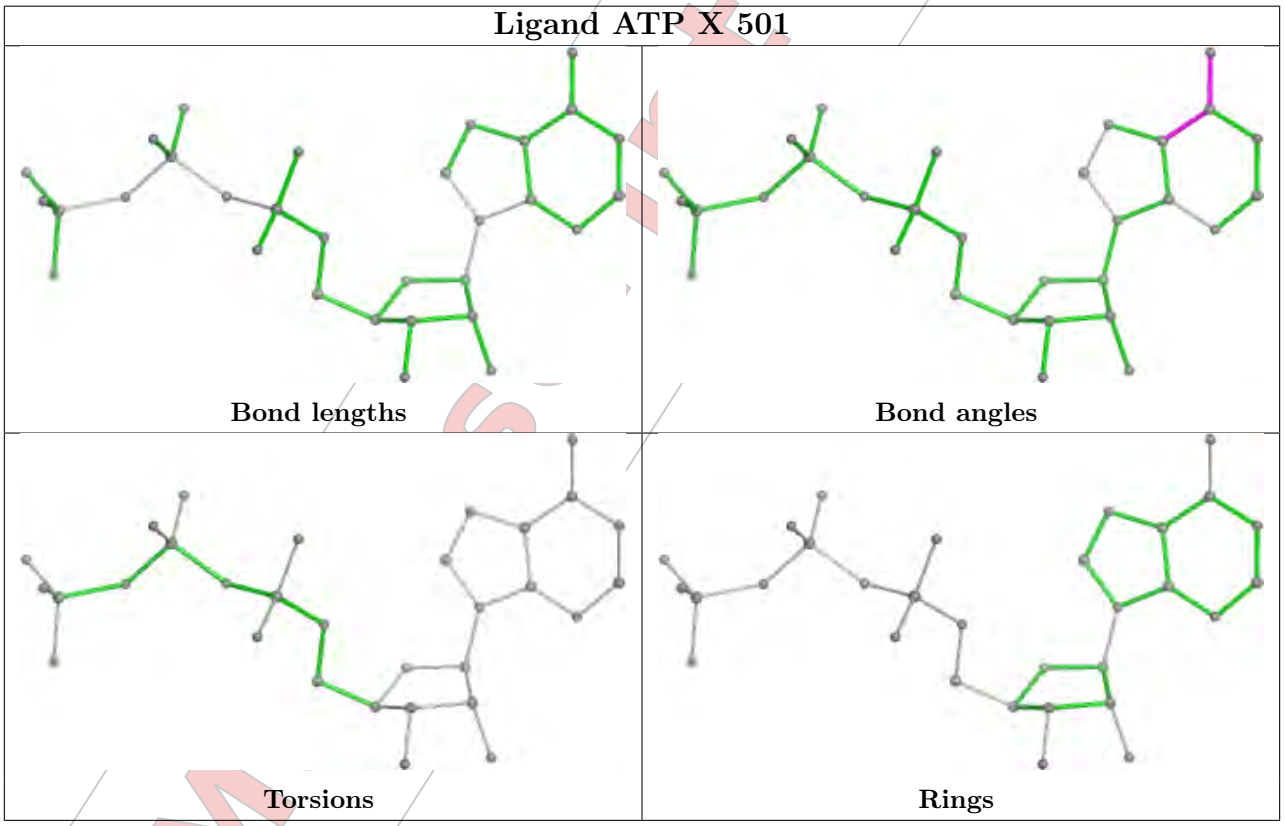
Mol	Chain	Res	Type	Atoms
40	X	502	GDP	C5'-O5'-PA-O1A
40	X	502	GDP	C4'-C5'-O5'-PA
42	A	1702	SPM	C7-C8-C9-N10
40	X	502	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

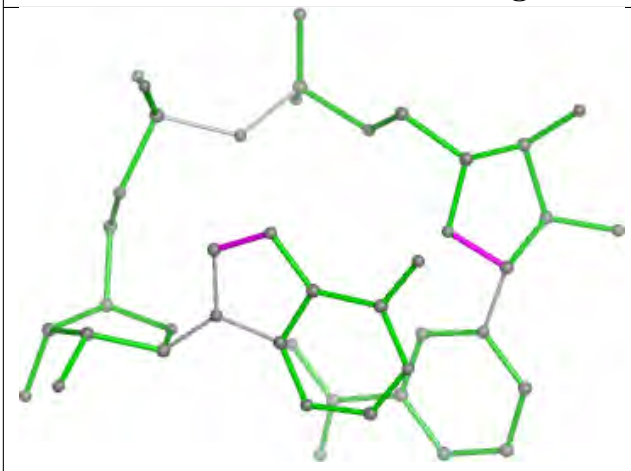
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

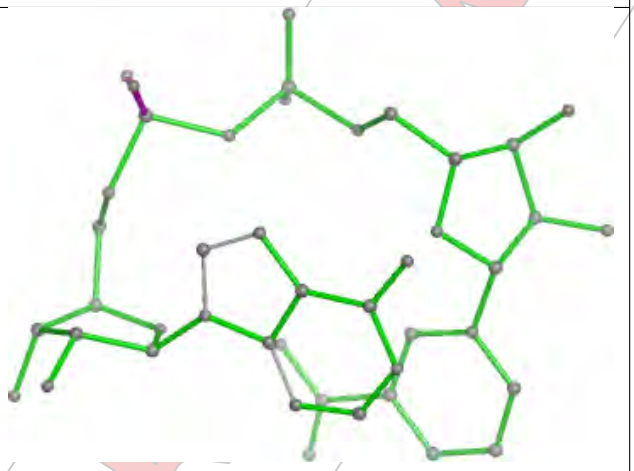
Ligand ATP X 501



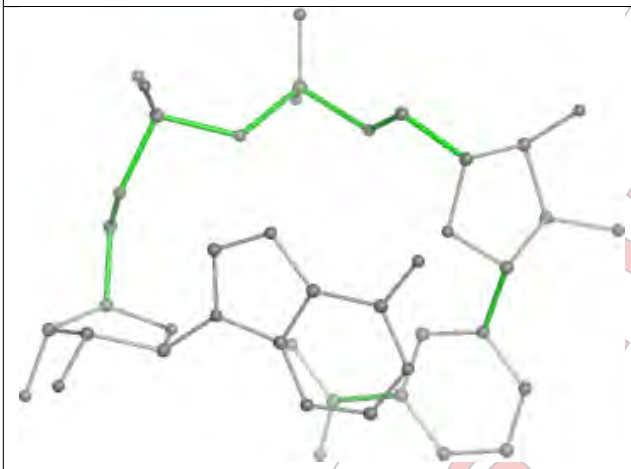
Ligand NAD A 1701



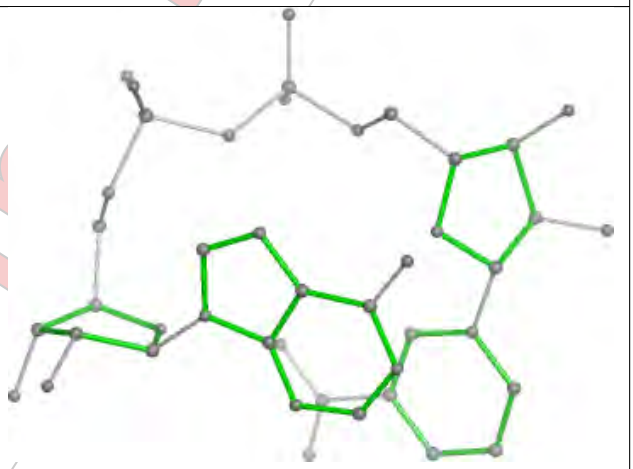
Bond lengths



Bond angles

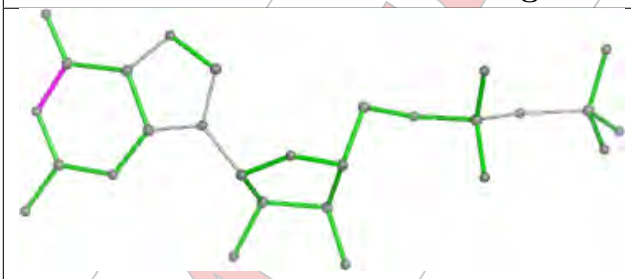


Torsions

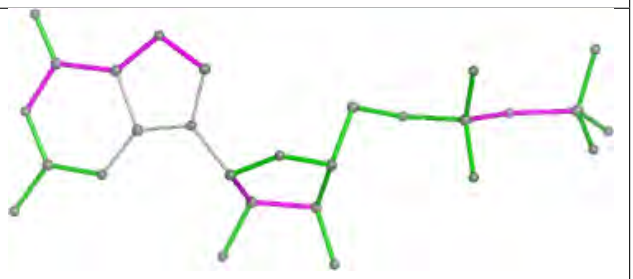


Rings

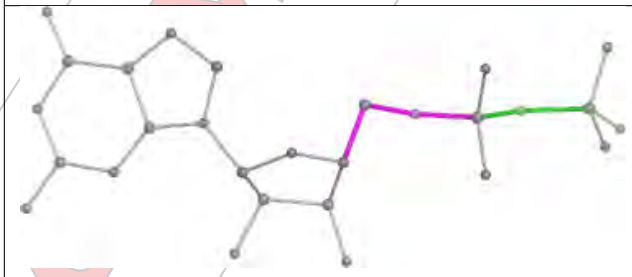
Ligand GDP X 502



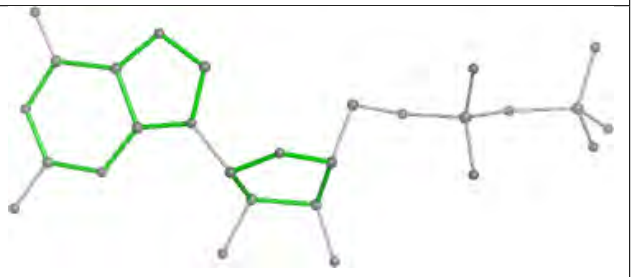
Bond lengths



Bond angles

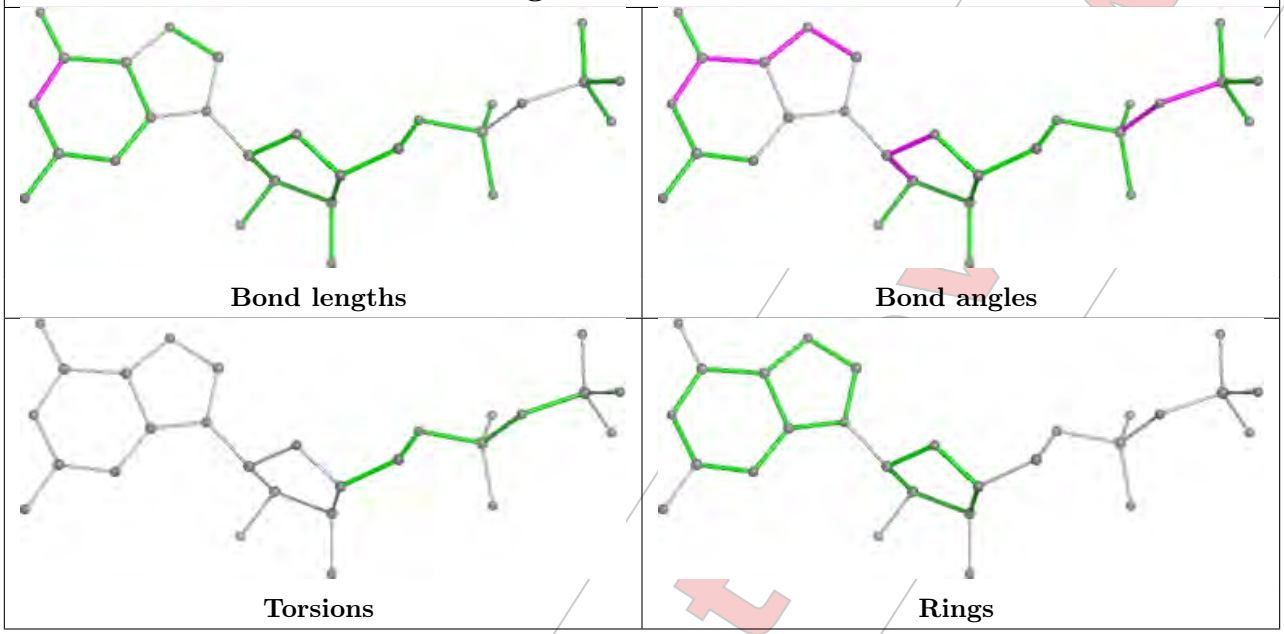


Torsions



Rings

Ligand GDP 7 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

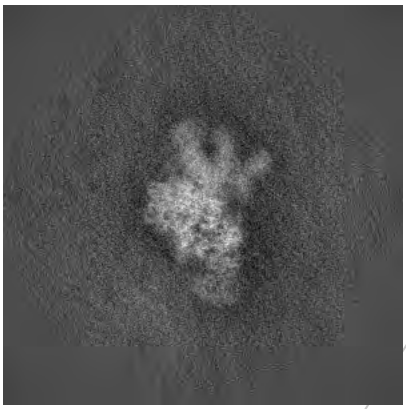
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51878. These allow visual inspection of the internal detail of the map and identification of artifacts.

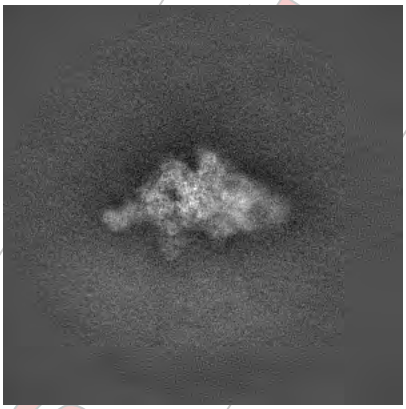
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

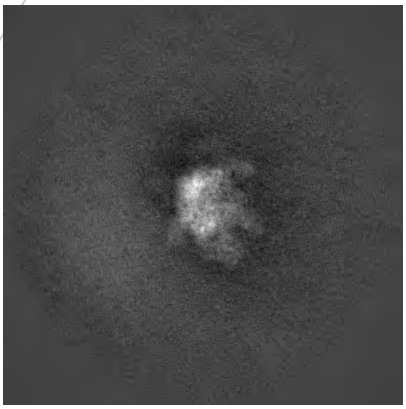
6.1.1 Primary map



X

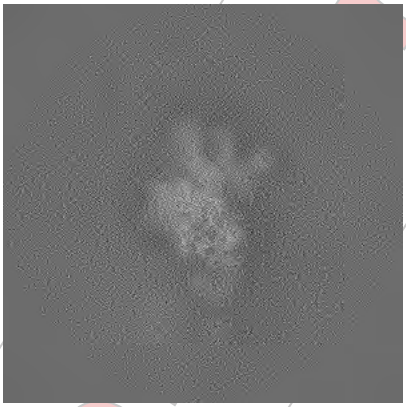


Y

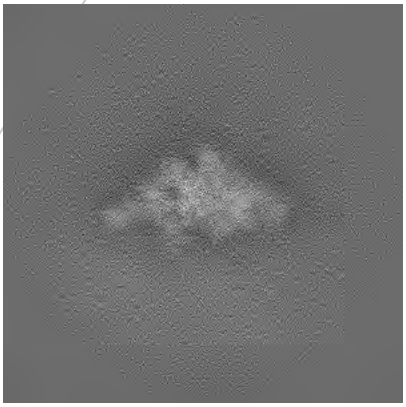


Z

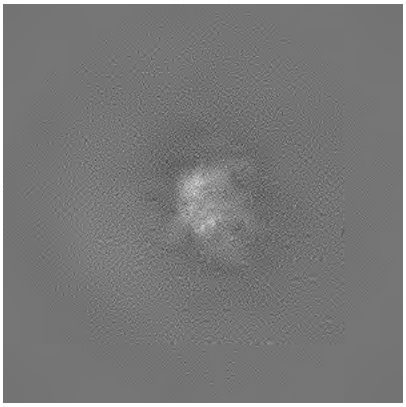
6.1.2 Raw map



X



Y

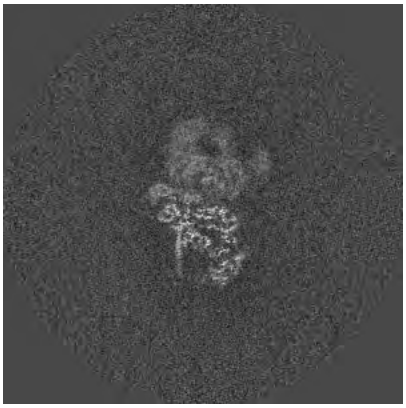


Z

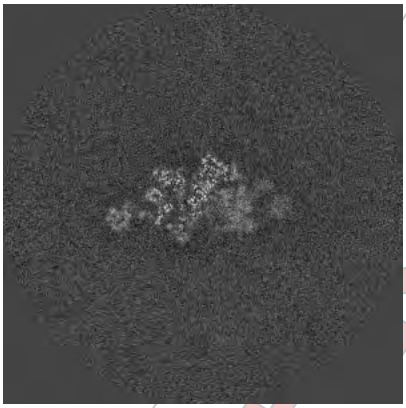
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

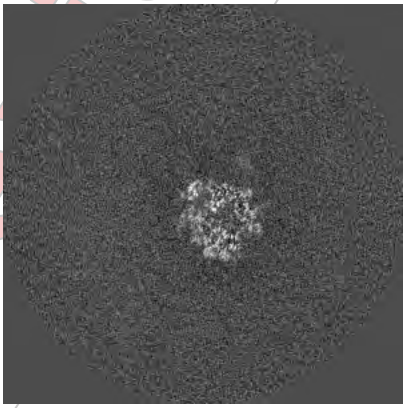
6.2.1 Primary map



X Index: 300

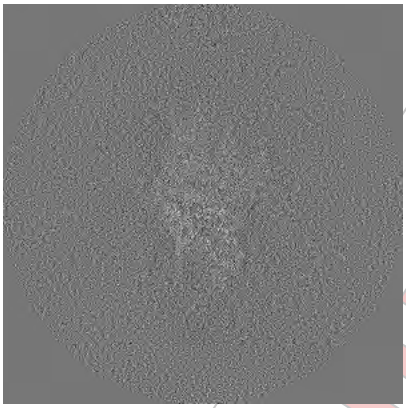


Y Index: 300

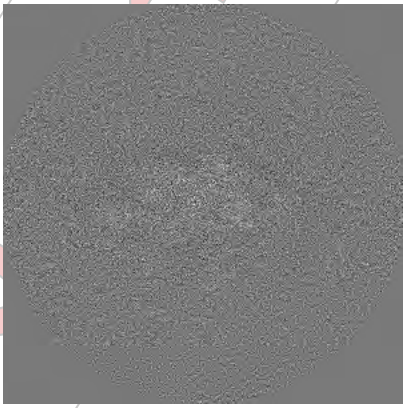


Z Index: 300

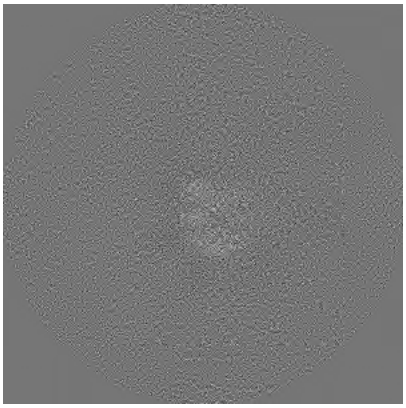
6.2.2 Raw map



X Index: 300



Y Index: 300

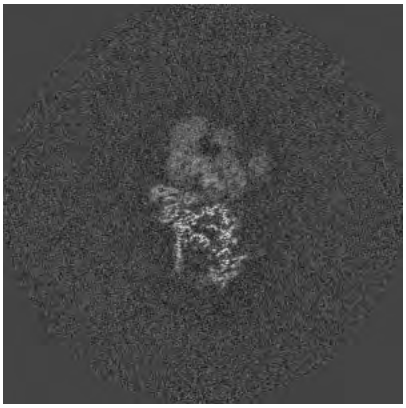


Z Index: 300

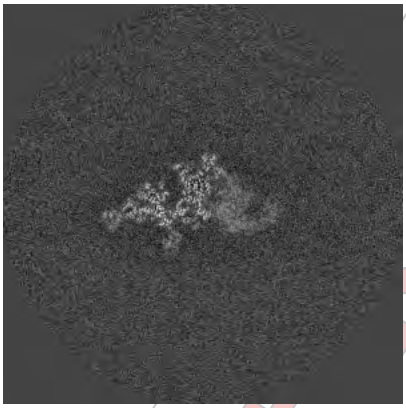
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

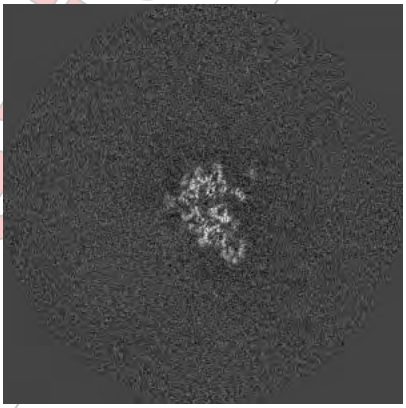
6.3.1 Primary map



X Index: 298

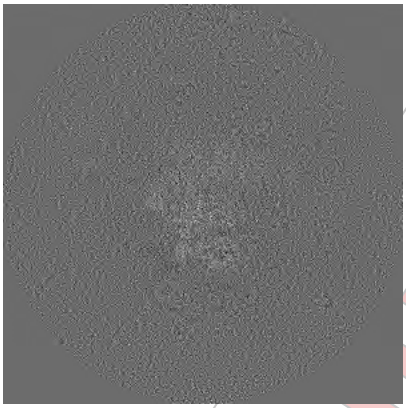


Y Index: 319

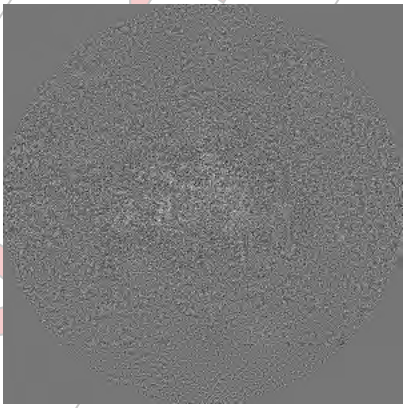


Z Index: 273

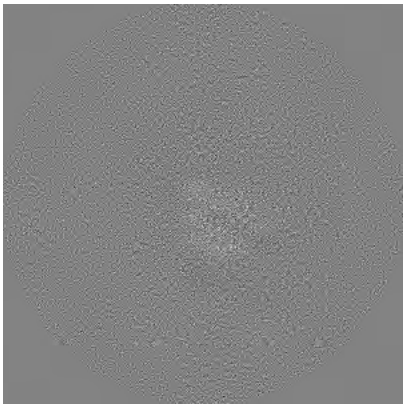
6.3.2 Raw map



X Index: 314



Y Index: 304

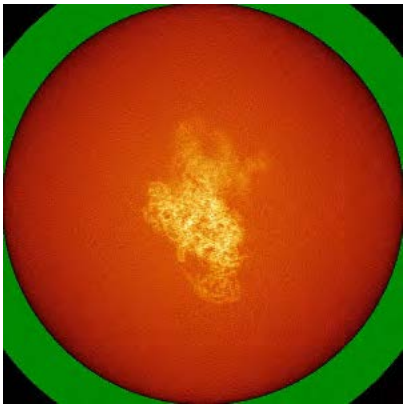


Z Index: 301

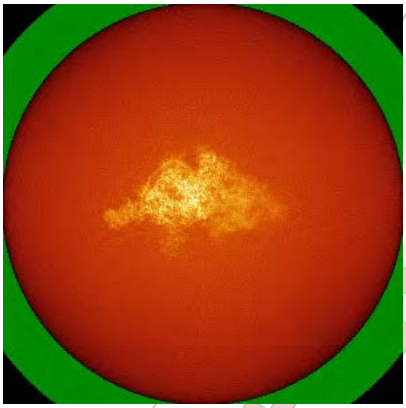
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

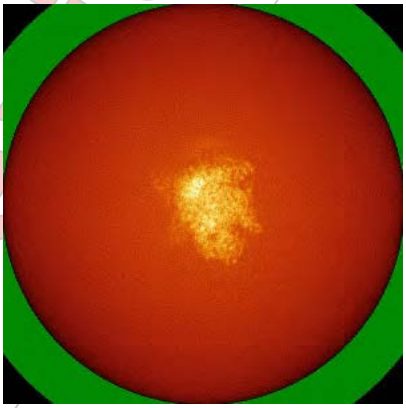
6.4.1 Primary map



X

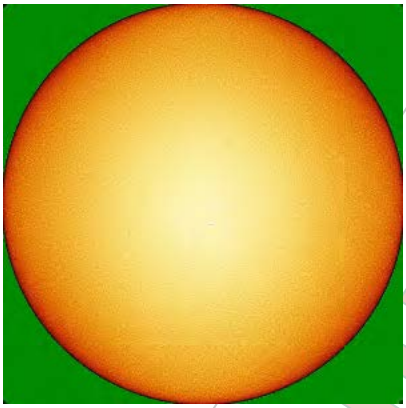


Y

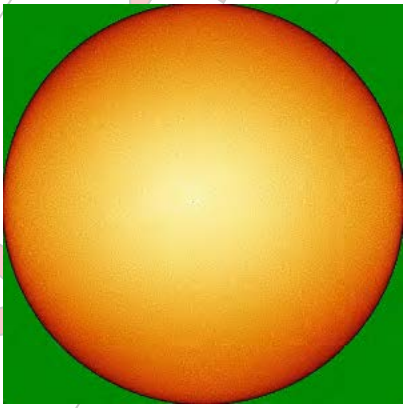


Z

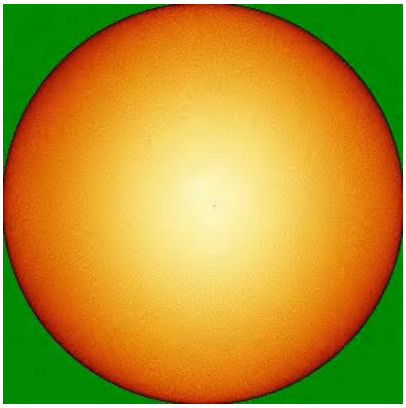
6.4.2 Raw map



X



Y

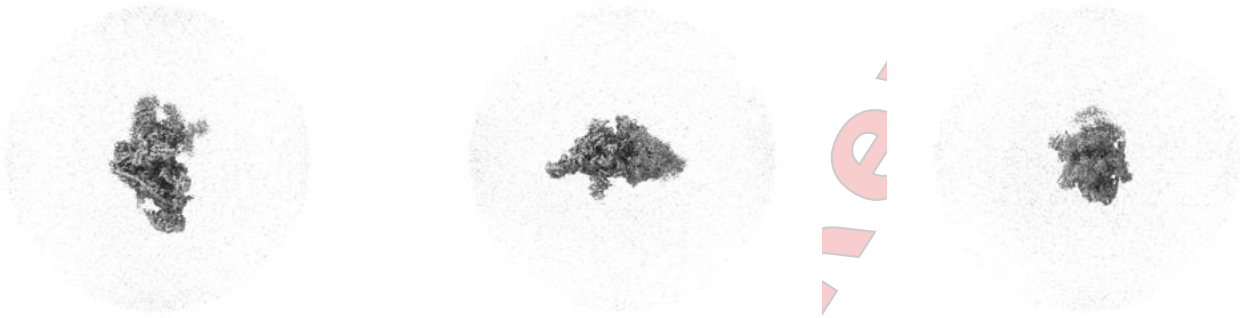


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

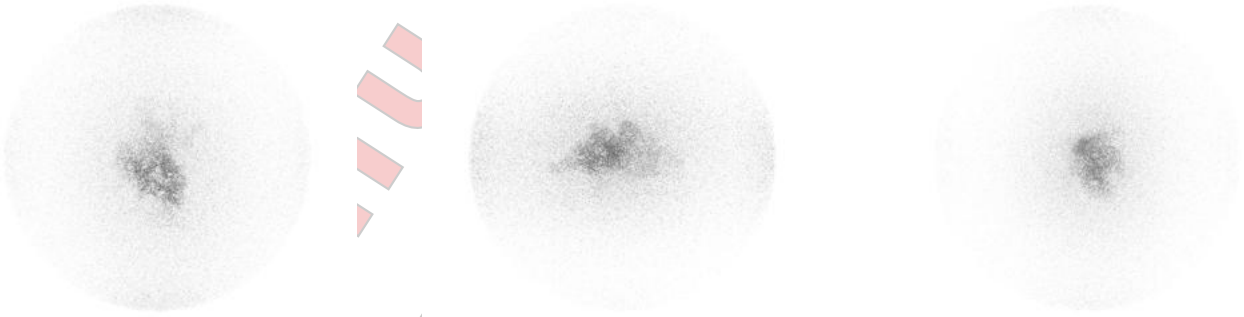
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

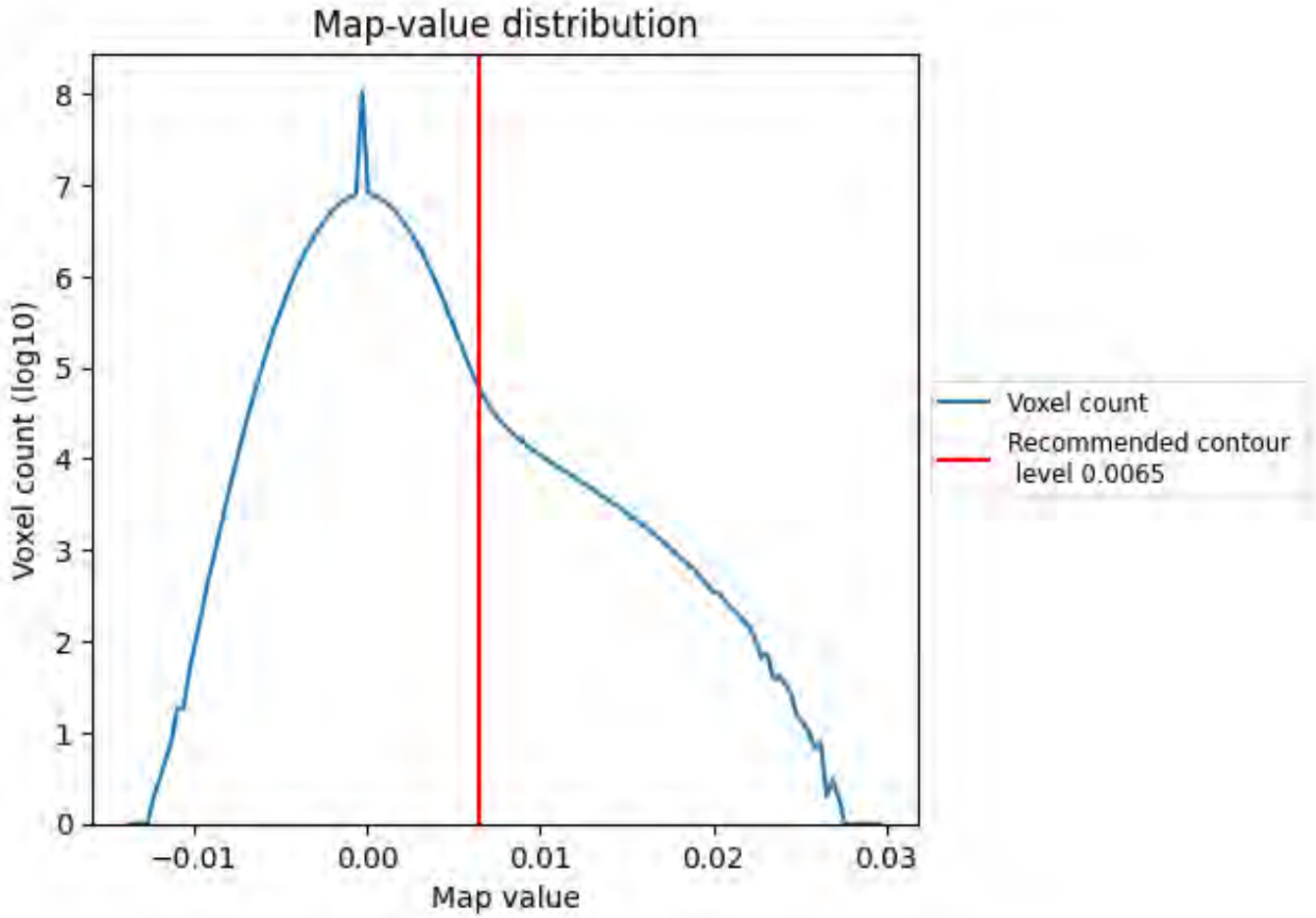
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

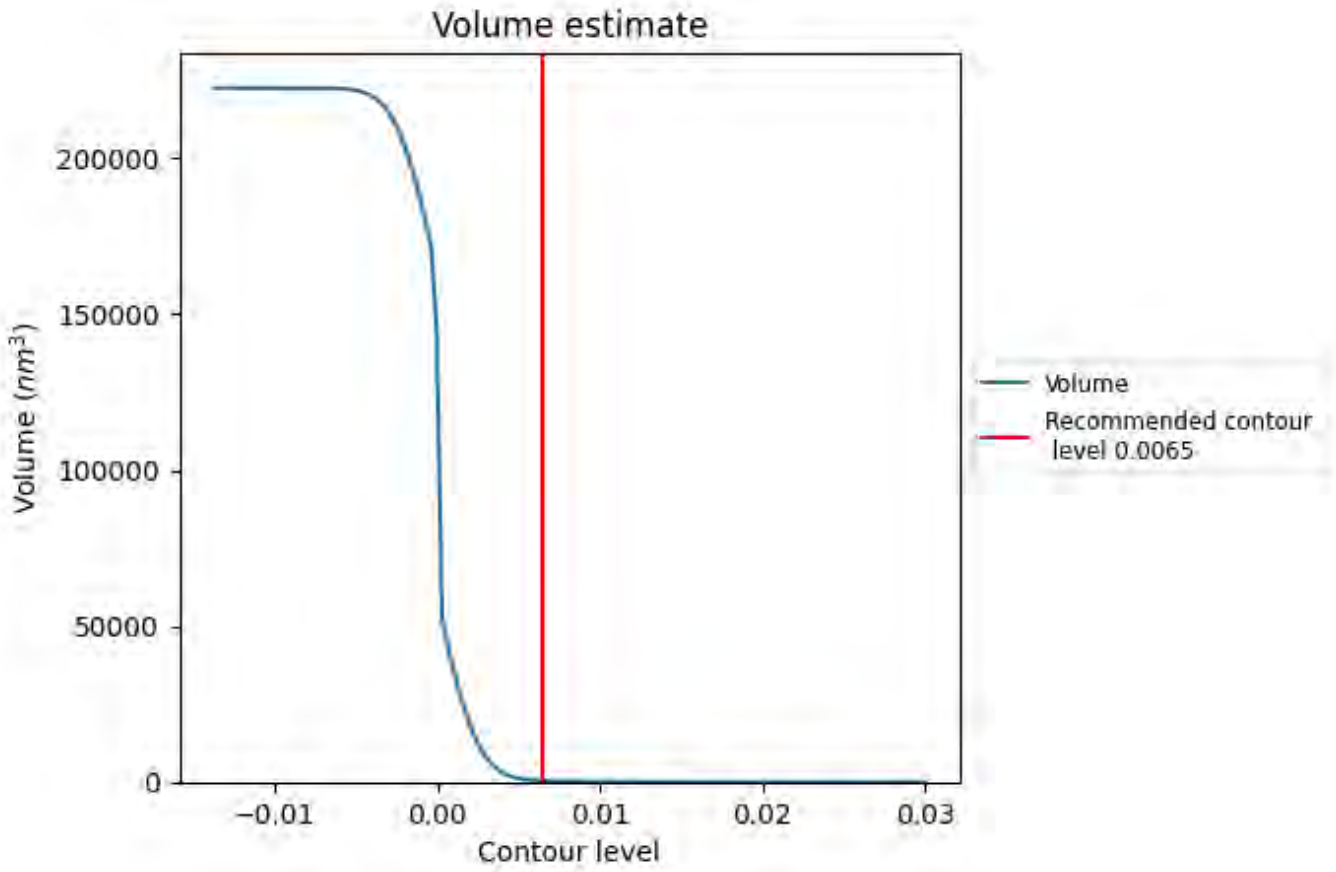
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

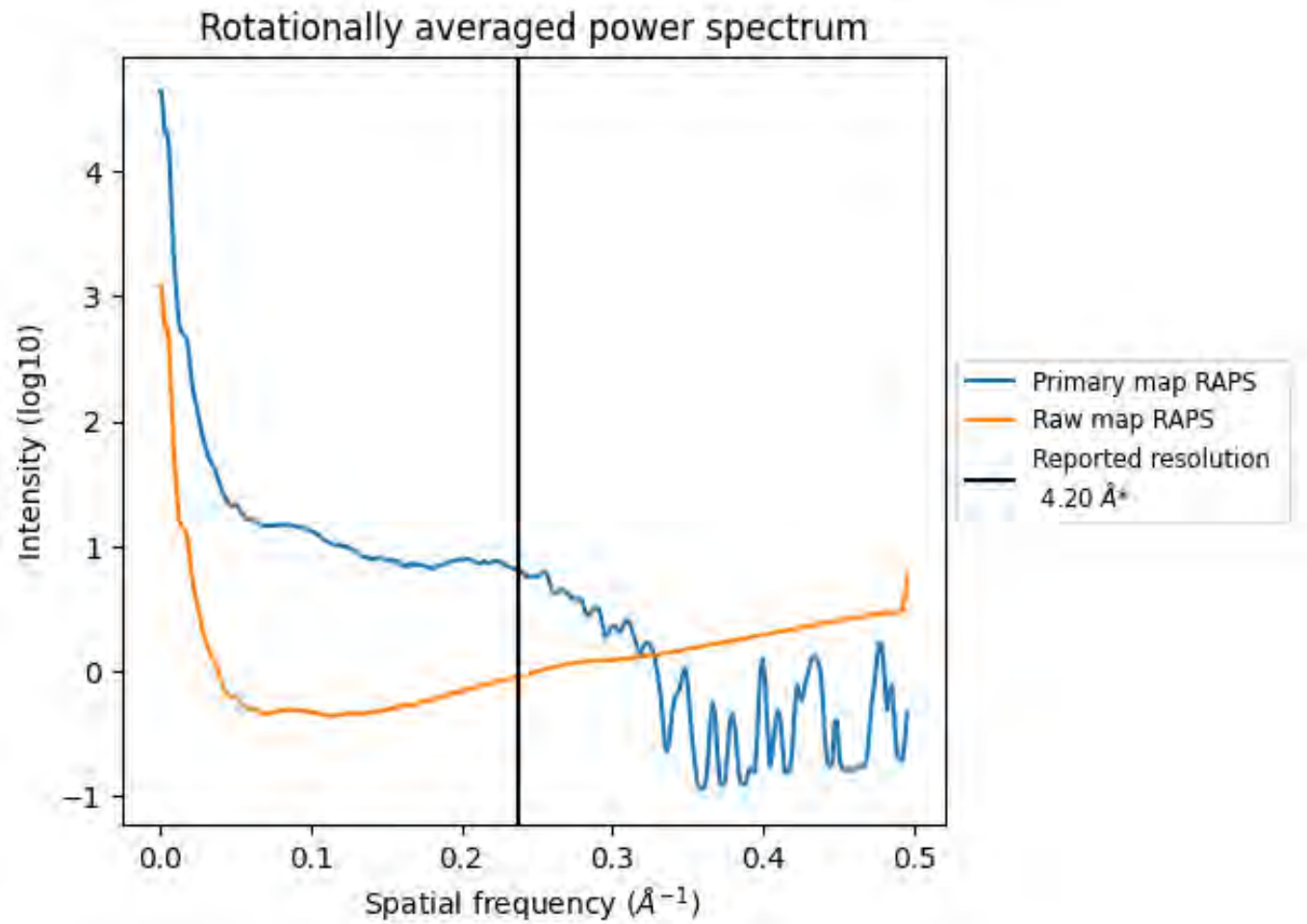
7.2 Volume estimate (i)



The volume at the recommended contour level is 394 nm^3; this corresponds to an approximate mass of 356 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

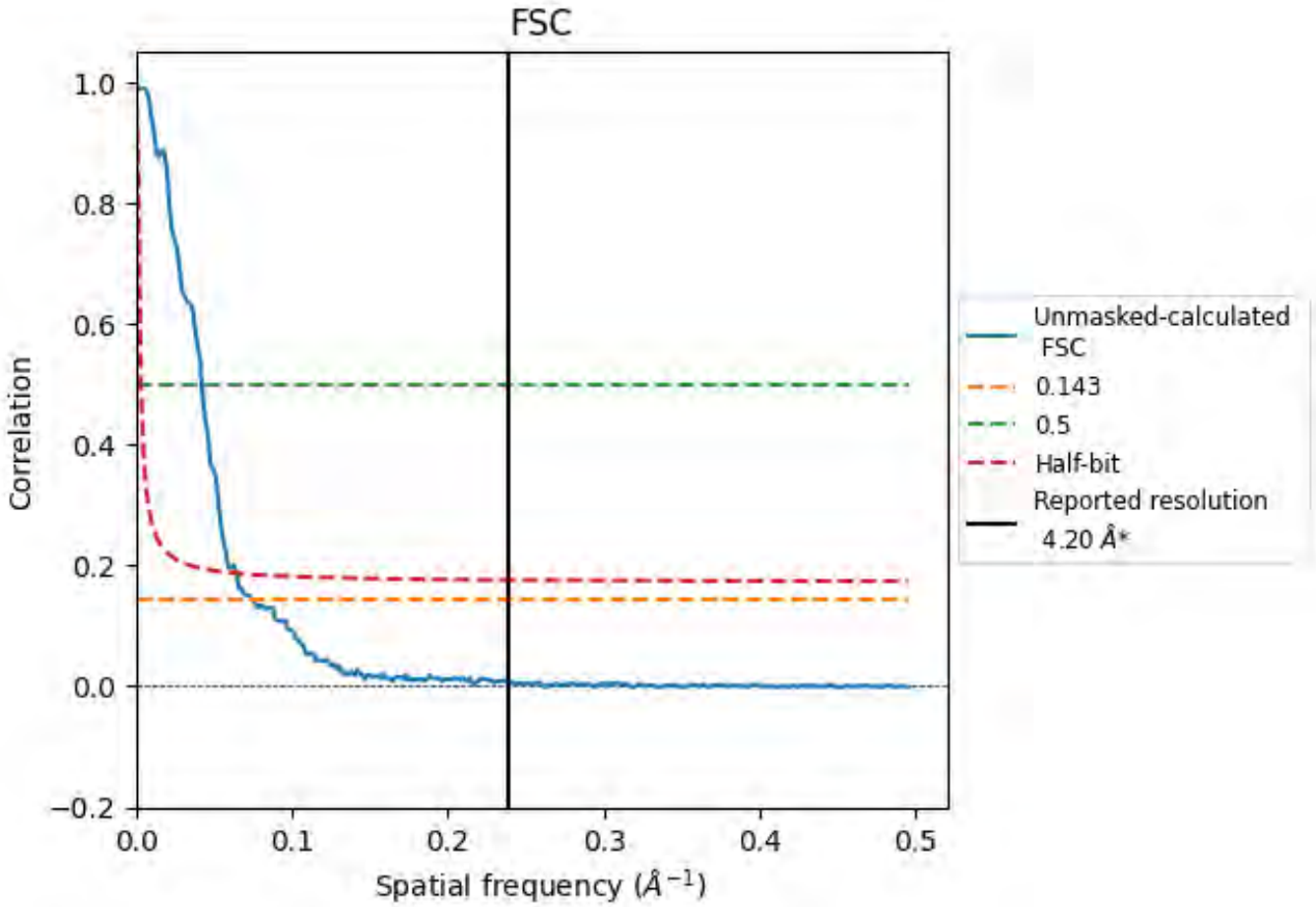


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

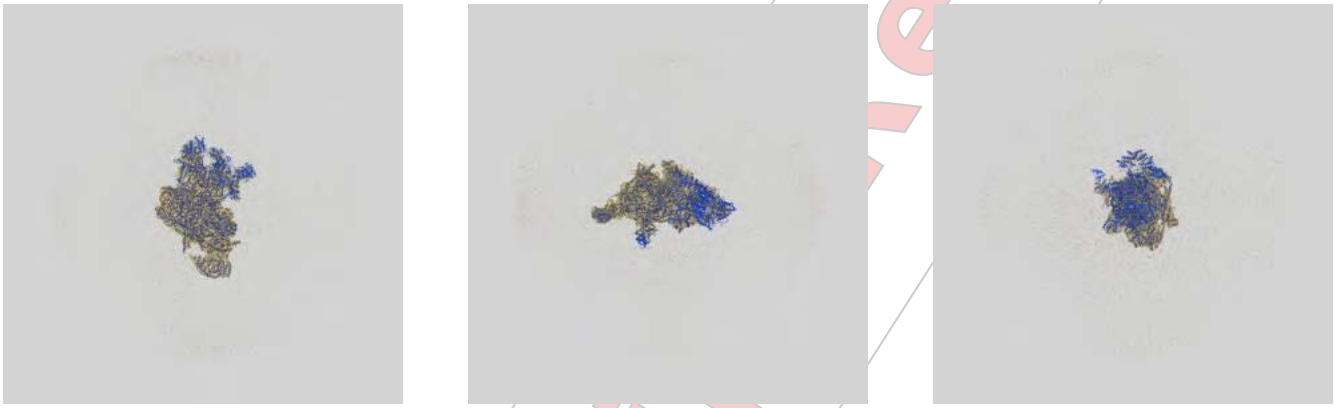
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	13.39	23.64	15.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 13.39 differs from the reported value 4.2 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51878 and PDB model 9H56. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay



X Y Z

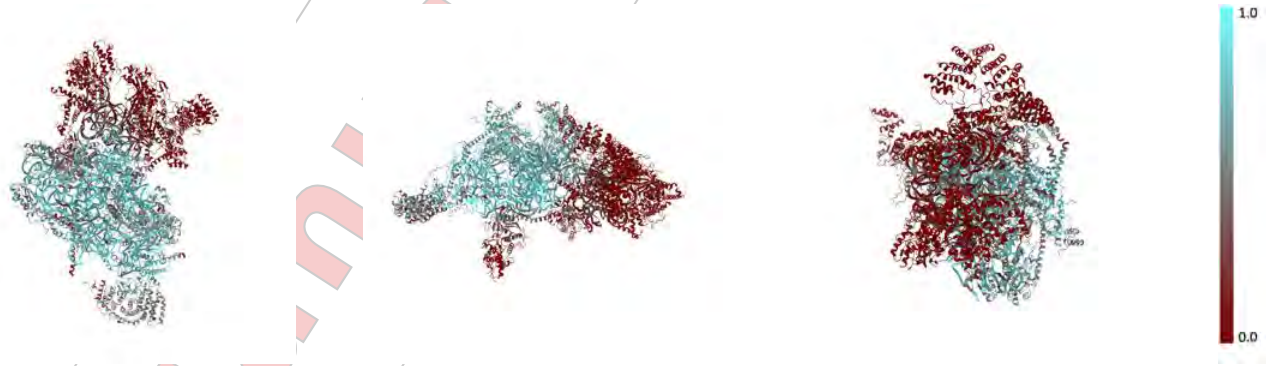
The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

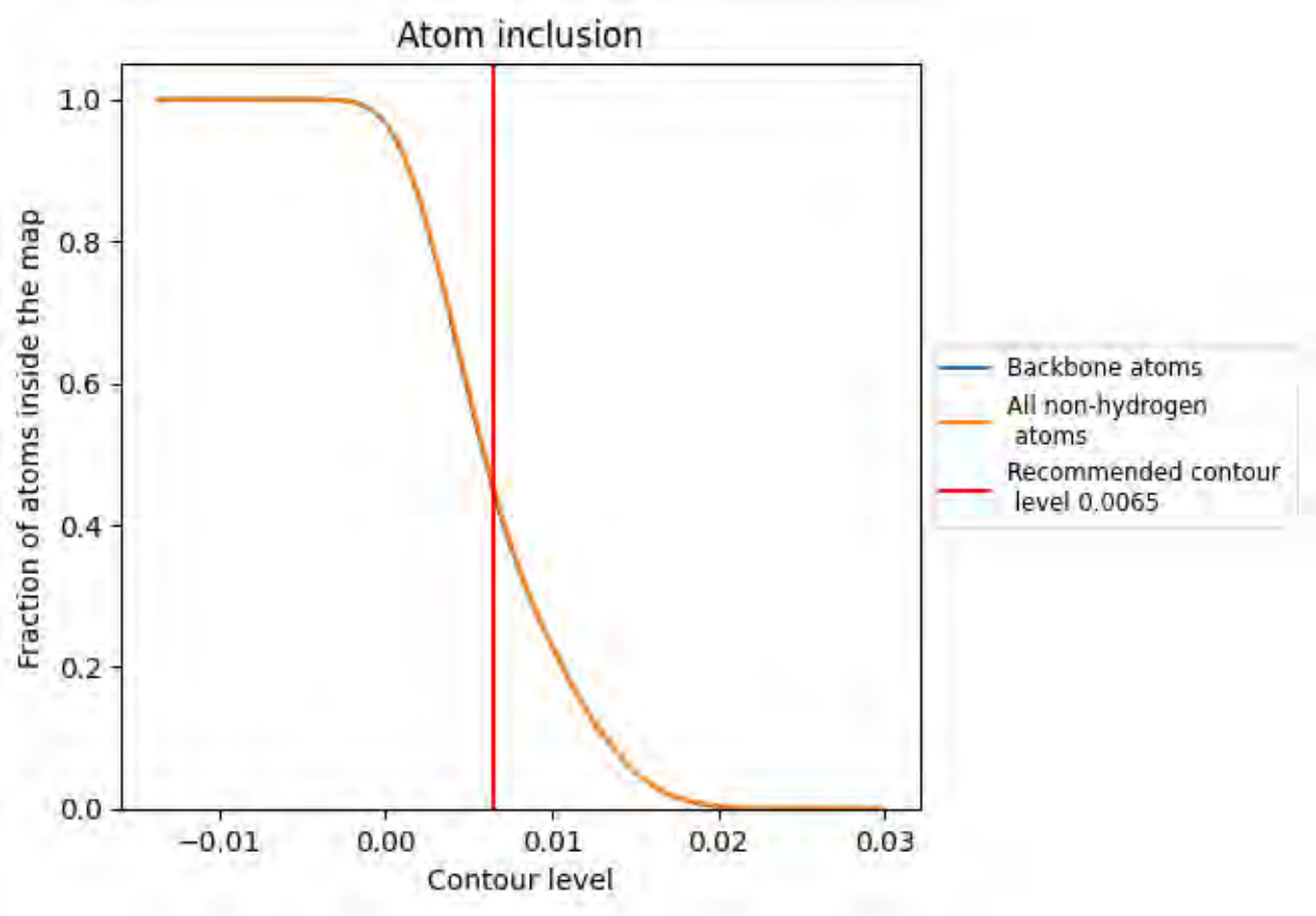
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0065).

9.4 Atom inclusion (i)



At the recommended contour level, 45% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4530	0.2510
0	0.6080	0.3640
1	0.0540	0.0120
3	0.5920	0.3710
4	0.0530	0.0110
7	0.2760	0.2480
9	0.3060	0.1860
A	0.6920	0.3360
B	0.7200	0.4360
C	0.1380	0.0470
D	0.5310	0.3440
E	0.5820	0.3510
F	0.1060	0.0210
G	0.2500	0.1260
H	0.0820	0.0350
I	0.5170	0.2820
J	0.6460	0.4460
K	0.1290	0.0150
L	0.6430	0.3950
M	0.7550	0.4870
N	0.7130	0.4510
O	0.7270	0.4420
P	0.6820	0.4050
R	0.6870	0.4130
S	0.6100	0.3490
T	0.7180	0.4360
U	0.6130	0.3360
V	0.4030	0.1990
W	0.6510	0.4000
X	0.0420	-0.0100
Y	0.0470	0.0270
Z	0.0840	0.0340
a	0.1320	0.1060
b	0.1350	0.0850
c	0.5770	0.3440
t	0.0050	0.0360

Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 12:53 am BST

PDB ID	:	9H5A
EMDB ID	:	EMD-51882
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit bound to METTL15 and RBFA (outward conformation) (State A6)
Deposited on	:	2024-10-22
Resolution	:	3.50 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ①) were used in the production of this report:

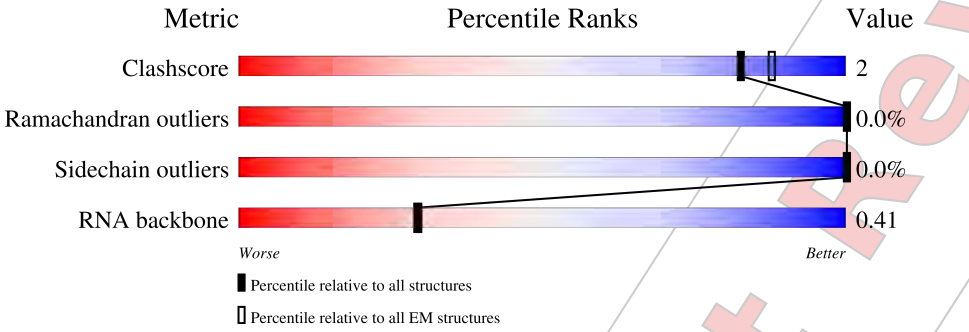
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	296	72% · 24%
2	C	167	36% 72% 7% 21%
3	D	430	16% 73% · 25%
4	E	125	7% 87% 5% 8%
5	F	242	53% 78% 5% 17%

Continued on next page...

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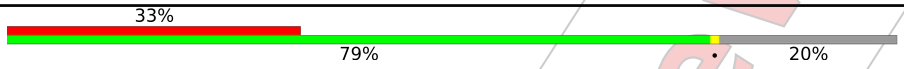
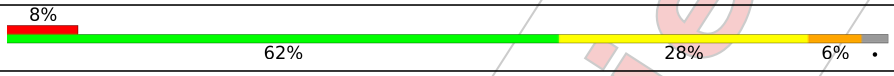
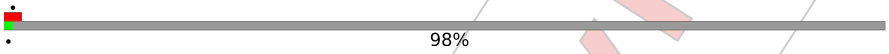
Mol	Chain	Length	Quality of chain
6	G	396	32% 72% 8% 21%
7	H	201	48% 67% 30%
8	I	194	68% 29%
9	J	138	75% 22%
10	K	128	41% 73% 6% 21%
11	L	257	5% 64% 32%
12	M	137	81% 6% 13%
13	N	130	82% 15%
14	O	258	72% 25%
15	P	142	65% 32%
16	Q	87	6% 99%
17	R	360	79% 18%
18	S	190	6% 68% 29%
19	T	173	93%
20	U	205	5% 81% 5% 14%
21	V	414	23% 81% 15%
22	W	187	52% 47%
23	X	398	78% 81% 7% 12%
24	Y	395	28% 30% 69%
25	Z	106	65% 89% 11%
26	0	218	14% 96%
27	1	323	72% 81% 15%
28	3	199	34% 65%
29	4	689	78% 82% 15%
30	a	343	33% 45% 55%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	b	407	
32	A	955	
33	9	698	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 128119 atoms, of which 59494 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	B	225	3642	1164	1814	331	323	10	0	0

- Molecule 2 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C	132	2171	699	1088	195	185	4	0	0

- Molecule 3 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	322	5189	1617	2614	483	462	13	0	0

- Molecule 4 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	E	115	1840	574	930	165	167	4	0	0

- Molecule 5 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	200	3343	1049	1698	297	288	11	0	0

- Molecule 6 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	G	314	5162	1643	2574	460	471	14	0	0

- Molecule 7 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	H	140	2335	745	1183	194	210	3	0	0

- Molecule 8 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	I	137	2075	642	1055	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 9 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	J	108	1724	521	885	169	143	6	0	0

- Molecule 10 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	K	101	1747	537	885	179	141	5	0	0

- Molecule 11 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	L	174	2993	925	1540	270	251	7	0	0

- Molecule 12 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	M	119	1905	594	964	184	157	6	0	0

- Molecule 13 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	110	Total	C	H	N	O	S	0	0
			1796	562	928	156	147	3		

- Molecule 14 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	O	194	Total	C	H	N	O	S	0	0
			3166	1019	1567	295	278	7		

- Molecule 15 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	97	Total	C	H	N	O	S	0	0
			1588	501	807	134	138	8		

- Molecule 16 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	87	Total	C	H	N	O	S	0	0
			1501	460	757	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 17 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	295	Total	C	H	N	O	S	0	0
			4837	1533	2428	413	455	8		

- Molecule 18 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	135	Total	C	H	N	O	S	0	0
			2226	716	1115	198	196	1		

- Molecule 19 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

- Molecule 20 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	U	176	Total	C	H	N	O	S	0	0
			2987	916	1499	301	267	4		

- Molecule 21 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	352	Total	C	H	N	O	S	0	0
			5771	1853	2887	480	539	12		

- Molecule 22 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	W	100	Total	C	H	N	O	S	0	0
			1591	498	802	141	146	4		

- Molecule 23 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	X	352	Total	C	H	N	O	S	0	0
			5693	1822	2844	499	517	11		

- Molecule 24 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Y	121	Total	C	H	N	O	S	0	0
			1993	662	970	168	191	2		

- Molecule 25 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	94	Total	C	H	N	O	S	0	0
			1612	510	815	143	140	4		

- Molecule 26 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	0	215	Total	C	H	N	O	S	0	0
			3582	1130	1795	339	313	5		

- Molecule 27 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	1	276	Total	C	H	N	O	S	0	0
			4506	1419	2268	381	427	11		

- Molecule 28 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	3	70	Total	C	H	N	O	S	0	0
			1322	401	697	134	89	1		

- Molecule 29 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	588	Total	C	H	N	O	S	0	0
			9532	3053	4764	808	879	28		

- Molecule 30 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	a	155	Total	C	H	N	O	S	0	0
			2436	765	1218	211	235	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	84	VAL	LYS	conflict	UNP Q8N0V3

- Molecule 31 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	b	324	Total	C	H	N	O	S	0	0
			5148	1605	2610	456	462	15		

- Molecule 32 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	A	922	Total	C	H	N	O	P	0	0
			29525	8783	9941	3524	6355	922		

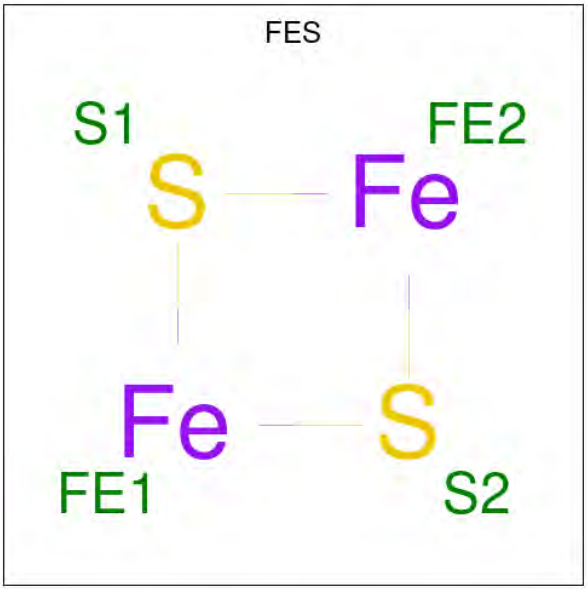
- Molecule 33 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	9	12	Total	C	H	N	O	S	0	0
			219	76	108	16	18	1		

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

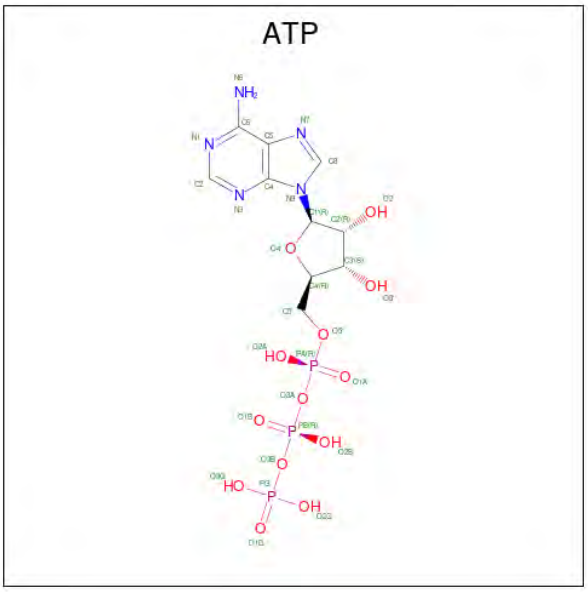
Mol	Chain	Residues	Atoms		AltConf
34	O	1	Total	Zn	0
			1	1	

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



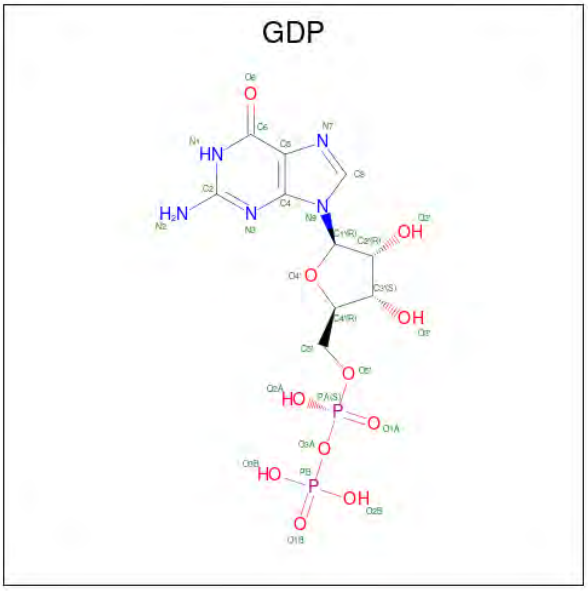
Mol	Chain	Residues	Atoms			AltConf
35	P	1	Total	Fe	S	0
			4	2	2	
35	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



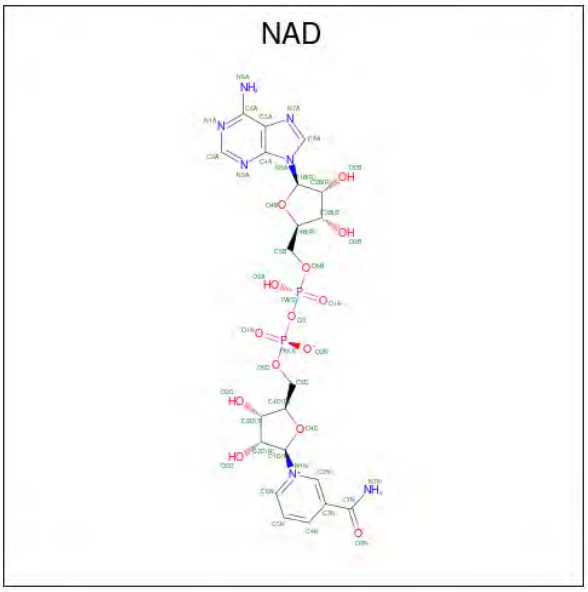
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
36	X	1	43	10	12	5	13	3	0

- Molecule 37 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



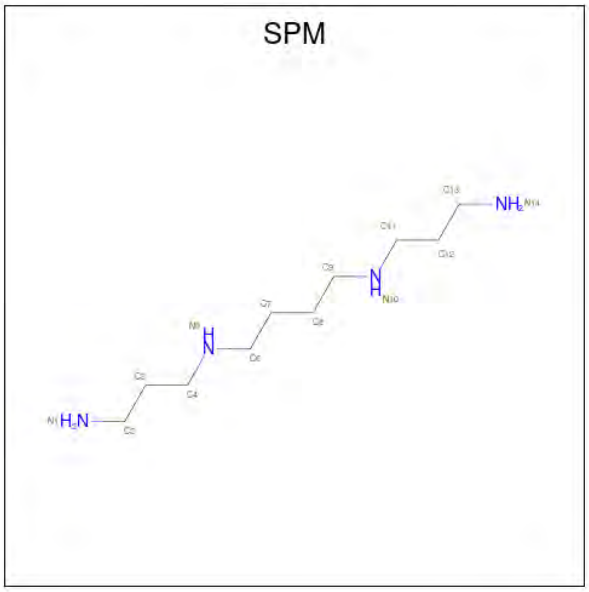
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
37	X	1	38	10	10	5	11	2	0

- Molecule 38 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
38	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 39 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
39	A	1	Total	C	N	0
			14	10	4	

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
40	A	13	Total Mg 13 13	0

- Molecule 41 is water.

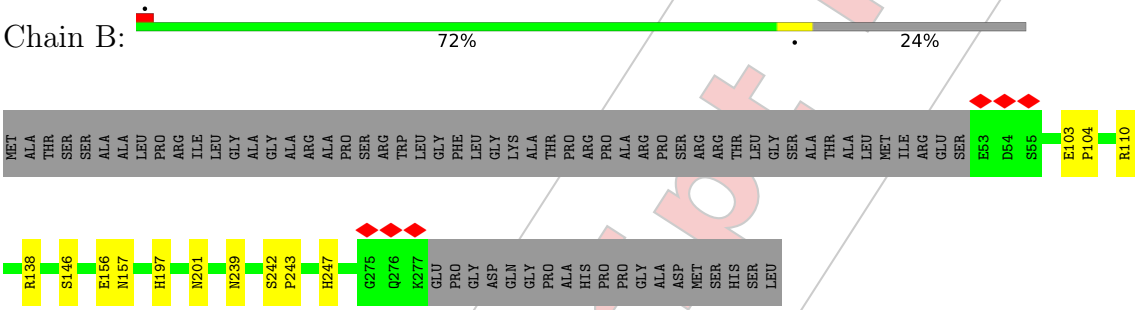
Mol	Chain	Residues	Atoms	AltConf
41	C	1	Total O 1 1	0
41	G	2	Total O 2 2	0
41	I	1	Total O 1 1	0
41	T	1	Total O 1 1	0
41	0	1	Total O 1 1	0
41	A	2	Total O 2 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

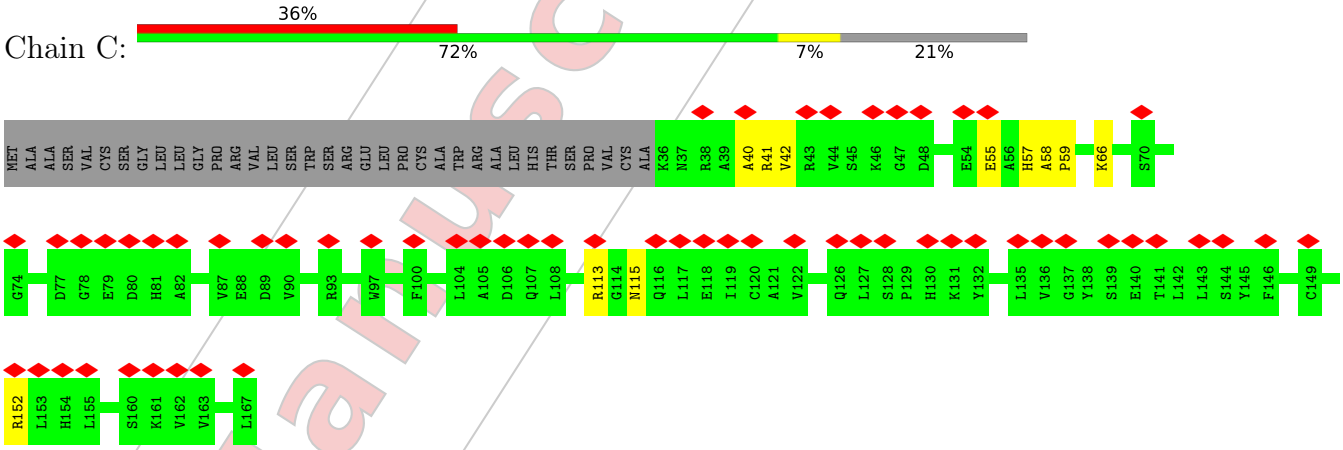
• Molecule 1: 28S ribosomal protein S2, mitochondrial

Chain B:



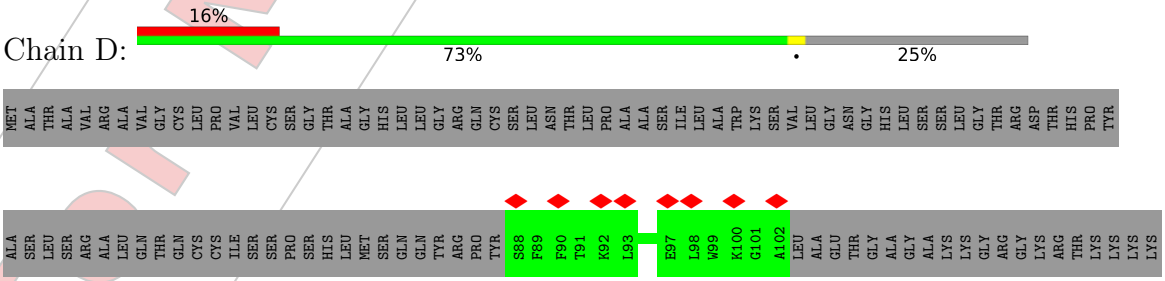
• Molecule 2: 28S ribosomal protein S24, mitochondrial

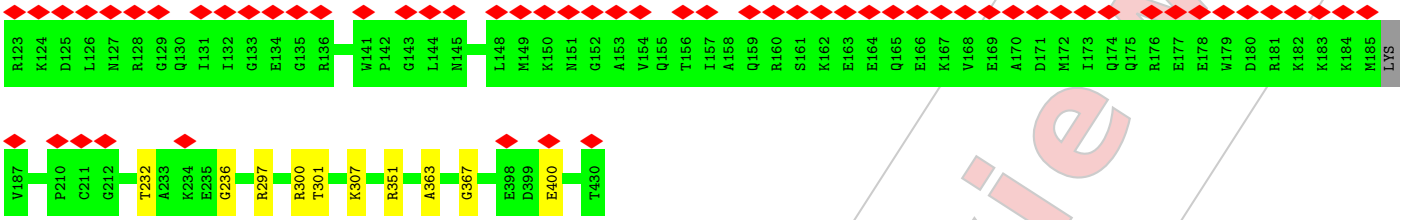
Chain C:



• Molecule 3: 28S ribosomal protein S5, mitochondrial

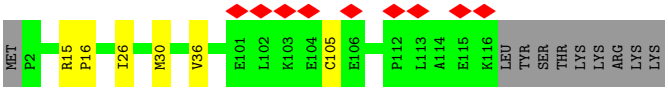
Chain D:





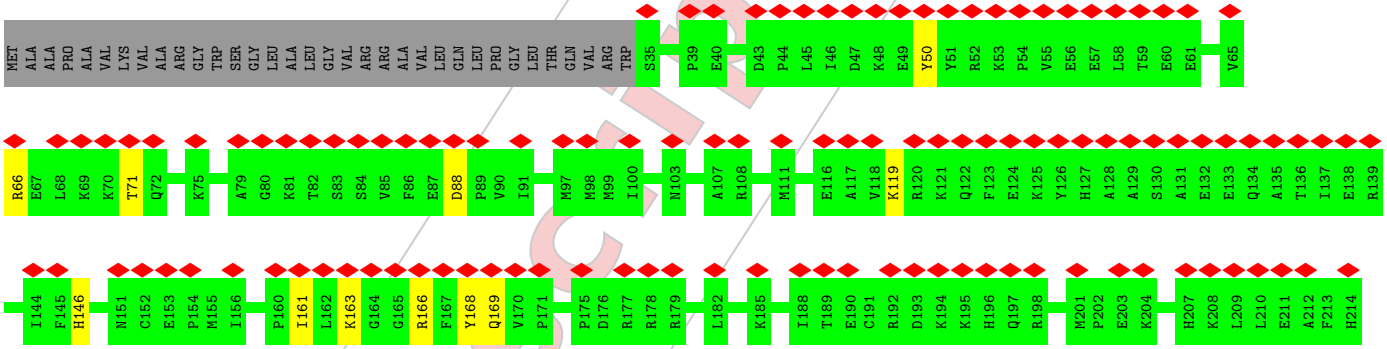
• Molecule 4: 28S ribosomal protein S6, mitochondrial

Chain E:



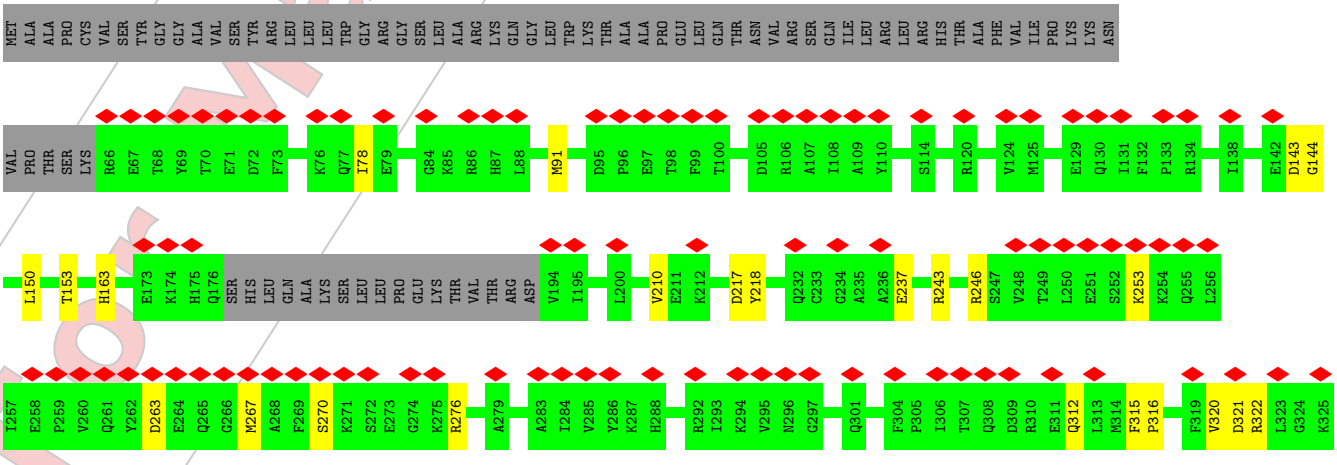
• Molecule 5: 28S ribosomal protein S7, mitochondrial

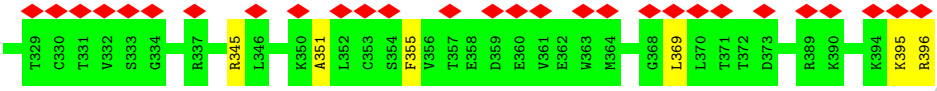
Chain F:



• Molecule 6: 28S ribosomal protein S9, mitochondrial

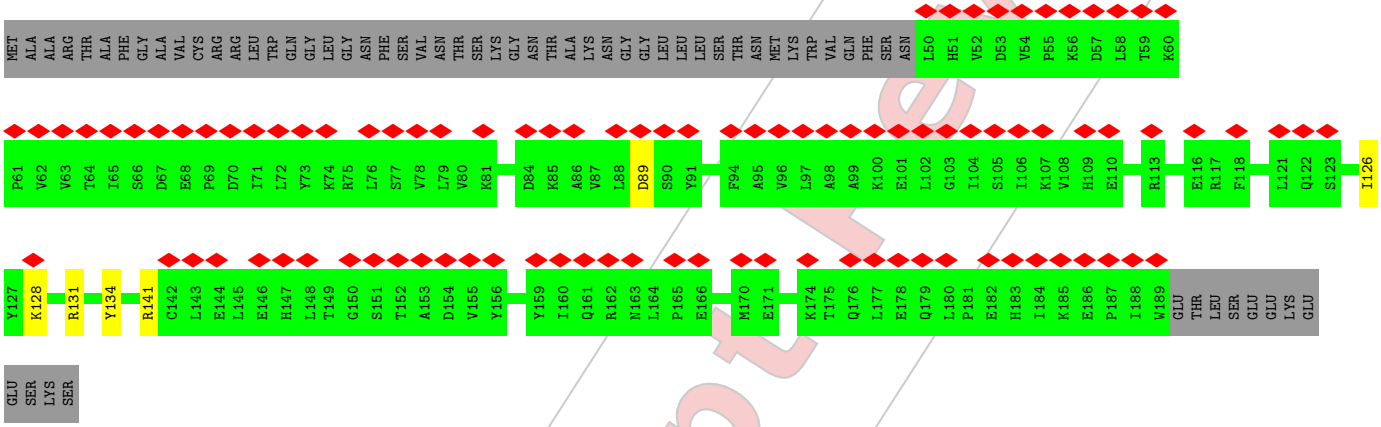
Chain G:





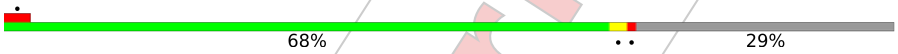
• Molecule 7: 28S ribosomal protein S10, mitochondrial

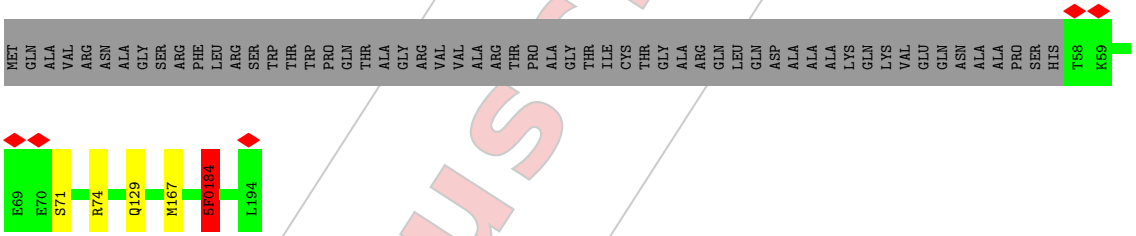
Chain H:



• Molecule 8: 28S ribosomal protein S11, mitochondrial

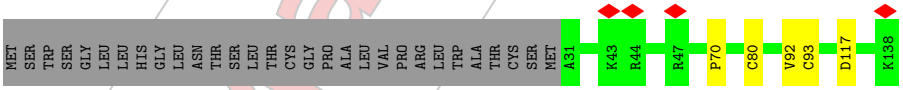
Chain I:





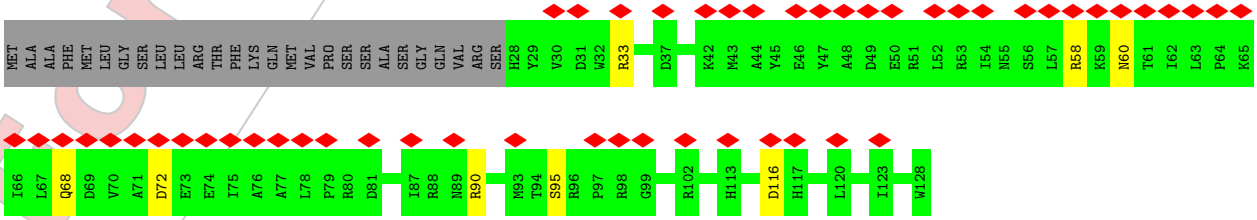
• Molecule 9: 28S ribosomal protein S12, mitochondrial

Chain J:



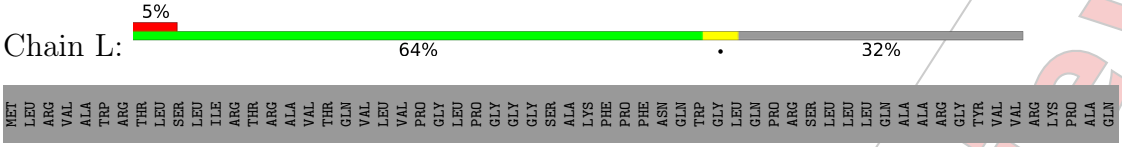
• Molecule 10: 28S ribosomal protein S14, mitochondrial

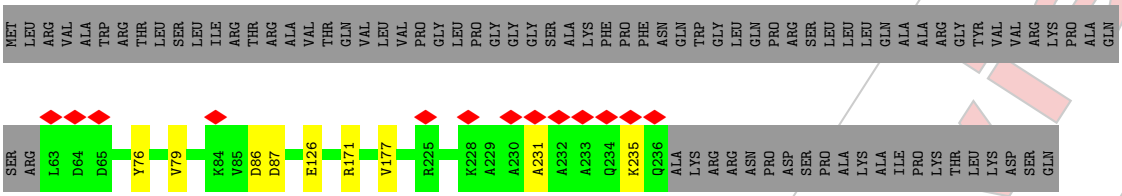
Chain K:



• Molecule 11: 28S ribosomal protein S15, mitochondrial

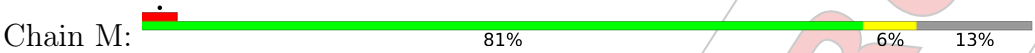
Chain L:





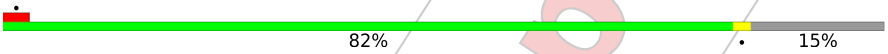
• Molecule 12: 28S ribosomal protein S16, mitochondrial

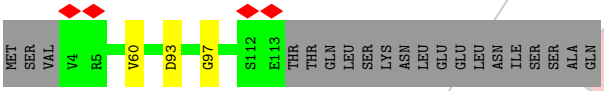
Chain M:



• Molecule 13: 28S ribosomal protein S17, mitochondrial

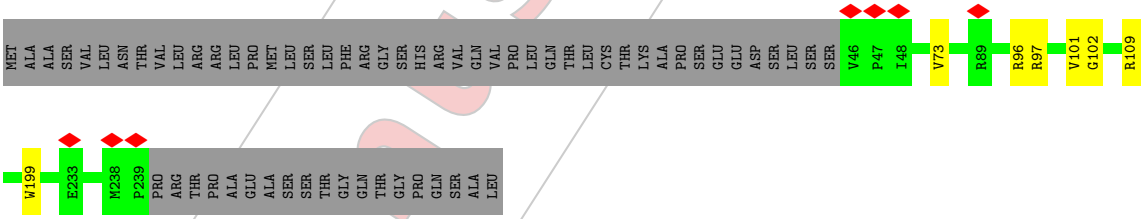
Chain N:





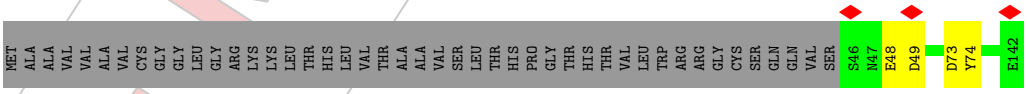
• Molecule 14: 28S ribosomal protein S18b, mitochondrial

Chain O:



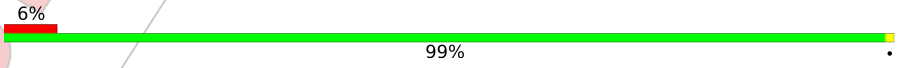
• Molecule 15: 28S ribosomal protein S18c, mitochondrial

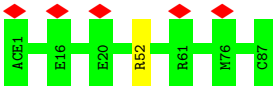
Chain P:



• Molecule 16: Small ribosomal subunit protein bS21m

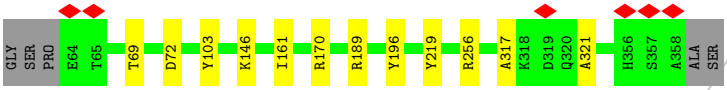
Chain Q:





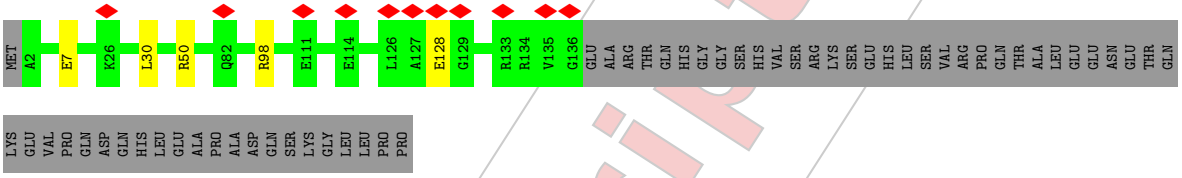
• Molecule 17: 28S ribosomal protein S22, mitochondrial

Chain R:



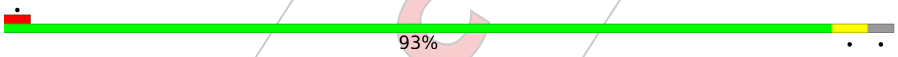
• Molecule 18: 28S ribosomal protein S23, mitochondrial

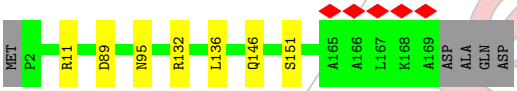
Chain S:



• Molecule 19: 28S ribosomal protein S25, mitochondrial

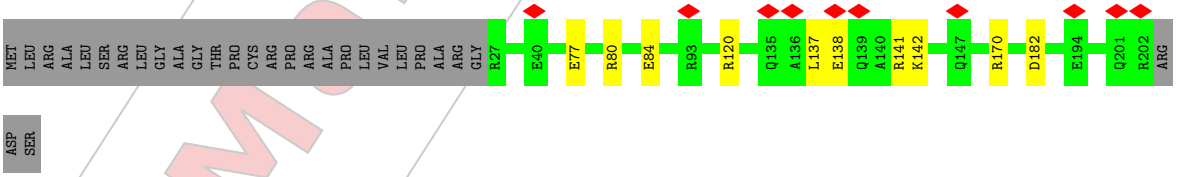
Chain T:





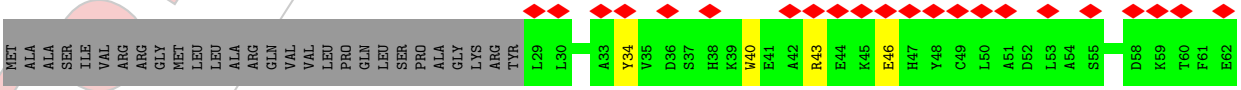
• Molecule 20: 28S ribosomal protein S26, mitochondrial

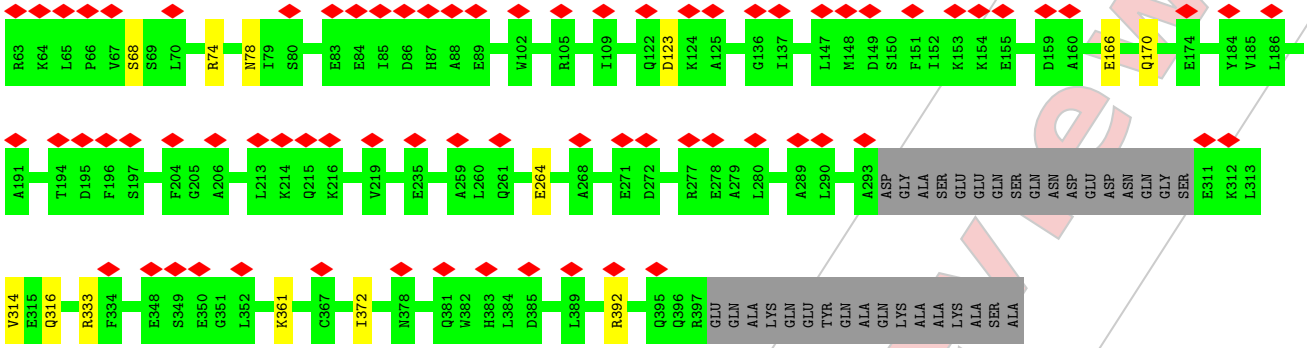
Chain U:



• Molecule 21: 28S ribosomal protein S27, mitochondrial

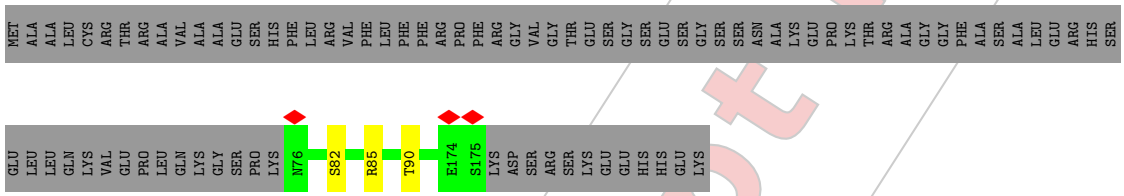
Chain V:





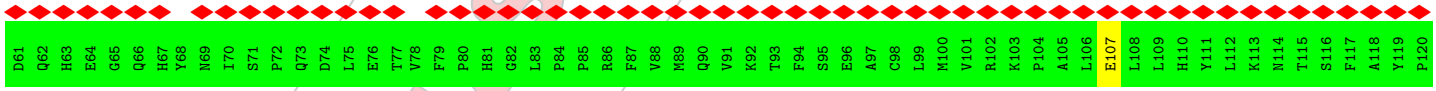
• Molecule 22: 28S ribosomal protein S28, mitochondrial

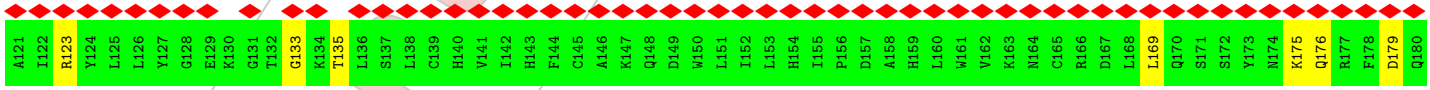
Chain W:

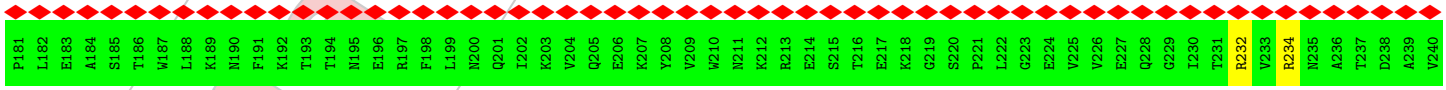


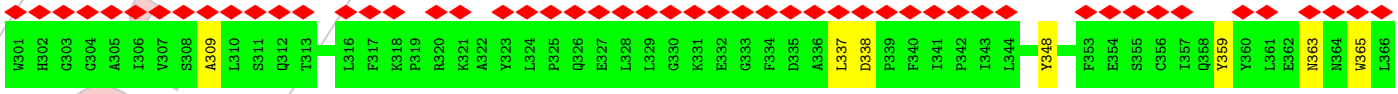
• Molecule 23: 28S ribosomal protein S29, mitochondrial

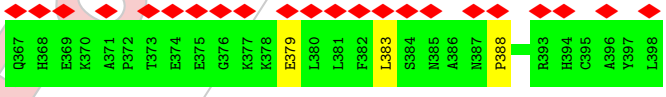
Chain X:





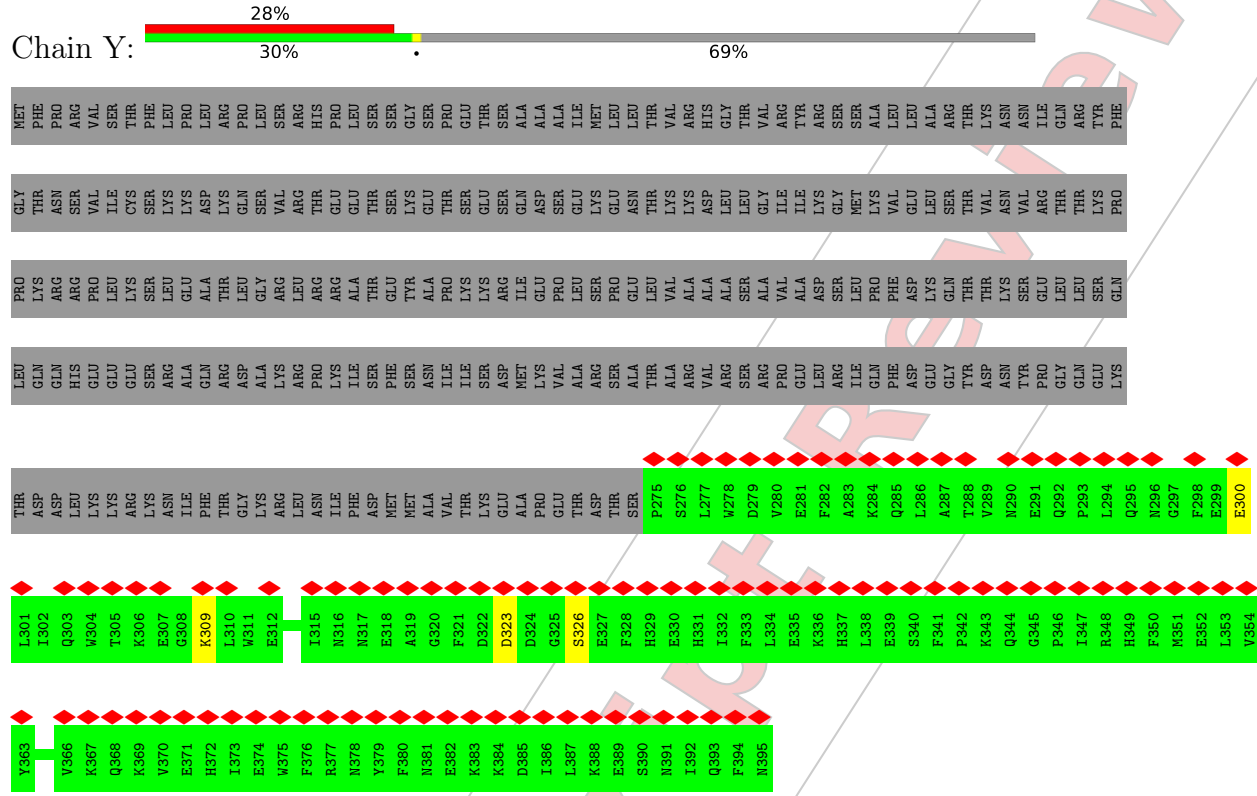






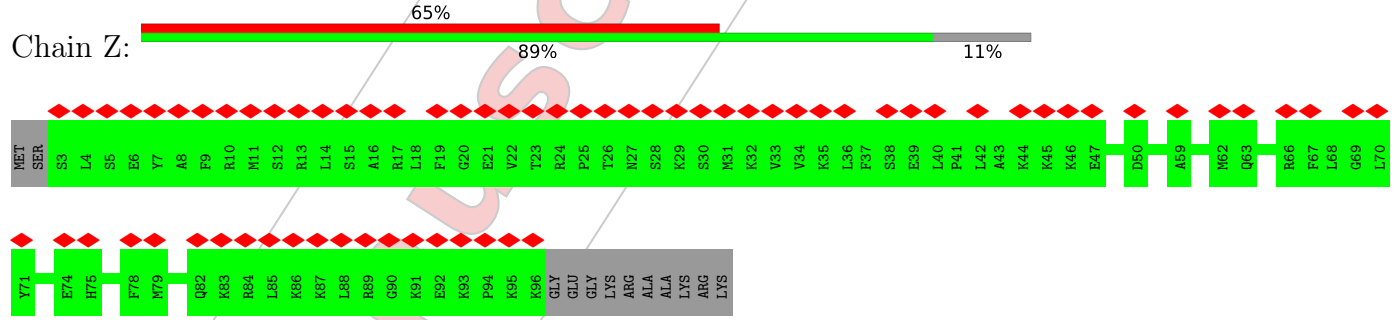
• Molecule 24: 28S ribosomal protein S31, mitochondrial

Chain Y:



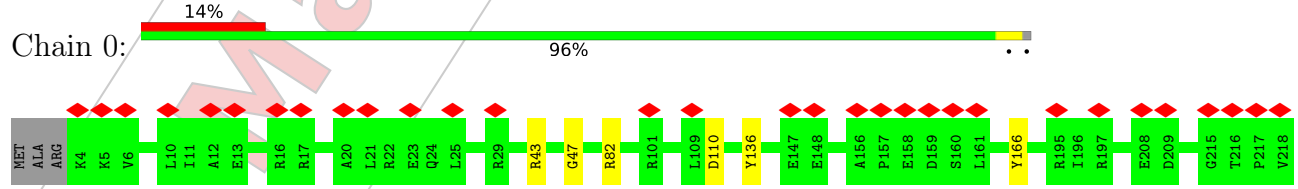
• Molecule 25: 28S ribosomal protein S33, mitochondrial

Chain Z:



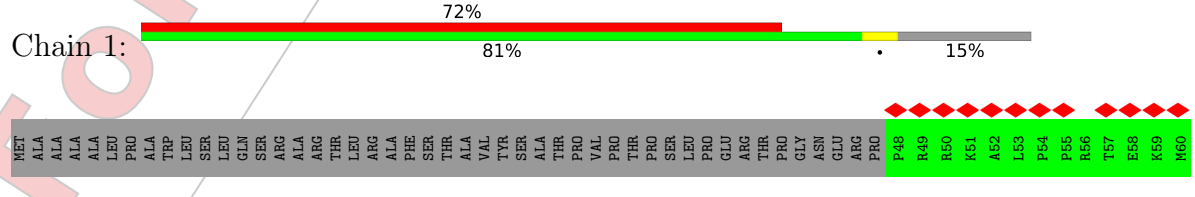
• Molecule 26: 28S ribosomal protein S34, mitochondrial

Chain 0:



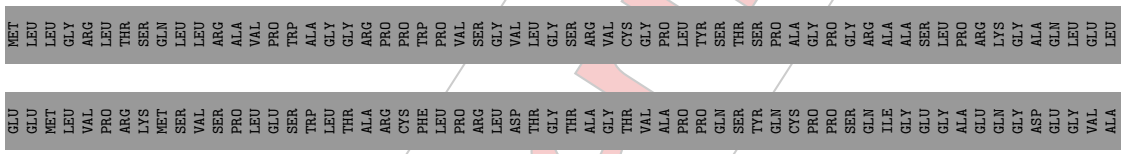
• Molecule 27: 28S ribosomal protein S35, mitochondrial

Chain 1:



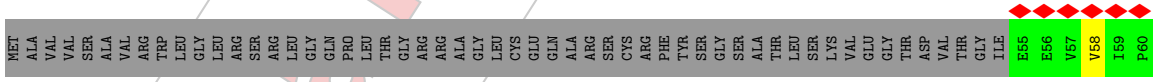
• Molecule 28: Aurora kinase A-interacting protein

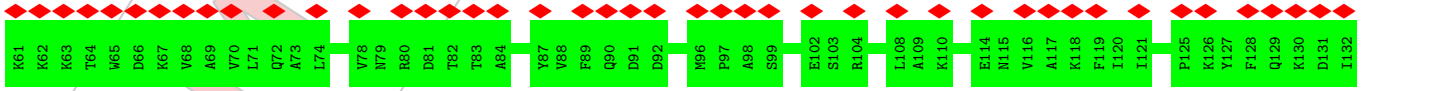
Chain 3:

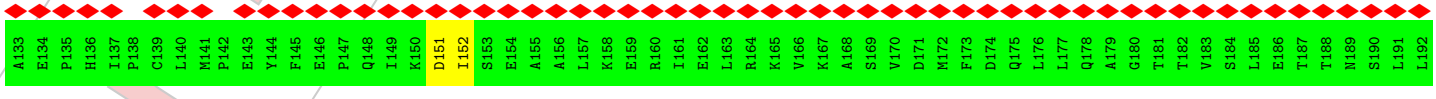


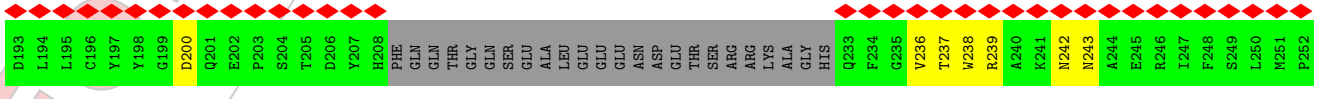
• Molecule 29: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

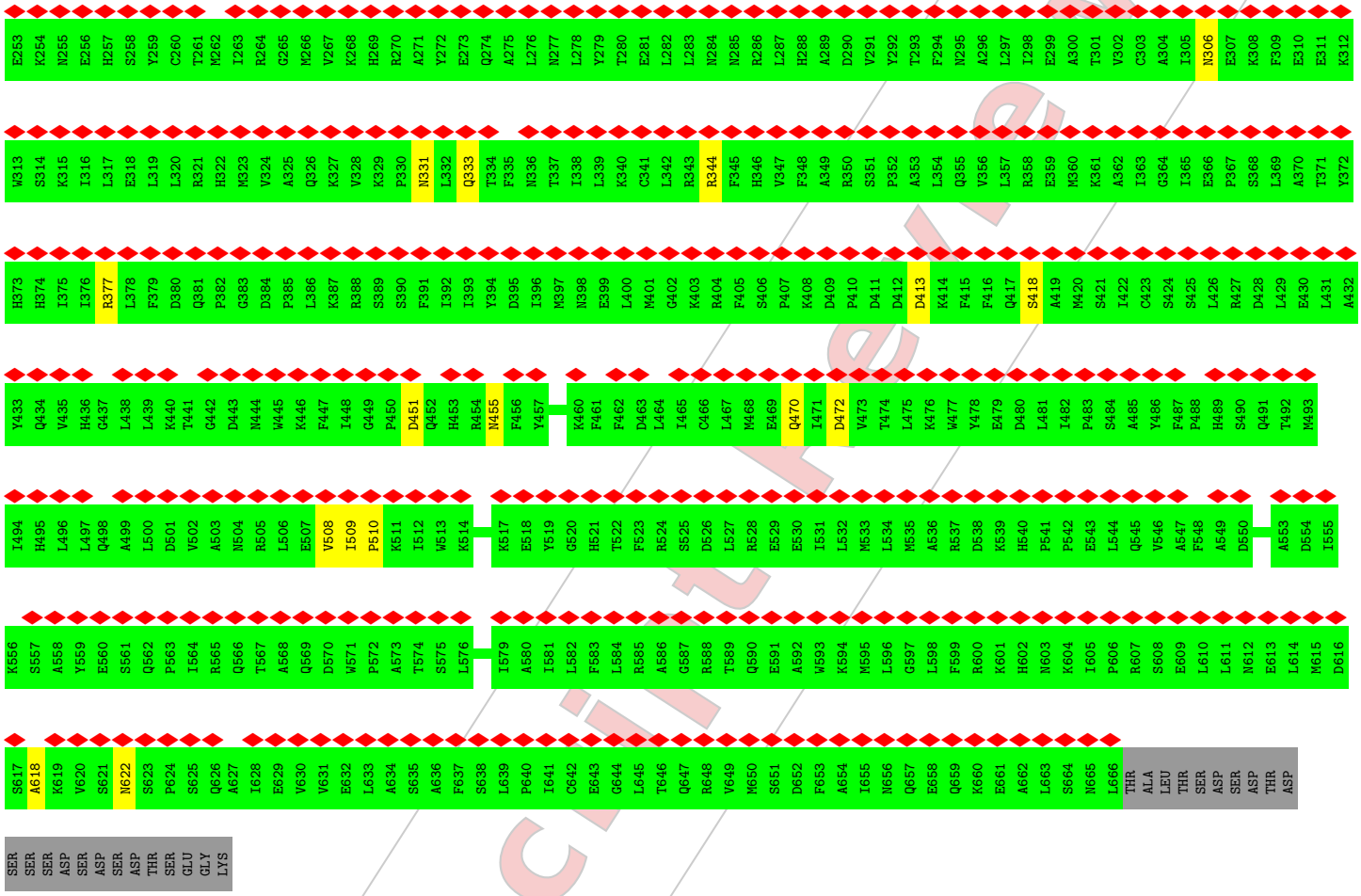
Chain 4:





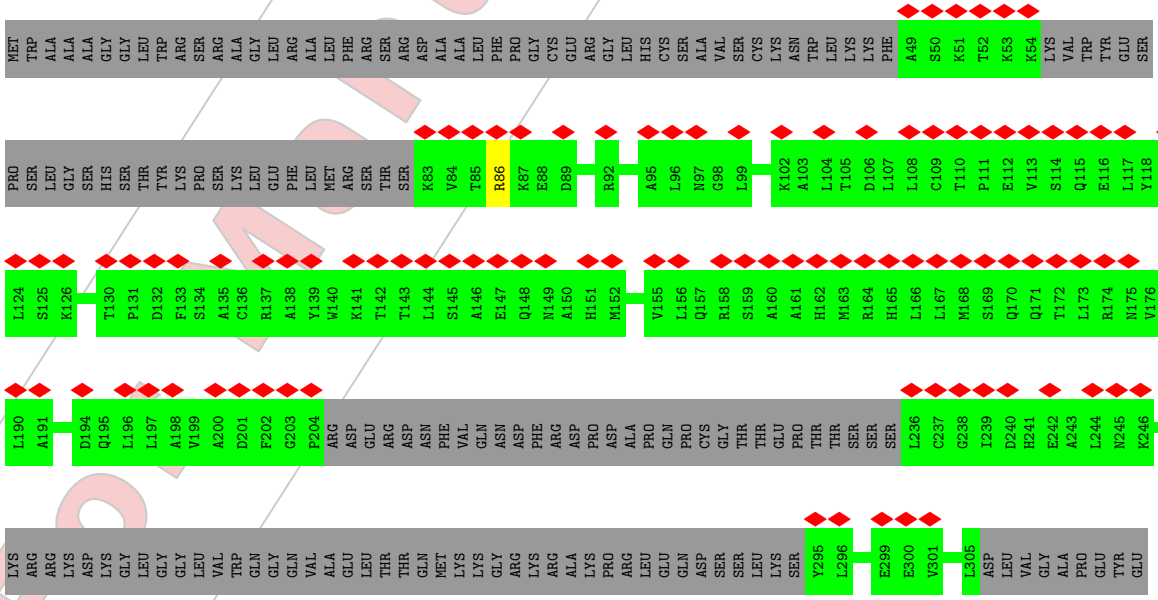


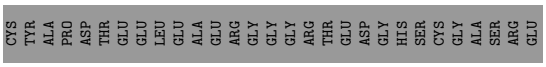




• Molecule 30: Putative ribosome-binding factor A, mitochondrial

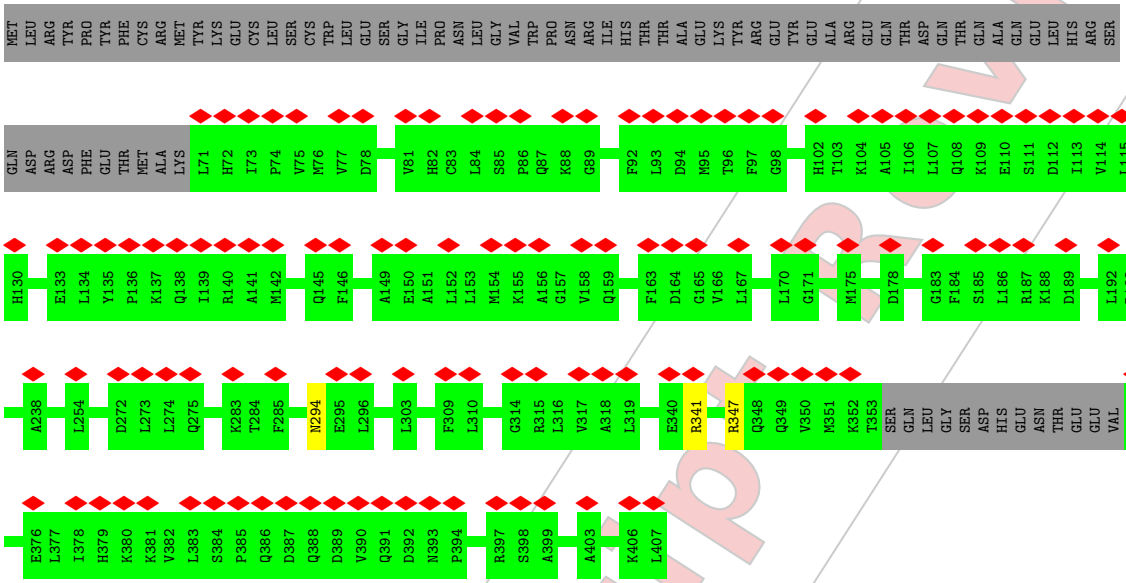
Chain a:





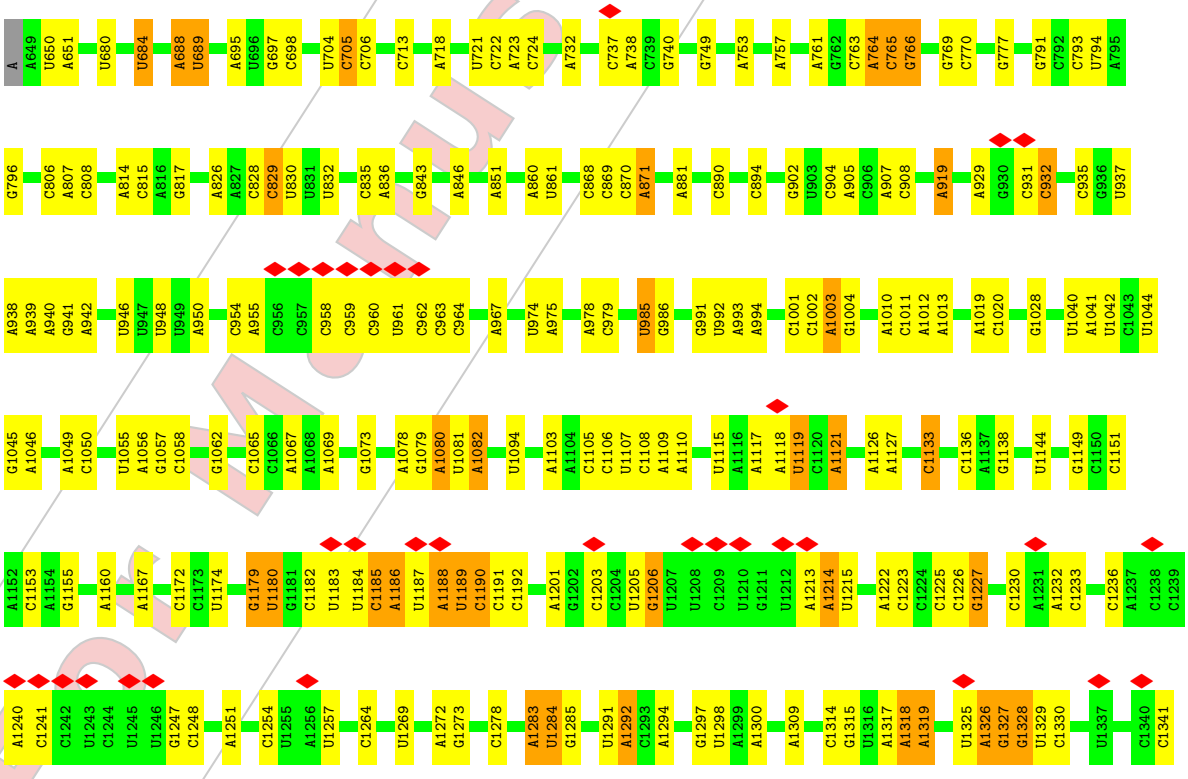
• Molecule 31: 12S rRNA N4-methylcytidine (m4C) methyltransferase

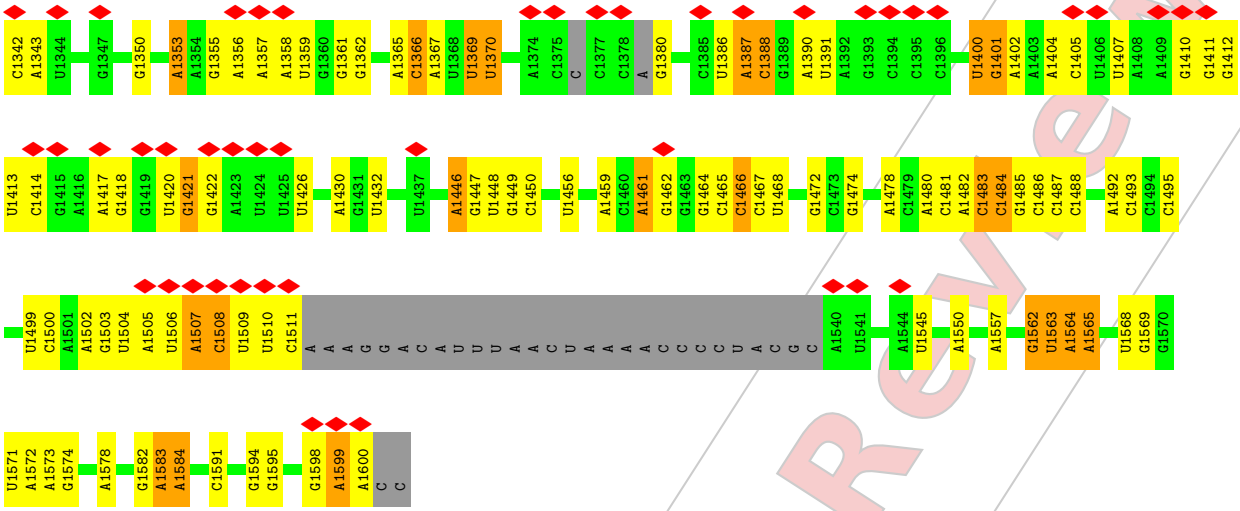
Chain b:



• Molecule 32: 12S mitochondrial rRNA

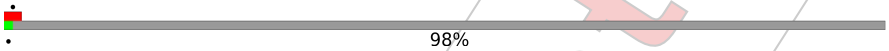
Chain A:

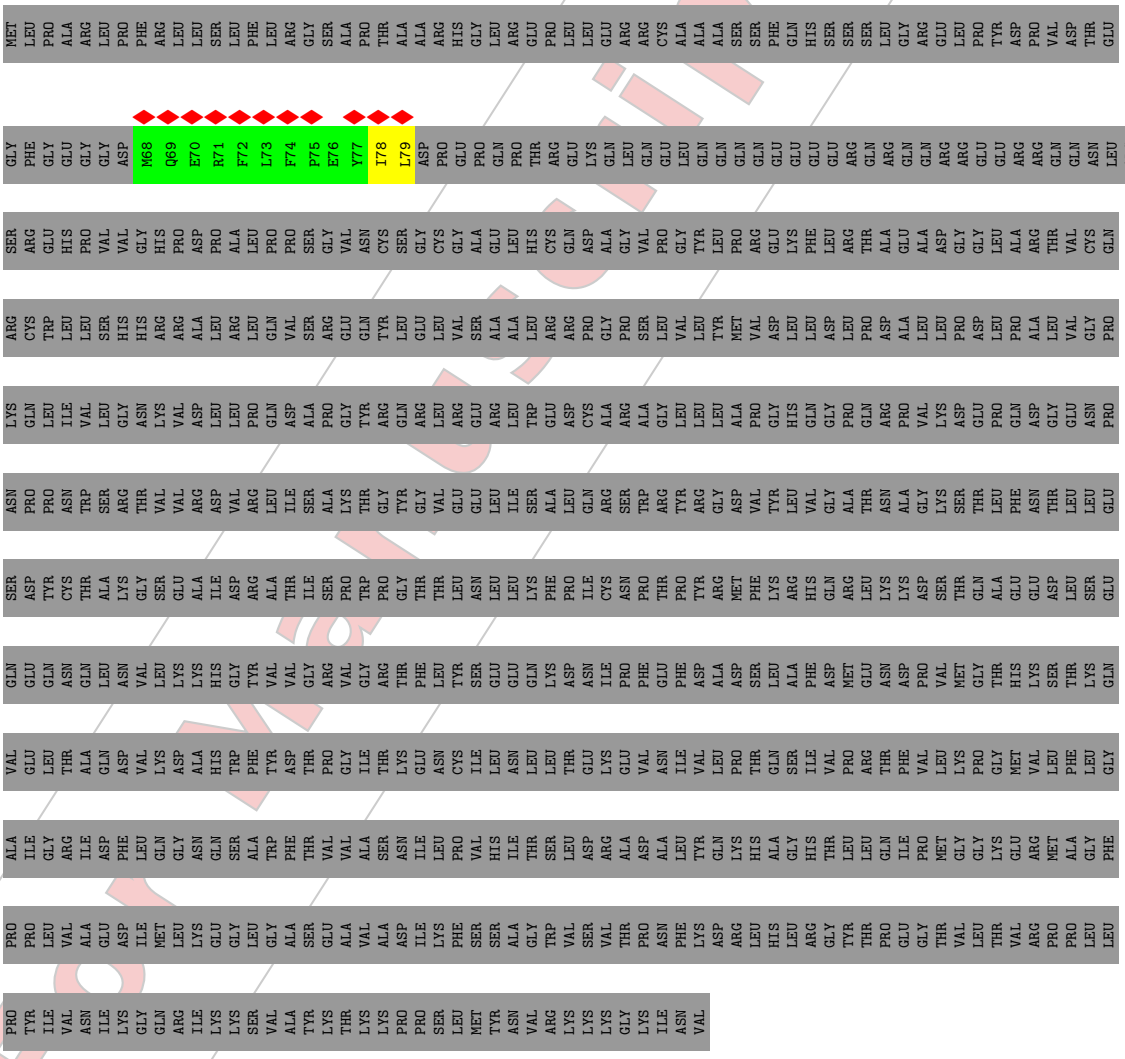




• Molecule 33: Nitric oxide-associated protein 1

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5590	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.011	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, B8T, SPM, ATP, GDP, NAD, ZN, 5MC, 5MU, ACE, FES, 5F0, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.25	0/1871	0.49	0/2531
2	C	0.30	0/1113	0.49	0/1505
3	D	0.24	0/2625	0.50	0/3518
4	E	0.24	0/926	0.52	0/1252
5	F	0.28	0/1681	0.48	0/2255
6	G	0.28	0/2643	0.51	0/3541
7	H	0.27	0/1178	0.47	0/1598
8	I	0.25	0/1030	0.51	0/1386
9	J	0.26	0/855	0.55	0/1148
10	K	0.23	0/880	0.57	0/1182
11	L	0.25	0/1477	0.48	0/1974
12	M	0.25	0/962	0.53	0/1293
13	N	0.24	0/886	0.49	0/1199
14	O	0.24	0/1655	0.48	0/2254
15	P	0.25	0/798	0.43	0/1070
16	Q	0.24	0/754	0.57	0/1003
17	R	0.24	0/2456	0.45	0/3317
18	S	0.25	0/1138	0.51	0/1533
19	T	0.25	0/1402	0.46	0/1883
20	U	0.27	0/1510	0.54	0/2025
21	V	0.23	0/2944	0.42	0/3978
22	W	0.25	0/801	0.52	0/1079
23	X	0.26	0/2921	0.45	0/3954
24	Y	0.24	0/1054	0.37	0/1421
25	Z	0.31	0/815	0.52	0/1087
26	0	0.24	0/1834	0.54	0/2484
27	1	0.24	0/2285	0.44	0/3090
28	3	0.24	0/636	0.59	0/839
29	4	0.24	0/4877	0.43	0/6598
30	a	0.36	0/1234	0.55	0/1665
31	b	0.28	0/2582	0.49	0/3480
32	A	0.24	0/21777	0.70	3/33897 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	9	0.27	0/114	0.50	0/152
All	All	0.25	0/71714	0.57	3/101191 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
5	F	0	1
6	G	0	1
8	I	0	1
23	X	0	2
31	b	0	2
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	1133	C	C4-C5-C6	7.63	121.21	117.40
32	A	1133	C	N3-C4-C5	6.37	124.45	121.90
32	A	1264	C	OP1-P-O3'	5.48	117.26	105.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	41	ARG	Sidechain
5	F	166	ARG	Sidechain
6	G	276	ARG	Sidechain
8	I	184	5F0	Mainchain
23	X	232	ARG	Sidechain
23	X	234	ARG	Sidechain
31	b	341	ARG	Sidechain
31	b	347	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1828	1814	1815	9	0
2	C	1083	1088	1088	7	0
3	D	2575	2614	2614	8	0
4	E	910	930	930	5	0
5	F	1645	1698	1699	6	0
6	G	2588	2574	2573	20	0
7	H	1152	1183	1183	4	0
8	I	1020	1055	1053	3	0
9	J	839	885	887	5	0
10	K	862	885	885	6	0
11	L	1453	1540	1540	5	0
12	M	941	964	964	8	0
13	N	868	928	928	2	0
14	O	1599	1567	1566	5	0
15	P	781	807	807	3	0
16	Q	744	757	758	1	0
17	R	2409	2428	2428	9	0
18	S	1111	1115	1115	4	0
19	T	1371	1396	1394	6	0
20	U	1488	1499	1499	8	0
21	V	2884	2887	2885	10	0
22	W	789	802	802	3	0
23	X	2849	2844	2844	18	0
24	Y	1023	970	970	4	0
25	Z	797	815	815	0	0
26	0	1787	1795	1796	5	0
27	1	2238	2268	2269	10	0
28	3	625	697	699	3	0
29	4	4768	4764	4766	16	0
30	a	1218	1218	1220	0	0
31	b	2538	2610	2610	0	0
32	A	19584	9941	9946	89	0
33	9	111	108	108	1	0
34	O	1	0	0	0	0
35	P	4	0	0	1	0
35	T	4	0	0	0	0
36	X	31	12	12	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	X	28	10	12	1	0
38	A	44	26	26	0	0
39	A	14	0	26	2	0
40	A	13	0	0	0	0
41	0	1	0	0	1	0
41	A	2	0	0	0	0
41	C	1	0	0	1	0
41	G	2	0	0	0	0
41	I	1	0	0	0	0
41	T	1	0	0	0	0
All	All	68625	59494	59532	234	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASN:ND2	32:A:1294:A:OP1	2.22	0.72
6:G:315:PHE:CD2	6:G:369:LEU:HD21	2.26	0.70
12:M:67:ALA:HB1	17:R:161:ILE:HG13	1.72	0.70
24:Y:326:SER:O	27:1:217:GLN:NE2	2.23	0.70
29:4:200:ASP:OD2	29:4:243:ASN:N	2.25	0.70
6:G:217:ASP:OD1	6:G:218:TYR:N	2.25	0.69
32:A:1203:C:O2	32:A:1362:G:N2	2.26	0.69
7:H:131:ARG:NH2	32:A:1450:C:O3'	2.27	0.67
9:J:117:ASP:OD2	32:A:894:C:N4	2.28	0.66
12:M:55:ASP:OD2	19:T:146:GLN:NE2	2.27	0.66
28:3:145:LYS:NZ	32:A:1583:MA6:O3'	2.26	0.66
9:J:80:CYS:SG	9:J:92:VAL:HG13	2.36	0.66
21:V:40:TRP:O	21:V:43:ARG:NH1	2.29	0.65
23:X:338:ASP:OD1	27:1:292:TYR:OH	2.15	0.65
29:4:451:ASP:OD1	29:4:455:ASN:ND2	2.30	0.64
23:X:379:GLU:O	23:X:383:LEU:HD23	1.97	0.64
15:P:48:GLU:O	22:W:85:ARG:NH1	2.31	0.63
29:4:470:GLN:NE2	29:4:472:ASP:OD2	2.32	0.63
5:F:71:THR:O	6:G:253:LYS:NZ	2.32	0.62
32:A:1583:MA6:H93	32:A:1584:MA6:N1	2.15	0.62
3:D:307:LYS:NZ	17:R:103:TYR:OH	2.32	0.62
14:O:97:ARG:NH1	32:A:871:A:OP2	2.33	0.61
32:A:1044:U:OP1	32:A:1110:A:O2'	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:50:TYR:O	5:F:66:ARG:NH2	2.33	0.61
18:S:50:ARG:NH1	32:A:1119:U:OP2	2.33	0.61
29:4:237:THR:O	29:4:237:THR:HG22	2.00	0.60
32:A:1369:U:O2'	32:A:1370:U:OP1	2.17	0.60
8:I:71:SER:O	8:I:74:ARG:NH1	2.33	0.60
26:0:136:TYR:OH	32:A:705:C:OP2	2.11	0.60
9:J:80:CYS:SG	9:J:93:CYS:O	2.62	0.58
11:L:86:ASP:OD1	11:L:87:ASP:N	2.36	0.58
32:A:688:A:O2'	32:A:689:U:OP2	2.19	0.58
29:4:239:ARG:O	29:4:242:ASN:ND2	2.36	0.58
19:T:132:ARG:NH1	19:T:136:LEU:O	2.37	0.58
17:R:219:TYR:O	17:R:256:ARG:NH2	2.37	0.58
4:E:15:ARG:NH1	20:U:182:ASP:OD1	2.36	0.57
2:C:152:ARG:NH1	24:Y:300:GLU:OE1	2.36	0.57
23:X:299:ASN:ND2	27:1:265:THR:OG1	2.38	0.57
10:K:60:ASN:OD1	10:K:68:GLN:NE2	2.37	0.56
3:D:363:ALA:O	3:D:367:GLY:N	2.37	0.56
32:A:688:A:OP2	32:A:829:C:N4	2.35	0.56
32:A:1365:A:OP1	32:A:1388:C:O2'	2.23	0.56
32:A:1179:G:H4'	32:A:1180:U:OP2	2.06	0.56
12:M:74:ARG:NH2	20:U:77:GLU:OE2	2.39	0.56
23:X:123:ARG:NH2	23:X:337:LEU:O	2.39	0.56
32:A:946:U:H5	39:A:1702:SPM:H71	1.71	0.55
32:A:1057:G:H4'	32:A:1578:A:H4'	1.89	0.55
16:Q:52:ARG:NH2	32:A:1591:C:OP1	2.39	0.55
17:R:317:ALA:O	17:R:321:ALA:N	2.39	0.55
1:B:138:ARG:NH1	18:S:30:LEU:O	2.40	0.55
32:A:843:G:N2	32:A:846:A:OP2	2.38	0.55
23:X:276:ARG:NH2	23:X:286:GLU:OE1	2.39	0.55
14:O:199:TRP:NE1	26:0:166:TYR:O	2.38	0.55
12:M:53:SER:H	12:M:67:ALA:HB3	1.72	0.54
32:A:1108:C:H4'	32:A:1109:A:OP2	2.07	0.54
5:F:88:ASP:OD2	5:F:146:HIS:NE2	2.38	0.54
2:C:115:ASN:ND2	24:Y:309:LYS:O	2.41	0.54
23:X:348:TYR:OH	36:X:501:ATP:O1B	2.16	0.54
6:G:150:LEU:O	6:G:153:THR:OG1	2.25	0.54
6:G:263:ASP:OD1	6:G:267:MET:N	2.40	0.54
27:1:255:ASN:N	27:1:259:GLU:OE1	2.37	0.54
21:V:74:ARG:O	21:V:78:ASN:ND2	2.38	0.53
8:I:184:5F0:CXT	32:A:1013:A:O2'	2.56	0.53
20:U:80:ARG:O	20:U:84:GLU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:11:ARG:NH2	32:A:932:C:N3	2.57	0.53
27:1:150:GLU:OE1	27:1:174:ARG:NH2	2.40	0.53
1:B:157:ASN:OD1	6:G:163:HIS:NE2	2.40	0.52
14:O:73:VAL:O	14:O:109:ARG:NH2	2.42	0.52
32:A:1080:A:O2'	32:A:1082:A:N7	2.38	0.52
10:K:90:ARG:NH1	10:K:95:SER:O	2.42	0.52
29:4:151:ASP:OD1	29:4:152:ILE:N	2.42	0.52
19:T:151:SER:OG	32:A:684:U:O2'	2.27	0.52
26:0:82:ARG:NH1	41:0:301:HOH:O	2.42	0.52
32:A:806:C:OP2	32:A:807:A:N6	2.42	0.52
6:G:237:GLU:OE1	6:G:237:GLU:N	2.42	0.52
32:A:1507:A:HO2'	32:A:1508:C:H6	1.58	0.52
29:4:306:ASN:OD1	29:4:344:ARG:NH2	2.43	0.52
6:G:210:VAL:HG12	6:G:210:VAL:O	2.10	0.51
6:G:312:GLN:OE1	6:G:345:ARG:NH1	2.43	0.51
8:I:129:GLN:NE2	8:I:167:MET:SD	2.84	0.50
23:X:107:GLU:OE2	27:1:313:LYS:NZ	2.37	0.50
26:0:43:ARG:O	26:0:47:GLY:N	2.37	0.50
32:A:1562:G:O2'	32:A:1563:U:OP2	2.26	0.50
2:C:113:ARG:NH2	41:C:201:HOH:O	2.43	0.50
29:4:331:ASN:ND2	29:4:333:GLN:OE1	2.45	0.50
32:A:1214:A:N7	32:A:1353:A:N6	2.59	0.50
18:S:98:ARG:NH2	18:S:128:GLU:OE1	2.44	0.50
21:V:68:SER:OG	21:V:392:ARG:NH2	2.44	0.50
32:A:688:A:O2'	32:A:689:U:P	2.69	0.50
21:V:46:GLU:OE2	21:V:74:ARG:NE	2.42	0.50
3:D:297:ARG:NH2	32:A:1118:A:N1	2.60	0.50
7:H:89:ASP:OD1	7:H:141:ARG:NH1	2.42	0.50
19:T:89:ASP:OD2	20:U:120:ARG:NH2	2.40	0.50
20:U:137:LEU:O	20:U:141:ARG:N	2.39	0.49
32:A:1400:U:O2'	32:A:1401:G:OP1	2.30	0.49
6:G:322:ARG:NH1	6:G:355:PHE:O	2.46	0.49
32:A:1369:U:HO2'	32:A:1370:U:P	2.33	0.49
1:B:156:GLU:OE1	6:G:163:HIS:ND1	2.46	0.49
3:D:301:THR:HG23	3:D:301:THR:O	2.13	0.49
32:A:1056:A:C2'	32:A:1057:G:H5'	2.44	0.48
29:4:413:ASP:N	29:4:413:ASP:OD1	2.46	0.48
2:C:42:VAL:HG21	2:C:55:GLU:HG2	1.94	0.48
23:X:292:ASN:ND2	37:X:502:GDP:O3'	2.45	0.48
32:A:1369:U:O2'	32:A:1370:U:P	2.71	0.48
6:G:143:ASP:OD1	6:G:144:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:123:GLN:O	12:M:127:ALA:N	2.44	0.47
23:X:359:TYR:O	23:X:363:ASN:ND2	2.46	0.47
21:V:123:ASP:OD1	21:V:123:ASP:N	2.48	0.47
32:A:1179:G:H5"	32:A:1180:U:O5'	2.14	0.47
32:A:1562:G:O2'	32:A:1563:U:P	2.72	0.47
1:B:243:PRO:O	1:B:247:HIS:ND1	2.44	0.47
32:A:1283:A:H3'	32:A:1284:U:H5"	1.97	0.47
29:4:618:ALA:O	29:4:622:ASN:N	2.46	0.47
21:V:314:VAL:HG22	21:V:316:GLN:H	1.79	0.46
32:A:1291:U:O2'	32:A:1292:A:P	2.73	0.46
32:A:1055:U:H2'	32:A:1056:A:O4'	2.15	0.46
14:O:96:ARG:NH2	32:A:919:A:OP2	2.45	0.46
11:L:231:ALA:O	11:L:235:LYS:N	2.40	0.46
21:V:34:TYR:HA	21:V:372:ILE:HD11	1.96	0.46
32:A:1318:A:H3'	32:A:1319:A:H5"	1.97	0.46
10:K:33:ARG:HE	32:A:1236:C:H5"	1.80	0.46
32:A:1563:U:O2	32:A:1564:A:N6	2.49	0.46
23:X:133:GLY:H	36:X:501:ATP:H8	1.63	0.46
32:A:1187:U:O3'	32:A:1188:A:O4'	2.34	0.46
5:F:119:LYS:NZ	23:X:365:TRP:O	2.42	0.46
6:G:270:SER:OG	6:G:351:ALA:O	2.32	0.46
23:X:175:LYS:O	23:X:176:GLN:HB2	2.15	0.46
11:L:126:GLU:HG2	11:L:177:VAL:HG11	1.98	0.46
15:P:49:ASP:OD2	22:W:82:SER:OG	2.32	0.46
17:R:69:THR:OG1	17:R:72:ASP:OD1	2.30	0.45
23:X:169:LEU:O	23:X:179:ASP:N	2.41	0.45
28:3:150:THR:HG22	28:3:150:THR:O	2.16	0.45
29:4:509:ILE:N	29:4:510:PRO:CD	2.79	0.45
32:A:1505:A:H2'	32:A:1506:U:O4'	2.16	0.45
15:P:73:ASP:OD1	15:P:74:TYR:N	2.50	0.45
5:F:161:ILE:HG22	5:F:163:LYS:H	1.81	0.45
3:D:300:ARG:NH1	32:A:1121:A:OP1	2.49	0.45
4:E:105:CYS:HB2	35:P:201:FES:S1	2.56	0.45
23:X:135:THR:HB	36:X:501:ATP:H1'	1.99	0.45
32:A:1503:G:H2'	32:A:1504:U:O4'	2.17	0.45
9:J:70:PRO:HB3	9:J:117:ASP:HB3	1.98	0.45
18:S:7:GLU:OE1	18:S:7:GLU:N	2.48	0.45
32:A:946:U:C5	39:A:1702:SPM:H71	2.50	0.45
21:V:166:GLU:O	21:V:170:GLN:HG2	2.16	0.45
32:A:985:U:H3	32:A:1003:A:H61	1.64	0.45
13:N:93:ASP:O	13:N:97:GLY:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:232:THR:N	3:D:236:GLY:O	2.45	0.44
32:A:1056:A:H2'	32:A:1057:G:H5'	2.00	0.44
32:A:1400:U:O2'	32:A:1401:G:P	2.75	0.44
6:G:78:ILE:HG22	6:G:78:ILE:O	2.17	0.44
10:K:58:ARG:NE	10:K:72:ASP:OD1	2.44	0.44
32:A:1506:U:O4	32:A:1507:A:N6	2.51	0.44
17:R:161:ILE:HG22	17:R:161:ILE:O	2.17	0.44
32:A:1205:U:C2	32:A:1206:G:C6	3.06	0.44
32:A:1326:A:H2'	32:A:1327:G:O4'	2.17	0.44
1:B:103:GLU:N	1:B:104:PRO:CD	2.81	0.44
6:G:320:VAL:O	6:G:321:ASP:OD1	2.36	0.44
32:A:1487:C:C4	32:A:1488:5MC:HM52	2.53	0.44
1:B:239:ASN:ND2	1:B:242:SER:OG	2.51	0.43
4:E:30:MET:HB2	20:U:170:ARG:HH21	1.83	0.43
33:9:78:ILE:O	33:9:79:LEU:C	2.56	0.43
6:G:243:ARG:O	6:G:246:ARG:NH1	2.51	0.43
32:A:1078:A:H2'	32:A:1079:G:H5"	2.00	0.43
32:A:1309:A:N6	32:A:1315:G:O6	2.52	0.43
32:A:1499:U:H2'	32:A:1500:C:O4'	2.19	0.43
32:A:764:A:O2'	32:A:765:C:OP2	2.33	0.43
32:A:1461:A:O3'	32:A:1462:G:C8	2.72	0.43
12:M:111:ARG:NH2	17:R:146:LYS:O	2.50	0.43
32:A:1133:C:N3	32:A:1133:C:N1	2.63	0.43
11:L:171:ARG:NH2	13:N:60:VAL:O	2.46	0.43
27:1:273:GLU:O	27:1:274:LYS:HB2	2.18	0.43
17:R:170:ARG:O	17:R:189:ARG:NH1	2.46	0.43
26:0:110:ASP:OD1	26:0:110:ASP:N	2.48	0.43
2:C:57:HIS:HB2	2:C:66:LYS:HD2	2.01	0.43
12:M:15:GLY:O	32:A:732:A:O2'	2.35	0.43
27:1:118:ALA:O	27:1:122:HIS:N	2.42	0.43
29:4:237:THR:O	29:4:237:THR:CG2	2.66	0.43
32:A:689:U:OP2	32:A:689:U:H3'	2.19	0.43
6:G:315:PHE:HD2	6:G:369:LEU:HD21	1.80	0.43
10:K:90:ARG:NH2	32:A:1236:C:OP2	2.44	0.42
29:4:236:VAL:HG12	29:4:238:TRP:H	1.84	0.42
32:A:1327:G:C2'	32:A:1328:G:H5'	2.49	0.42
32:A:1355:G:C8	32:A:1356:A:N7	2.87	0.42
4:E:26:ILE:HG23	4:E:36:VAL:HG21	2.00	0.42
32:A:1328:G:H2'	32:A:1329:U:O4'	2.20	0.42
32:A:1407:U:O2'	32:A:1446:A:O2'	2.23	0.42
32:A:948:U:OP2	32:A:1045:G:N1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:1504:U:H2'	32:A:1505:A:C8	2.54	0.42
3:D:400:GLU:OE1	19:T:95:ASN:ND2	2.50	0.42
32:A:1483:C:H4'	32:A:1484:C:H5'	2.02	0.42
6:G:91:MET:HB3	27:1:115:THR:HG21	2.02	0.42
29:4:508:VAL:HG12	29:4:508:VAL:O	2.20	0.42
32:A:1487:C:C5	32:A:1488:5MC:HM52	2.55	0.42
32:A:1365:A:H2	32:A:1421:G:H22	1.68	0.42
7:H:128:LYS:HD3	32:A:1227:G:OP1	2.20	0.42
12:M:67:ALA:HB2	17:R:196:TYR:CE1	2.55	0.42
32:A:765:C:H5'	32:A:766:G:OP2	2.19	0.42
11:L:76:TYR:O	11:L:79:VAL:HG22	2.19	0.41
32:A:1361:G:O2'	32:A:1449:G:OP1	2.33	0.41
32:A:1189:U:H1'	32:A:1190:C:OP1	2.20	0.41
32:A:1599:A:N3	32:A:1599:A:H2'	2.35	0.41
21:V:361:LYS:HG2	21:V:361:LYS:O	2.20	0.41
32:A:1564:A:O2'	32:A:1565:A:P	2.78	0.41
1:B:146:SER:OG	1:B:197:HIS:ND1	2.41	0.41
23:X:388:PRO:HB3	36:X:501:ATP:O1B	2.19	0.41
32:A:1019:A:H4'	32:A:1020:C:OP2	2.21	0.41
32:A:1465:C:H2'	32:A:1466:C:C1'	2.50	0.41
32:A:764:A:O2'	32:A:765:C:P	2.79	0.41
4:E:15:ARG:HB3	4:E:16:PRO:HD3	2.02	0.41
7:H:134:TYR:OH	10:K:116:ASP:OD1	2.30	0.41
24:Y:323:ASP:OD2	27:1:217:GLN:NE2	2.51	0.41
20:U:138:GLU:O	20:U:142:LYS:N	2.45	0.41
23:X:265:ILE:HG12	23:X:265:ILE:O	2.20	0.41
29:4:377:ARG:NE	29:4:418:SER:OG	2.54	0.41
2:C:40:ALA:HB3	2:C:59:PRO:HG3	2.03	0.41
32:A:1365:A:H5'	32:A:1366:C:O4'	2.20	0.41
32:A:1387:A:H4'	32:A:1388:C:O5'	2.21	0.41
3:D:351:ARG:NH2	32:A:1118:A:O2'	2.54	0.41
6:G:315:PHE:HB3	6:G:316:PRO:HD3	2.02	0.41
6:G:395:LYS:O	6:G:396:ARG:OXT	2.39	0.41
32:A:698:C:O2'	32:A:851:A:N7	2.46	0.41
2:C:58:ALA:HB1	2:C:59:PRO:CD	2.51	0.41
20:U:84:GLU:HG2	20:U:84:GLU:O	2.21	0.41
23:X:268:LEU:O	23:X:294:ARG:NH2	2.47	0.41
28:3:165:LYS:NZ	32:A:1149:G:OP2	2.46	0.41
23:X:264:GLY:N	23:X:309:ALA:O	2.50	0.40
5:F:168:TYR:O	5:F:169:GLN:C	2.59	0.40
21:V:264:GLU:OE2	21:V:333:ARG:NH2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:58:VAL:O	29:4:58:VAL:HG23	2.21	0.40
1:B:110:ARG:NH2	22:W:90:THR:O	2.51	0.40
9:J:80:CYS:SG	9:J:93:CYS:N	2.95	0.40
14:O:101:VAL:HG12	14:O:102:GLY:N	2.35	0.40
32:A:1185:C:HO2'	32:A:1186:A:P	2.43	0.40
32:A:1291:U:HO2'	32:A:1292:A:P	2.43	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	223/296 (75%)	215 (96%)	8 (4%)	0	100	100
2	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
3	D	316/430 (74%)	306 (97%)	10 (3%)	0	100	100
4	E	113/125 (90%)	110 (97%)	3 (3%)	0	100	100
5	F	198/242 (82%)	194 (98%)	4 (2%)	0	100	100
6	G	310/396 (78%)	298 (96%)	12 (4%)	0	100	100
7	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	19	53
8	I	134/194 (69%)	128 (96%)	6 (4%)	0	100	100
9	J	106/138 (77%)	98 (92%)	8 (8%)	0	100	100
10	K	99/128 (77%)	99 (100%)	0	0	100	100
11	L	172/257 (67%)	166 (96%)	6 (4%)	0	100	100
12	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
13	N	108/130 (83%)	102 (94%)	6 (6%)	0	100	100
14	O	192/258 (74%)	186 (97%)	6 (3%)	0	100	100
15	P	95/142 (67%)	95 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
17	R	293/360 (81%)	287 (98%)	6 (2%)	0	100	100
18	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
19	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
20	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
21	V	348/414 (84%)	341 (98%)	7 (2%)	0	100	100
22	W	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
23	X	350/398 (88%)	340 (97%)	10 (3%)	0	100	100
24	Y	119/395 (30%)	118 (99%)	1 (1%)	0	100	100
25	Z	92/106 (87%)	91 (99%)	1 (1%)	0	100	100
26	0	213/218 (98%)	208 (98%)	5 (2%)	0	100	100
27	1	274/323 (85%)	259 (94%)	15 (6%)	0	100	100
28	3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
29	4	584/689 (85%)	568 (97%)	16 (3%)	0	100	100
30	a	147/343 (43%)	140 (95%)	7 (5%)	0	100	100
31	b	320/407 (79%)	301 (94%)	18 (6%)	1 (0%)	37	68
33	9	10/698 (1%)	9 (90%)	1 (10%)	0	100	100
All	All	5925/8633 (69%)	5749 (97%)	174 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	126	ILE
31	b	294	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	198/249 (80%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	115/143 (80%)	115 (100%)	0	100	100
3	D	272/357 (76%)	272 (100%)	0	100	100
4	E	97/107 (91%)	97 (100%)	0	100	100
5	F	179/209 (86%)	178 (99%)	1 (1%)	84	91
6	G	273/342 (80%)	273 (100%)	0	100	100
7	H	130/180 (72%)	130 (100%)	0	100	100
8	I	104/146 (71%)	104 (100%)	0	100	100
9	J	93/118 (79%)	93 (100%)	0	100	100
10	K	91/113 (80%)	91 (100%)	0	100	100
11	L	158/226 (70%)	158 (100%)	0	100	100
12	M	97/113 (86%)	97 (100%)	0	100	100
13	N	96/115 (84%)	96 (100%)	0	100	100
14	O	175/230 (76%)	175 (100%)	0	100	100
15	P	88/123 (72%)	88 (100%)	0	100	100
16	Q	78/78 (100%)	78 (100%)	0	100	100
17	R	264/318 (83%)	264 (100%)	0	100	100
18	S	116/164 (71%)	116 (100%)	0	100	100
19	T	153/157 (98%)	153 (100%)	0	100	100
20	U	152/174 (87%)	152 (100%)	0	100	100
21	V	317/364 (87%)	317 (100%)	0	100	100
22	W	87/158 (55%)	87 (100%)	0	100	100
23	X	311/351 (89%)	311 (100%)	0	100	100
24	Y	112/357 (31%)	112 (100%)	0	100	100
25	Z	87/95 (92%)	87 (100%)	0	100	100
26	0	188/190 (99%)	188 (100%)	0	100	100
27	1	254/291 (87%)	254 (100%)	0	100	100
28	3	65/166 (39%)	65 (100%)	0	100	100
29	4	526/609 (86%)	526 (100%)	0	100	100
30	a	133/288 (46%)	132 (99%)	1 (1%)	79	88
31	b	274/350 (78%)	274 (100%)	0	100	100
33	9	12/600 (2%)	12 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5295/7481 (71%)	5293 (100%)	2 (0%)	100 100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	221	LYS
30	a	86	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
11	L	162	GLN
16	Q	4	HIS
21	V	145	ASN
21	V	170	GLN
23	X	292	ASN
24	Y	290	ASN
29	4	285	ASN
30	a	241	HIS
30	a	245	ASN
31	b	130	HIS
31	b	241	GLN
31	b	379	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	A	915/955 (95%)	266 (29%)	11 (1%)

All (266) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	A	650	U
32	A	651	A
32	A	680	U
32	A	684	U
32	A	688	A
32	A	689	U
32	A	695	A

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Mol	Chain	Res	Type
32	A	697	G
32	A	704	U
32	A	705	C
32	A	706	C
32	A	713	C
32	A	718	A
32	A	721	U
32	A	722	C
32	A	723	A
32	A	724	C
32	A	737	C
32	A	738	A
32	A	740	G
32	A	749	G
32	A	753	A
32	A	757	A
32	A	761	A
32	A	763	C
32	A	764	A
32	A	765	C
32	A	766	G
32	A	769	G
32	A	770	C
32	A	777	G
32	A	791	G
32	A	793	C
32	A	794	U
32	A	796	G
32	A	808	C
32	A	814	A
32	A	815	C
32	A	817	G
32	A	826	A
32	A	828	C
32	A	829	C
32	A	830	U
32	A	832	U
32	A	835	C
32	A	836	A
32	A	860	A
32	A	861	U
32	A	868	C

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Mol	Chain	Res	Type
32	A	869	C
32	A	870	C
32	A	871	A
32	A	881	A
32	A	890	C
32	A	902	G
32	A	904	C
32	A	905	A
32	A	907	A
32	A	908	C
32	A	919	A
32	A	929	A
32	A	931	C
32	A	932	C
32	A	935	C
32	A	937	U
32	A	938	A
32	A	939	A
32	A	940	A
32	A	941	G
32	A	942	A
32	A	950	A
32	A	954	C
32	A	955	A
32	A	958	C
32	A	959	C
32	A	960	C
32	A	961	U
32	A	962	C
32	A	963	C
32	A	964	C
32	A	967	A
32	A	974	U
32	A	975	A
32	A	978	A
32	A	979	C
32	A	985	U
32	A	986	G
32	A	991	G
32	A	992	U
32	A	993	A
32	A	994	A

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Mol	Chain	Res	Type
32	A	1001	C
32	A	1002	C
32	A	1003	A
32	A	1004	G
32	A	1010	A
32	A	1011	C
32	A	1012	A
32	A	1028	G
32	A	1040	U
32	A	1041	A
32	A	1042	U
32	A	1046	A
32	A	1049	A
32	A	1050	C
32	A	1058	C
32	A	1062	G
32	A	1065	C
32	A	1067	A
32	A	1069	A
32	A	1073	G
32	A	1080	A
32	A	1081	U
32	A	1082	A
32	A	1094	U
32	A	1103	A
32	A	1105	C
32	A	1106	C
32	A	1107	U
32	A	1115	U
32	A	1117	A
32	A	1119	U
32	A	1121	A
32	A	1126	A
32	A	1127	A
32	A	1136	C
32	A	1138	G
32	A	1144	U
32	A	1151	C
32	A	1153	C
32	A	1155	G
32	A	1160	A
32	A	1167	A

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Mol	Chain	Res	Type
32	A	1172	C
32	A	1174	U
32	A	1180	U
32	A	1182	C
32	A	1183	U
32	A	1184	U
32	A	1185	C
32	A	1186	A
32	A	1188	A
32	A	1189	U
32	A	1190	C
32	A	1191	C
32	A	1192	C
32	A	1201	A
32	A	1206	G
32	A	1213	A
32	A	1214	A
32	A	1215	U
32	A	1222	A
32	A	1223	C
32	A	1225	C
32	A	1226	C
32	A	1227	G
32	A	1230	C
32	A	1232	A
32	A	1233	C
32	A	1240	A
32	A	1241	C
32	A	1247	G
32	A	1248	C
32	A	1251	A
32	A	1254	C
32	A	1257	U
32	A	1269	U
32	A	1272	A
32	A	1273	G
32	A	1278	C
32	A	1283	A
32	A	1284	U
32	A	1285	G
32	A	1292	A
32	A	1297	G

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Mol	Chain	Res	Type
32	A	1298	U
32	A	1300	A
32	A	1314	C
32	A	1317	A
32	A	1318	A
32	A	1319	A
32	A	1325	U
32	A	1326	A
32	A	1327	G
32	A	1328	G
32	A	1330	C
32	A	1341	C
32	A	1342	C
32	A	1343	A
32	A	1350	G
32	A	1353	A
32	A	1357	A
32	A	1358	A
32	A	1359	U
32	A	1366	C
32	A	1367	A
32	A	1370	U
32	A	1380	G
32	A	1386	U
32	A	1387	A
32	A	1388	C
32	A	1390	A
32	A	1391	U
32	A	1400	U
32	A	1401	G
32	A	1402	A
32	A	1405	C
32	A	1411	G
32	A	1412	G
32	A	1413	U
32	A	1414	C
32	A	1417	A
32	A	1418	G
32	A	1420	U
32	A	1421	G
32	A	1422	G
32	A	1426	U

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Mol	Chain	Res	Type
32	A	1430	A
32	A	1432	U
32	A	1446	A
32	A	1447	G
32	A	1448	U
32	A	1456	U
32	A	1459	A
32	A	1461	A
32	A	1464	G
32	A	1466	C
32	A	1467	C
32	A	1468	U
32	A	1472	G
32	A	1474	G
32	A	1478	A
32	A	1480	A
32	A	1481	C
32	A	1482	A
32	A	1483	C
32	A	1484	C
32	A	1485	G
32	A	1492	A
32	A	1493	C
32	A	1495	C
32	A	1502	A
32	A	1507	A
32	A	1508	C
32	A	1509	U
32	A	1510	U
32	A	1511	C
32	A	1545	U
32	A	1550	A
32	A	1557	A
32	A	1562	G
32	A	1563	U
32	A	1564	A
32	A	1565	A
32	A	1568	U
32	A	1569	G
32	A	1571	U
32	A	1572	A
32	A	1573	A

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Mol	Chain	Res	Type
32	A	1574	G
32	A	1582	G
32	A	1594	G
32	A	1595	G
32	A	1598	G
32	A	1599	A
32	A	1600	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	A	931	C
32	A	1179	G
32	A	1189	U
32	A	1284	U
32	A	1369	U
32	A	1387	A
32	A	1390	A
32	A	1400	U
32	A	1404	A
32	A	1410	G
32	A	1564	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	MA6	A	1583	32	18,26,27	1.00	2 (11%)	19,38,41	3.37	3 (15%)
32	5MC	A	1488	32	18,22,23	0.52	0	26,32,35	0.48	0
8	5F0	I	184	8	8,8,9	0.58	0	7,9,11	1.03	1 (14%)
32	B8T	A	1486	32	19,22,23	3.31	8 (42%)	26,31,34	0.85	1 (3%)
32	5MU	A	1076	32	19,22,23	0.44	0	28,32,35	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	MA6	A	1584	32	18,26,27	1.00	2 (11%)	19,38,41	3.23	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	A	1583	32	-	5/7/29/30	0/3/3/3
32	5MC	A	1488	32	-	0/7/25/26	0/2/2/2
8	5F0	I	184	8	-	0/9/9/10	-
32	B8T	A	1486	32	-	0/7/27/28	0/2/2/2
32	5MU	A	1076	32	-	0/7/25/26	0/2/2/2
32	MA6	A	1584	32	-	1/7/29/30	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	1486	B8T	C4-N3	7.65	1.46	1.32
32	A	1486	B8T	C2-N3	5.97	1.48	1.36
32	A	1486	B8T	C6-C5	5.93	1.48	1.35
32	A	1486	B8T	C4-N4	4.82	1.45	1.35
32	A	1486	B8T	C2-N1	4.51	1.49	1.40
32	A	1486	B8T	C5-C4	3.50	1.48	1.40
32	A	1486	B8T	C6-N1	3.48	1.46	1.38
32	A	1486	B8T	O2-C2	-2.99	1.18	1.23
32	A	1583	MA6	C5-C4	-2.58	1.34	1.40
32	A	1584	MA6	C5-C4	-2.51	1.34	1.40
32	A	1583	MA6	C2-N3	2.43	1.36	1.32
32	A	1584	MA6	C2-N3	2.42	1.36	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	1583	MA6	N1-C6-N6	-13.14	103.23	117.06
32	A	1584	MA6	N1-C6-N6	-12.77	103.62	117.06
32	A	1583	MA6	N3-C2-N1	-5.54	120.02	128.68
32	A	1584	MA6	N3-C2-N1	-5.47	120.13	128.68
8	I	184	5F0	O-C-CB	-2.47	118.22	125.43
32	A	1486	B8T	C6-C5-C4	2.43	119.93	116.96
32	A	1583	MA6	C3'-C2'-C1'	2.23	104.34	100.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	1583	MA6	O4'-C4'-C5'-O5'
32	A	1583	MA6	C5-C6-N6-C9
32	A	1583	MA6	C3'-C4'-C5'-O5'
32	A	1583	MA6	N1-C6-N6-C9
32	A	1583	MA6	C5-C6-N6-C10
32	A	1584	MA6	C5-C6-N6-C9

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	1583	MA6	2	0
32	A	1488	5MC	2	0
8	I	184	5F0	1	0
32	A	1584	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	ATP	X	501	-	26,33,33	0.63	0	31,52,52	1.08	4 (12%)
35	FES	T	201	19	0,4,4	-	-	-		
38	NAD	A	1701	40	42,48,48	0.91	2 (4%)	50,73,73	0.95	2 (4%)
39	SPM	A	1702	-	13,13,13	0.34	0	12,12,12	0.97	0
35	FES	P	201	15	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	GDP	X	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.17	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	X	501	-	-	3/18/38/38	0/3/3/3
39	SPM	A	1702	-	-	4/11/11/11	-
38	NAD	A	1701	40	-	4/26/62/62	0/5/5/5
35	FES	T	201	19	-	-	0/1/1/1
35	FES	P	201	15	-	-	0/1/1/1
37	GDP	X	502	-	-	4/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A	1701	NAD	O4D-C1D	-2.62	1.37	1.41
38	A	1701	NAD	C8A-N7A	-2.61	1.30	1.34
37	X	502	GDP	C6-N1	-2.56	1.34	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	502	GDP	PA-O3A-PB	-3.54	120.69	132.83
38	A	1701	NAD	O4D-C1D-C2D	-2.73	102.94	106.93
37	X	502	GDP	C8-N7-C5	2.44	107.63	102.99
36	X	501	ATP	C5-C6-N6	2.35	123.92	120.35
37	X	502	GDP	C5-C6-N1	2.34	118.08	113.95
36	X	501	ATP	O4'-C1'-C2'	-2.18	103.73	106.93
38	A	1701	NAD	O2A-PA-O1A	2.05	122.37	112.24
36	X	501	ATP	O2'-C2'-C3'	-2.04	105.22	111.82
36	X	501	ATP	PB-O3B-PG	2.01	139.71	132.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	A	1701	NAD	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
37	X	502	GDP	C3'-C4'-C5'-O5'
39	A	1702	SPM	C3-C4-N5-C6
39	A	1702	SPM	C6-C7-C8-C9
37	X	502	GDP	O4'-C4'-C5'-O5'
39	A	1702	SPM	C7-C8-C9-N10
38	A	1701	NAD	C5D-O5D-PN-O3
38	A	1701	NAD	C5D-O5D-PN-O1N
37	X	502	GDP	PB-O3A-PA-O2A
39	A	1702	SPM	N5-C6-C7-C8
37	X	502	GDP	PB-O3A-PA-O1A
36	X	501	ATP	C5'-O5'-PA-O3A
36	X	501	ATP	O4'-C4'-C5'-O5'
38	A	1701	NAD	PA-O3-PN-O1N
36	X	501	ATP	C5'-O5'-PA-O1A

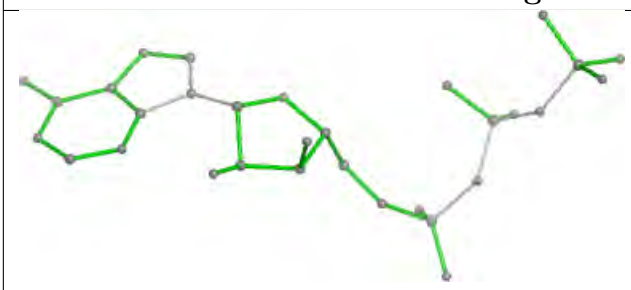
There are no ring outliers.

4 monomers are involved in 8 short contacts:

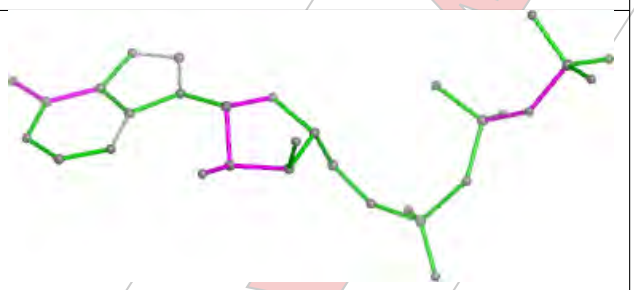
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	X	501	ATP	4	0
39	A	1702	SPM	2	0
35	P	201	FES	1	0
37	X	502	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

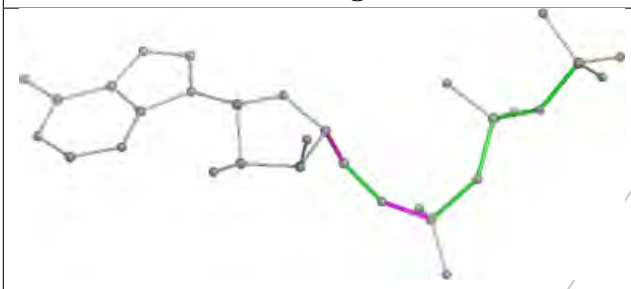
Ligand ATP X 501



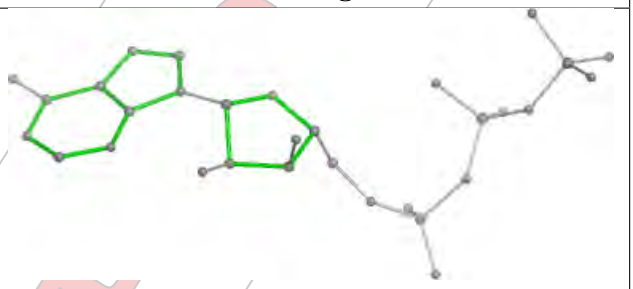
Bond lengths



Bond angles

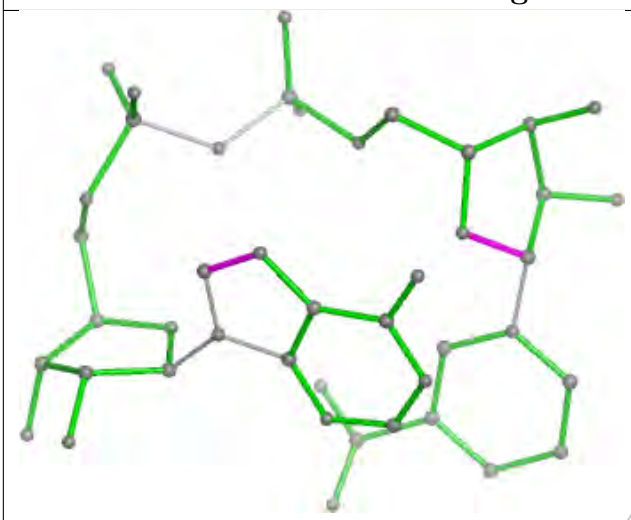


Torsions

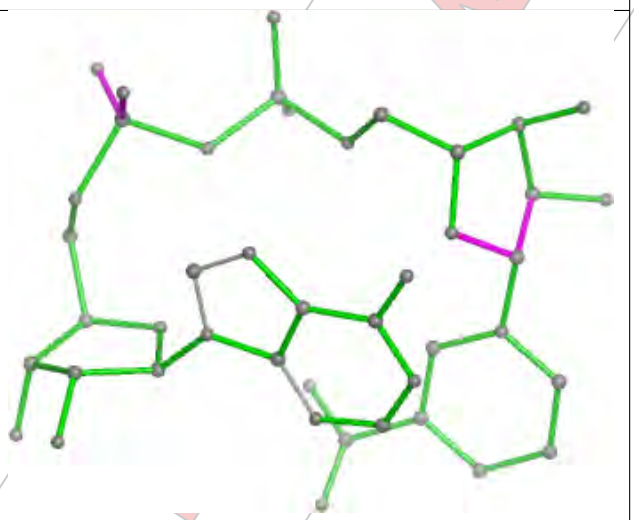


Rings

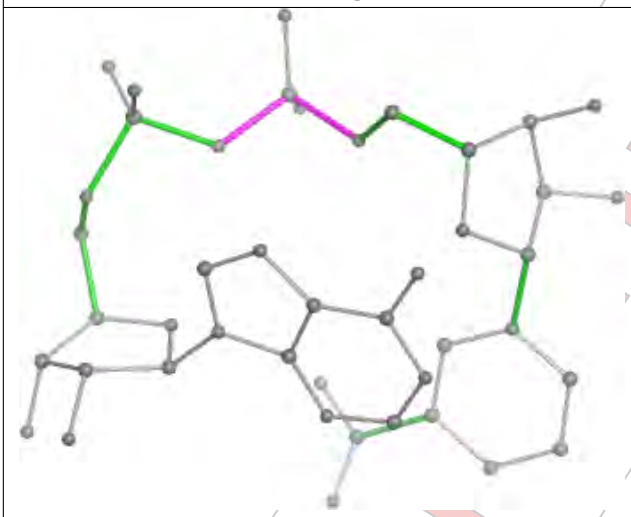
Ligand NAD A 1701



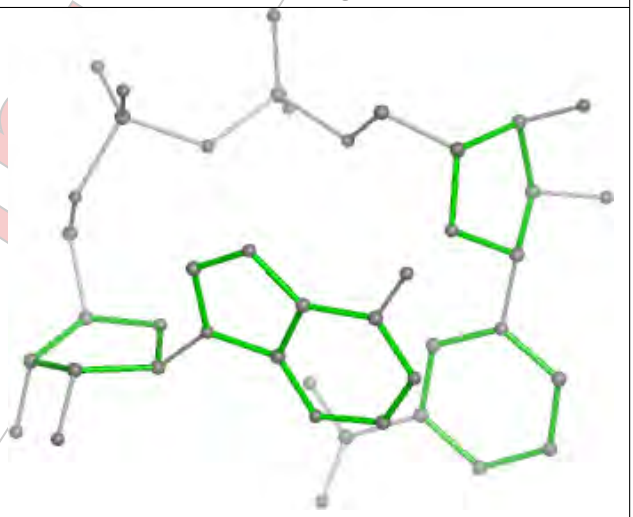
Bond lengths



Bond angles

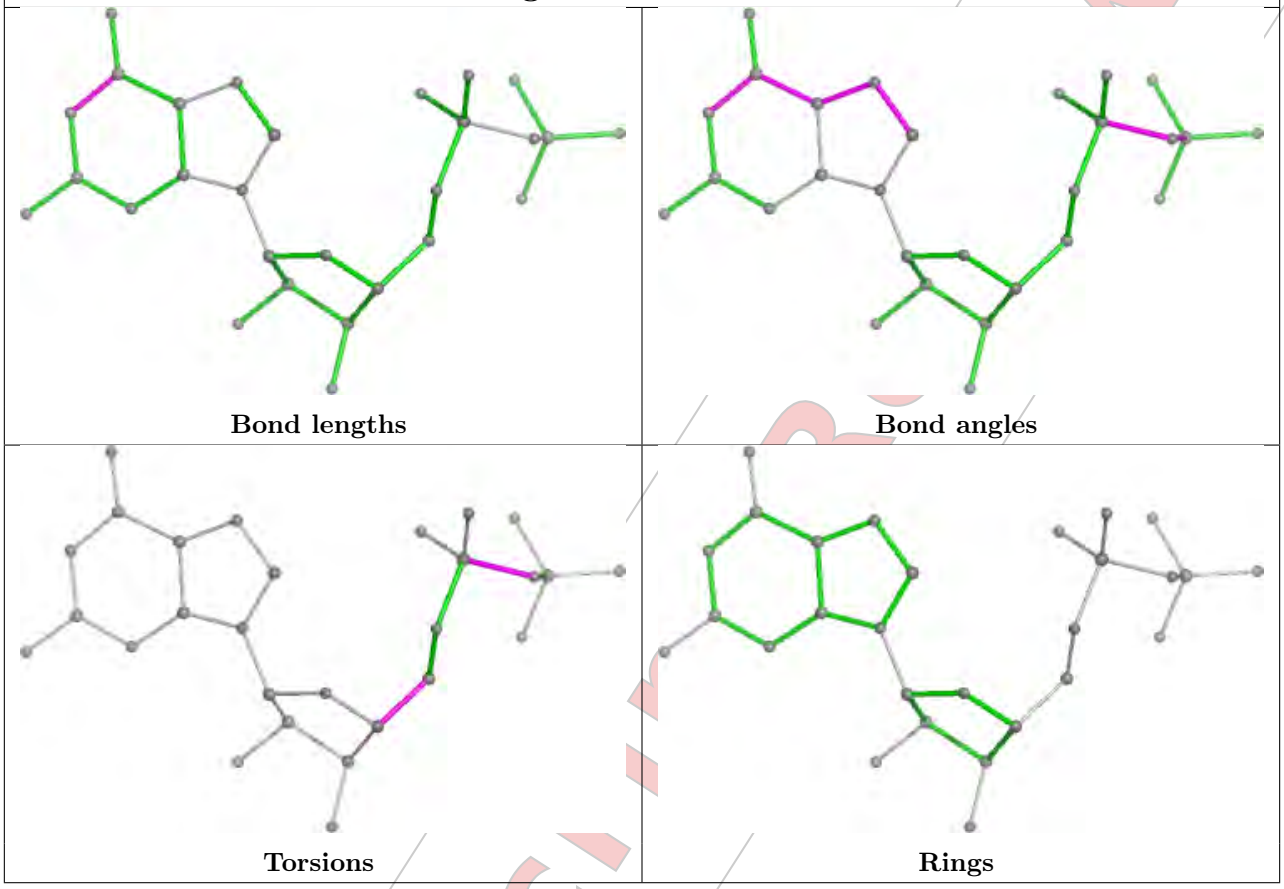


Torsions



Rings

Ligand GDP X 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1486:B8T	O3'	1487:C	P	4.48
1	A	1485:G	O3'	1486:B8T	P	3.07

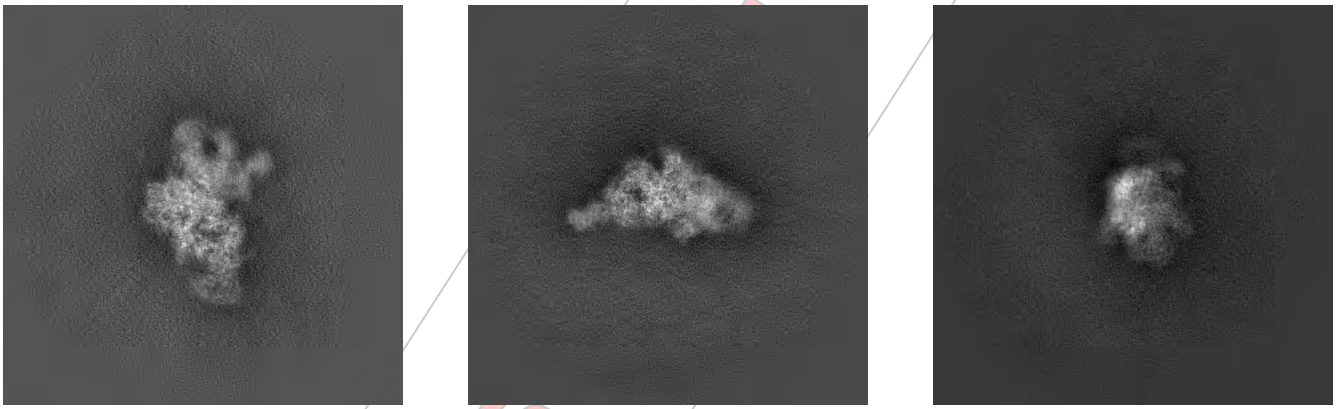
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51882. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

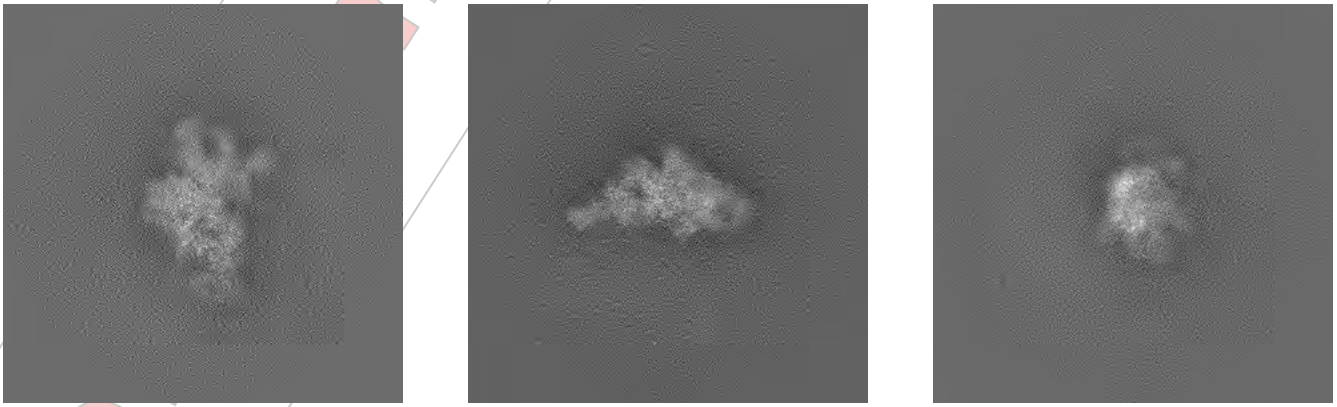
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

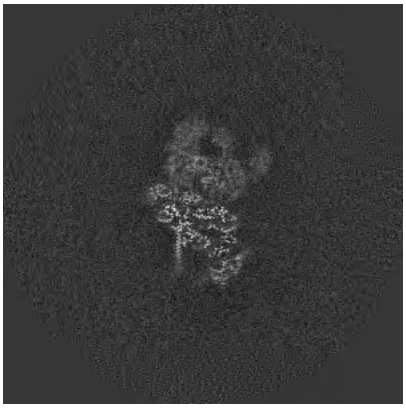


X Y Z

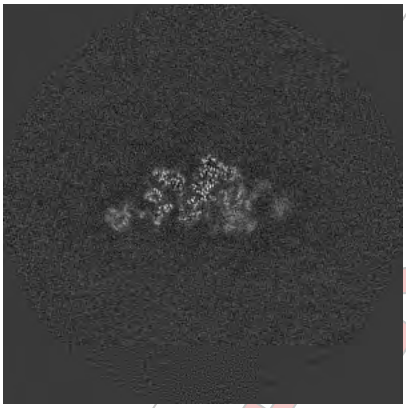
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

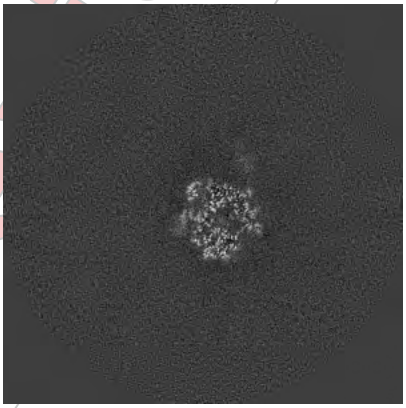
6.2.1 Primary map



X Index: 300

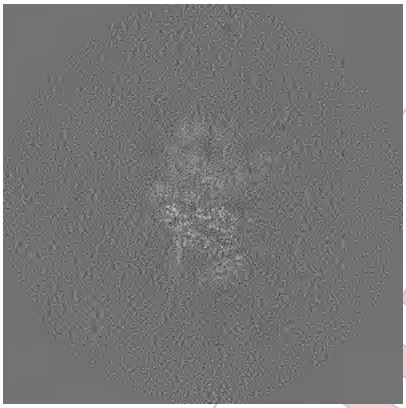


Y Index: 300

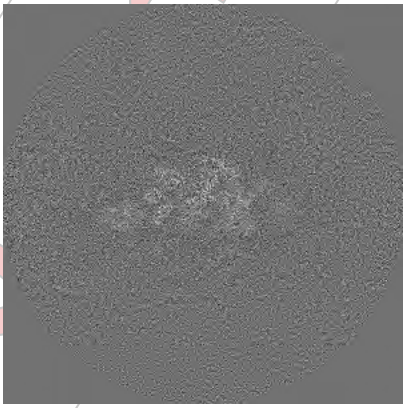


Z Index: 300

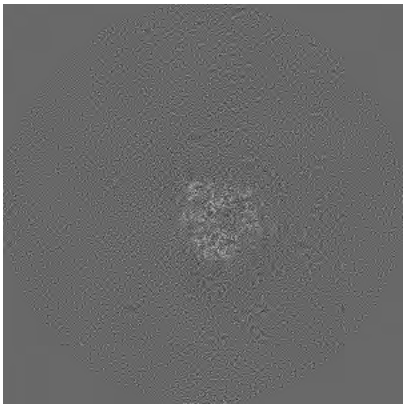
6.2.2 Raw map



X Index: 300



Y Index: 300

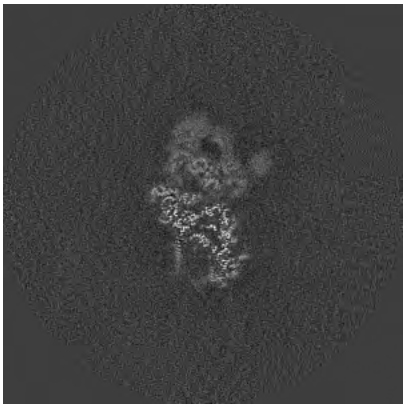


Z Index: 300

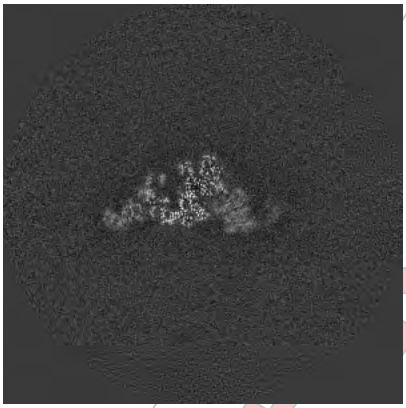
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

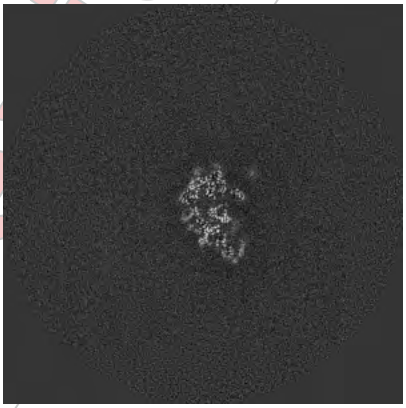
6.3.1 Primary map



X Index: 297

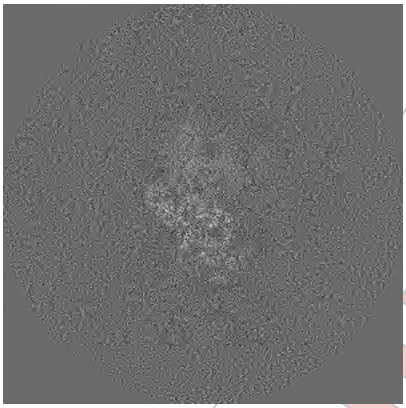


Y Index: 312

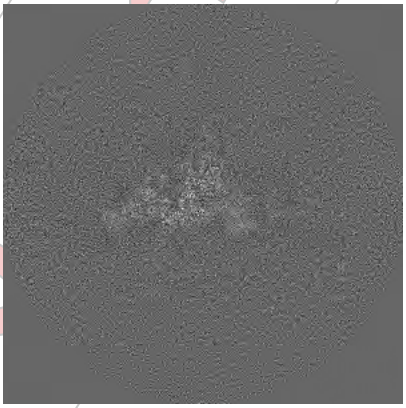


Z Index: 273

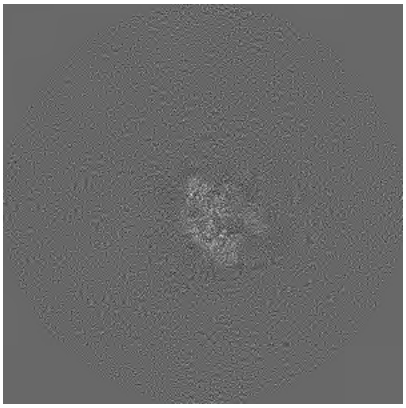
6.3.2 Raw map



X Index: 305



Y Index: 312

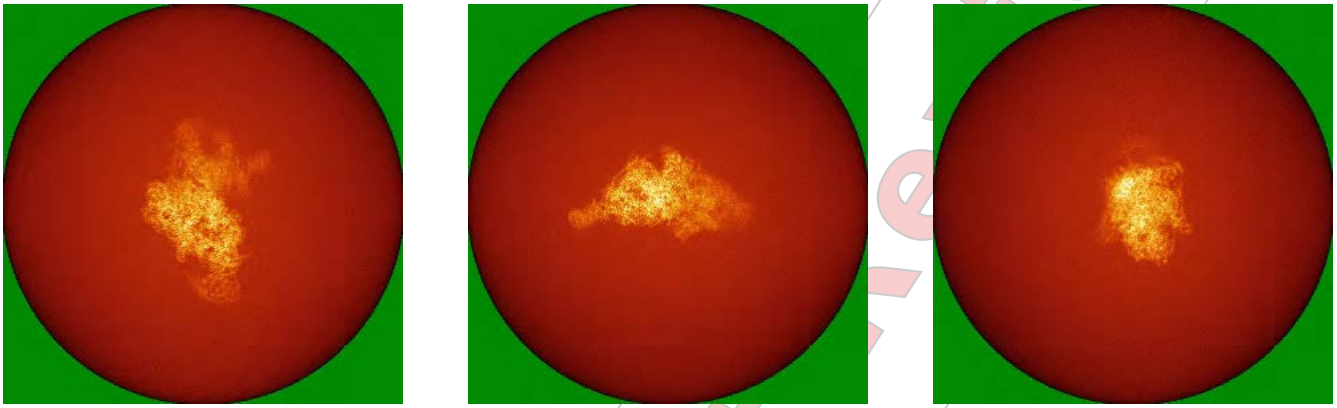


Z Index: 292

The images above show the largest variance slices of the map in three orthogonal directions.

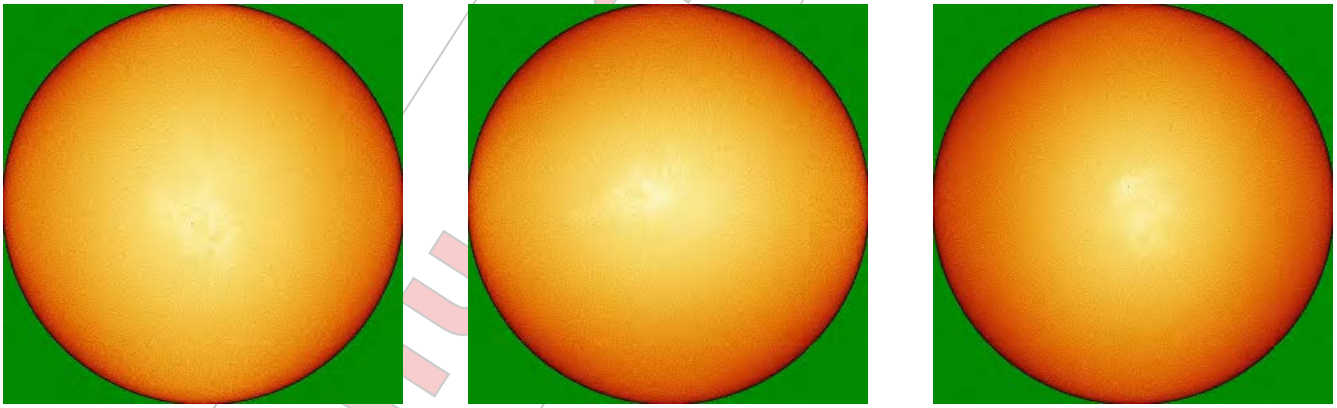
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

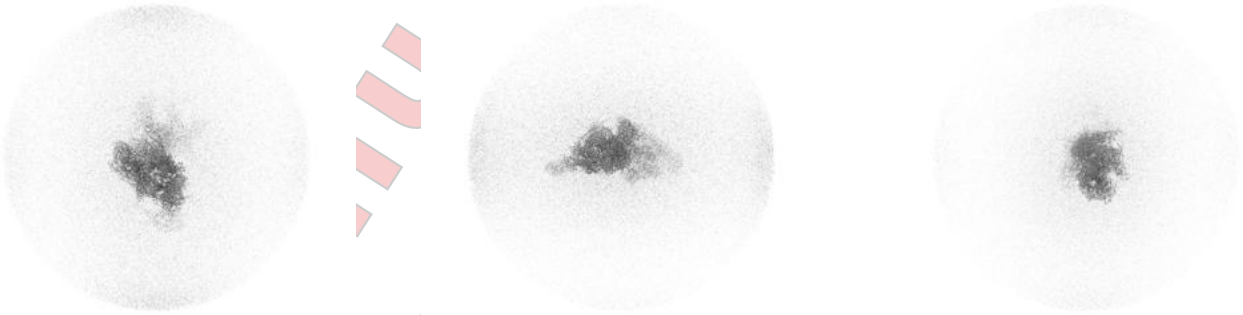
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

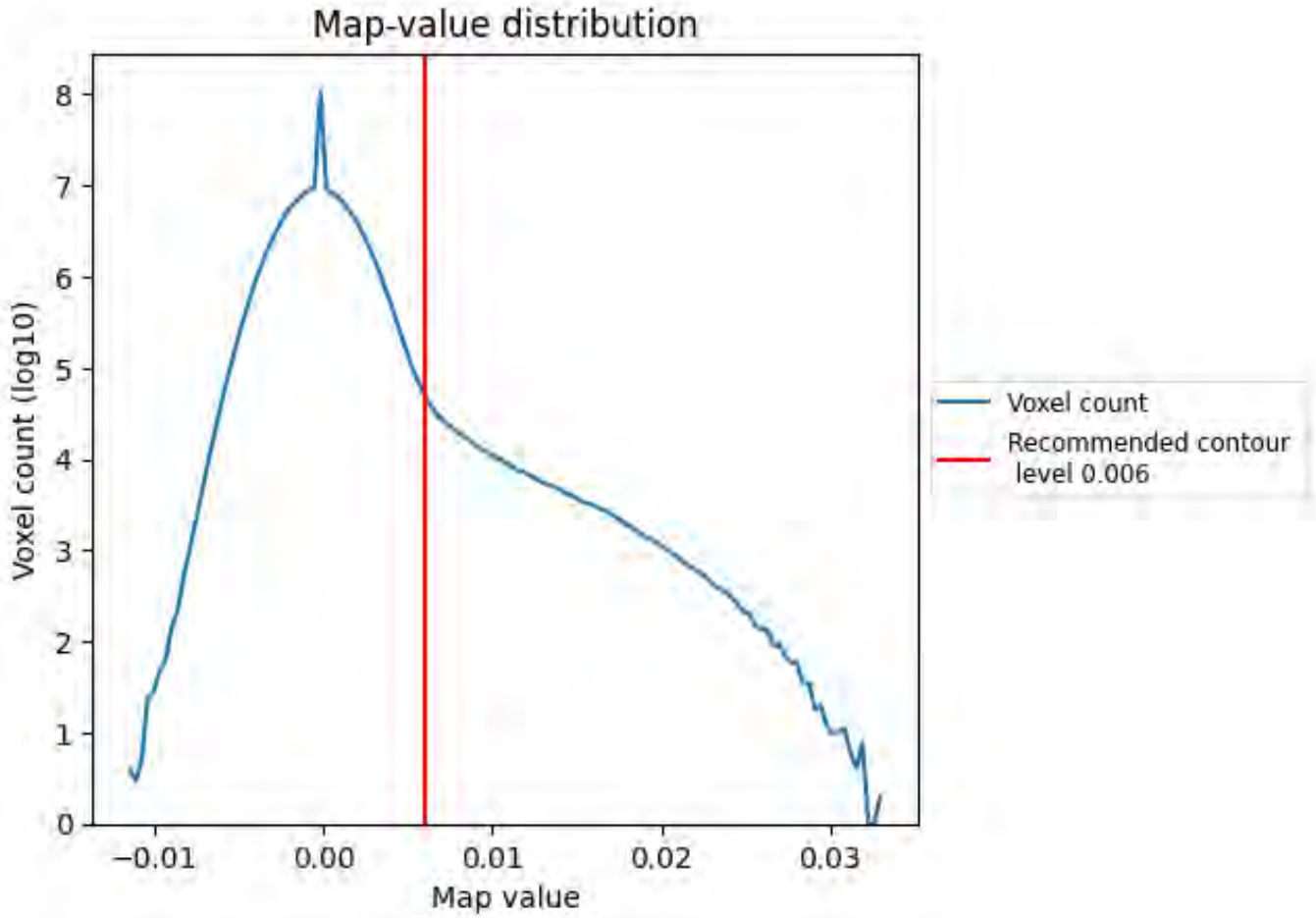
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

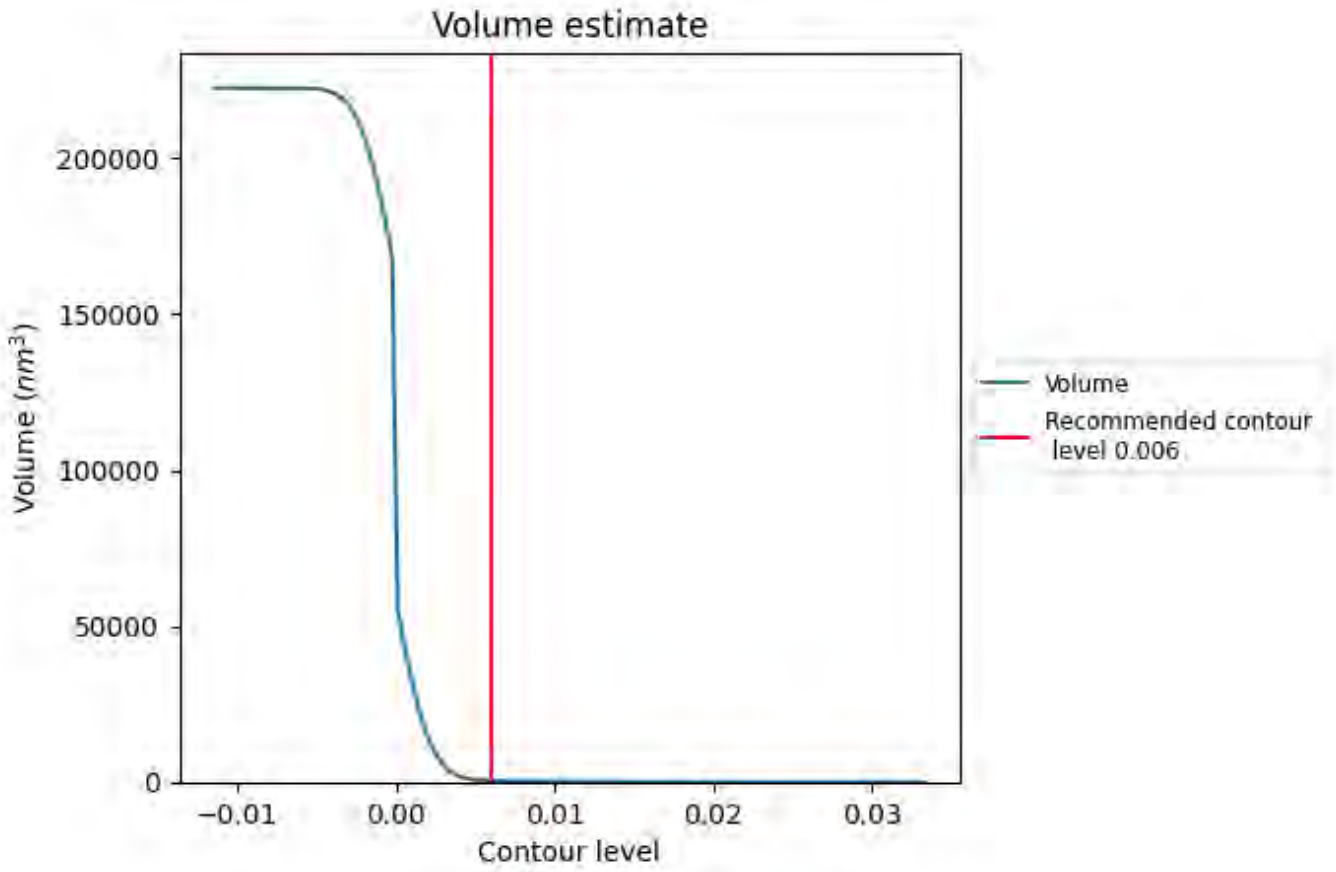
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

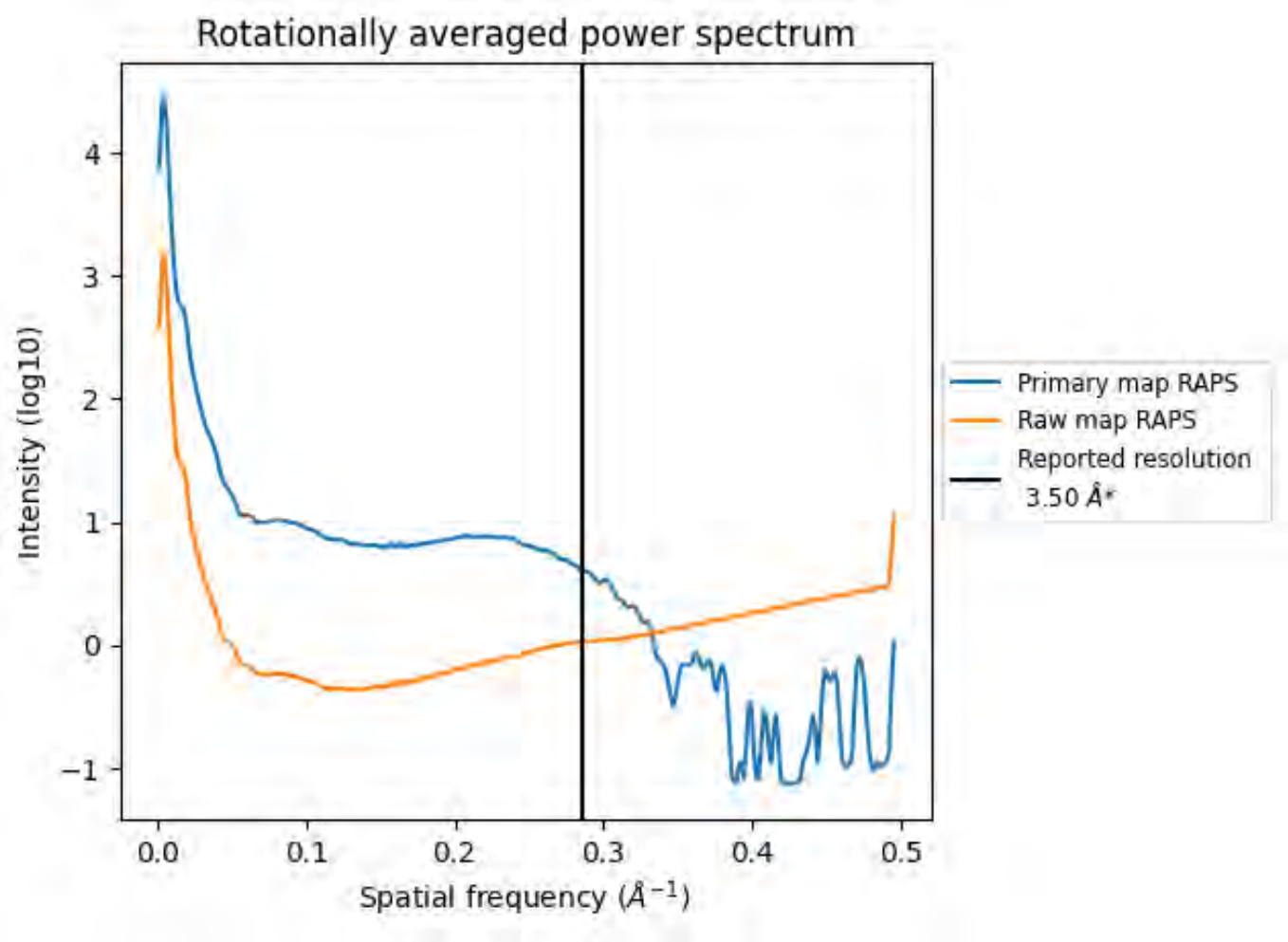
7.2 Volume estimate



The volume at the recommended contour level is 431 nm^3; this corresponds to an approximate mass of 389 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

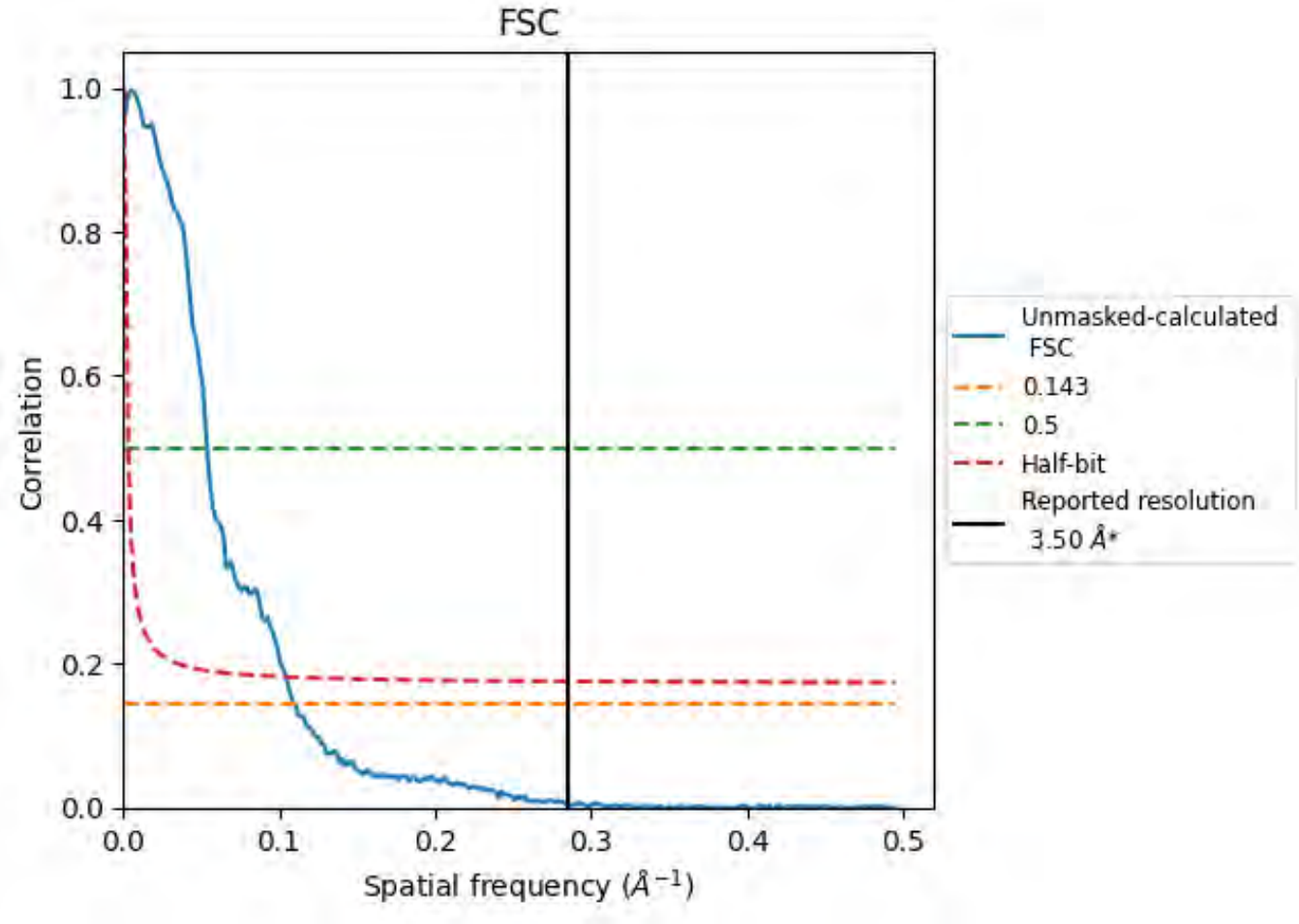


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

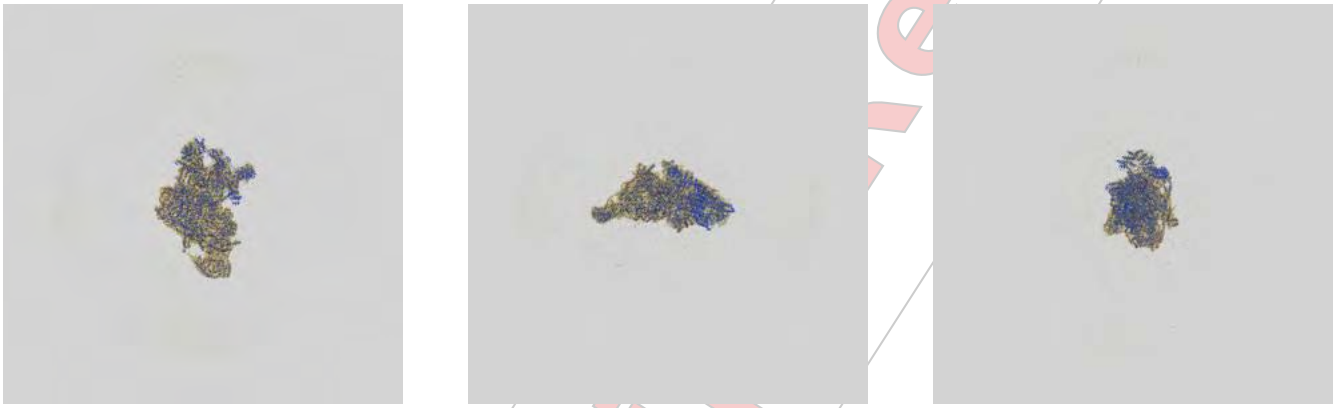
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.09	18.59	9.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.09 differs from the reported value 3.5 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51882 and PDB model 9H5A. Per-residue inclusion information can be found in section 3 on page 14.

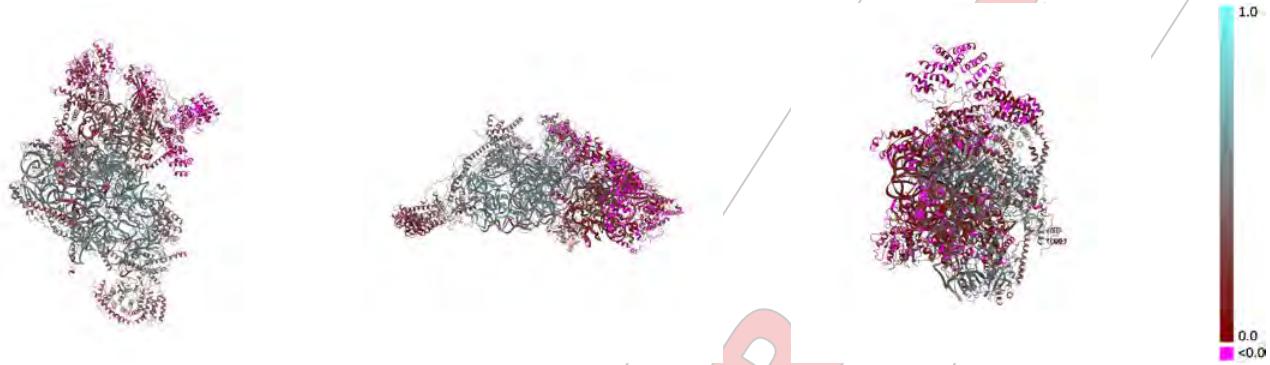
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

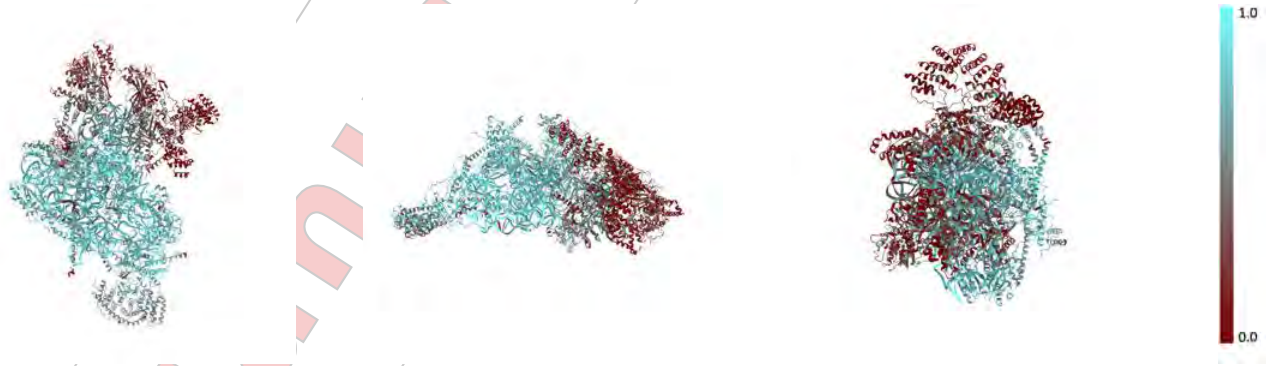
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

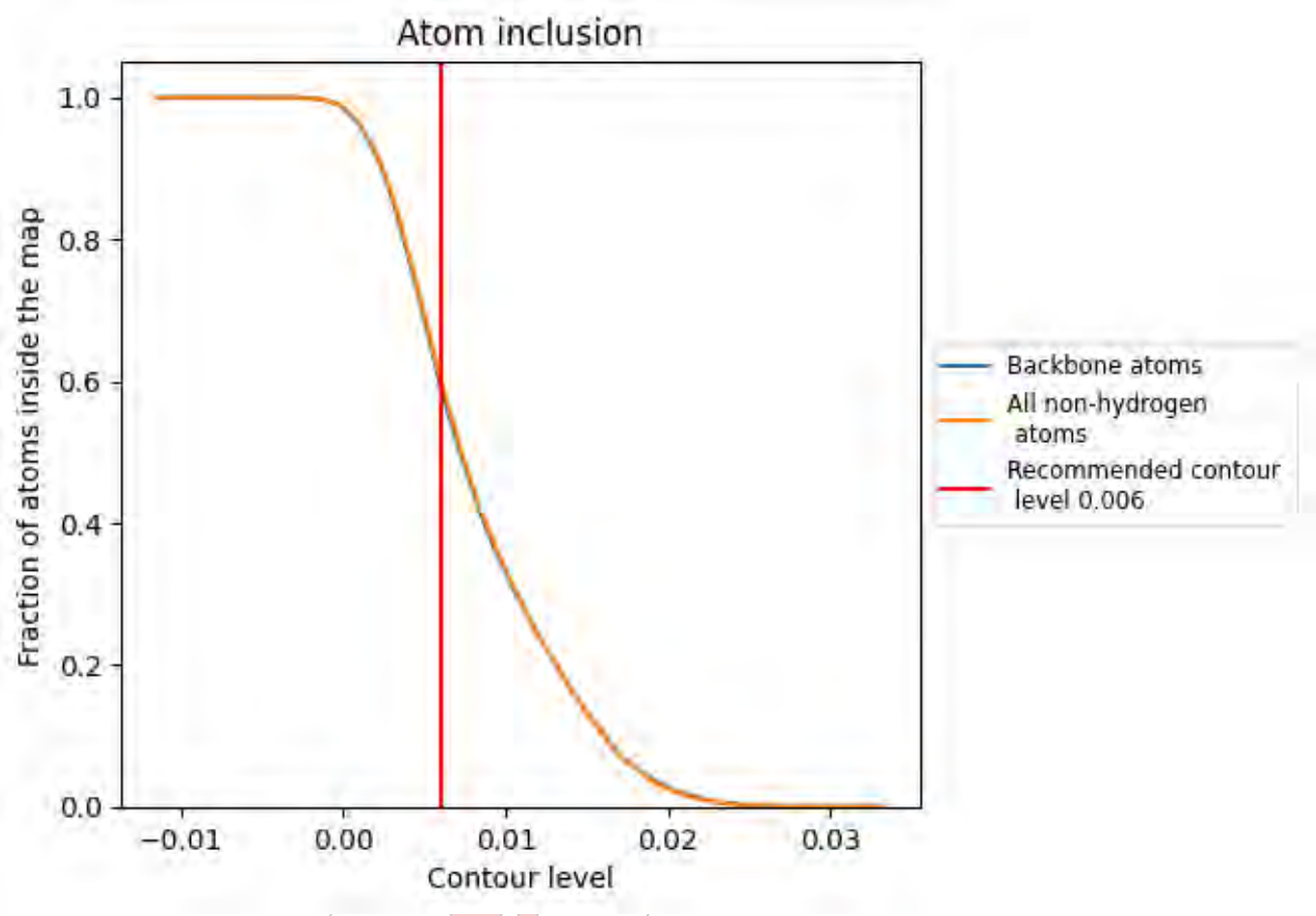
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.3410
0	0.6690	0.3920
1	0.1890	0.1210
3	0.7600	0.4620
4	0.1230	0.0580
9	0.2040	0.0820
A	0.8250	0.4300
B	0.8250	0.4980
C	0.4300	0.3090
D	0.6680	0.4340
E	0.7490	0.4680
F	0.3280	0.1800
G	0.4770	0.2620
H	0.2990	0.1860
I	0.7560	0.4410
J	0.7990	0.4920
K	0.4030	0.2100
L	0.7580	0.4630
M	0.8270	0.5160
N	0.8250	0.5240
O	0.8270	0.4950
P	0.7890	0.4720
Q	0.7540	0.4570
R	0.7830	0.4740
S	0.7330	0.4140
T	0.8050	0.4990
U	0.6980	0.3870
V	0.5190	0.2430
W	0.7570	0.4770
X	0.1770	0.1010
Y	0.1550	0.0980
Z	0.2790	0.1680
a	0.3100	0.1730
b	0.4590	0.2310

Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 12:10 am BST

PDB ID	:	9H57
EMDB ID	:	EMD-51879
Title	:	Structure of human mitochondrial ribosome small subunit bound to METTL15 and mS37 (State A7*)
Deposited on	:	2024-10-22
Resolution	:	4.00 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

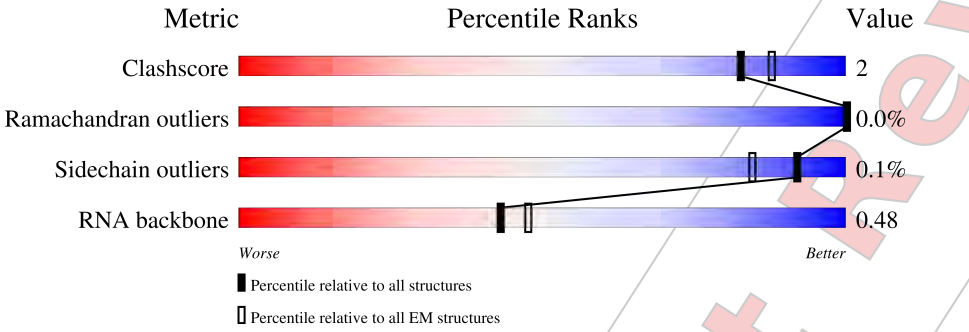
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	955	9% 71% 23%
2	B	296	46% 73% 24%
3	C	167	50% 77% 21%
4	D	430	49% 77% 20%
5	E	125	58% 92% 6%

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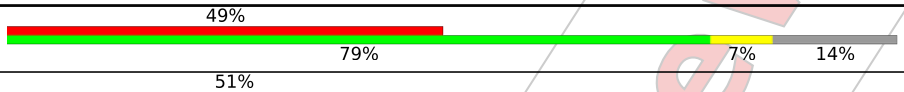
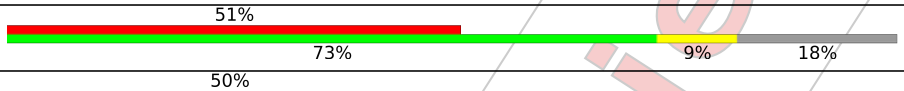
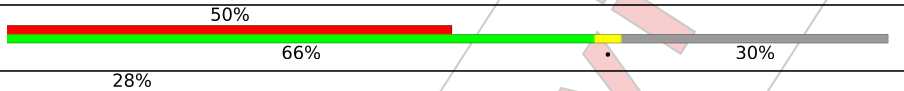
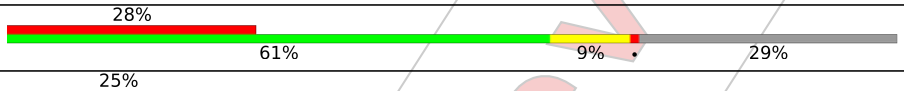
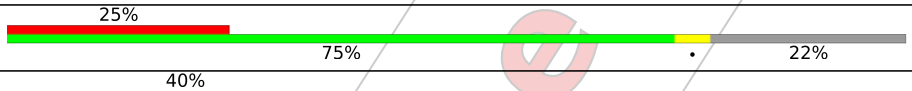
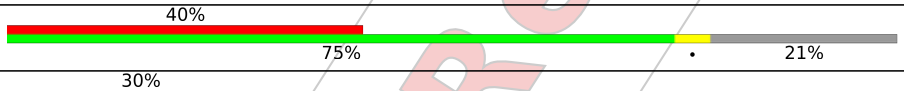
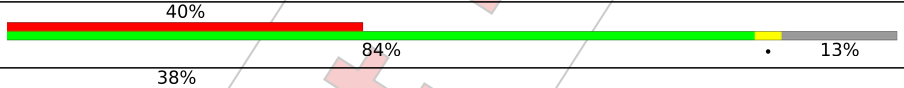
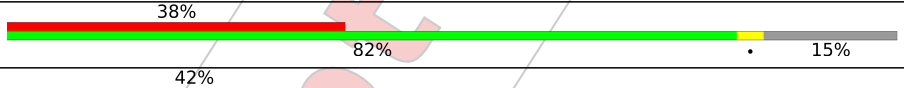
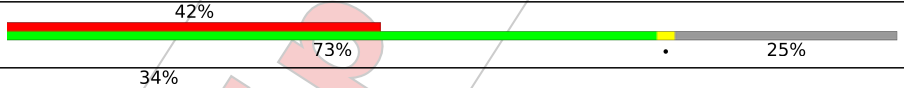
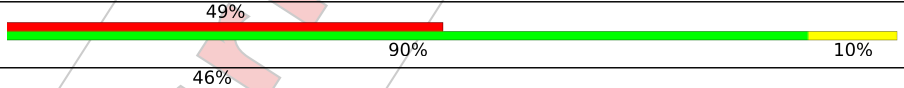
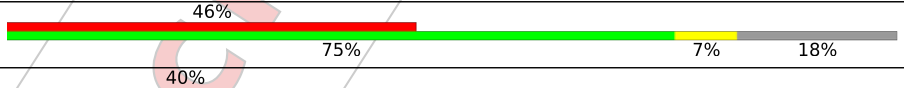
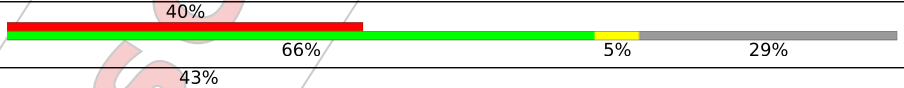
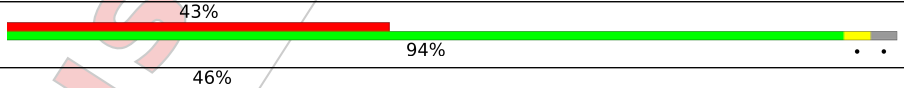
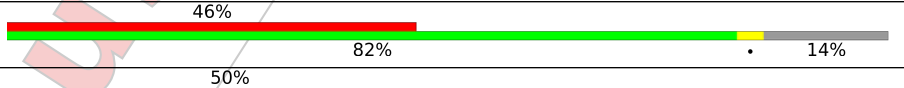
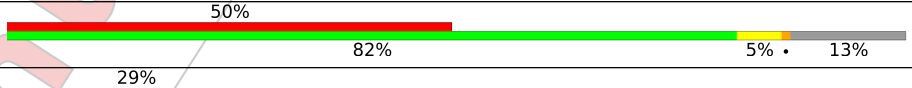
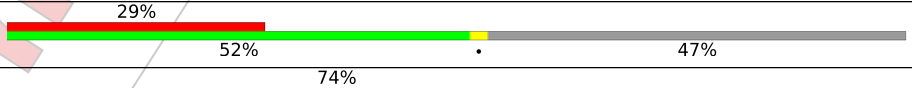
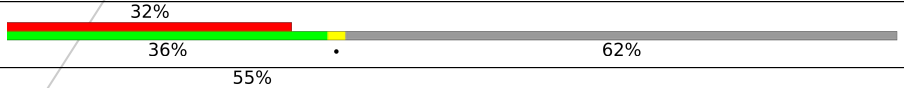
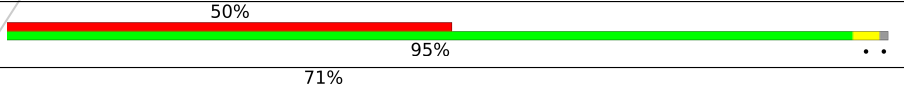
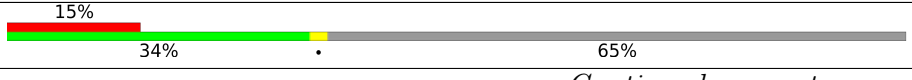
Mol	Chain	Length	Quality of chain
6	F	242	
7	G	396	
8	H	201	
9	I	194	
10	J	138	
11	K	128	
12	L	257	
13	M	137	
14	N	130	
15	O	258	
16	P	142	
17	Q	87	
18	R	360	
19	S	190	
20	T	173	
21	U	205	
22	V	414	
23	W	187	
24	X	398	
25	Y	395	
26	Z	106	
27	0	218	
28	1	323	
29	2	118	
30	3	199	

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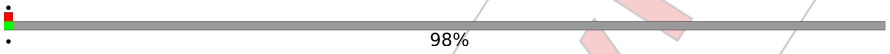
Mol	Chain	Length	Quality of chain
31	4	689	
32	b	407	
33	9	698	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 128748 atoms, of which 59808 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	929	29753	8850	10021	3551	6402	929	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	225	3643	1164	1815	331	323	10	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	132	2171	699	1088	195	185	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	343	5535	1713	2804	518	487	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	122	1972	614	1000	177	177	4	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	208	3494	1104	1769	312	298	11	0	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	324	5303	1684	2649	473	483	14	0	0

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	140	2335	745	1183	194	210	3	0	0

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	137	2080	642	1060	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	108	1726	521	887	169	143	6	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	101	1747	537	885	179	141	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	174	2993	925	1540	270	251	7	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1907	594	965	185	157	6		

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	110	Total	C	H	N	O	S	0	0
			1796	562	928	156	147	3		

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	194	Total	C	H	N	O	S	0	0
			3165	1019	1566	295	278	7		

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	97	Total	C	H	N	O	S	0	0
			1587	501	806	134	138	8		

- Molecule 17 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	87	Total	C	H	N	O	S	0	0
			1501	460	757	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	295	Total	C	H	N	O	S	0	0
			4837	1533	2428	413	455	8		

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	135	Total	C	H	N	O	S	0	0
			2226	716	1115	198	196	1		

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	168	Total	C	H	N	O	S	0	0
			2765	877	1394	239	244	11		

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	176	Total	C	H	N	O	S	0	0
			2987	916	1499	301	267	4		

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	362	Total	C	H	N	O	S	0	0
			5930	1904	2961	495	558	12		

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	100	Total	C	H	N	O	S	0	0
			1591	498	802	141	146	4		

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	352	Total	C	H	N	O	S	0	0
			5693	1822	2844	499	517	11		

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	149	Total	C	H	N	O	S	0	0
			2443	801	1197	207	234	4		

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	86	Total	C	H	N	O	S	0	0
			1464	468	734	128	130	4		

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	0	215	Total	C	H	N	O	S	0	0
			3583	1130	1796	339	313	5		

- Molecule 28 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	276	Total	C	H	N	O	S	0	0
			4507	1419	2269	381	427	11		

- Molecule 29 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	2	118	Total	C	H	N	O	S	0	0
			1903	579	968	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 30 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	3	70	Total	C	H	N	O	S	0	0
			1324	401	699	134	89	1		

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	588	Total	C	H	N	O	S	0	0
			9534	3053	4766	808	879	28		

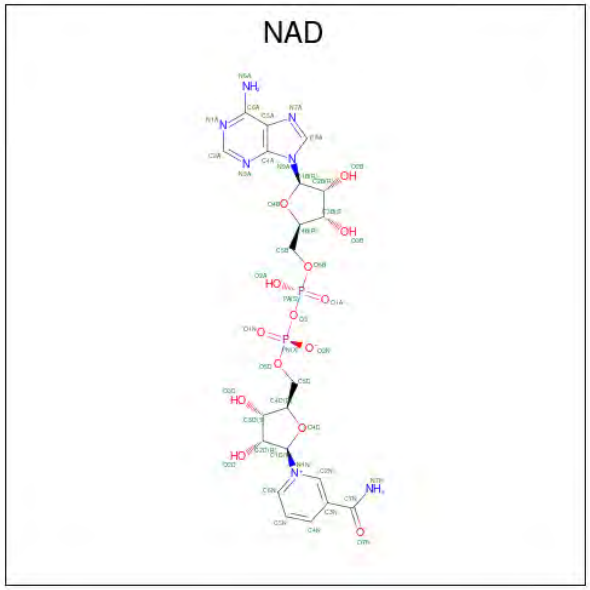
- Molecule 32 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	b	307	Total	C	H	N	O	S	0	0
			4850	1517	2457	426	437	13		

- Molecule 33 is a protein called Nitric oxide-associated protein 1.

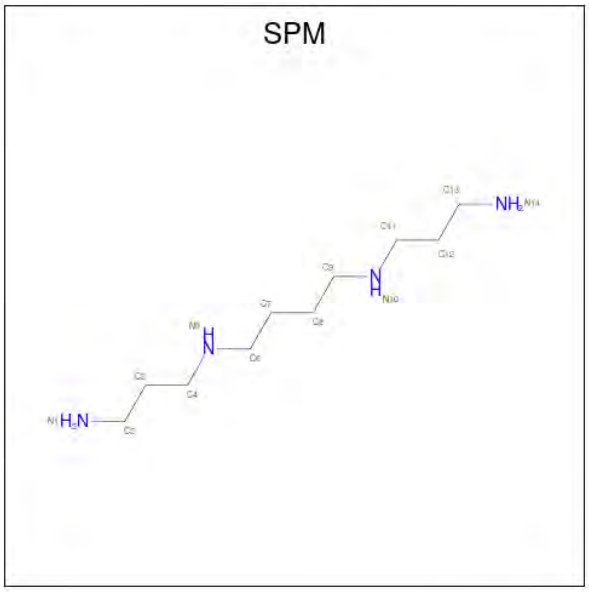
Mol	Chain	Residues	Atoms						AltConf	Trace
33	9	12	Total	C	H	N	O	S	0	0
			219	76	108	16	18	1		

- Molecule 34 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
34	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 35 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).

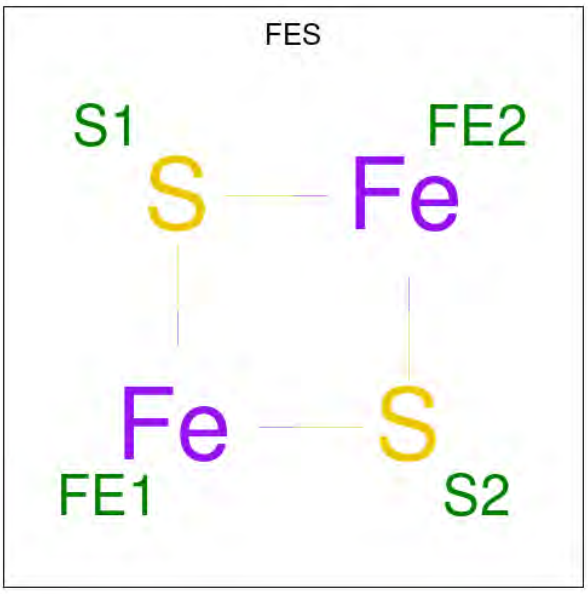


Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C N 14 10 4	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
36	B	1	Total Mg 1 1	0
36	3	1	Total Mg 1 1	0

- Molecule 37 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

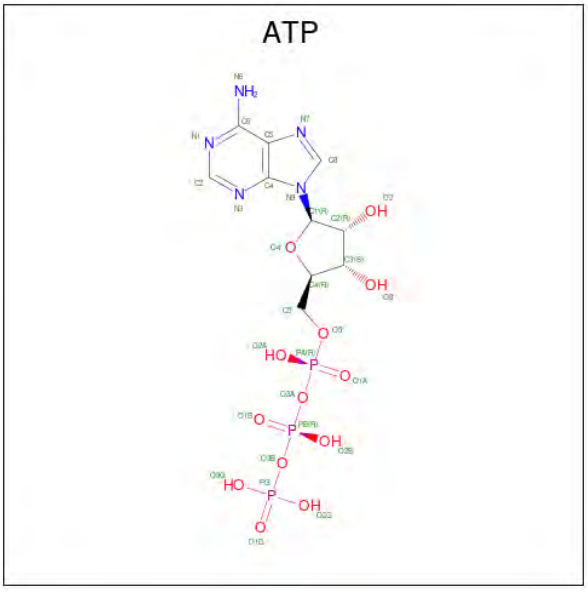


Mol	Chain	Residues	Atoms	AltConf
37	M	1	Total Fe S 4 2 2	0
37	P	1	Total Fe S 4 2 2	0

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

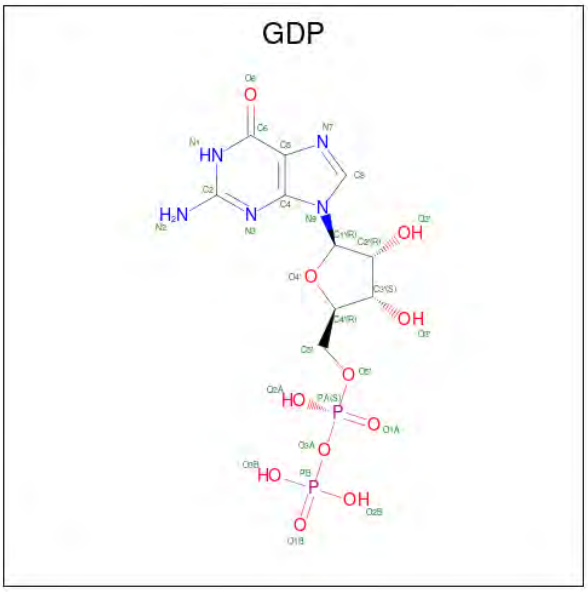
Mol	Chain	Residues	Atoms	AltConf
38	O	1	Total Zn 1 1	0

- Molecule 39 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
39	X	1	Total C H N O P 43 10 12 5 13 3	0

- Molecule 40 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						AltConf
40	X	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

- Molecule 41 is water.

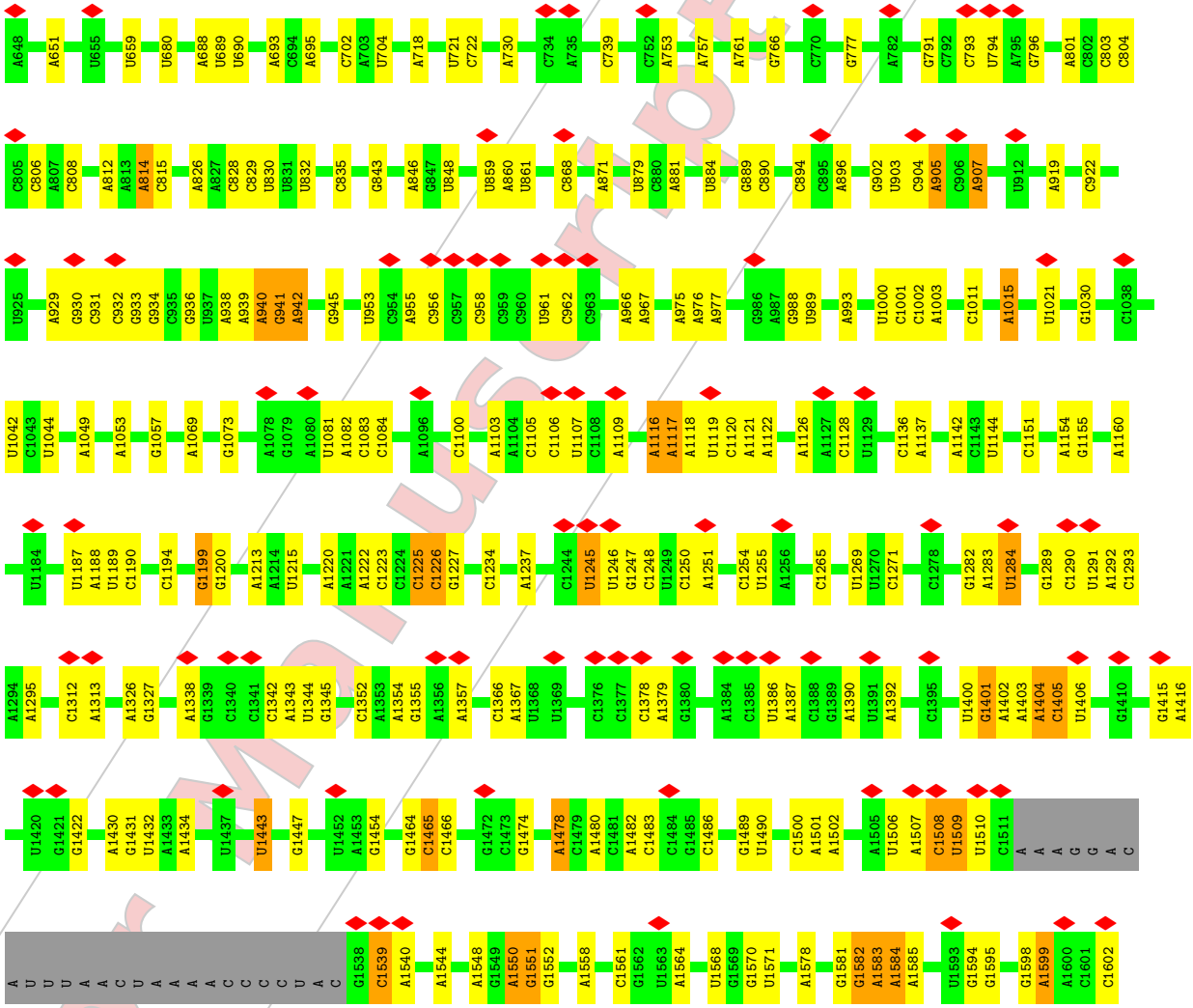
Mol	Chain	Residues	Atoms		AltConf
41	A	2	Total	O	0
			2	2	
41	C	2	Total	O	0
			2	2	
41	G	1	Total	O	0
			1	1	
41	T	1	Total	O	0
			1	1	
41	0	1	Total	O	0
			1	1	
41	2	1	Total	O	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 12S mitochondrial rRNA

Chain A:

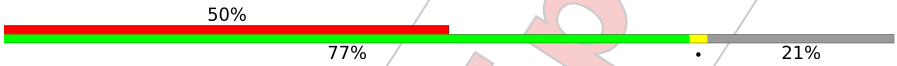


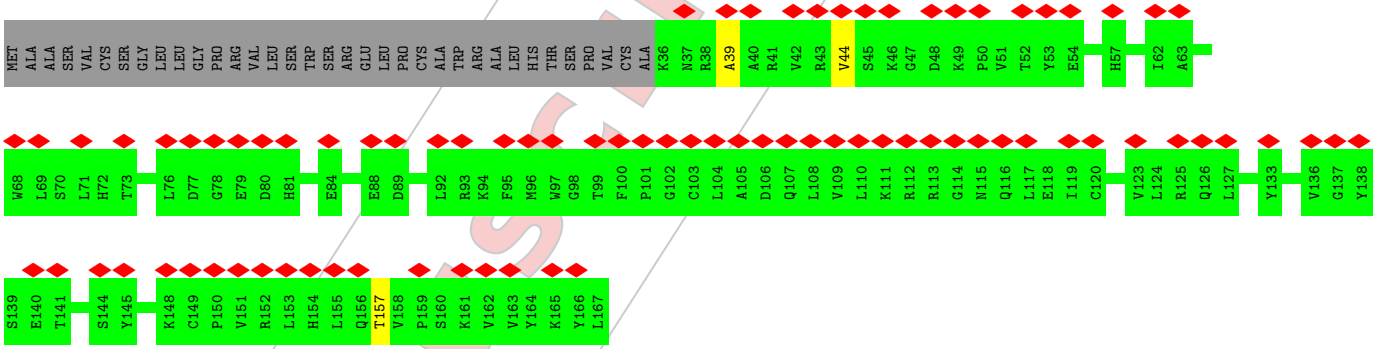
• Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:

• Molecule 3: 28S ribosomal protein S24, mitochondrial

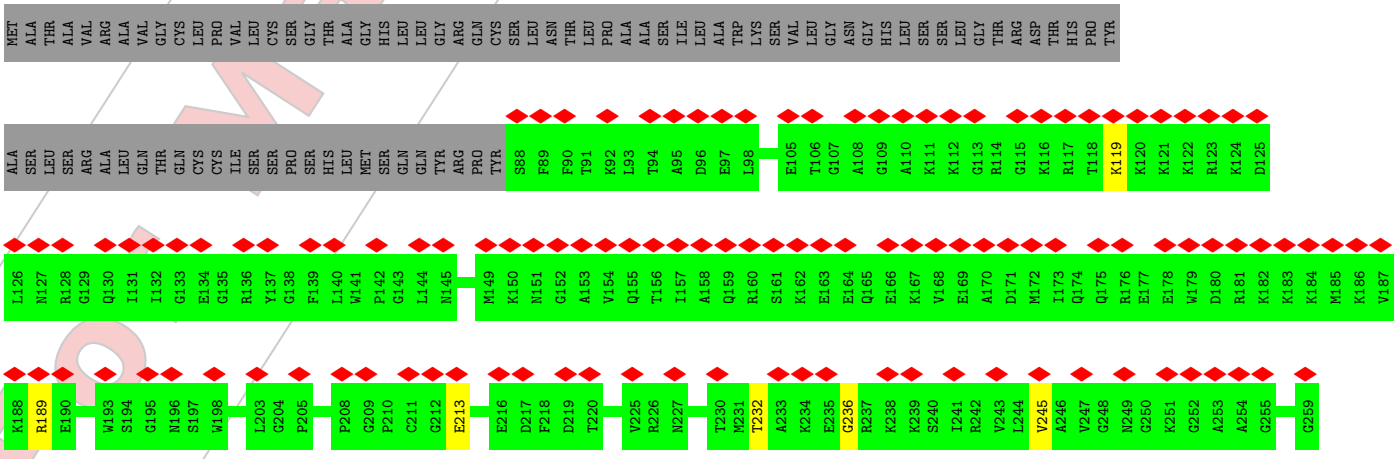
Chain C:

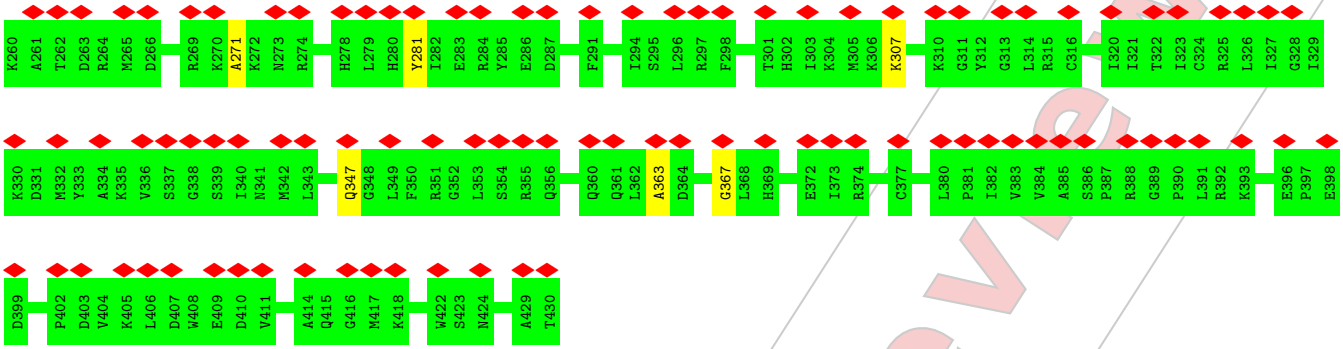




• Molecule 4: 28S ribosomal protein S5, mitochondrial

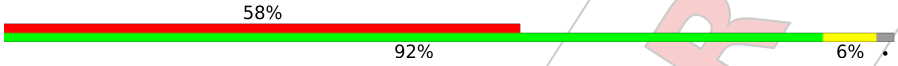
Chain D:

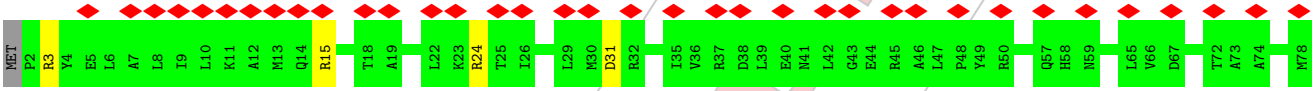


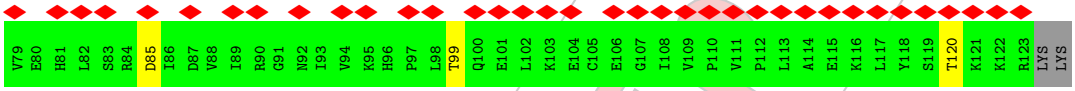


• Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain E:

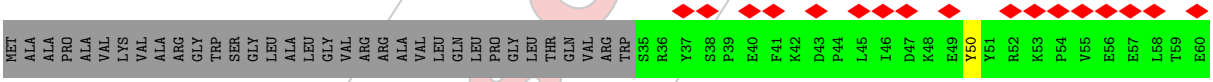


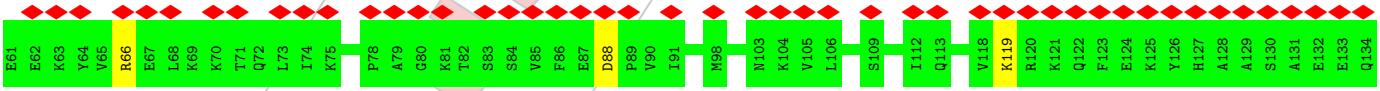


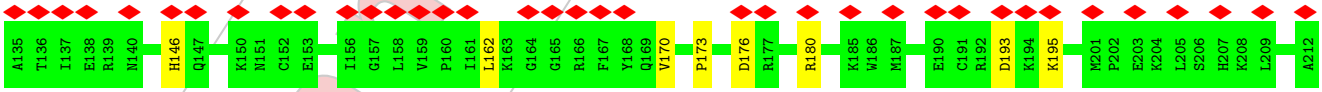


• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:

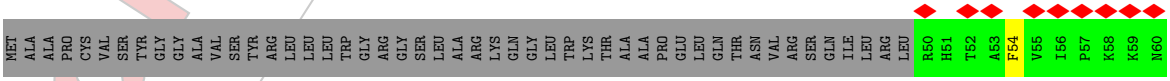


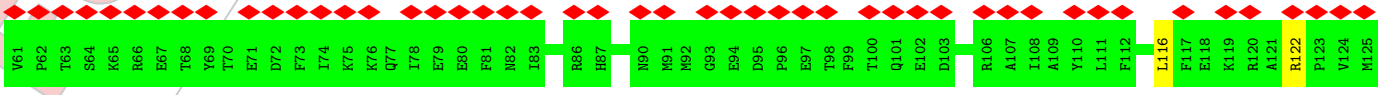


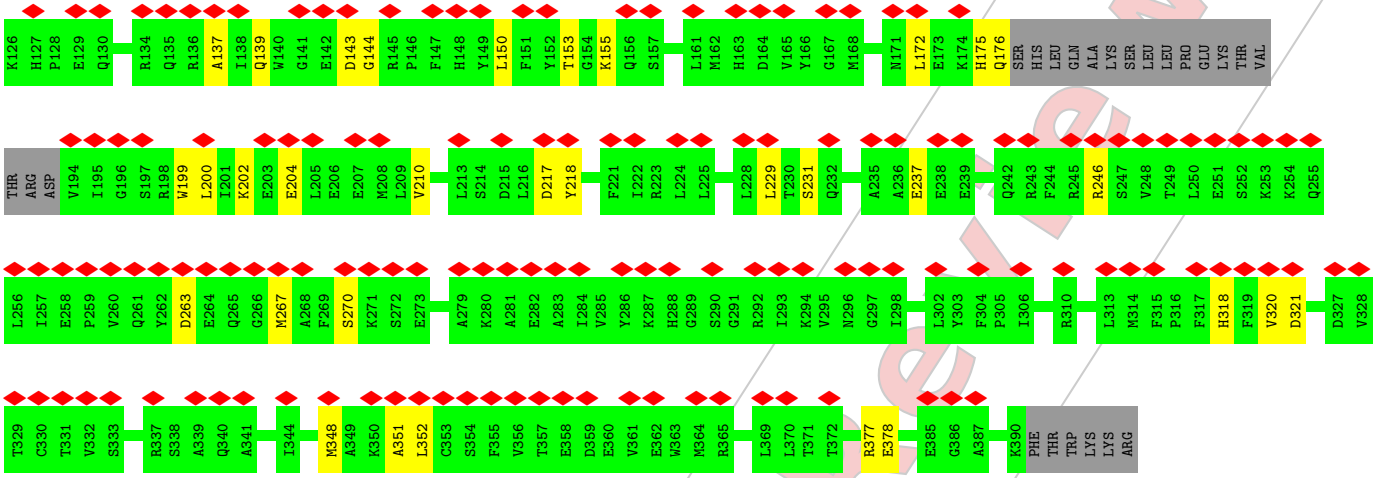


• Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G:

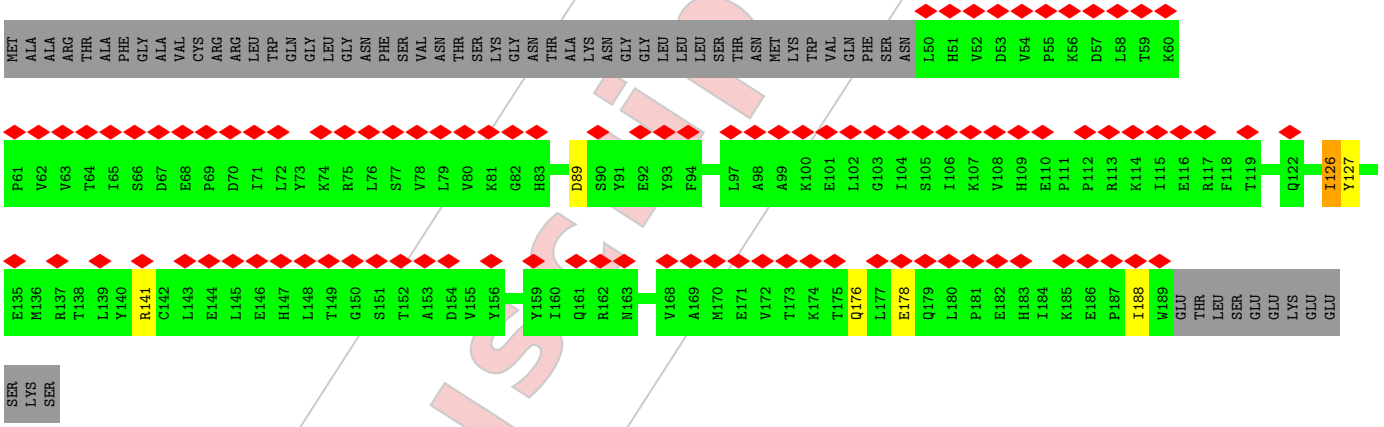






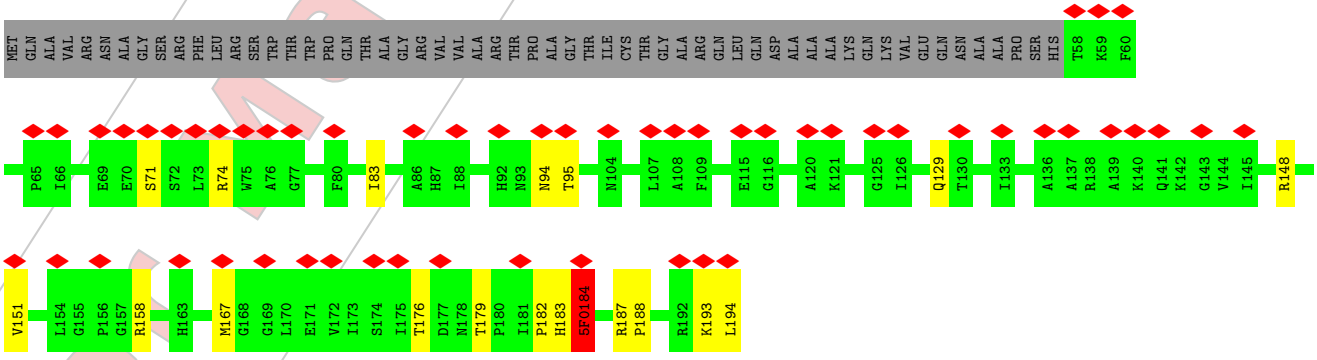
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



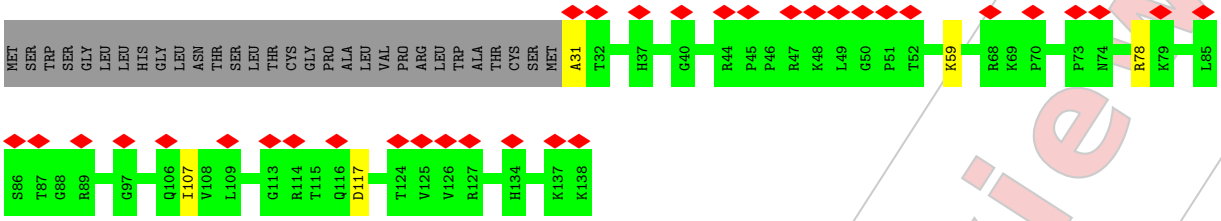
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



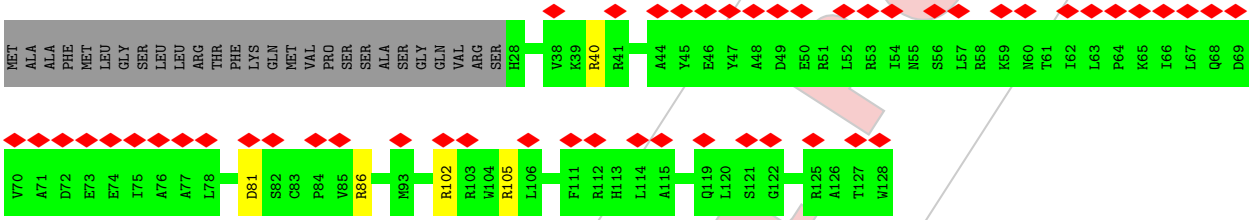
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:



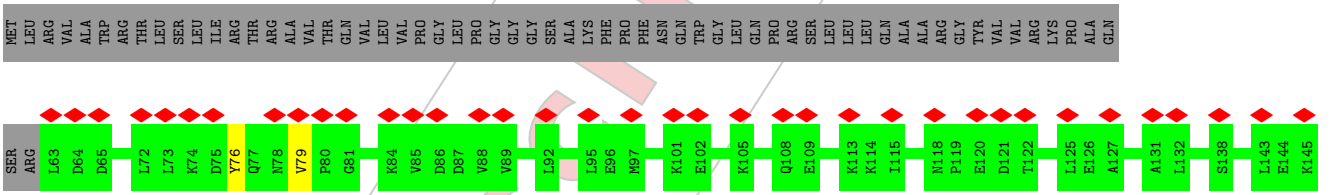
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:



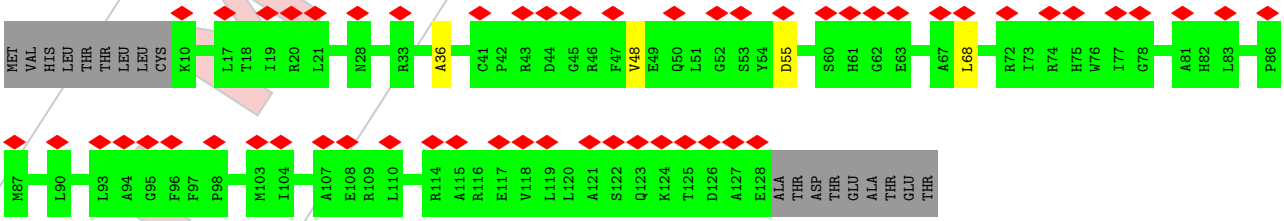
• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L:



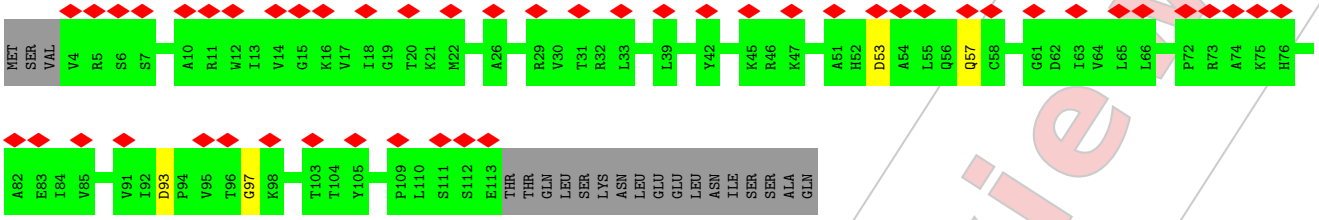
• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain M:



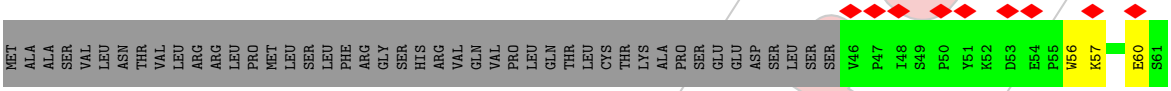
• Molecule 14: 28S ribosomal protein S17, mitochondrial

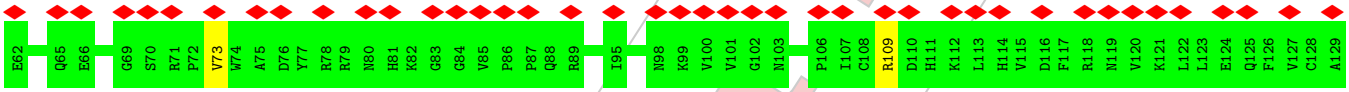
Chain N:

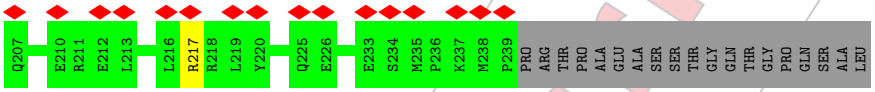


• Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain O:

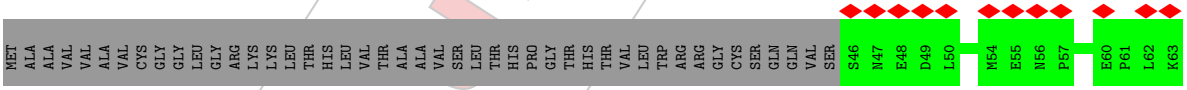


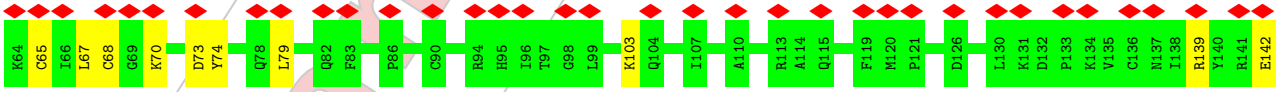




• Molecule 16: 28S ribosomal protein S18c, mitochondrial

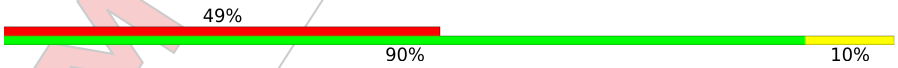
Chain P:

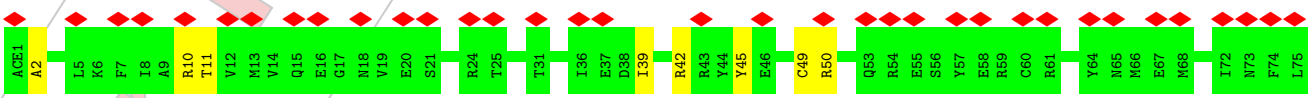


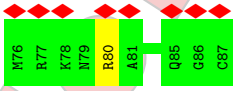


• Molecule 17: Small ribosomal subunit protein bS21m

Chain Q:

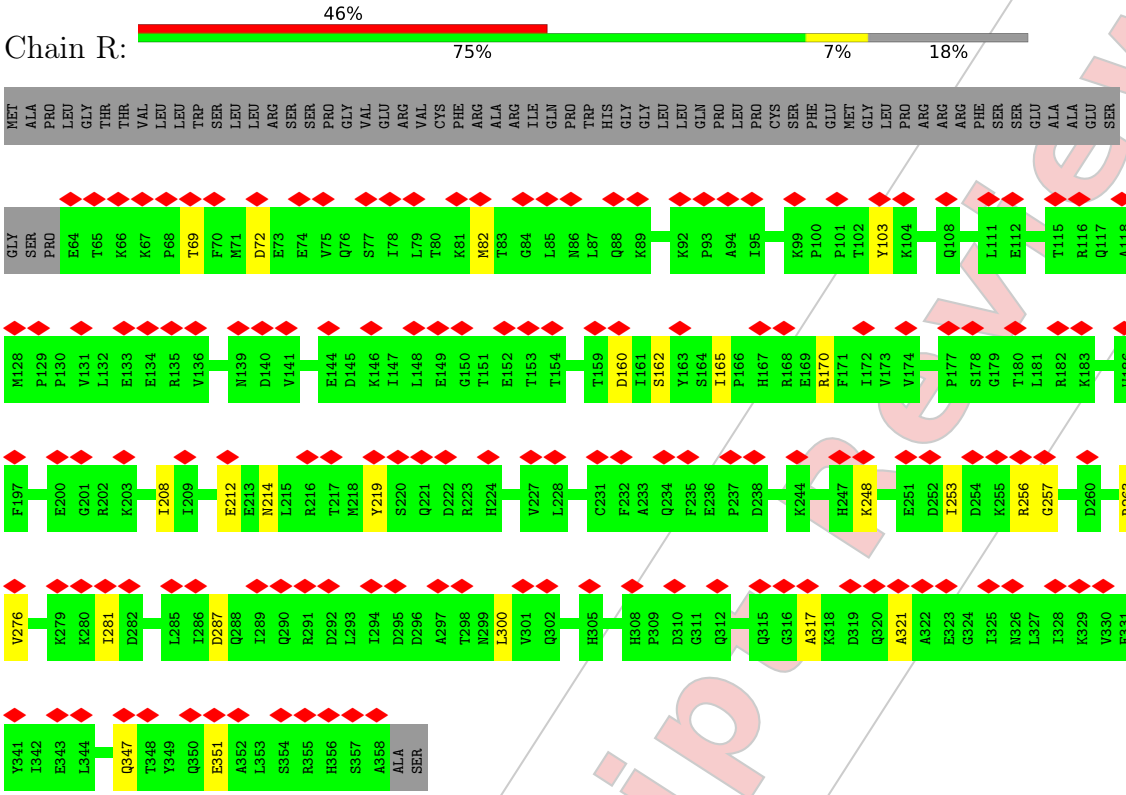






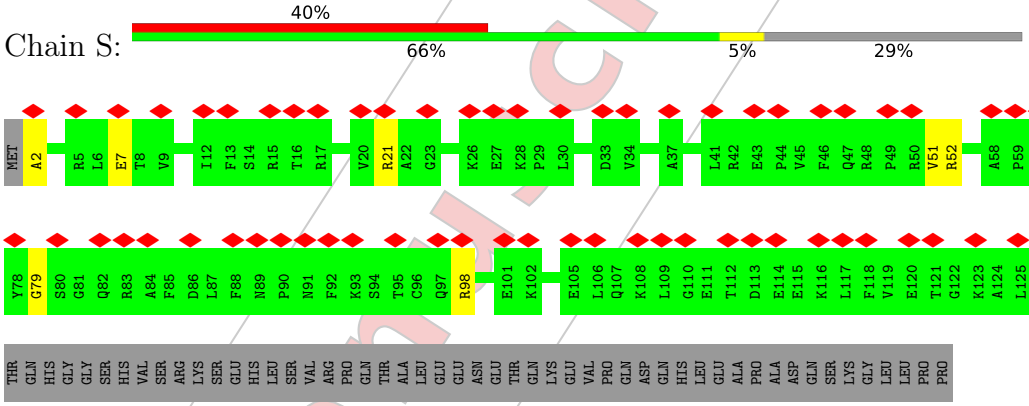
• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:



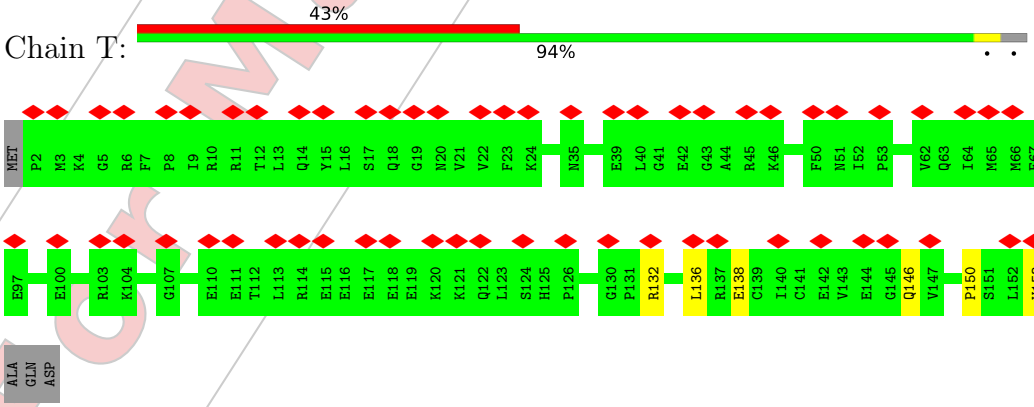
• Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S:



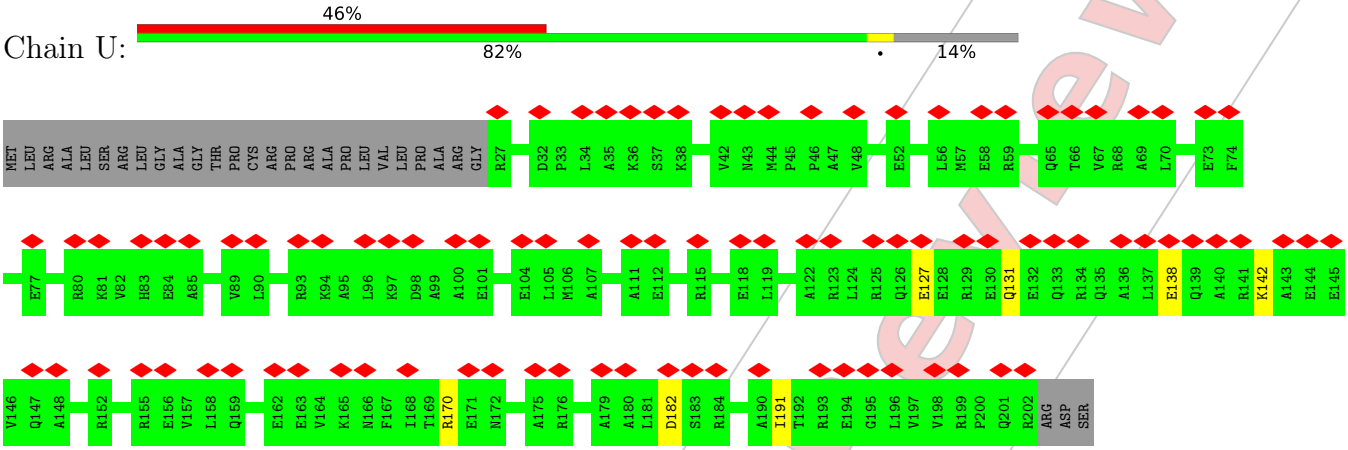
• Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T:



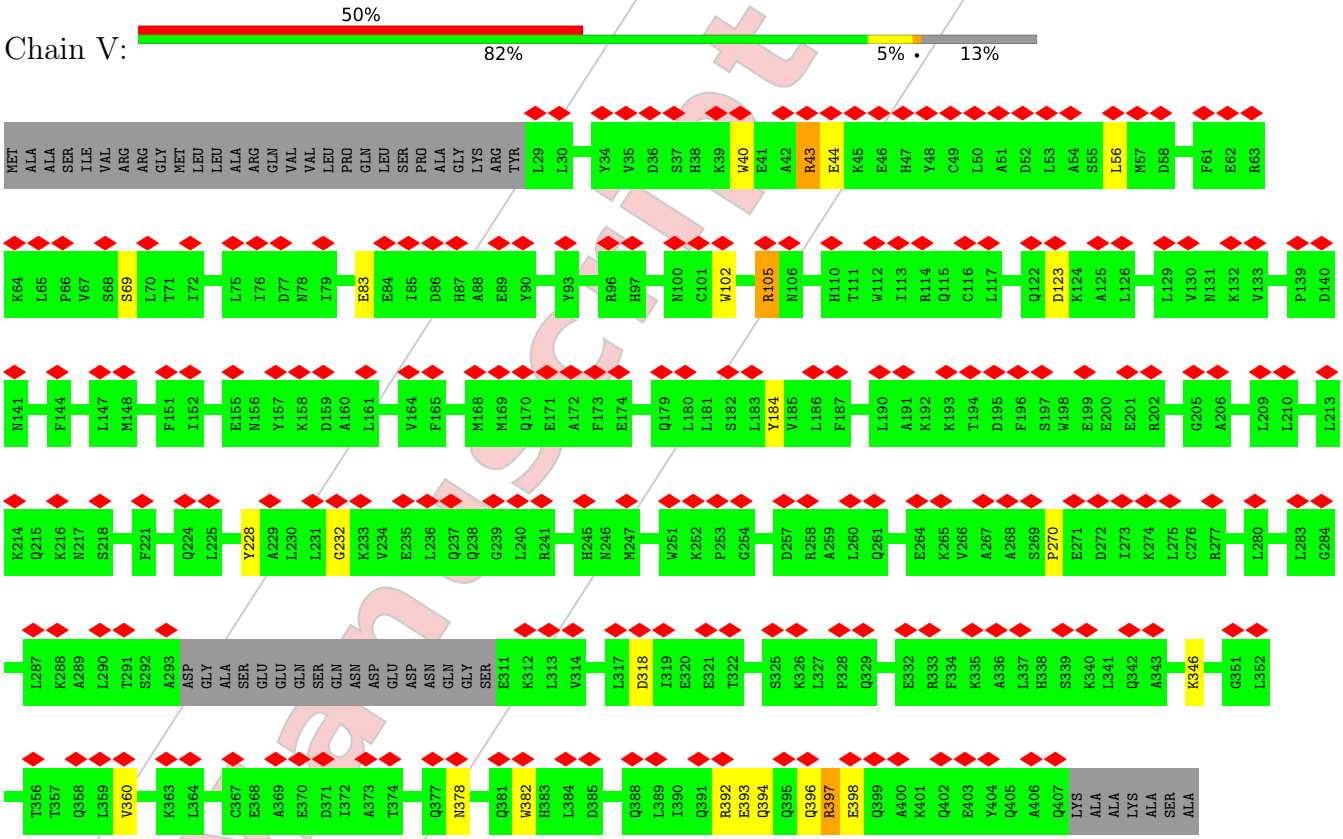
• Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U:



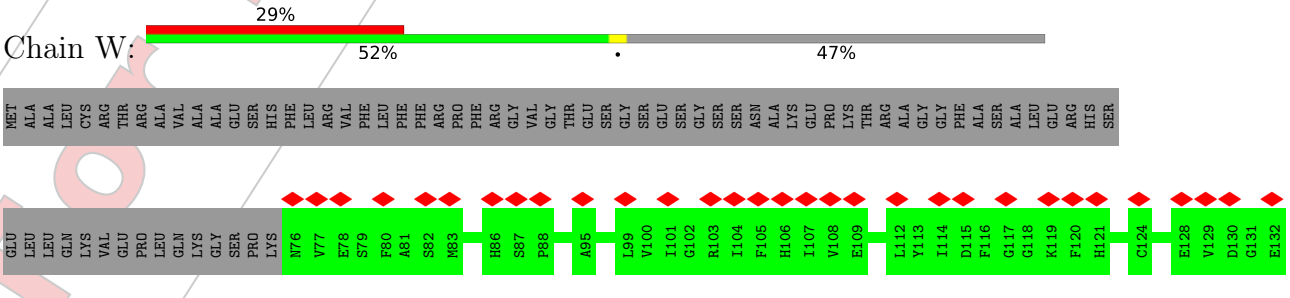
• Molecule 22: 28S ribosomal protein S27, mitochondrial

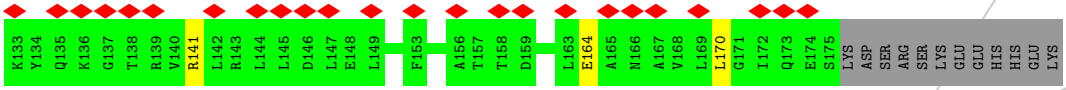
Chain V:



• Molecule 23: 28S ribosomal protein S28, mitochondrial

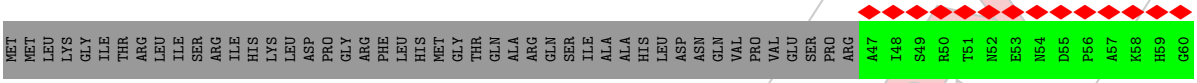
Chain W:

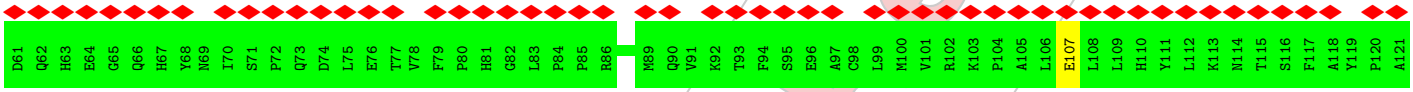


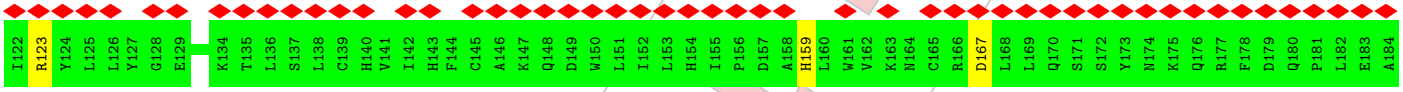


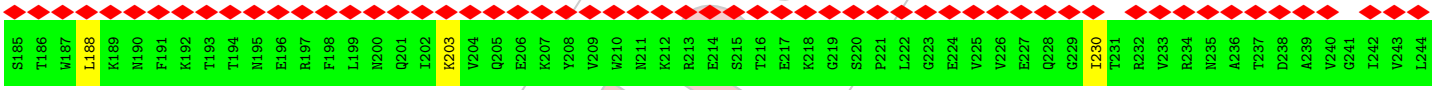
• Molecule 24: 28S ribosomal protein S29, mitochondrial

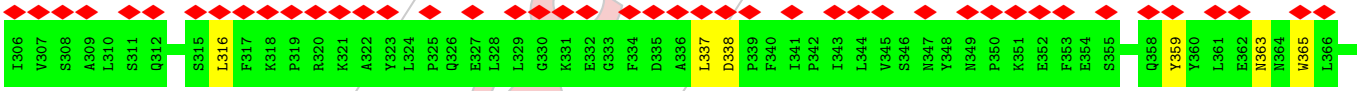
Chain X:

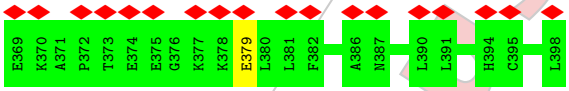






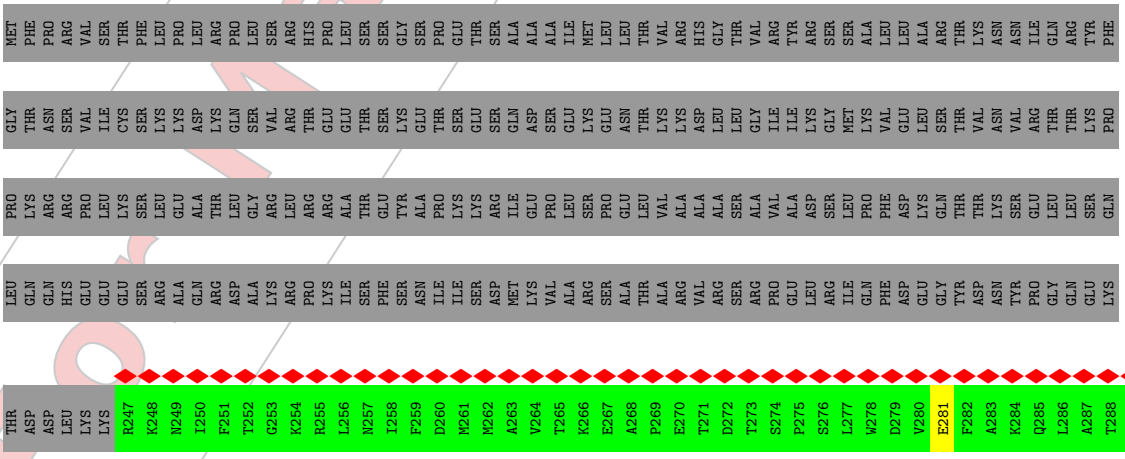


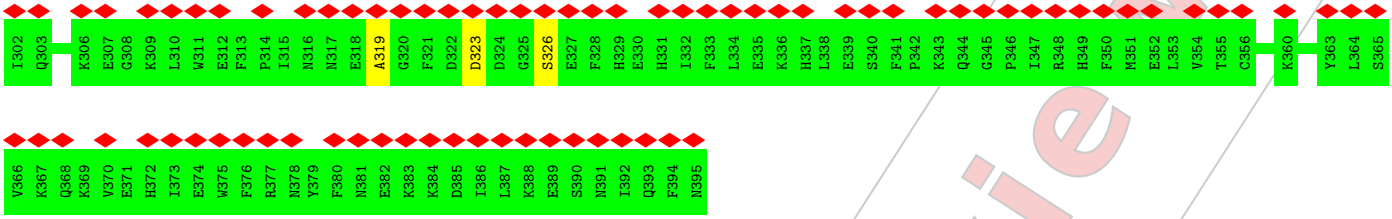




• Molecule 25: 28S ribosomal protein S31, mitochondrial

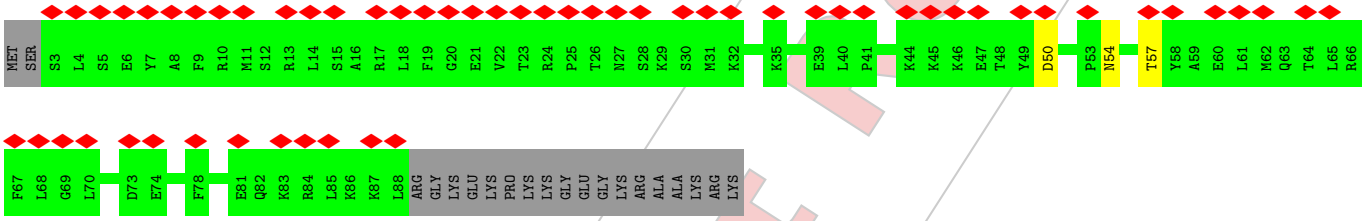
Chain Y:





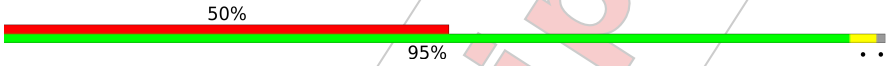
• Molecule 26: 28S ribosomal protein S33, mitochondrial

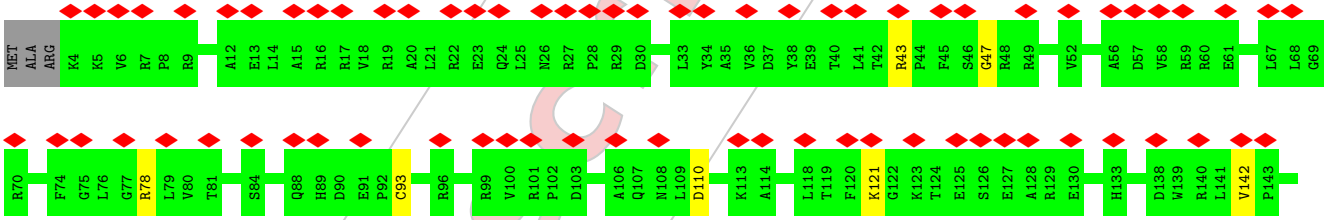
Chain Z:

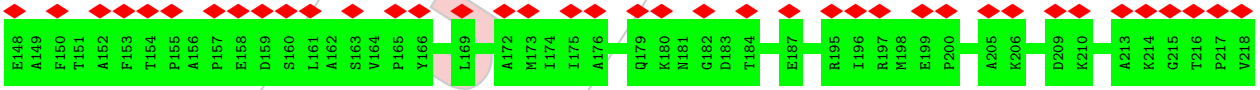


• Molecule 27: 28S ribosomal protein S34, mitochondrial

Chain 0:

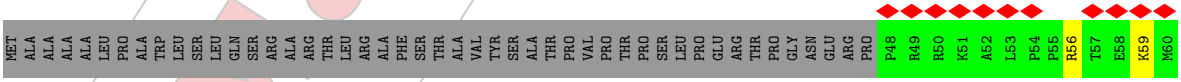


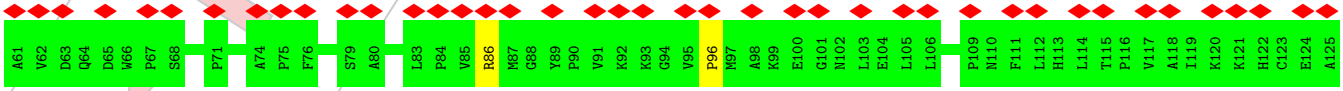


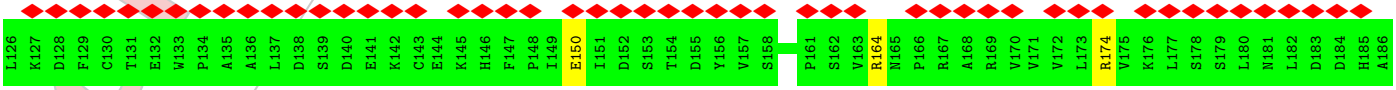


• Molecule 28: 28S ribosomal protein S35, mitochondrial

Chain 1:

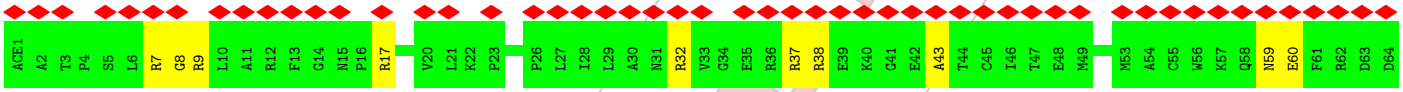






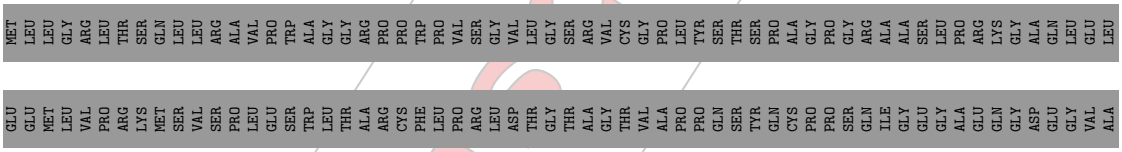
• Molecule 29: Small ribosomal subunit protein mS37

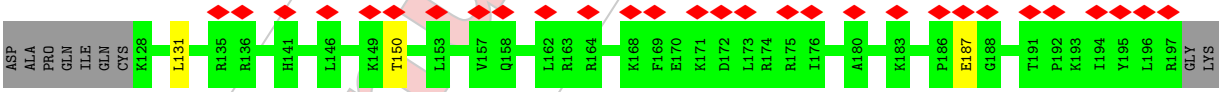
Chain 2:



• Molecule 30: Aurora kinase A-interacting protein

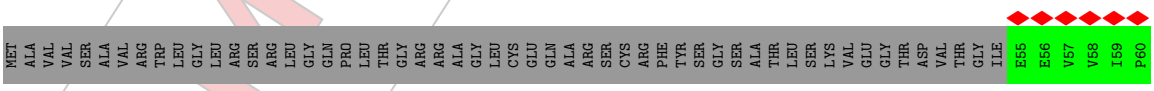
Chain 3:

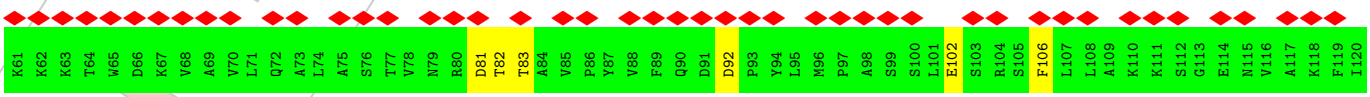


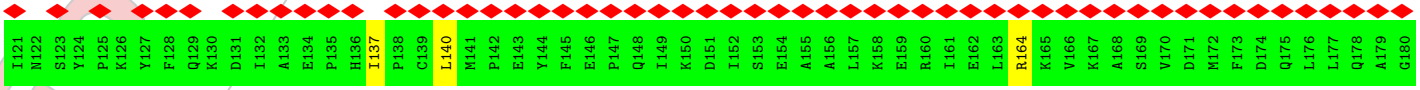


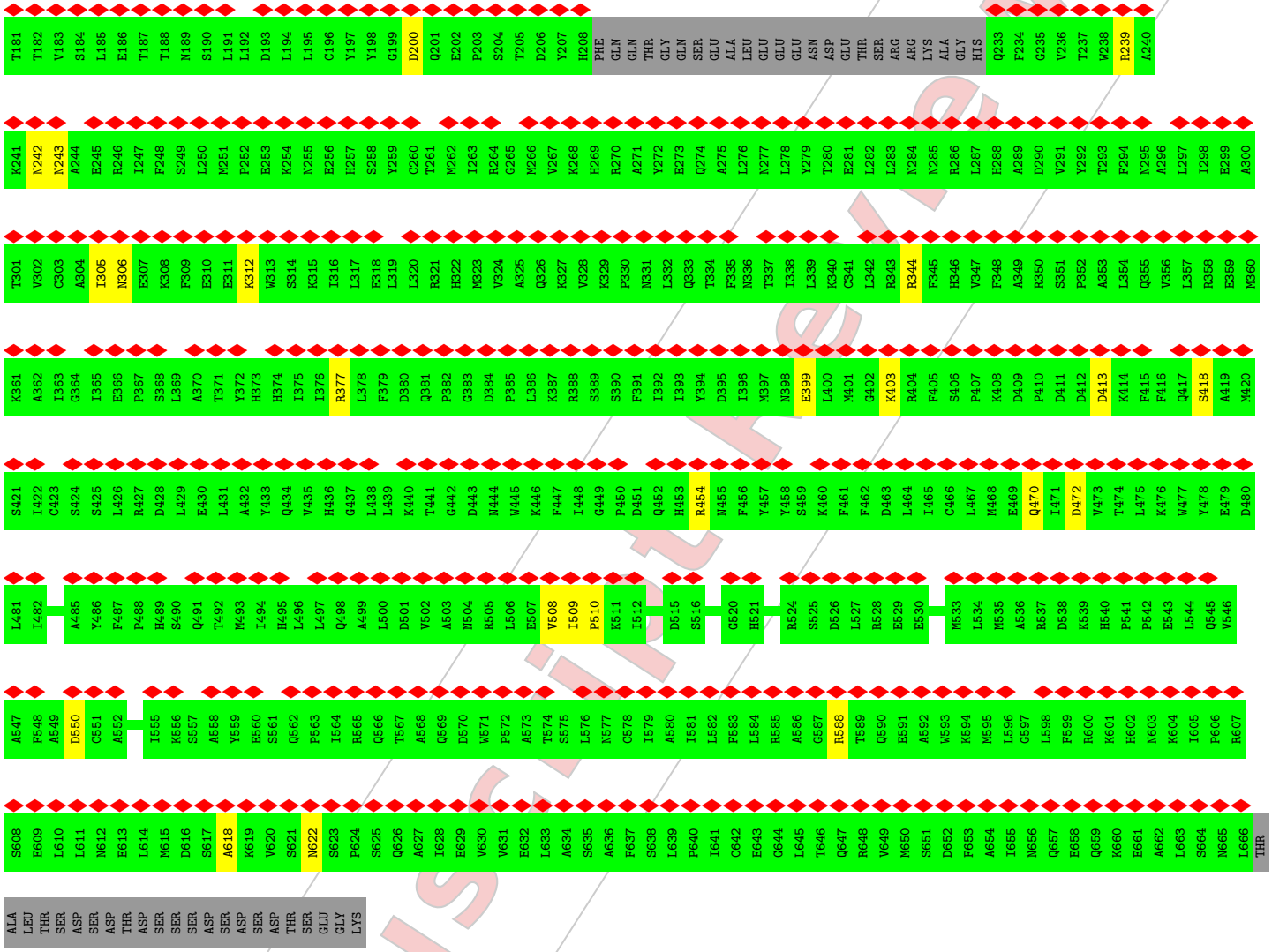
• Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain 4:



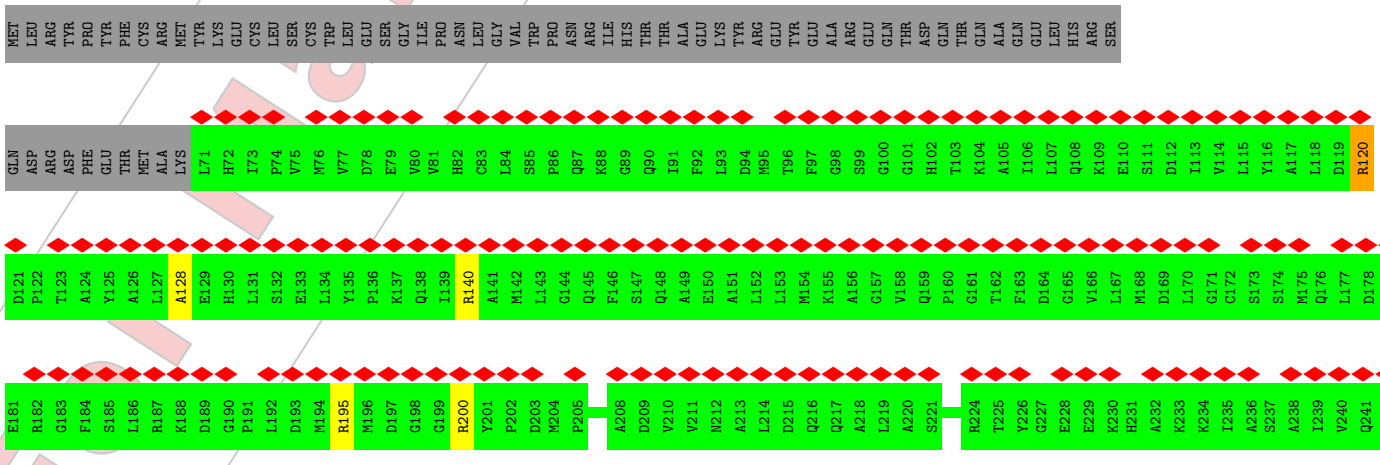


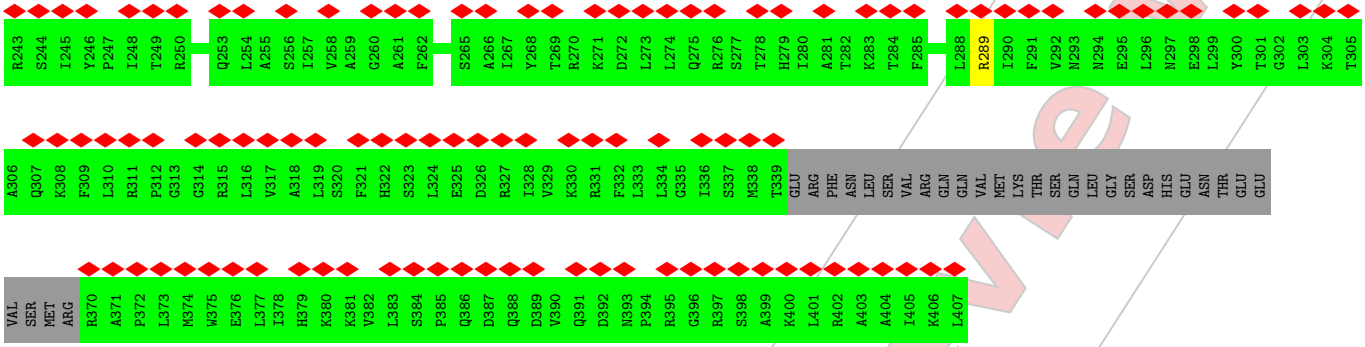




• Molecule 32: 12S rRNA N4-methylcytidine (m4C) methyltransferase

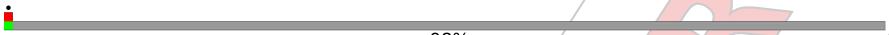
Chain b:

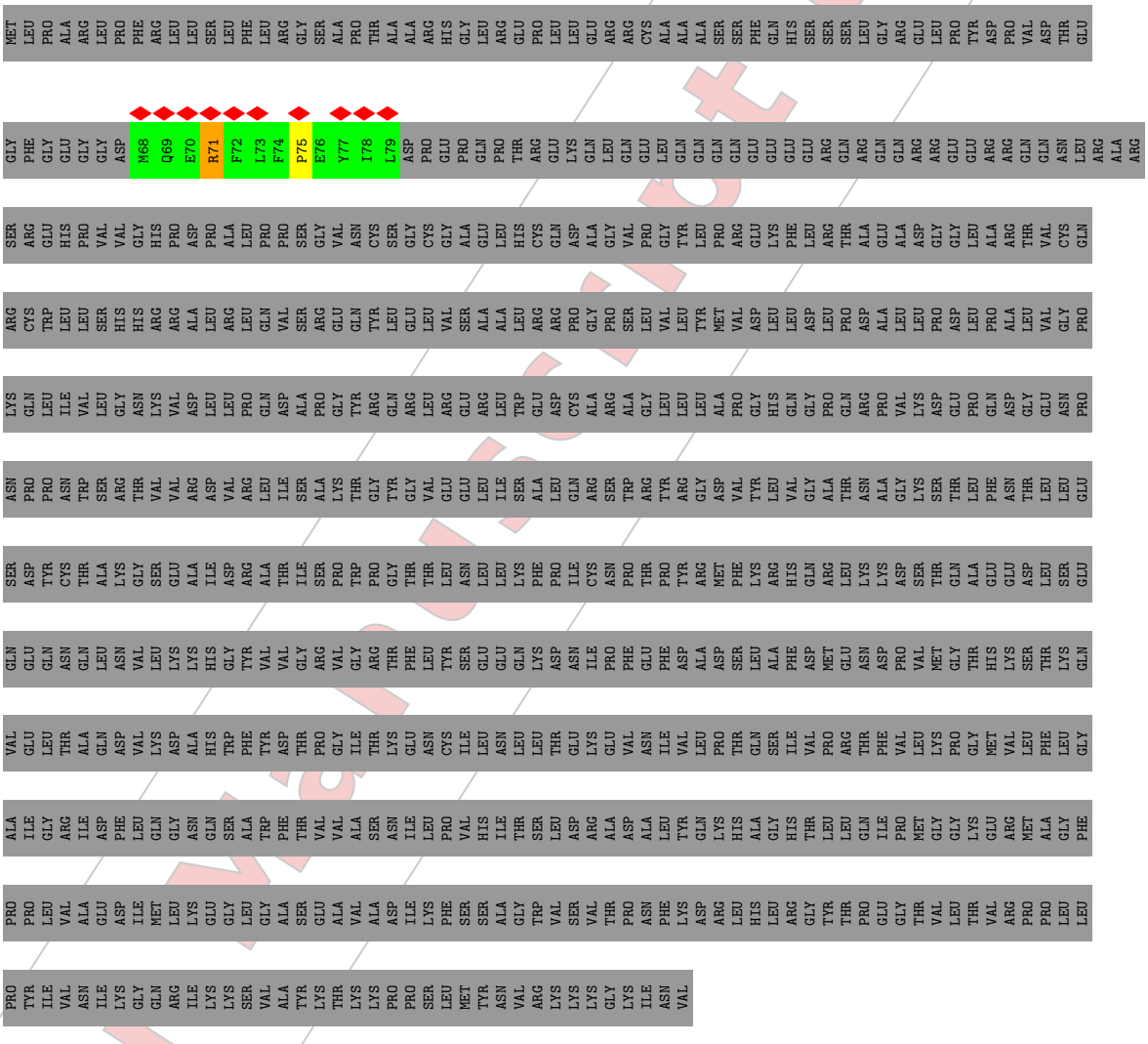




• Molecule 33: Nitric oxide-associated protein 1

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 5F0, 5MC, B8T, ACE, FES, SPM, GDP, MA6, MG, ATP, NAD, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.19	0/21945	0.69	0/34162
2	B	0.24	0/1871	0.48	0/2531
3	C	0.24	0/1113	0.47	0/1505
4	D	0.24	0/2783	0.51	0/3724
5	E	0.24	0/989	0.52	0/1335
6	F	0.24	0/1767	0.46	0/2373
7	G	0.26	0/2710	0.50	0/3635
8	H	0.23	0/1178	0.46	0/1598
9	I	0.31	0/1030	0.54	0/1386
10	J	0.25	0/855	0.55	0/1148
11	K	0.22	0/880	0.58	0/1182
12	L	0.24	0/1477	0.48	0/1974
13	M	0.24	0/963	0.53	0/1295
14	N	0.24	0/886	0.49	0/1199
15	O	0.24	0/1655	0.48	0/2254
16	P	0.25	0/798	0.43	0/1070
17	Q	0.24	0/754	0.55	0/1003
18	R	0.24	0/2456	0.45	0/3317
19	S	0.25	0/1138	0.51	0/1533
20	T	0.26	0/1402	0.46	0/1883
21	U	0.23	0/1510	0.53	0/2025
22	V	0.27	0/3030	0.43	0/4093
23	W	0.25	0/801	0.52	0/1079
24	X	0.24	0/2921	0.43	0/3954
25	Y	0.24	0/1280	0.39	0/1725
26	Z	0.24	0/747	0.46	0/1000
27	0	0.24	0/1834	0.54	0/2484
28	1	0.24	0/2285	0.44	0/3090
29	2	0.31	0/947	0.55	0/1266
30	3	0.25	0/636	0.63	0/839
31	4	0.24	0/4877	0.43	0/6598
32	b	0.40	0/2436	0.58	1/3287 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	9	0.56	0/114	0.76	0/152
All	All	0.24	0/72068	0.56	1/101699 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1
22	V	0	3
29	2	0	3
32	b	0	5
33	9	0	1
All	All	0	13

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	128	ALA	CA-C-O	-5.87	107.76	120.10

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	2	37	ARG	Sidechain
29	2	38	ARG	Sidechain
29	2	84	ARG	Sidechain
33	9	71	ARG	Sidechain
9	I	184	5F0	Mainchain
22	V	105	ARG	Sidechain
22	V	392	ARG	Sidechain
22	V	397	ARG	Sidechain
32	b	120	ARG	Sidechain
32	b	140	ARG	Sidechain
32	b	195	ARG	Sidechain
32	b	200	ARG	Sidechain
32	b	289	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19732	10021	10021	81	0
2	B	1828	1815	1815	5	0
3	C	1083	1088	1088	4	0
4	D	2731	2804	2804	10	0
5	E	972	1000	1001	5	0
6	F	1725	1769	1769	12	0
7	G	2654	2649	2649	22	0
8	H	1152	1183	1183	4	0
9	I	1020	1060	1053	40	0
10	J	839	887	887	4	0
11	K	862	885	885	4	0
12	L	1453	1540	1540	2	0
13	M	942	965	965	3	0
14	N	868	928	928	2	0
15	O	1599	1566	1565	4	0
16	P	781	806	806	6	0
17	Q	744	757	758	13	0
18	R	2409	2428	2428	14	0
19	S	1111	1115	1115	7	0
20	T	1371	1394	1394	4	0
21	U	1488	1499	1499	5	0
22	V	2969	2961	2961	14	0
23	W	789	802	802	2	0
24	X	2849	2844	2844	16	0
25	Y	1246	1197	1197	6	0
26	Z	730	734	734	2	0
27	0	1787	1796	1796	4	0
28	1	2238	2269	2269	10	0
29	2	935	968	969	11	0
30	3	625	699	699	3	0
31	4	4768	4766	4766	20	0
32	b	2393	2457	2457	0	0
33	9	111	108	108	2	0
34	A	44	26	26	0	0
35	A	14	0	26	1	0
36	3	1	0	0	0	0
36	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	M	4	0	0	0	0
37	P	4	0	0	0	0
38	O	1	0	0	0	0
39	X	31	12	12	0	0
40	X	28	10	12	0	0
41	0	1	0	0	0	0
41	2	1	0	0	0	0
41	A	2	0	0	0	0
41	C	2	0	0	0	0
41	G	1	0	0	0	0
41	T	1	0	0	0	0
All	All	68940	59808	59831	259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:A:C1'	9:I:182:PRO:HB3	1.82	1.10
1:A:977:A:H1'	9:I:182:PRO:HB3	1.01	0.99
1:A:977:A:H1'	9:I:182:PRO:CB	1.96	0.96
1:A:989:U:OP1	9:I:94:ASN:ND2	2.00	0.95
9:I:179:THR:HG21	17:Q:39:ILE:HD13	1.55	0.89
1:A:975:A:H2	9:I:183:HIS:HB2	1.42	0.83
6:F:238:HIS:HA	29:2:43:ALA:HB3	1.61	0.82
18:R:347:GLN:NE2	18:R:351:GLU:OE2	2.21	0.73
11:K:81:ASP:OD1	11:K:86:ARG:NH1	2.22	0.73
16:P:139:ARG:NH2	16:P:142:GLU:OE1	2.22	0.72
29:2:102:ASN:OD1	29:2:103:LYS:N	2.24	0.71
29:2:7:ARG:O	29:2:9:ARG:NH1	2.24	0.71
1:A:1583:MA6:H93	1:A:1584:MA6:H92	1.73	0.70
20:T:132:ARG:NH1	20:T:136:LEU:O	2.23	0.70
1:A:894:C:N4	10:J:117:ASP:OD2	2.25	0.69
1:A:1490:U:O2	1:A:1582:G:N2	2.25	0.69
9:I:179:THR:HG21	17:Q:39:ILE:CD1	2.21	0.69
7:G:318:HIS:NE2	24:X:379:GLU:OE2	2.27	0.68
9:I:71:SER:O	9:I:74:ARG:NH1	2.26	0.68
6:F:50:TYR:O	6:F:66:ARG:NH2	2.27	0.68
8:H:126:ILE:HG22	8:H:127:TYR:H	1.59	0.67
1:A:1234:C:O3'	11:K:40:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:470:GLN:NE2	31:4:472:ASP:OD2	2.27	0.67
1:A:976:A:H1'	9:I:183:HIS:CD2	2.30	0.66
25:Y:326:SER:O	28:1:217:GLN:NE2	2.28	0.65
15:O:73:VAL:O	15:O:109:ARG:NH2	2.30	0.65
1:A:1015:A:C4	9:I:183:HIS:CE1	2.84	0.64
15:O:217:ARG:NH1	22:V:318:ASP:OD2	2.31	0.63
16:P:65:CYS:N	16:P:68:CYS:SG	2.73	0.62
1:A:1015:A:C5	9:I:183:HIS:CE1	2.87	0.62
1:A:976:A:H2	9:I:182:PRO:HB2	1.65	0.60
1:A:1582:G:H3'	1:A:1583:MA6:H8	1.84	0.60
7:G:210:VAL:HG12	7:G:210:VAL:O	2.01	0.60
5:E:3:ARG:HB3	5:E:99:THR:HG21	1.84	0.60
1:A:1581:G:N1	1:A:1584:MA6:OP2	2.34	0.60
1:A:975:A:C2	9:I:183:HIS:HB2	2.31	0.59
4:D:363:ALA:O	4:D:367:GLY:N	2.35	0.59
4:D:281:TYR:OH	19:S:21:ARG:NH1	2.34	0.59
31:4:239:ARG:O	31:4:242:ASN:ND2	2.35	0.59
1:A:976:A:N3	9:I:182:PRO:HA	2.18	0.58
1:A:1464:G:H4'	6:F:241:TRP:HZ2	1.70	0.57
31:4:306:ASN:OD1	31:4:344:ARG:NH2	2.38	0.57
1:A:1116:A:O5'	2:B:100:ARG:NH2	2.37	0.56
1:A:1084:C:H4'	9:I:194:LEU:HB2	1.85	0.56
29:2:8:GLY:O	29:2:17:ARG:NH2	2.39	0.56
7:G:150:LEU:O	7:G:153:THR:OG1	2.25	0.55
16:P:67:LEU:HD21	16:P:79:LEU:HD11	1.88	0.55
22:V:270:PRO:O	22:V:346:LYS:NZ	2.38	0.55
31:4:399:GLU:OE2	31:4:403:LYS:NZ	2.40	0.55
24:X:338:ASP:OD1	28:1:292:TYR:OH	2.24	0.55
22:V:184:TYR:HB2	22:V:360:VAL:HG21	1.87	0.54
31:4:200:ASP:OD2	31:4:243:ASN:N	2.40	0.54
1:A:1015:A:C4	9:I:183:HIS:HE1	2.22	0.54
3:C:157:THR:OG1	31:4:92:ASP:OD1	2.26	0.54
1:A:1464:G:H2'	1:A:1465:C:C6	2.43	0.54
21:U:138:GLU:O	21:U:142:LYS:N	2.37	0.53
1:A:1053:A:N1	1:A:1100:C:O2'	2.40	0.53
13:M:55:ASP:OD2	20:T:146:GLN:NE2	2.41	0.53
19:S:98:ARG:NH2	19:S:128:GLU:OE1	2.41	0.53
1:A:1583:MA6:C9	1:A:1584:MA6:H92	2.38	0.53
24:X:299:ASN:ND2	28:1:265:THR:OG1	2.41	0.53
9:I:129:GLN:NE2	9:I:167:MET:SD	2.81	0.53
17:Q:49:CYS:SG	17:Q:50:ARG:NH1	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:199:TRP:CH2	7:G:229:LEU:HD12	2.44	0.52
12:L:212:ARG:NH2	30:3:187:GLU:O	2.43	0.52
29:2:100:LEU:H	29:2:100:LEU:HD23	1.74	0.52
16:P:70:LYS:O	16:P:103:LYS:NZ	2.42	0.52
1:A:1583:MA6:H8	1:A:1583:MA6:OP2	2.09	0.52
10:J:78:ARG:NH2	10:J:117:ASP:OD2	2.42	0.52
1:A:945:G:OP2	35:A:1702:SPM:H71	2.10	0.52
9:I:187:ARG:HG3	17:Q:45:TYR:CD1	2.45	0.52
16:P:73:ASP:OD1	16:P:74:TYR:N	2.41	0.52
22:V:43:ARG:NH1	22:V:44:GLU:O	2.43	0.52
1:A:1478:A:C2	30:3:131:LEU:HD21	2.45	0.51
6:F:119:LYS:NZ	24:X:365:TRP:O	2.36	0.51
28:1:59:LYS:NZ	31:4:82:THR:OG1	2.40	0.51
1:A:1489:G:O2'	1:A:1583:MA6:O2'	2.28	0.51
1:A:843:G:N2	1:A:846:A:OP2	2.44	0.51
1:A:1599:A:OP2	29:2:32:ARG:NH1	2.41	0.51
2:B:239:ASN:ND2	2:B:242:SER:OG	2.44	0.50
9:I:188:PRO:HB2	17:Q:45:TYR:N	2.26	0.50
4:D:232:THR:N	4:D:236:GLY:O	2.42	0.50
23:W:141:ARG:NH2	23:W:170:LEU:O	2.44	0.50
5:E:120:THR:HG21	19:S:51:VAL:HG21	1.94	0.49
29:2:79:ARG:O	29:2:83:ALA:N	2.39	0.49
18:R:253:ILE:O	18:R:257:GLY:N	2.45	0.49
1:A:976:A:N3	9:I:183:HIS:N	2.59	0.49
9:I:184:5F0:C1	9:I:184:5F0:O	2.60	0.49
27:0:43:ARG:O	27:0:47:GLY:N	2.38	0.49
9:I:183:HIS:O	9:I:184:5F0:CB	2.55	0.49
1:A:1015:A:C5	9:I:183:HIS:HE1	2.30	0.49
1:A:1265:C:P	3:C:39:ALA:HB2	2.53	0.49
6:F:240:ARG:O	29:2:43:ALA:N	2.46	0.49
20:T:132:ARG:N	20:T:138:GLU:OE2	2.44	0.49
1:A:976:A:OP1	17:Q:2:ALA:N	2.45	0.49
1:A:1199:G:N1	1:A:1422:G:OP2	2.45	0.49
31:4:413:ASP:N	31:4:413:ASP:OD1	2.46	0.49
6:F:88:ASP:OD2	6:F:146:HIS:NE2	2.45	0.49
18:R:208:ILE:O	18:R:214:ASN:ND2	2.44	0.49
1:A:934:G:O6	10:J:31:ALA:N	2.46	0.48
15:O:56:TRP:O	15:O:60:GLU:OE1	2.31	0.48
25:Y:296:ASN:OD1	25:Y:298:PHE:N	2.43	0.48
14:N:93:ASP:O	14:N:97:GLY:N	2.40	0.48
22:V:393:GLU:HA	22:V:397:ARG:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1283:A:H3'	1:A:1284:U:H5"	1.96	0.48
1:A:940:A:H5'	1:A:941:G:OP2	2.13	0.48
9:I:176:THR:HA	17:Q:10:ARG:O	2.14	0.47
7:G:155:LYS:NZ	7:G:217:ASP:OD2	2.31	0.47
9:I:94:ASN:OD1	9:I:95:THR:N	2.47	0.47
18:R:212:GLU:OE1	18:R:248:LYS:NZ	2.32	0.47
22:V:123:ASP:OD1	22:V:123:ASP:N	2.46	0.47
25:Y:292:GLN:OE1	31:4:454:ARG:NH2	2.40	0.47
9:I:176:THR:HG23	17:Q:11:THR:OG1	2.14	0.47
31:4:377:ARG:NE	31:4:418:SER:OG	2.47	0.47
19:S:7:GLU:OE1	19:S:7:GLU:N	2.44	0.47
1:A:1500:C:H2'	1:A:1501:A:O4'	2.15	0.47
1:A:1539:C:H3'	1:A:1540:A:H5'	1.96	0.47
1:A:1550:A:O2'	1:A:1551:G:P	2.72	0.47
31:4:550:ASP:OD1	31:4:588:ARG:NH2	2.48	0.47
4:D:232:THR:OG1	4:D:236:GLY:N	2.48	0.47
1:A:1506:U:O4	1:A:1507:A:N6	2.47	0.47
7:G:116:LEU:O	7:G:122:ARG:NH2	2.42	0.46
18:R:317:ALA:O	18:R:321:ALA:N	2.49	0.46
1:A:1583:MA6:H2'	1:A:1584:MA6:H8	1.97	0.46
7:G:237:GLU:OE1	7:G:237:GLU:N	2.44	0.46
5:E:15:ARG:NH1	21:U:182:ASP:OD1	2.44	0.46
22:V:83:GLU:N	22:V:83:GLU:OE1	2.48	0.46
24:X:276:ARG:NH2	24:X:286:GLU:OE1	2.48	0.46
9:I:83:ILE:O	9:I:148:ARG:NH2	2.49	0.46
19:S:75:TYR:O	19:S:79:GLY:N	2.49	0.46
28:1:56:ARG:NH1	31:4:83:THR:OG1	2.47	0.46
2:B:180:ARG:NH1	2:B:185:PRO:O	2.48	0.46
3:C:44:VAL:HG13	3:C:44:VAL:O	2.16	0.46
8:H:89:ASP:OD1	8:H:141:ARG:NH1	2.42	0.46
25:Y:281:GLU:OE2	31:4:164:ARG:NH2	2.44	0.46
24:X:123:ARG:NH2	24:X:337:LEU:O	2.49	0.45
1:A:1057:G:H4'	1:A:1578:A:H4'	1.99	0.45
14:N:53:ASP:OD2	14:N:57:GLN:N	2.48	0.45
9:I:151:VAL:HG11	9:I:158:ARG:HG3	1.99	0.45
9:I:188:PRO:HD2	17:Q:45:TYR:HB2	1.99	0.45
11:K:105:ARG:NH1	26:Z:50:ASP:O	2.49	0.45
27:0:110:ASP:OD1	27:0:110:ASP:N	2.47	0.45
31:4:618:ALA:O	31:4:622:ASN:N	2.47	0.45
1:A:976:A:C2	9:I:182:PRO:HB2	2.48	0.45
29:2:59:ASN:O	29:2:60:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:305:ILE:O	31:4:312:LYS:NZ	2.43	0.45
1:A:702:C:OP1	1:A:848:U:O2'	2.35	0.45
2:B:243:PRO:O	2:B:247:HIS:ND1	2.48	0.45
18:R:69:THR:OG1	18:R:72:ASP:OD1	2.34	0.45
24:X:263:ASP:OD1	24:X:264:GLY:N	2.49	0.45
7:G:320:VAL:O	7:G:321:ASP:OD1	2.34	0.45
30:3:150:THR:HG22	30:3:150:THR:O	2.17	0.45
31:4:102:GLU:O	31:4:106:PHE:N	2.46	0.45
9:I:184:5F0:O1	17:Q:42:ARG:NH2	2.30	0.45
28:1:86:ARG:NH1	28:1:96:PRO:O	2.50	0.44
7:G:200:LEU:HD12	7:G:246:ARG:HG2	1.98	0.44
1:A:1465:C:H4'	6:F:162:LEU:HD22	2.00	0.44
7:G:172:LEU:HD13	7:G:231:SER:OG	2.17	0.44
1:A:1245:U:H2'	1:A:1342:C:H41	1.82	0.44
26:Z:54:ASN:ND2	26:Z:57:THR:OG1	2.50	0.44
7:G:200:LEU:HD12	7:G:246:ARG:CG	2.47	0.44
7:G:270:SER:OG	7:G:351:ALA:O	2.33	0.44
1:A:1293:C:N4	17:Q:80:ARG:O	2.49	0.44
7:G:200:LEU:HG	7:G:204:GLU:HB3	2.00	0.44
4:D:245:VAL:HG22	4:D:271:ALA:HB1	1.99	0.44
1:A:976:A:C1'	9:I:183:HIS:CD2	3.00	0.43
16:P:67:LEU:HD23	21:U:191:ILE:HD12	2.00	0.43
24:X:359:TYR:O	24:X:363:ASN:ND2	2.51	0.43
4:D:307:LYS:NZ	18:R:103:TYR:OH	2.49	0.43
1:A:1265:C:OP1	3:C:39:ALA:HB2	2.19	0.43
1:A:1443:U:OP2	11:K:102:ARG:HD2	2.19	0.43
4:D:189:ARG:CD	7:G:54:PHE:HB2	2.48	0.43
27:0:93:CYS:SG	27:0:121:LYS:N	2.85	0.43
31:4:509:ILE:N	31:4:510:PRO:CD	2.81	0.43
1:A:1116:A:H5'	1:A:1117:A:OP2	2.18	0.43
1:A:1550:A:HO2'	1:A:1551:G:P	2.40	0.43
1:A:1550:A:O2'	1:A:1551:G:OP1	2.33	0.43
6:F:193:ASP:OD2	6:F:195:LYS:NZ	2.44	0.43
12:L:76:TYR:O	12:L:79:VAL:HG22	2.18	0.43
1:A:1084:C:H4'	9:I:194:LEU:CB	2.48	0.43
7:G:137:ALA:O	7:G:139:GLN:OE1	2.37	0.43
24:X:188:LEU:HB3	24:X:230:ILE:HD11	2.00	0.43
1:A:941:G:H4'	1:A:942:A:O5'	2.18	0.43
1:A:976:A:N3	9:I:182:PRO:CA	2.82	0.42
5:E:24:ARG:NH1	5:E:85:ASP:OD1	2.52	0.42
1:A:905:A:O2'	1:A:907:A:OP1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:G:O6	1:A:1122:A:N6	2.51	0.42
1:A:1400:U:C2	1:A:1405:C:N4	2.87	0.42
1:A:1508:C:H4'	1:A:1509:U:OP1	2.19	0.42
8:H:176:GLN:NE2	8:H:178:GLU:OE2	2.52	0.42
18:R:263:ARG:NH2	18:R:287:ASP:OD1	2.52	0.42
21:U:127:GLU:O	21:U:131:GLN:N	2.52	0.42
1:A:1254:C:H4'	1:A:1255:U:H5'	2.01	0.42
24:X:273:THR:HG23	24:X:316:LEU:HD13	2.01	0.42
31:4:508:VAL:HG12	31:4:508:VAL:O	2.19	0.42
6:F:223:LYS:O	6:F:227:HIS:ND1	2.44	0.42
5:E:31:ASP:OD1	21:U:170:ARG:NH2	2.53	0.42
17:Q:80:ARG:NH2	23:W:164:GLU:OE1	2.53	0.42
24:X:167:ASP:OD1	24:X:167:ASP:N	2.52	0.42
24:X:265:ILE:HD11	24:X:337:LEU:HD21	2.02	0.42
1:A:1283:A:O2'	4:D:347:GLN:OE1	2.38	0.42
1:A:1415:G:OP2	1:A:1415:G:N2	2.45	0.42
13:M:36:ALA:O	13:M:48:VAL:N	2.51	0.42
15:O:57:LYS:HA	15:O:60:GLU:OE2	2.20	0.42
24:X:107:GLU:OE2	28:1:313:LYS:NZ	2.48	0.42
7:G:202:LYS:HA	7:G:218:TYR:CD1	2.55	0.42
8:H:188:ILE:O	8:H:188:ILE:HG13	2.20	0.42
22:V:396:GLN:HE22	33:9:71:ARG:HB3	1.84	0.42
24:X:268:LEU:HD21	24:X:293:LEU:HD23	2.02	0.42
7:G:143:ASP:OD1	7:G:144:GLY:N	2.53	0.41
25:Y:319:ALA:O	28:1:164:ARG:NH2	2.53	0.41
1:A:976:A:C2	9:I:182:PRO:CB	3.03	0.41
20:T:150:PRO:HA	20:T:153:VAL:O	2.20	0.41
1:A:1431:G:O2'	1:A:1432:U:OP2	2.38	0.41
28:1:56:ARG:NH1	31:4:81:ASP:OD2	2.53	0.41
1:A:1083:C:O3'	9:I:193:LYS:HB2	2.21	0.41
24:X:159:HIS:ND1	24:X:267:ALA:HB2	2.36	0.41
1:A:1508:C:O2'	1:A:1509:U:P	2.79	0.41
1:A:1432:U:OP1	7:G:378:GLU:N	2.53	0.41
2:B:59:ASN:OD1	2:B:64:ASN:ND2	2.54	0.41
6:F:173:PRO:HG3	29:2:77:ALA:HB1	2.02	0.41
7:G:175:HIS:CE1	7:G:176:GLN:HG3	2.55	0.41
18:R:276:VAL:HG22	18:R:281:ILE:HG21	2.03	0.41
22:V:40:TRP:O	22:V:43:ARG:NE	2.54	0.41
1:A:1084:C:OP1	9:I:193:LYS:HG3	2.20	0.41
1:A:1366:C:H3'	1:A:1367:A:H5'	2.02	0.41
4:D:213:GLU:OE2	19:S:2:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:170:ARG:O	18:R:189:ARG:NH1	2.50	0.41
18:R:219:TYR:O	18:R:256:ARG:NH2	2.54	0.41
27:0:78:ARG:NH2	27:0:142:VAL:O	2.54	0.41
1:A:1116:A:OP2	19:S:52:ARG:NH1	2.54	0.41
1:A:1454:G:OP2	7:G:377:ARG:NH1	2.46	0.41
18:R:162:SER:HB2	18:R:165:ILE:HD12	2.02	0.41
28:1:150:GLU:OE1	28:1:174:ARG:NH2	2.54	0.41
1:A:1225:C:H1'	1:A:1226:C:OP2	2.21	0.40
1:A:1401:G:H22	1:A:1404:A:C5'	2.34	0.40
1:A:1401:G:C2	1:A:1403:A:OP2	2.74	0.40
6:F:176:ASP:OD2	6:F:180:ARG:NH1	2.55	0.40
7:G:263:ASP:OD1	7:G:267:MET:N	2.54	0.40
22:V:56:LEU:HD11	33:9:75:PRO:HG2	2.03	0.40
29:2:87:ARG:O	29:2:91:GLU:N	2.54	0.40
24:X:203:LYS:O	24:X:250:GLN:NE2	2.54	0.40
31:4:137:ILE:HG21	31:4:140:LEU:HD12	2.03	0.40
1:A:812:A:O2'	1:A:814:A:N1	2.54	0.40
1:A:976:A:C1'	9:I:183:HIS:HD2	2.34	0.40
1:A:1598:G:HO2'	1:A:1599:A:P	2.43	0.40
4:D:119:LYS:HD3	4:D:119:LYS:O	2.21	0.40
6:F:170:VAL:HG23	6:F:236:LEU:O	2.21	0.40
22:V:228:TYR:O	22:V:232:GLY:N	2.44	0.40
22:V:378:ASN:O	22:V:382:TRP:N	2.47	0.40
22:V:394:GLN:HA	22:V:398:GLU:HB2	2.02	0.40
1:A:976:A:H1'	9:I:183:HIS:HD2	1.84	0.40
7:G:348:MET:O	7:G:352:LEU:N	2.55	0.40
9:I:187:ARG:NE	17:Q:45:TYR:CD2	2.89	0.40
10:J:59:LYS:HE2	10:J:107:ILE:HG21	2.04	0.40
13:M:68:LEU:O	18:R:160:ASP:HA	2.20	0.40
18:R:82:MET:HE2	18:R:300:LEU:N	2.37	0.40
22:V:69:SER:HB2	22:V:105:ARG:HG2	2.04	0.40
25:Y:323:ASP:OD1	25:Y:323:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	223/296 (75%)	216 (97%)	7 (3%)	0	100	100
3	C	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
4	D	341/430 (79%)	333 (98%)	8 (2%)	0	100	100
5	E	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
6	F	206/242 (85%)	203 (98%)	3 (2%)	0	100	100
7	G	320/396 (81%)	309 (97%)	11 (3%)	0	100	100
8	H	138/201 (69%)	137 (99%)	0	1 (1%)	19	55
9	I	134/194 (69%)	122 (91%)	12 (9%)	0	100	100
10	J	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
11	K	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
12	L	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
13	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
14	N	108/130 (83%)	104 (96%)	4 (4%)	0	100	100
15	O	192/258 (74%)	185 (96%)	7 (4%)	0	100	100
16	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
17	Q	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
18	R	293/360 (81%)	288 (98%)	5 (2%)	0	100	100
19	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
20	T	166/173 (96%)	166 (100%)	0	0	100	100
21	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
22	V	358/414 (86%)	354 (99%)	4 (1%)	0	100	100
23	W	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
24	X	350/398 (88%)	347 (99%)	3 (1%)	0	100	100
25	Y	147/395 (37%)	146 (99%)	1 (1%)	0	100	100
26	Z	84/106 (79%)	82 (98%)	2 (2%)	0	100	100
27	0	213/218 (98%)	210 (99%)	3 (1%)	0	100	100
28	1	274/323 (85%)	265 (97%)	9 (3%)	0	100	100
29	2	116/118 (98%)	116 (100%)	0	0	100	100
30	3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	4	584/689 (85%)	570 (98%)	14 (2%)	0	100	100
32	b	303/407 (74%)	288 (95%)	15 (5%)	0	100	100
33	9	10/698 (1%)	8 (80%)	2 (20%)	0	100	100
All	All	5957/8408 (71%)	5819 (98%)	137 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	126	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	198/249 (80%)	198 (100%)	0	100	100
3	C	115/143 (80%)	115 (100%)	0	100	100
4	D	286/357 (80%)	286 (100%)	0	100	100
5	E	104/107 (97%)	104 (100%)	0	100	100
6	F	185/209 (88%)	185 (100%)	0	100	100
7	G	282/342 (82%)	282 (100%)	0	100	100
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	104/146 (71%)	104 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	158/226 (70%)	158 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	175/230 (76%)	175 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	78/78 (100%)	78 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100
19	S	116/164 (71%)	116 (100%)	0	100	100
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	V	325/364 (89%)	323 (99%)	2 (1%)	84	88
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	311 (100%)	0	100	100
25	Y	137/357 (38%)	137 (100%)	0	100	100
26	Z	80/95 (84%)	80 (100%)	0	100	100
27	0	188/190 (99%)	188 (100%)	0	100	100
28	1	254/291 (87%)	254 (100%)	0	100	100
29	2	100/100 (100%)	100 (100%)	0	100	100
30	3	65/166 (39%)	65 (100%)	0	100	100
31	4	526/609 (86%)	526 (100%)	0	100	100
32	b	257/350 (73%)	256 (100%)	1 (0%)	89	91
33	9	12/600 (2%)	12 (100%)	0	100	100
All	All	5307/7293 (73%)	5304 (100%)	3 (0%)	92	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	V	43	ARG
22	V	102	TRP
32	b	120	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	156	GLN
4	D	347	GLN
7	G	127	HIS
8	H	109	HIS
8	H	125	HIS
9	I	98	GLN

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Mol	Chain	Res	Type
9	I	183	HIS
18	R	167	HIS
18	R	299	ASN
22	V	145	ASN
25	Y	290	ASN
26	Z	54	ASN
28	1	122	HIS
31	4	285	ASN
31	4	295	ASN
31	4	540	HIS
32	b	176	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	924/955 (96%)	194 (20%)	6 (0%)

All (194) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	651	A
1	A	659	U
1	A	680	U
1	A	688	A
1	A	689	U
1	A	690	U
1	A	693	A
1	A	695	A
1	A	704	U
1	A	718	A
1	A	721	U
1	A	722	C
1	A	730	A
1	A	739	C
1	A	753	A
1	A	757	A
1	A	761	A
1	A	766	G
1	A	777	G
1	A	791	G
1	A	793	C

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Mol	Chain	Res	Type
1	A	794	U
1	A	796	G
1	A	801	A
1	A	803	C
1	A	804	C
1	A	806	C
1	A	808	C
1	A	814	A
1	A	815	C
1	A	826	A
1	A	828	C
1	A	829	C
1	A	830	U
1	A	832	U
1	A	835	C
1	A	859	U
1	A	860	A
1	A	861	U
1	A	868	C
1	A	871	A
1	A	879	U
1	A	881	A
1	A	884	U
1	A	889	G
1	A	890	C
1	A	896	A
1	A	902	G
1	A	903	U
1	A	904	C
1	A	905	A
1	A	907	A
1	A	919	A
1	A	922	C
1	A	929	A
1	A	930	G
1	A	931	C
1	A	932	C
1	A	933	G
1	A	938	A
1	A	939	A
1	A	940	A
1	A	941	G

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Mol	Chain	Res	Type
1	A	942	A
1	A	953	U
1	A	955	A
1	A	956	C
1	A	958	C
1	A	961	U
1	A	962	C
1	A	966	A
1	A	967	A
1	A	988	G
1	A	993	A
1	A	1000	U
1	A	1001	C
1	A	1002	C
1	A	1003	A
1	A	1011	C
1	A	1015	A
1	A	1030	G
1	A	1042	U
1	A	1044	U
1	A	1049	A
1	A	1069	A
1	A	1073	G
1	A	1081	U
1	A	1082	A
1	A	1103	A
1	A	1105	C
1	A	1106	C
1	A	1107	U
1	A	1109	A
1	A	1116	A
1	A	1117	A
1	A	1118	A
1	A	1119	U
1	A	1120	C
1	A	1121	A
1	A	1126	A
1	A	1128	C
1	A	1136	C
1	A	1137	A
1	A	1142	A
1	A	1144	U

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Mol	Chain	Res	Type
1	A	1151	C
1	A	1154	A
1	A	1155	G
1	A	1160	A
1	A	1187	U
1	A	1188	A
1	A	1189	U
1	A	1190	C
1	A	1194	C
1	A	1199	G
1	A	1200	G
1	A	1213	A
1	A	1215	U
1	A	1220	A
1	A	1222	A
1	A	1223	C
1	A	1225	C
1	A	1226	C
1	A	1227	G
1	A	1237	A
1	A	1245	U
1	A	1246	U
1	A	1247	G
1	A	1248	C
1	A	1250	C
1	A	1251	A
1	A	1269	U
1	A	1271	C
1	A	1282	G
1	A	1284	U
1	A	1289	G
1	A	1290	C
1	A	1291	U
1	A	1292	A
1	A	1295	A
1	A	1312	C
1	A	1313	A
1	A	1326	A
1	A	1327	G
1	A	1338	A
1	A	1343	A
1	A	1344	U

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Mol	Chain	Res	Type
1	A	1345	G
1	A	1352	C
1	A	1354	A
1	A	1355	G
1	A	1357	A
1	A	1378	C
1	A	1379	A
1	A	1386	U
1	A	1387	A
1	A	1390	A
1	A	1392	A
1	A	1401	G
1	A	1402	A
1	A	1404	A
1	A	1405	C
1	A	1406	U
1	A	1416	A
1	A	1430	A
1	A	1434	A
1	A	1443	U
1	A	1447	G
1	A	1466	C
1	A	1474	G
1	A	1478	A
1	A	1480	A
1	A	1482	A
1	A	1483	C
1	A	1502	A
1	A	1509	U
1	A	1510	U
1	A	1539	C
1	A	1544	A
1	A	1548	A
1	A	1551	G
1	A	1552	G
1	A	1558	A
1	A	1561	C
1	A	1564	A
1	A	1568	U
1	A	1570	G
1	A	1571	U
1	A	1582	G

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Mol	Chain	Res	Type
1	A	1585	A
1	A	1594	G
1	A	1595	G
1	A	1599	A
1	A	1602	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1021	U
1	A	1081	U
1	A	1225	C
1	A	1465	C
1	A	1508	C
1	A	1550	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MU	A	1076	1	19,22,23	0.39	0	28,32,35	0.49	0
1	5MC	A	1488	1	18,22,23	0.53	0	26,32,35	0.56	0
9	5F0	I	184	9	8,8,9	0.55	0	7,9,11	1.17	1 (14%)
1	MA6	A	1583	1	18,26,27	1.00	2 (11%)	19,38,41	3.32	4 (21%)
1	B8T	A	1486	1	19,22,23	3.34	8 (42%)	26,31,34	0.85	1 (3%)
1	MA6	A	1584	1	18,26,27	1.02	2 (11%)	19,38,41	3.18	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	A	1076	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1488	1	-	0/7/25/26	0/2/2/2
9	5F0	I	184	9	-	0/9/9/10	-
1	MA6	A	1583	1	-	2/7/29/30	0/3/3/3
1	B8T	A	1486	1	-	0/7/27/28	0/2/2/2
1	MA6	A	1584	1	-	2/7/29/30	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1486	B8T	C4-N3	7.69	1.46	1.32
1	A	1486	B8T	C2-N3	6.07	1.48	1.36
1	A	1486	B8T	C6-C5	5.95	1.48	1.35
1	A	1486	B8T	C4-N4	4.83	1.45	1.35
1	A	1486	B8T	C2-N1	4.68	1.50	1.40
1	A	1486	B8T	C5-C4	3.51	1.48	1.40
1	A	1486	B8T	C6-N1	3.51	1.46	1.38
1	A	1486	B8T	O2-C2	-2.94	1.18	1.23
1	A	1583	MA6	C2-N3	2.49	1.36	1.32
1	A	1584	MA6	C2-N3	2.49	1.36	1.32
1	A	1584	MA6	C5-C4	-2.48	1.34	1.40
1	A	1583	MA6	C5-C4	-2.47	1.34	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1584	MA6	N1-C6-N6	-12.49	103.91	117.06
1	A	1583	MA6	N1-C6-N6	-12.39	104.02	117.06
1	A	1584	MA6	N3-C2-N1	-5.37	120.29	128.68
1	A	1583	MA6	N3-C2-N1	-5.32	120.37	128.68
1	A	1583	MA6	O4'-C4'-C5'	3.20	119.90	109.37
1	A	1583	MA6	C5'-C4'-C3'	3.07	126.67	115.18
9	I	184	5F0	O-C-CB	-2.74	117.45	125.43
1	A	1486	B8T	C6-C5-C4	2.53	120.06	116.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1583	MA6	O4'-C4'-C5'-O5'
1	A	1583	MA6	C4'-C5'-O5'-P
1	A	1584	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1584	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	184	5F0	3	0
1	A	1583	MA6	6	0
1	A	1584	MA6	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	NAD	A	1701	-	42,48,48	0.88	2 (4%)	50,73,73	0.84	1 (2%)
40	GDP	X	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.17	3 (10%)
37	FES	M	201	13	0,4,4	-	-	-		
35	SPM	A	1702	-	13,13,13	0.35	0	12,12,12	0.97	0
37	FES	P	201	16	0,4,4	-	-	-		
39	ATP	X	501	-	26,33,33	0.59	0	31,52,52	0.89	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	NAD	A	1701	-	-	0/26/62/62	0/5/5/5
40	GDP	X	502	-	-	2/12/32/32	0/3/3/3
37	FES	M	201	13	-	-	0/1/1/1
35	SPM	A	1702	-	-	0/11/11/11	-
37	FES	P	201	16	-	-	0/1/1/1
39	ATP	X	501	-	-	1/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	A	1701	NAD	C8A-N7A	-2.56	1.30	1.34
40	X	502	GDP	C6-N1	-2.45	1.34	1.37
34	A	1701	NAD	O4D-C1D	-2.37	1.37	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	X	502	GDP	PA-O3A-PB	-3.41	121.14	132.83
40	X	502	GDP	C8-N7-C5	2.52	107.80	102.99
34	A	1701	NAD	PN-O3-PA	-2.50	124.26	132.83
40	X	502	GDP	C5-C6-N1	2.33	118.07	113.95
39	X	501	ATP	C5-C6-N6	2.31	123.86	120.35
39	X	501	ATP	PB-O3B-PG	2.06	139.91	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	X	502	GDP	PA-O3A-PB-O1B
39	X	501	ATP	C3'-C4'-C5'-O5'
40	X	502	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

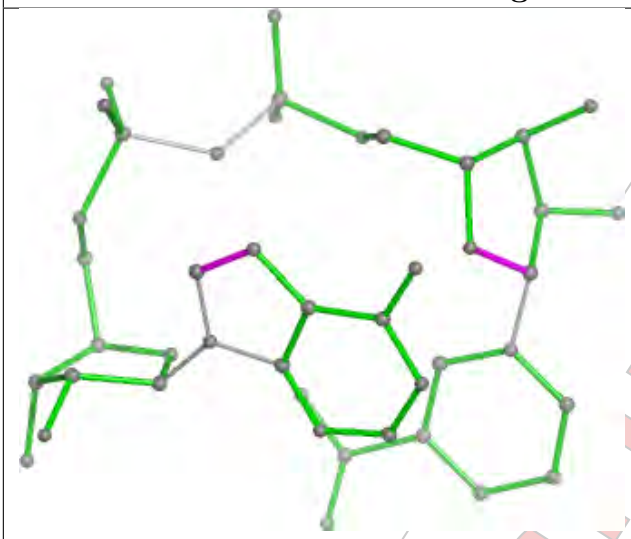
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	1702	SPM	1	0

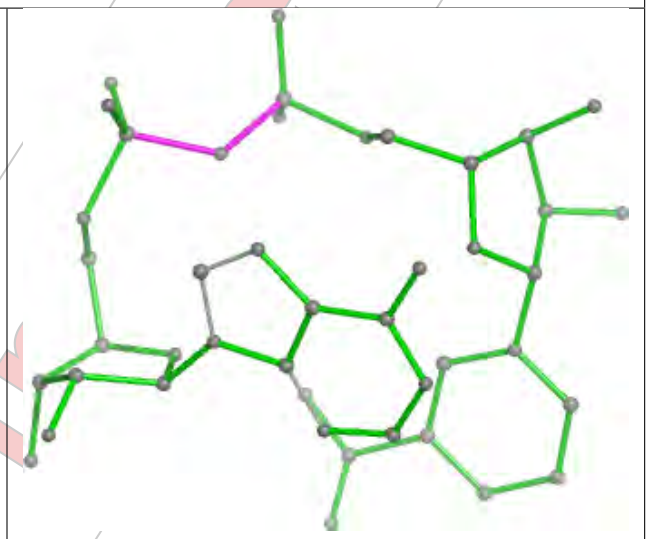
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

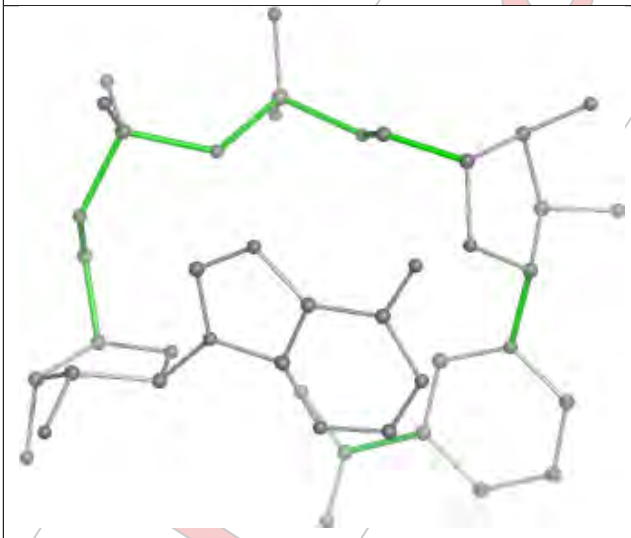
Ligand NAD A 1701



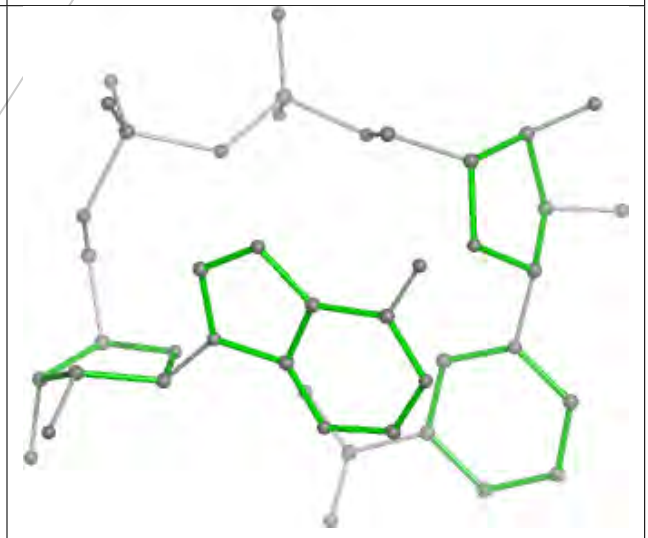
Bond lengths



Bond angles

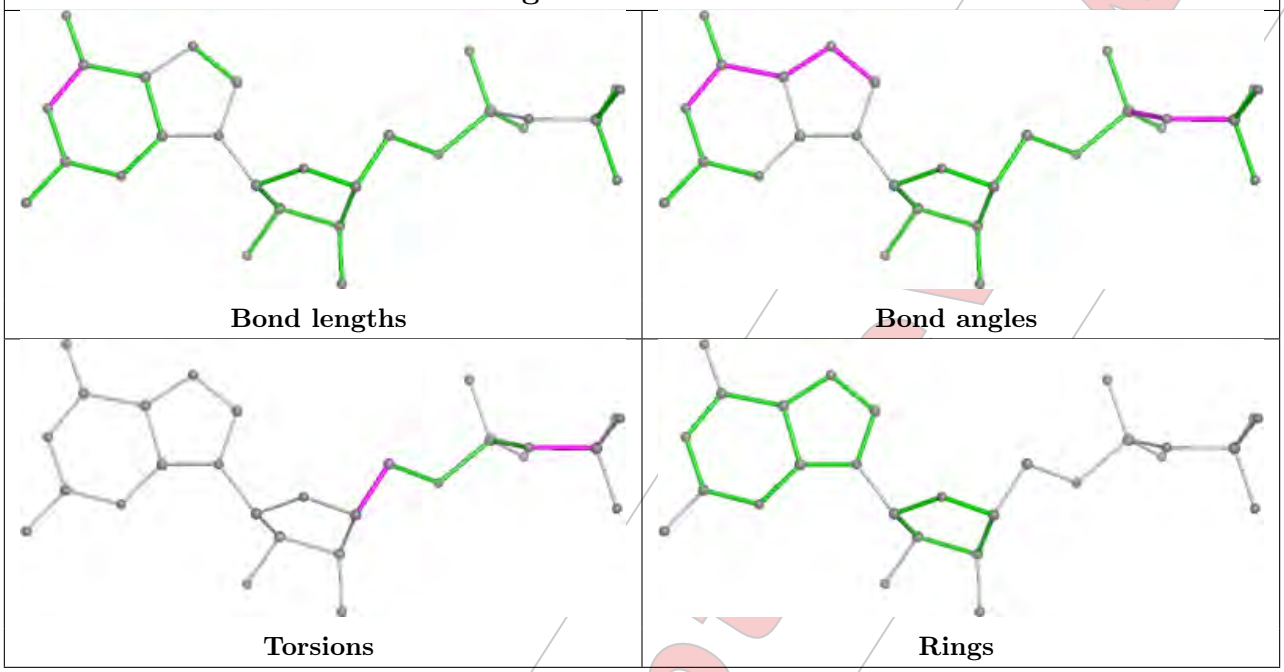


Torsions

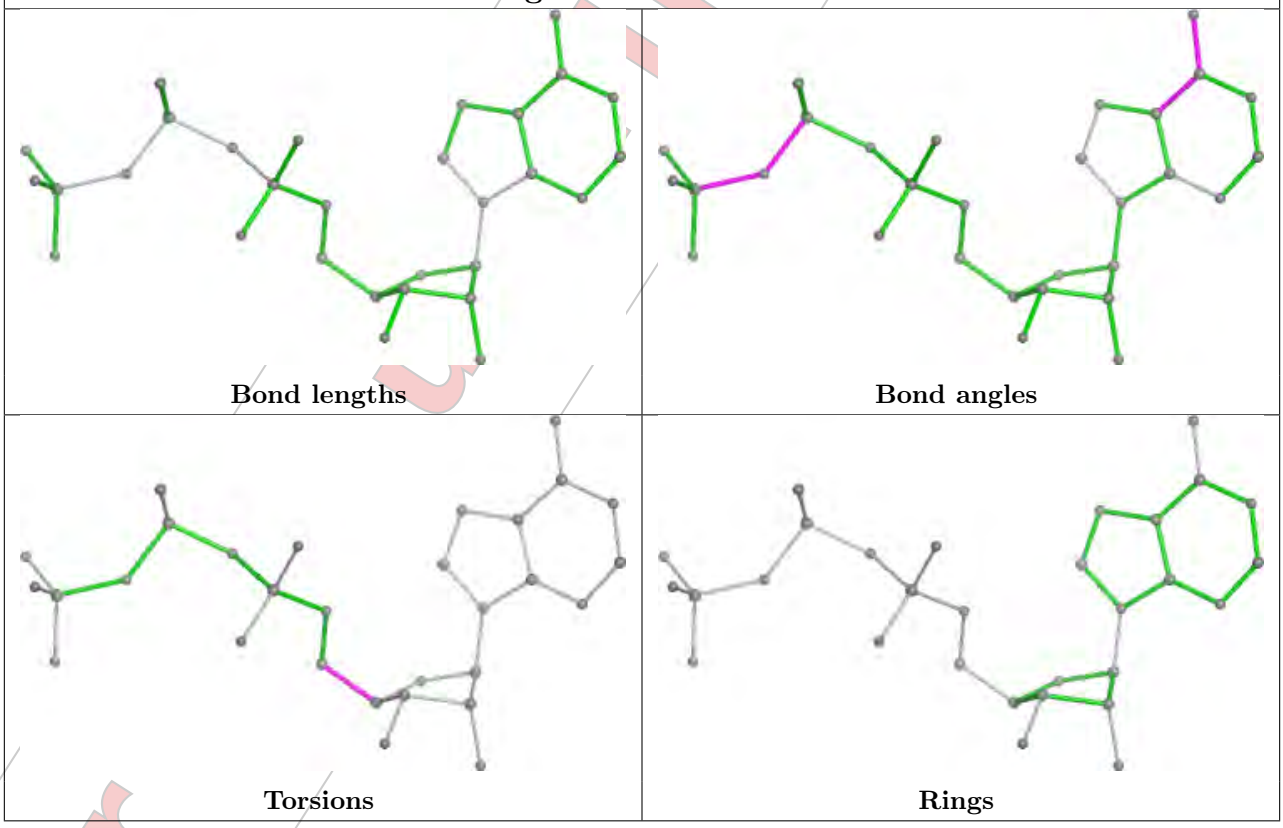


Rings

Ligand GDP X 502



Ligand ATP X 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

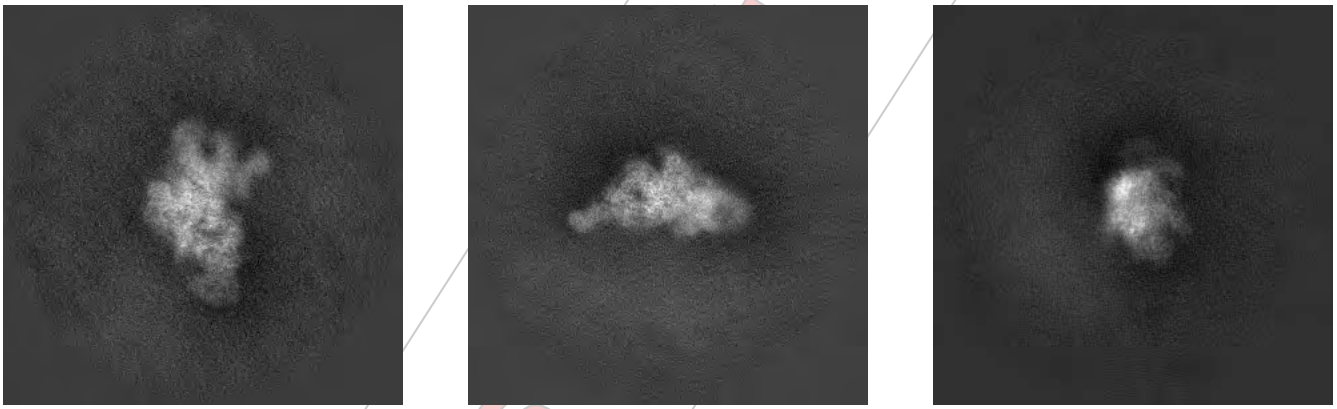
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51879. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

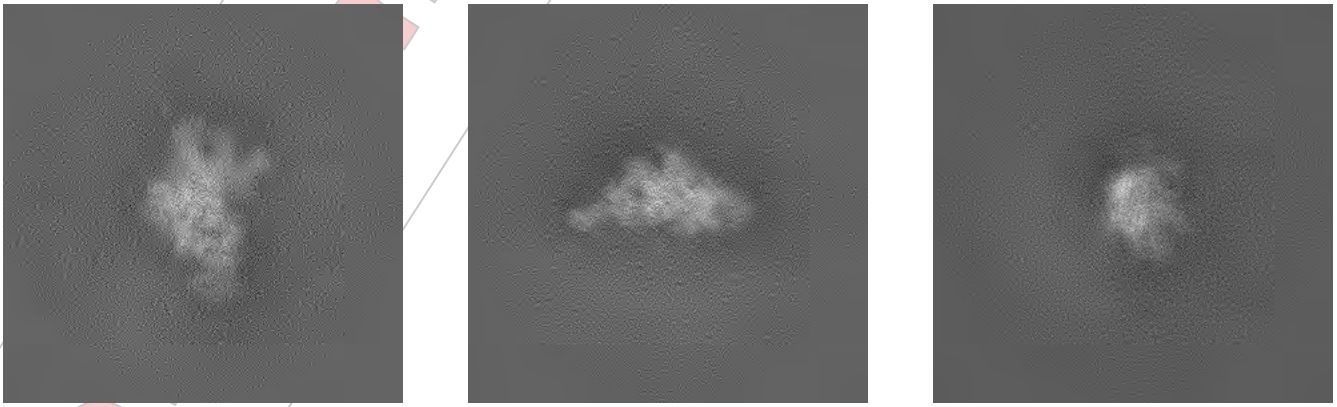
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

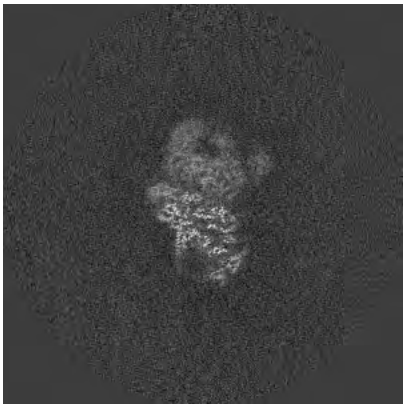


X Y Z

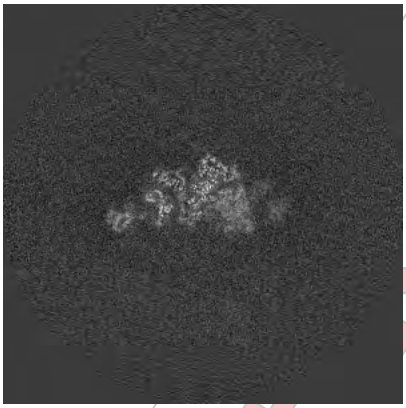
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

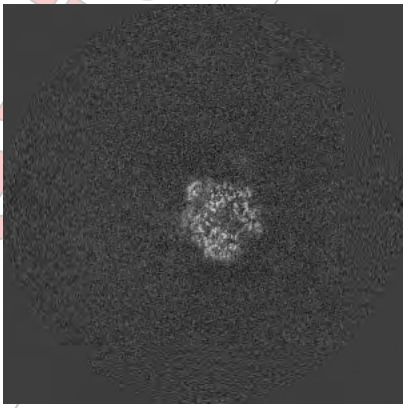
6.2.1 Primary map



X Index: 300

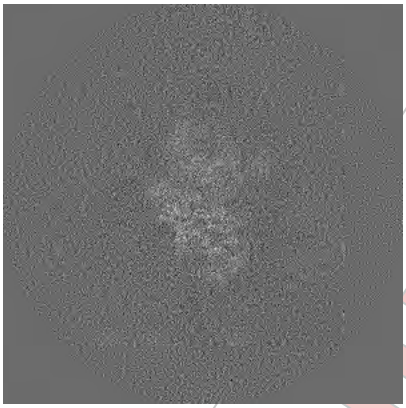


Y Index: 300

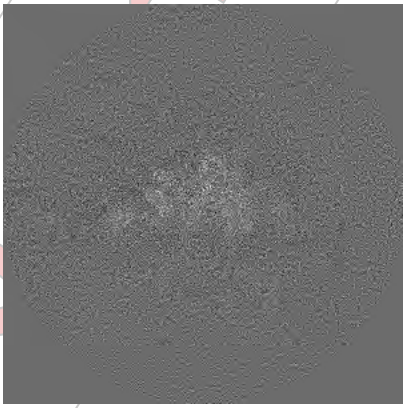


Z Index: 300

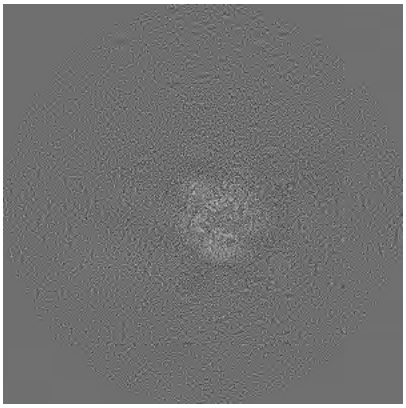
6.2.2 Raw map



X Index: 300



Y Index: 300

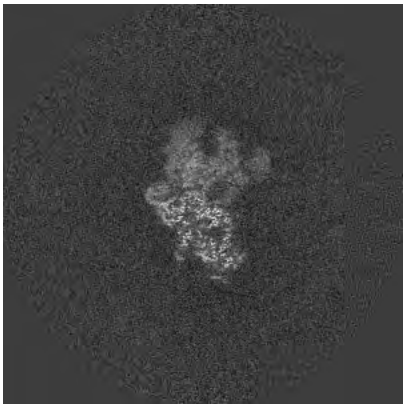


Z Index: 300

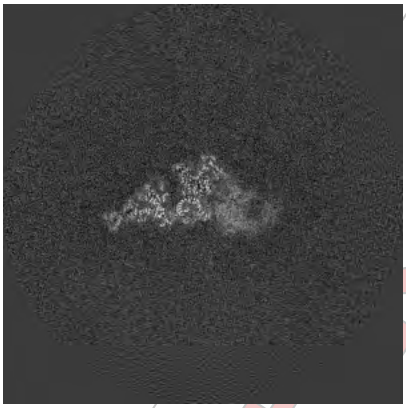
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

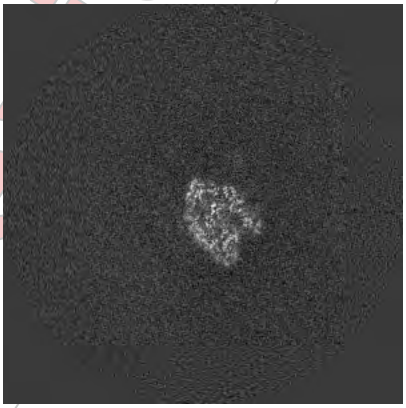
6.3.1 Primary map



X Index: 305

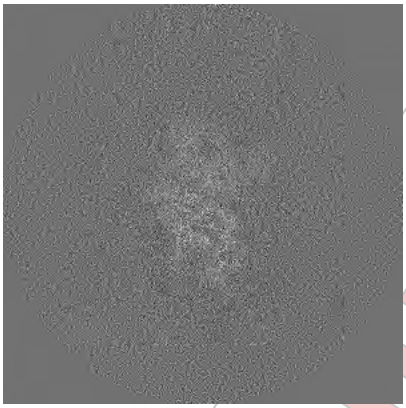


Y Index: 317

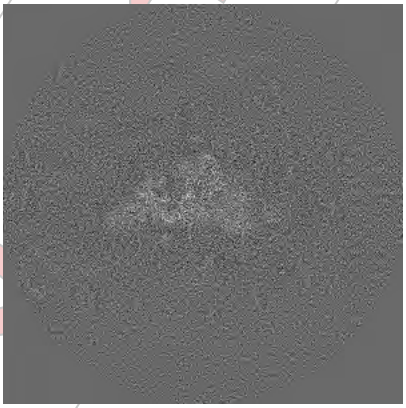


Z Index: 295

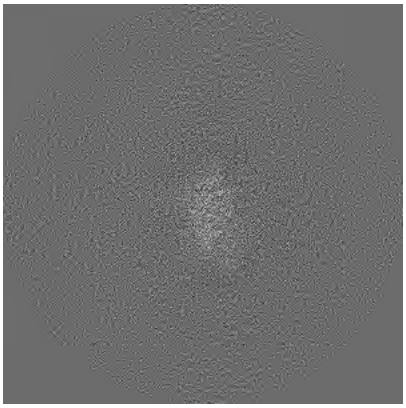
6.3.2 Raw map



X Index: 298



Y Index: 312

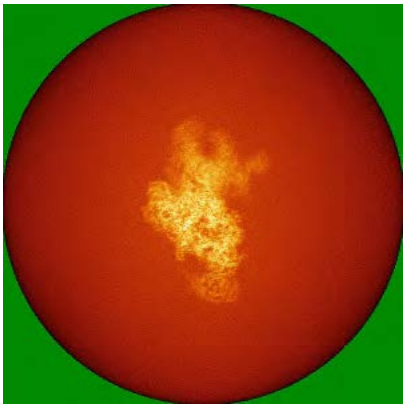


Z Index: 285

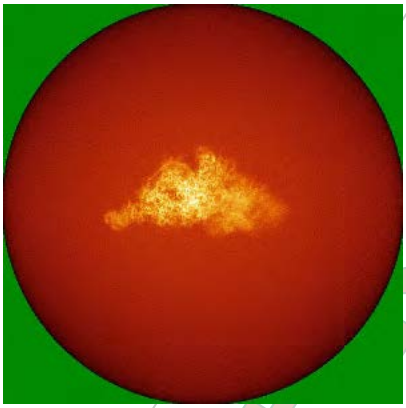
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

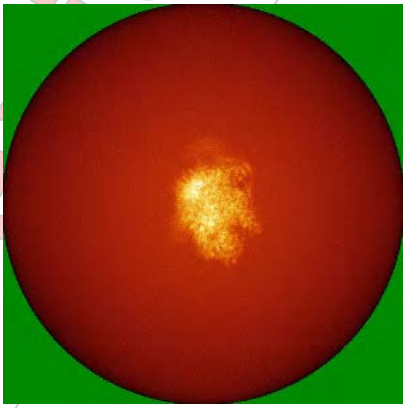
6.4.1 Primary map



X

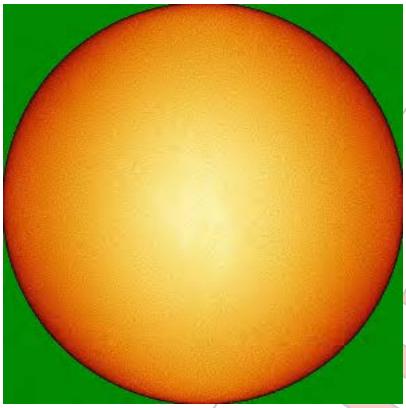


Y

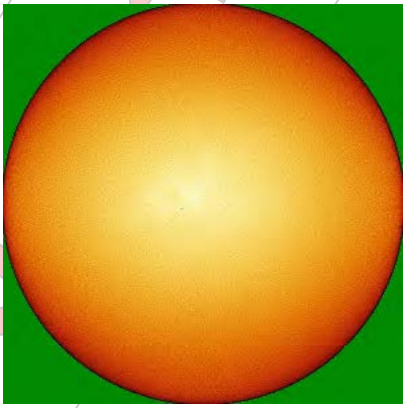


Z

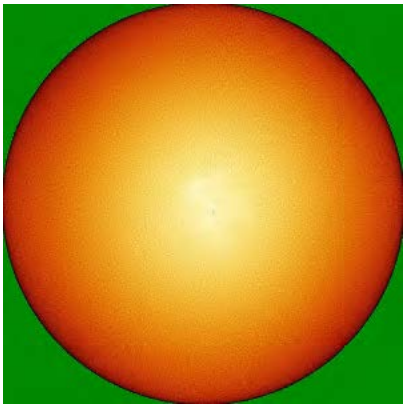
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

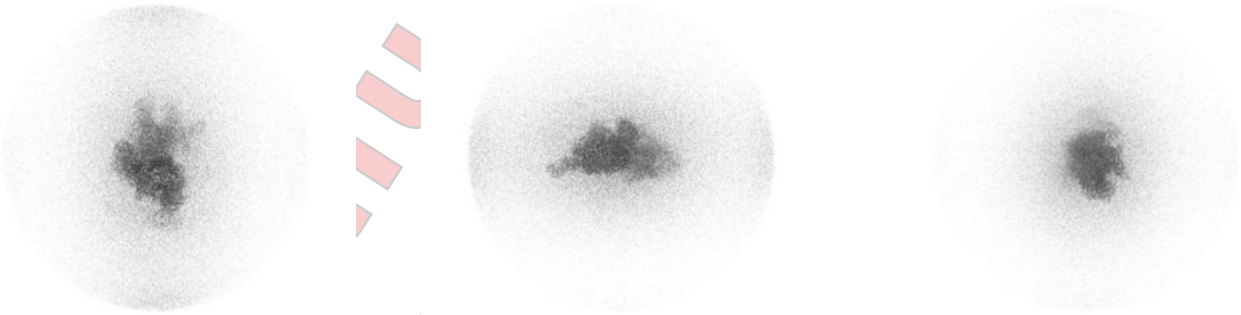
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

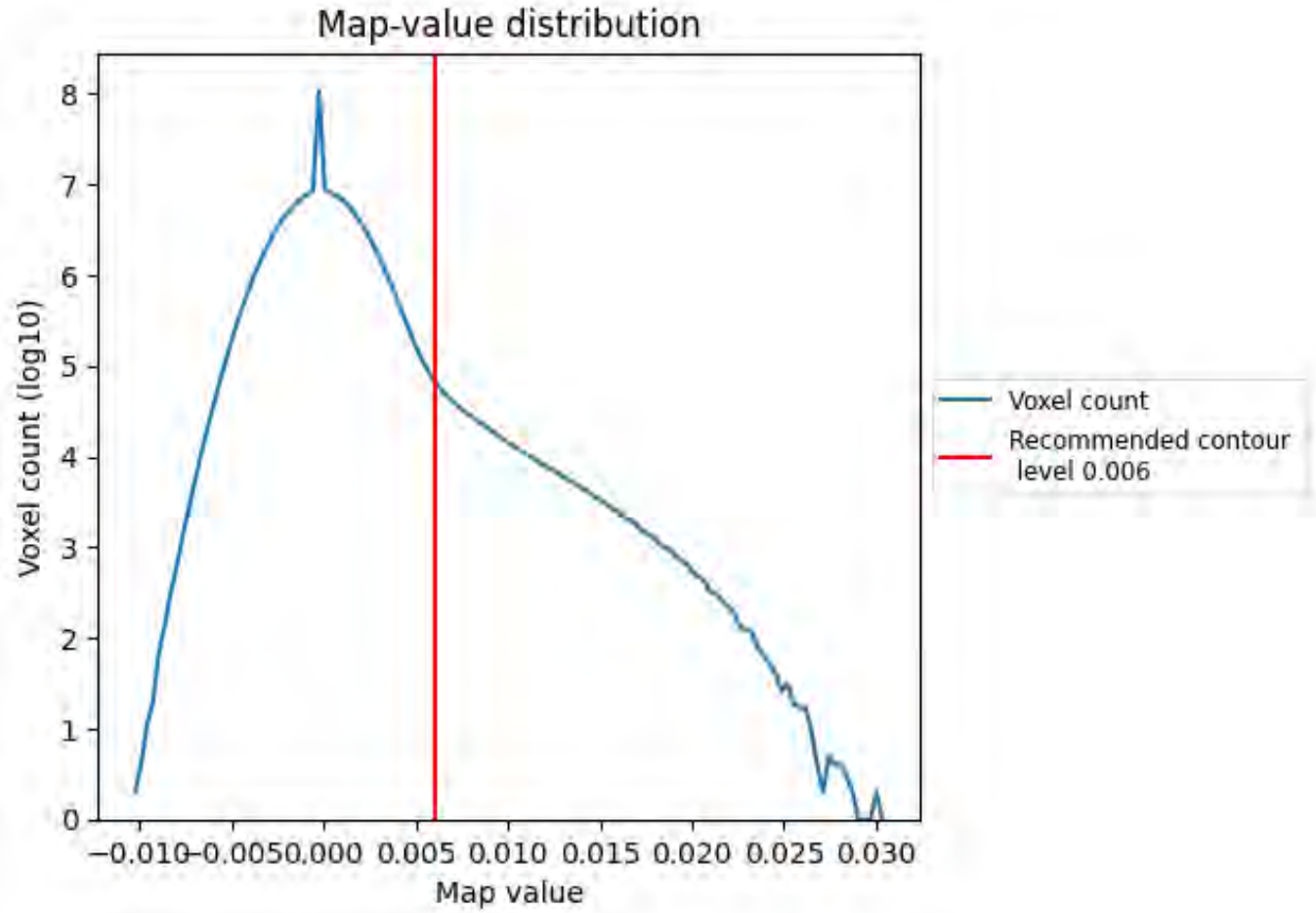
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

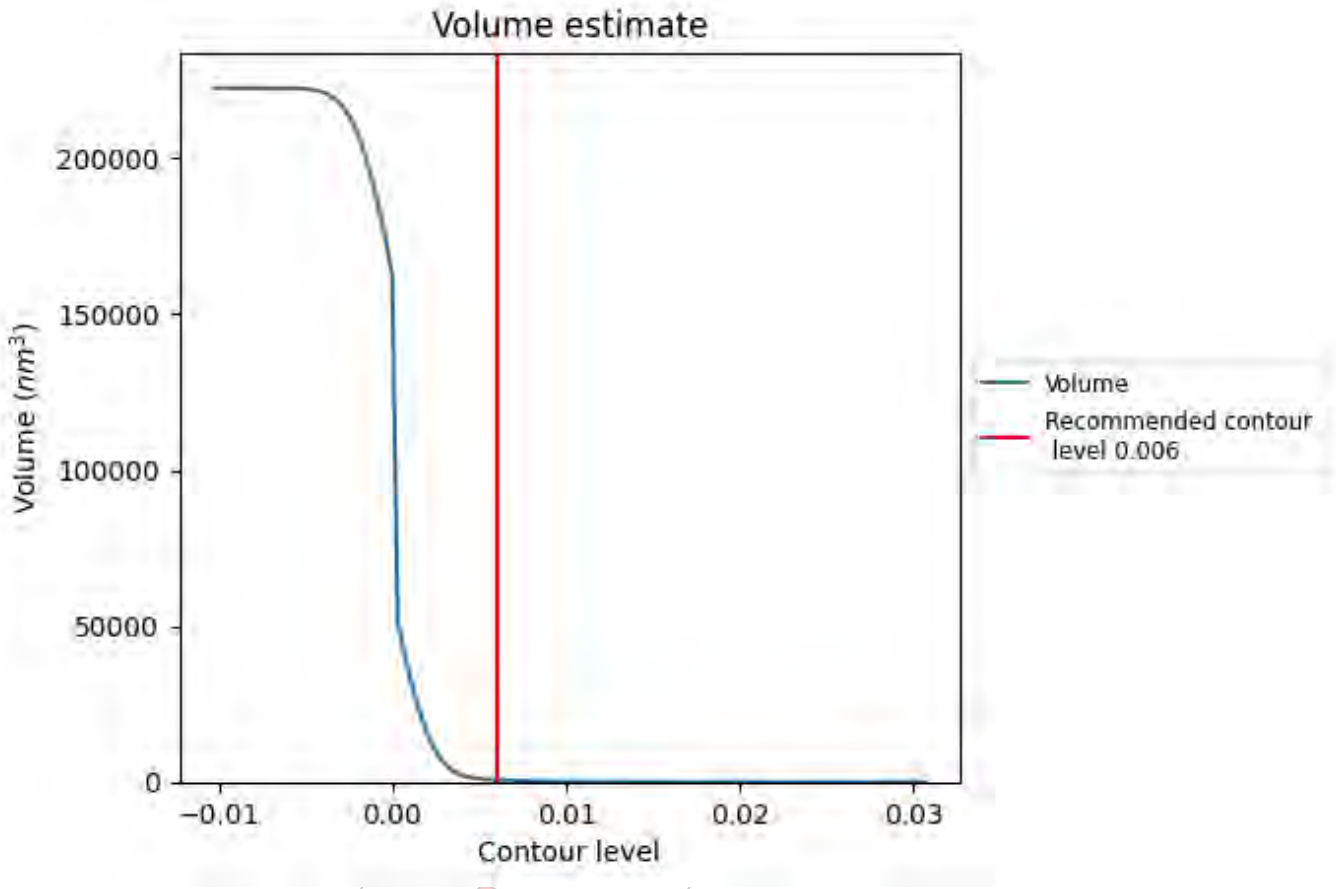
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

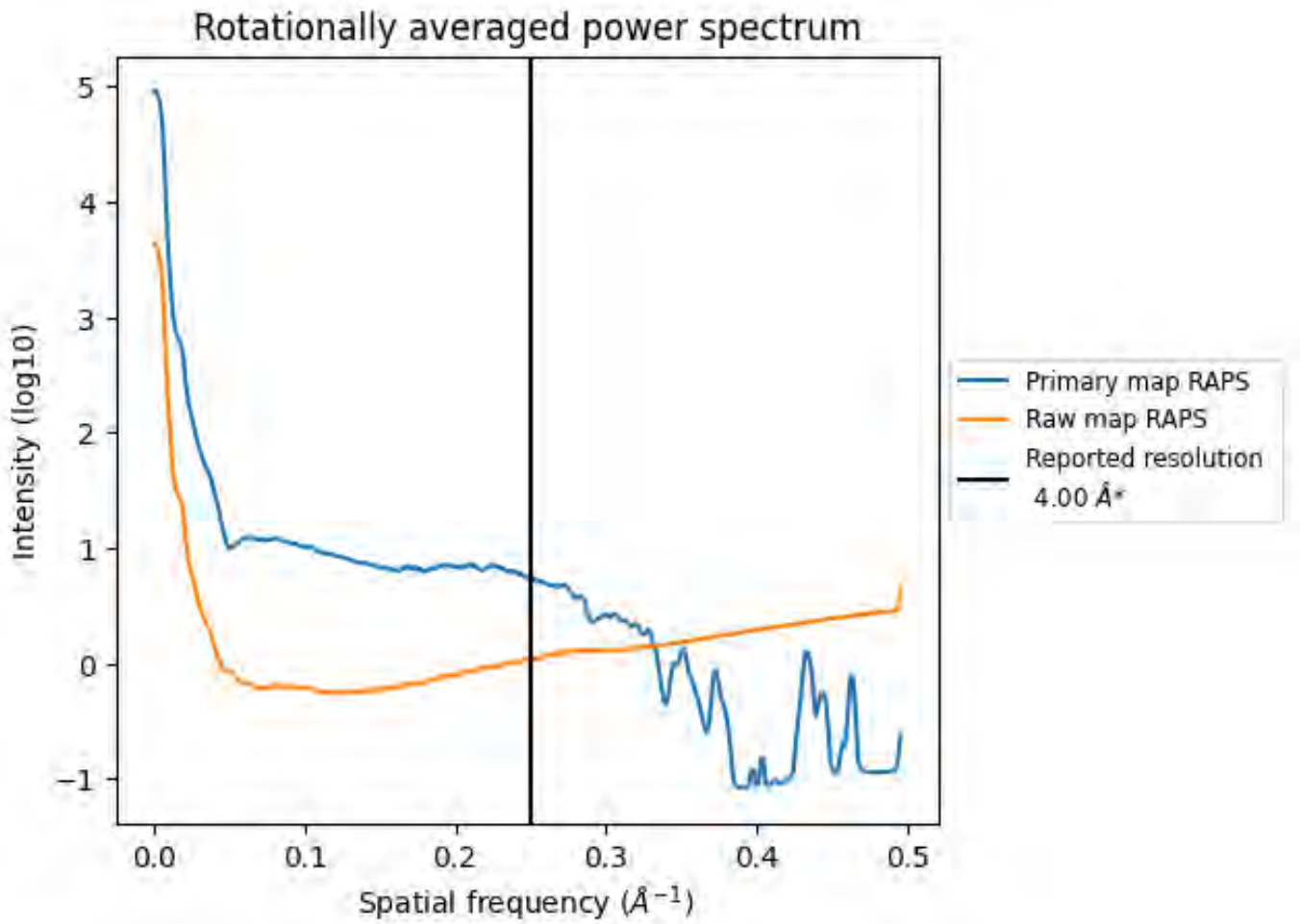
7.2 Volume estimate (i)



The volume at the recommended contour level is 591 nm^3; this corresponds to an approximate mass of 534 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

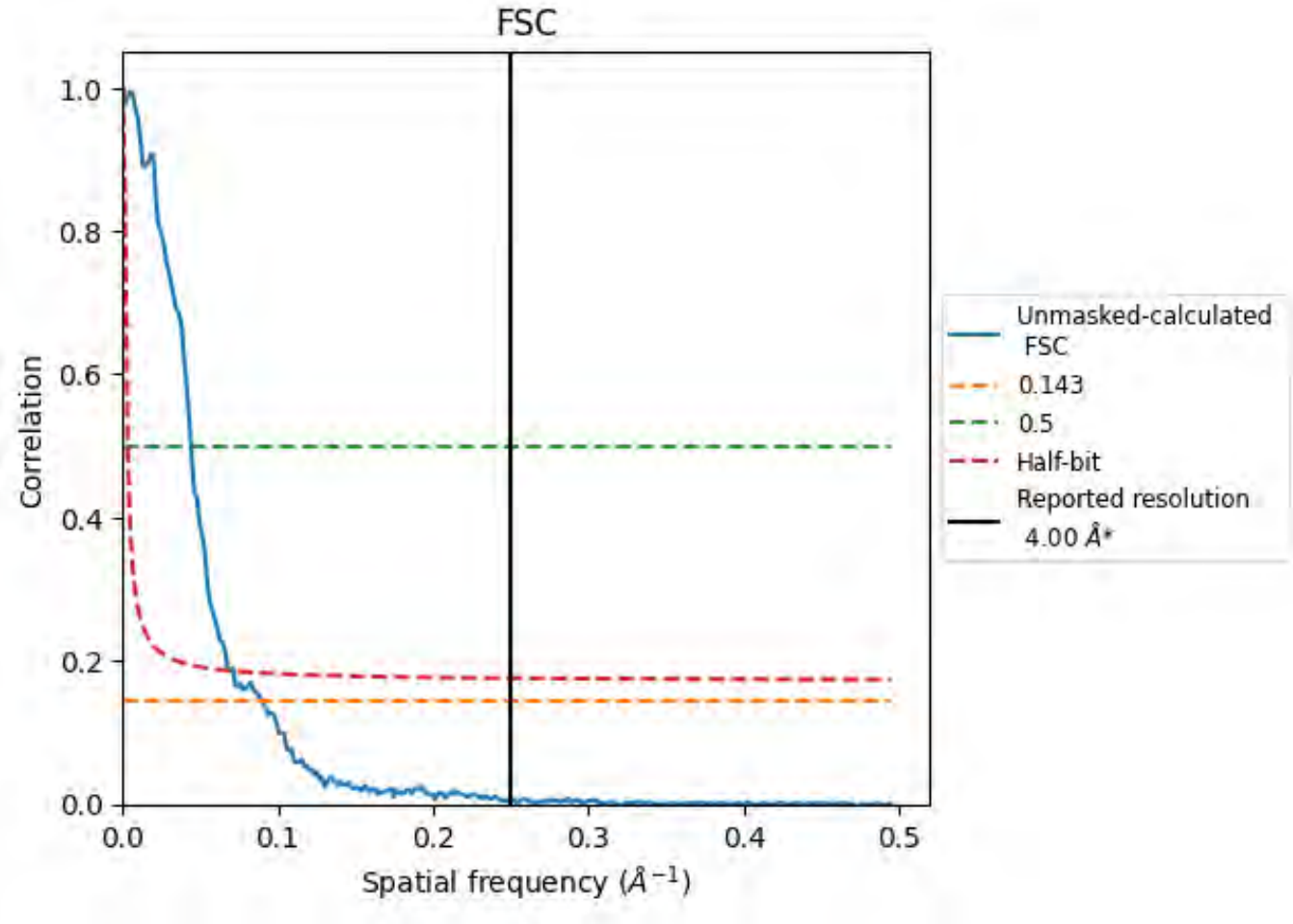


*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

8.2 Resolution estimates (i)

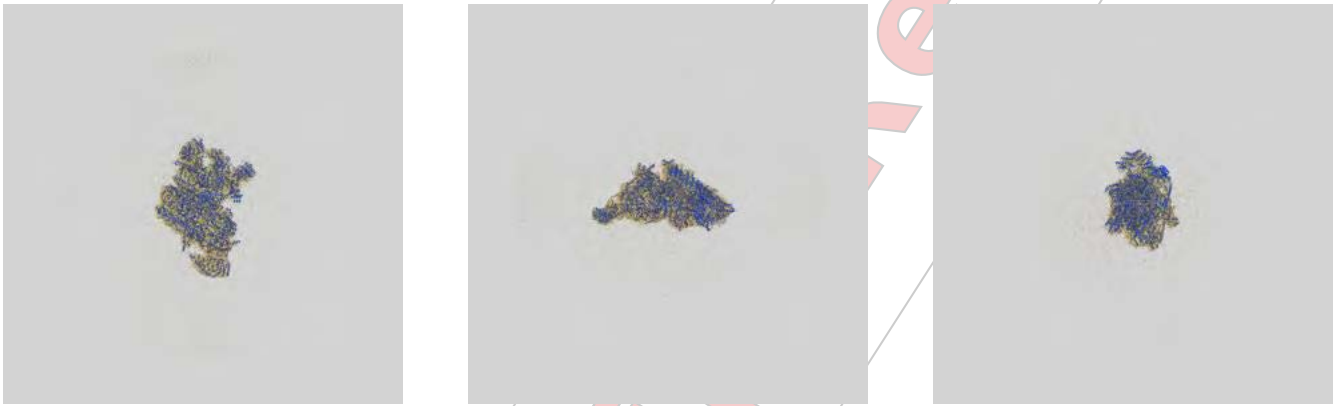
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.10	22.73	14.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 11.10 differs from the reported value 4.0 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51879 and PDB model 9H57. Per-residue inclusion information can be found in section 3 on page 14.

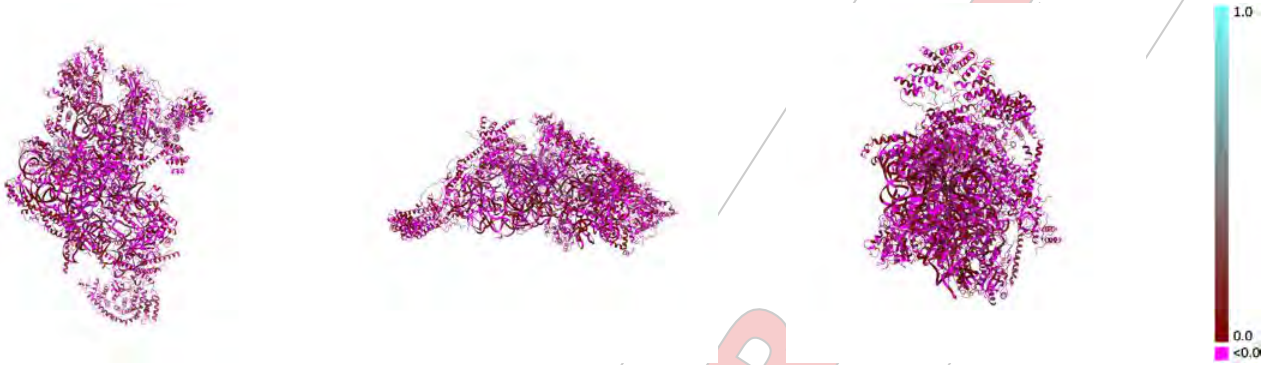
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

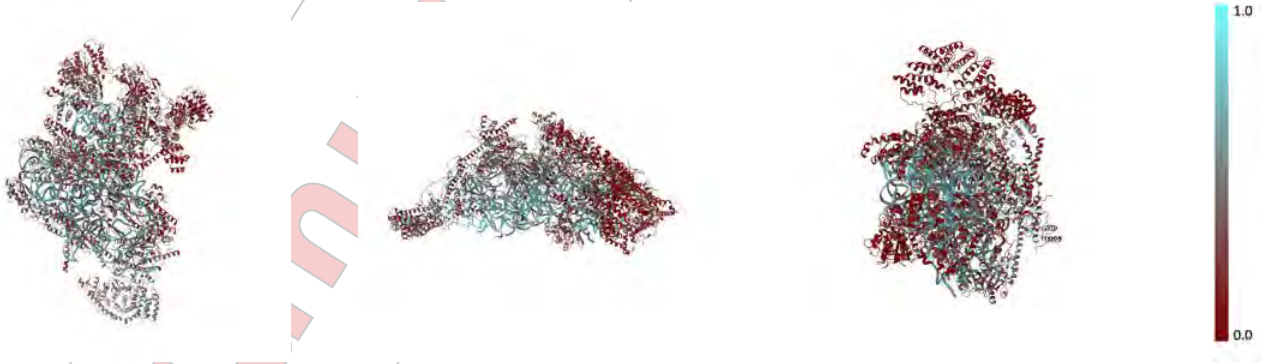
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

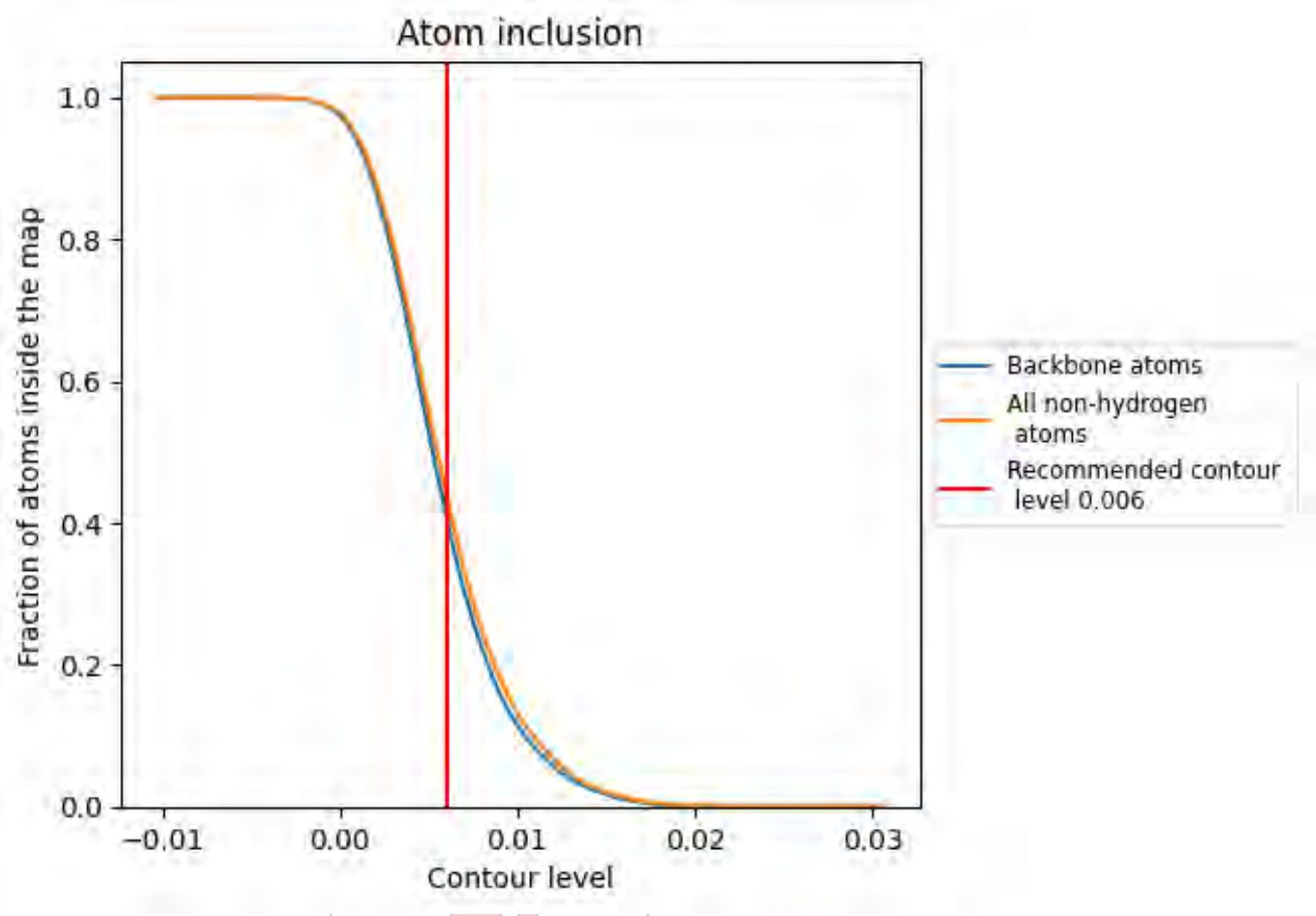
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 41% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4410	0.0240
0	0.4270	0.0360
1	0.1880	0.0010
2	0.1990	-0.0090
3	0.4560	-0.0000
4	0.1410	0.0210
9	0.2410	0.0530
A	0.6560	0.0410
B	0.3830	-0.0430
C	0.3410	-0.0090
D	0.3460	-0.0070
E	0.3920	0.0140
F	0.3620	0.0580
G	0.3550	0.0280
H	0.2780	0.0140
I	0.4640	0.0760
J	0.5040	0.0280
K	0.4200	0.0030
L	0.4740	0.0490
M	0.4700	0.0050
N	0.4700	0.0540
O	0.4210	0.0220
P	0.4290	-0.0230
Q	0.4390	-0.0050
R	0.3930	-0.0030
S	0.3880	0.0030
T	0.4560	0.0400
U	0.4370	0.0480
V	0.3800	0.0290
W	0.3680	-0.0500
X	0.2040	0.0180
Y	0.1620	0.0380
Z	0.3100	0.0240
b	0.1860	0.0280