Full wwPDB EM Validation Report ⓘ

Jul 28, 2026 – 02:06 PM JST

PDB ID	:	44EW / pdb_000044ew
EMDB ID	:	EMD-82546
Title	:	Ribosomal RNA modification enzyme
Deposited on	:	2026-07-27
Resolution	:	2.19 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.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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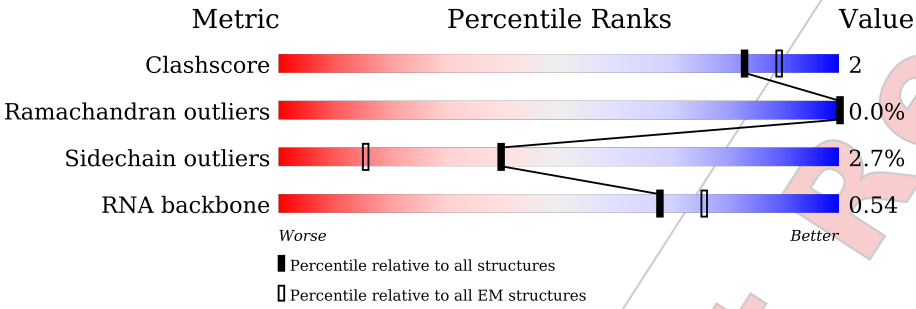
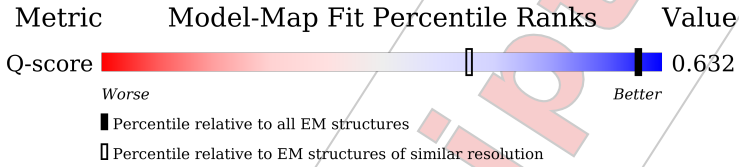
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.19 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2745 (1.70 - 2.69)

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	2904	79% 15% • 5%
2	1	120	88% 11% •

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Mol	Chain	Length	Quality of chain
3	2	1542	74% 22%
4	A	273	92% 7%
5	B	209	95%
6	C	201	94% 6%
7	D	179	84% 13%
8	E	177	92% 6%
9	F	149	48% 74% 23%
10	G	142	92% 8%
11	H	123	91% 9%
12	I	144	92% 8%
13	J	136	95%
14	K	127	83% 10% 7%
15	L	117	88% 11%
16	M	115	90% 9%
17	N	118	97%
18	O	103	96%
19	P	110	99%
20	Q	100	83% 9% 7%
21	R	104	93% 5%
22	S	94	90% 10%
23	T	85	84% 5% 12%
24	U	78	99%
25	V	63	89% 5% 5%
26	W	59	95%
27	X	70	9% 73% 13% 14%

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Mol	Chain	Length	Quality of chain
28	Y	178	81% 7% 11%
28	Z	178	76% 9% 15%
29	a	57	89% 7%
30	b	55	93% 7%
31	c	46	91% 9%
32	d	65	92% 6%
33	e	38	84% 16%
34	f	241	12% 76% 16% 7%
35	g	233	79% 9% 12%
36	h	206	92% 7%
37	i	167	87% 5% 7%
38	j	131	66% 15% 19%
39	k	179	12% 68% 16% 16%
40	l	130	91% 8%
41	m	130	6% 81% 16%
42	n	103	20% 71% 23%
43	o	129	81% 10% 9%
44	p	124	90% 9%
45	q	118	81% 14%
46	r	101	84% 12%
47	s	89	90% 8%
48	t	82	94% 6%
49	u	84	87% 7% 5%
50	v	75	79% 8% 12%
51	w	92	71% 15% 14%

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Mol	Chain	Length	Quality of chain
52	x	87	86% 13%
53	y	71	34% 80% 18%

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2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 141151 atoms, of which 0 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	0	2747	58988	26314	10873	19055	2746	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	120	2566	1144	468	835	119	0	0

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	1521	32638	14557	5991	10569	1521	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	271	2082	1288	423	364	7	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	208	1559	976	287	292	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	201	1552	974	283	290	5	0	0

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- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	177	1410	899	249	256	6	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	173	1295	814	237	242	2	0	0

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	149	1111	699	197	214	1	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	142	1129	714	212	199	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	123	947	593	181	167	6	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	144	1053	654	207	190	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	136	1074	686	205	177	6	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein bL17.

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 15 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	L	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 16 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 17 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	N	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 20 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

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Mol	Chain	Residues	Atoms				AltConf	Trace
21	R	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 23 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 26 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 28 is a protein called RlmH.

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Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	158	Total 1245	C 799	N 219	O 222	S 5	0	0
28	Z	152	Total 1190	C 765	N 207	O 214	S 4	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	55	Total 434	C 263	N 92	O 78	S 1	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	b	51	Total 417	C 269	N 76	O 72	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	46	Total 377	C 228	N 90	O 57	S 2	0	0

- Molecule 32 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	64	Total 504	C 323	N 105	O 74	S 2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	38	Total 302	C 185	N 65	O 48	S 4	0	0

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	224	Total 1753	C 1109	N 315	O 321	S 8	0	0

- Molecule 35 is a protein called 30S ribosomal protein S3.

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Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 38 is a protein called Small ribosomal subunit protein bS6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 42 is a protein called 30S ribosomal protein S10.

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 43 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 44 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 49 is a protein called 30S ribosomal protein S17.

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 54 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).

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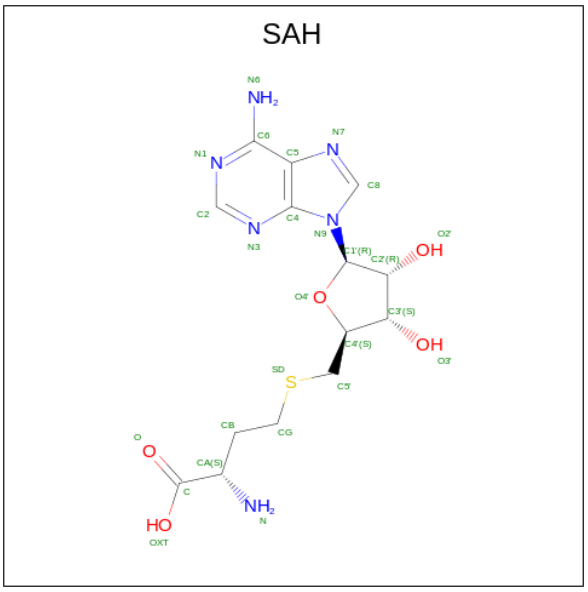

Mol	Chain	Residues	Atoms					AltConf
54	Y	1	Total	C	N	O	S	0
			26	14	6	5	1	
54	Z	1	Total	C	N	O	S	0
			26	14	6	5	1	

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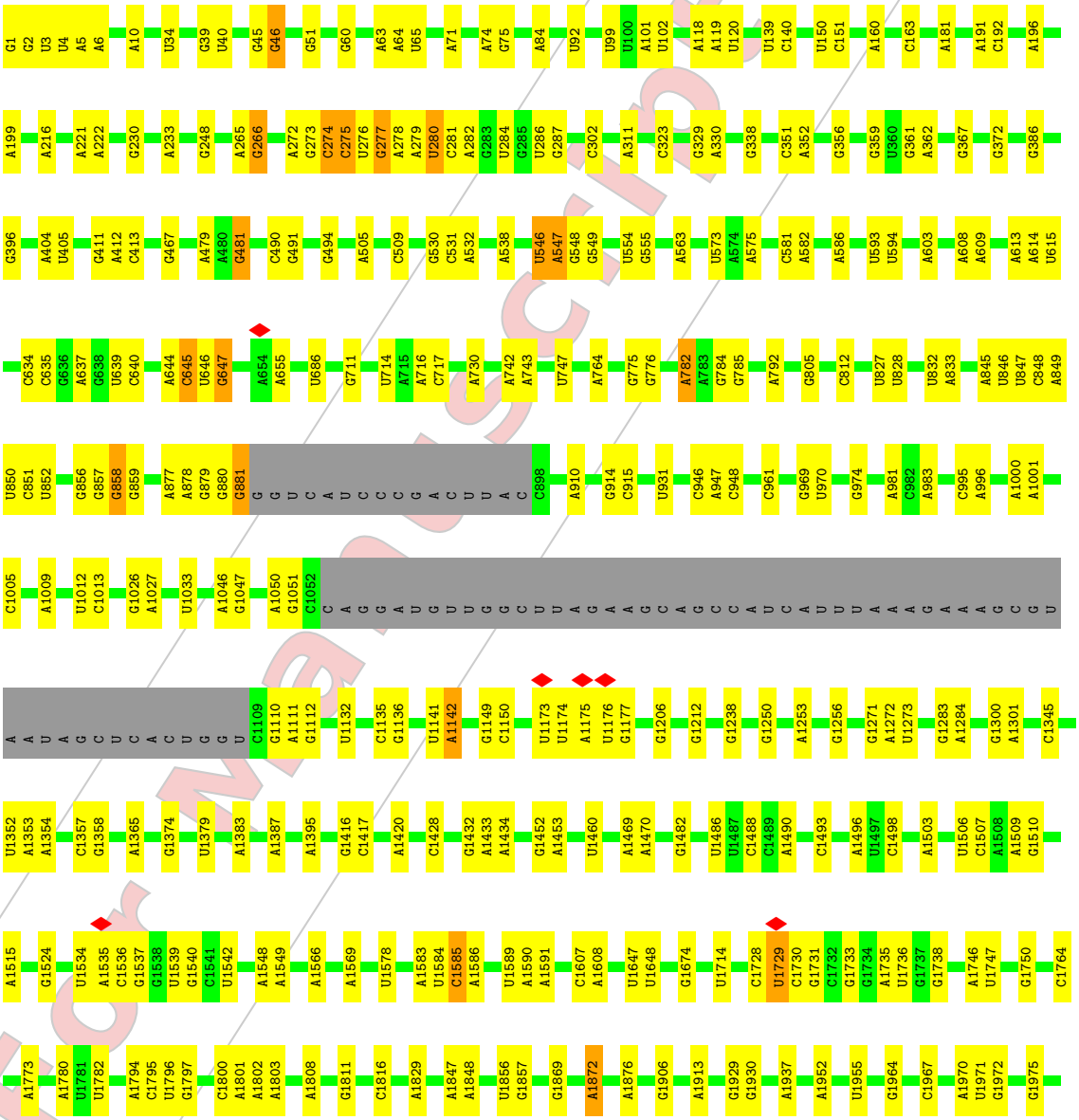
3 Residue-property plots (i)

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: 23S rRNA

Chain 0: 



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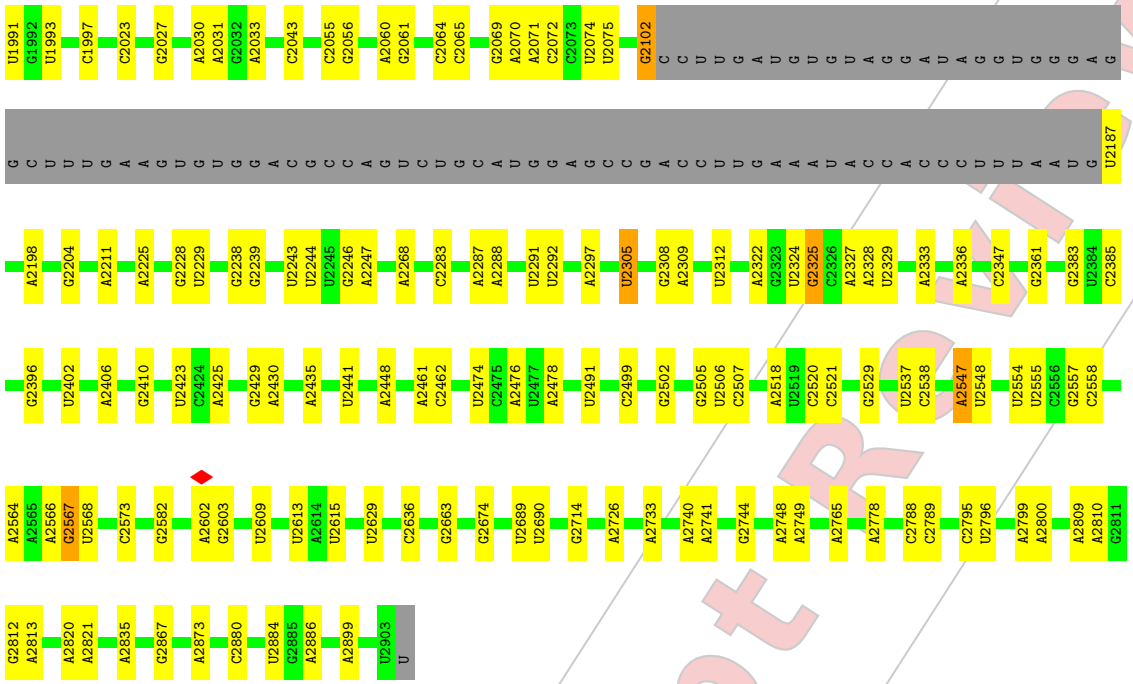


• Molecule 2: 5S rRNA

Chain 1:

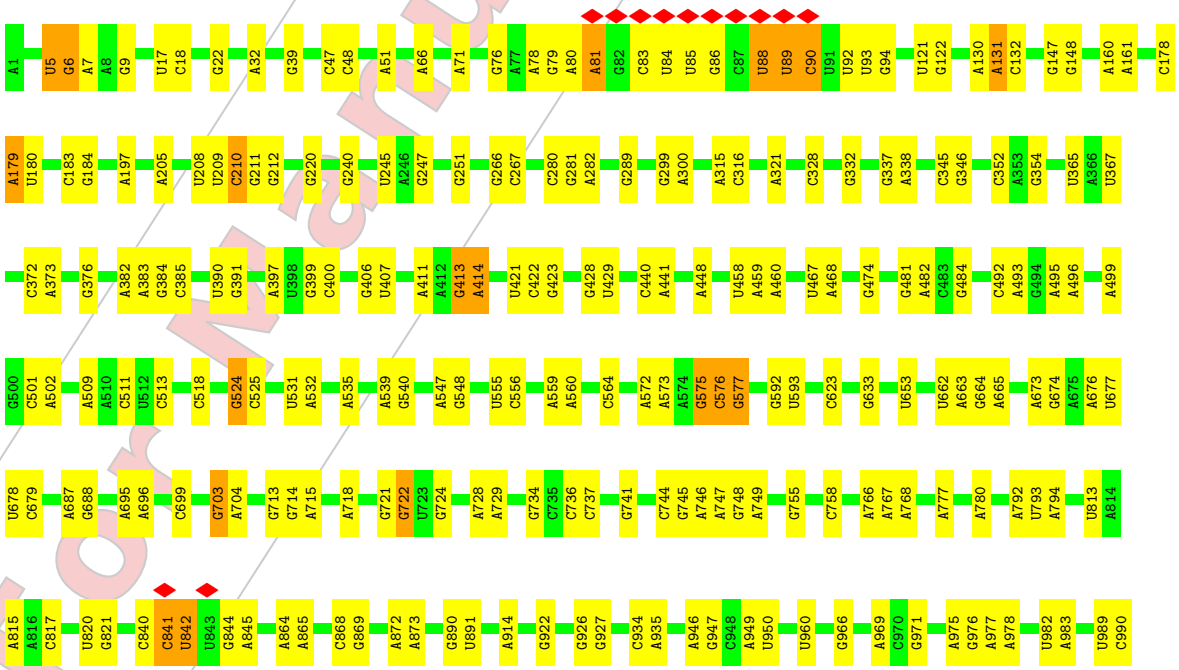




• Molecule 3: 16S rRNA

Chain 2:





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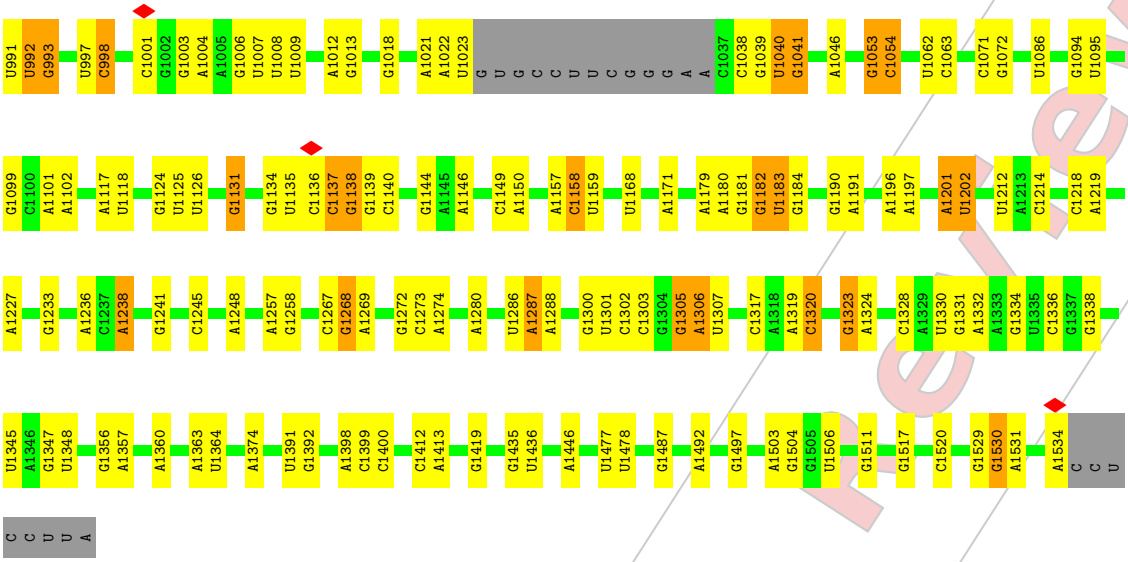
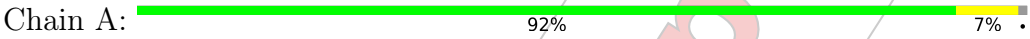
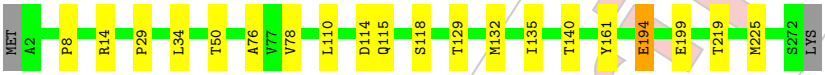


• Molecule 4: Large ribosomal subunit protein uL2





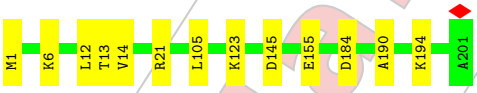
• Molecule 5: Large ribosomal subunit protein uL3



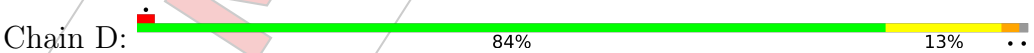


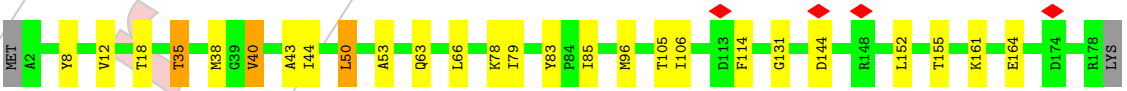
• Molecule 6: 50S ribosomal protein L4



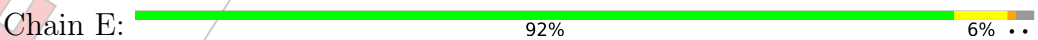


• Molecule 7: Large ribosomal subunit protein uL5





• Molecule 8: Large ribosomal subunit protein uL6



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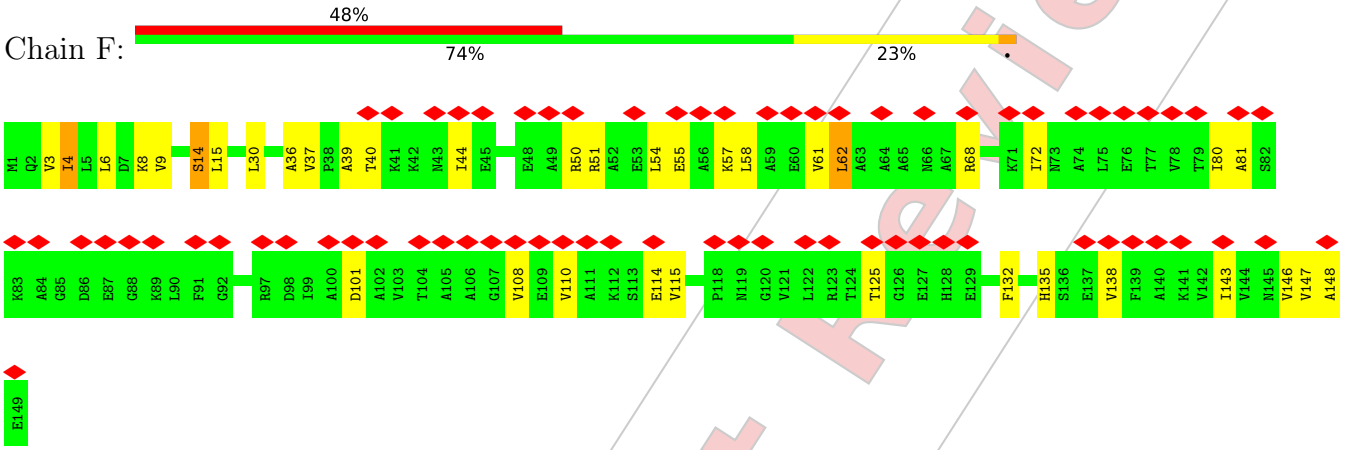
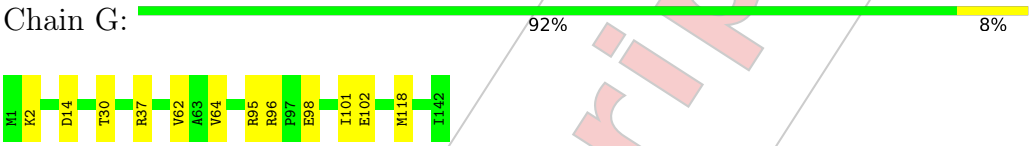
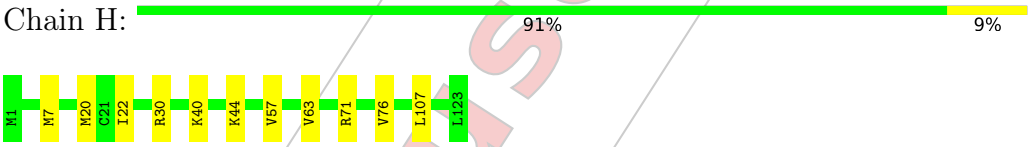
• Molecule 9: 50S ribosomal protein L9



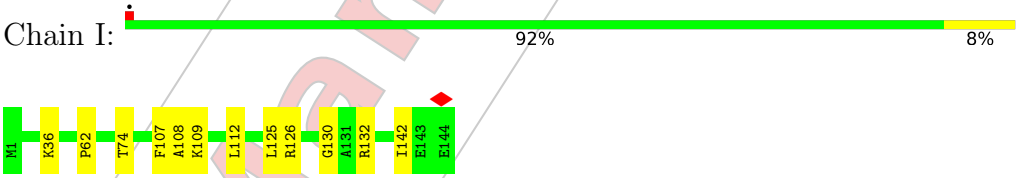
• Molecule 10: 50S ribosomal protein L13



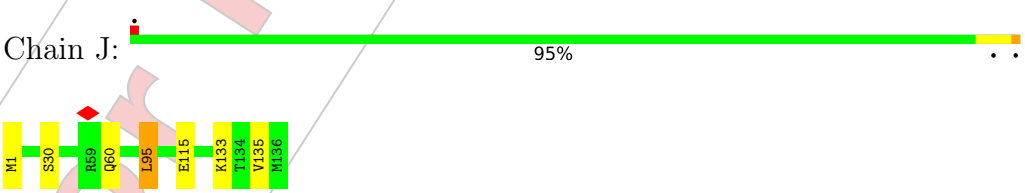
• Molecule 11: 50S ribosomal protein L14



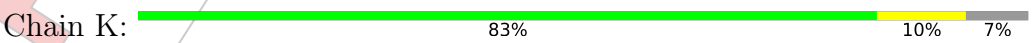
• Molecule 12: 50S ribosomal protein L15



• Molecule 13: 50S ribosomal protein L16



• Molecule 14: Large ribosomal subunit protein bL17



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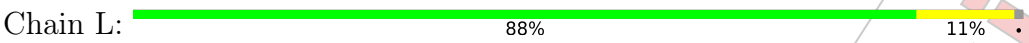
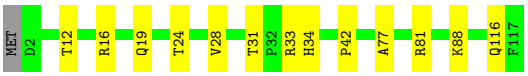
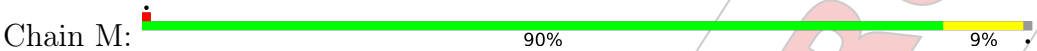
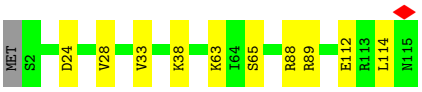
• Molecule 15: Large ribosomal subunit protein uL18





• Molecule 16: Large ribosomal subunit protein bL19





• Molecule 17: Large ribosomal subunit protein bL20





• Molecule 18: 50S ribosomal protein L21



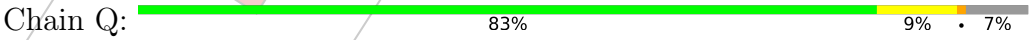


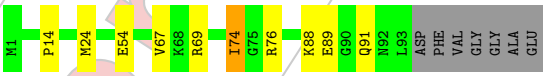
• Molecule 19: 50S ribosomal protein L22



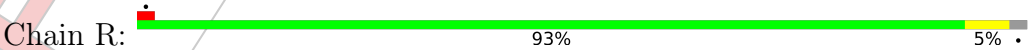


• Molecule 20: Large ribosomal subunit protein uL23





• Molecule 21: 50S ribosomal protein L24



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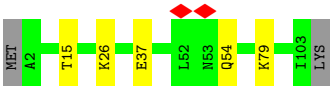


• Molecule 22: 50S ribosomal protein L25

Chain S:

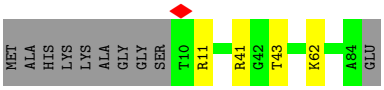




• Molecule 23: Large ribosomal subunit protein bL27

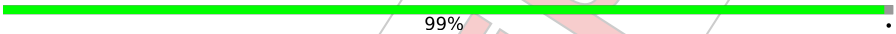
Chain T:





• Molecule 24: Large ribosomal subunit protein bL28

Chain U:





• Molecule 25: Large ribosomal subunit protein uL29

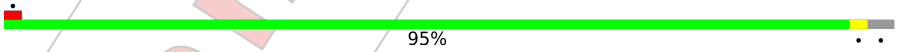
Chain V:

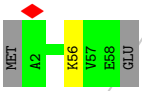




• Molecule 26: Large ribosomal subunit protein uL30

Chain W:

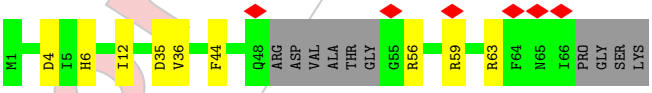




• Molecule 27: 50S ribosomal protein L31

Chain X:





• Molecule 28: RlmH

Chain Y:



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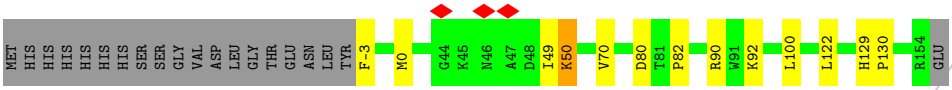
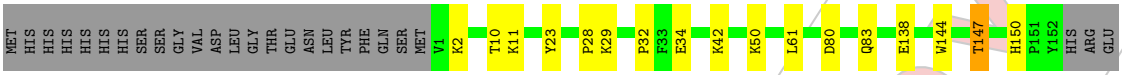
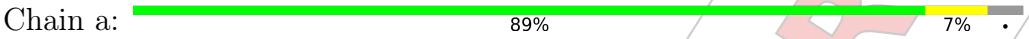


• Molecule 28: RlmH



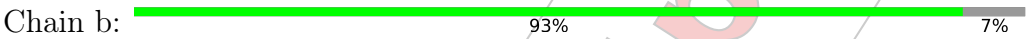


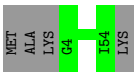
• Molecule 29: Large ribosomal subunit protein bL32



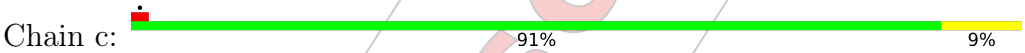


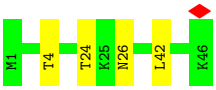
• Molecule 30: Large ribosomal subunit protein bL33



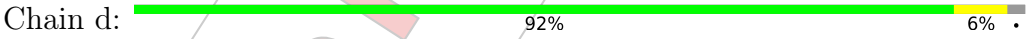


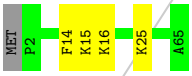
• Molecule 31: 50S ribosomal protein L34



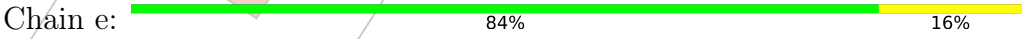


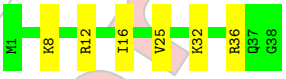
• Molecule 32: Large ribosomal subunit protein bL35





• Molecule 33: 50S ribosomal protein L36





• Molecule 34: 30S ribosomal protein S2



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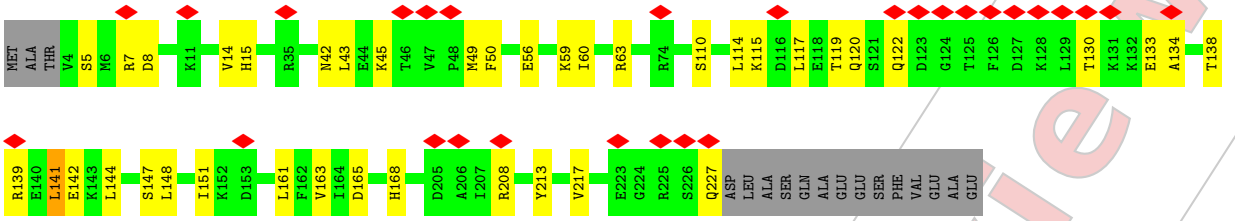
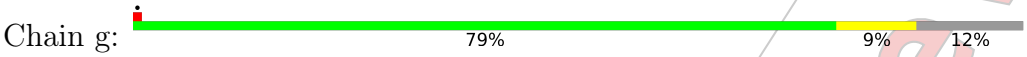
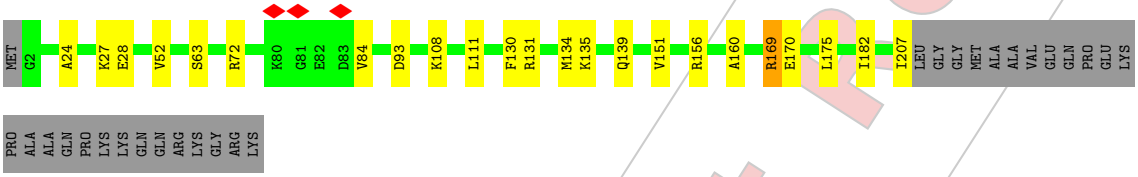
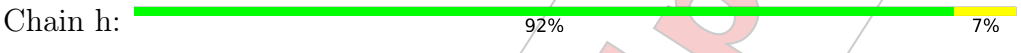


• Molecule 35: 30S ribosomal protein S3



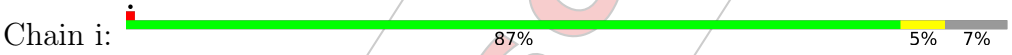


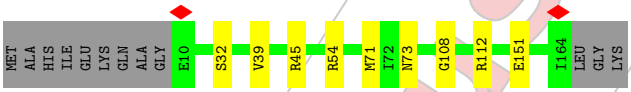
• Molecule 36: 30S ribosomal protein S4





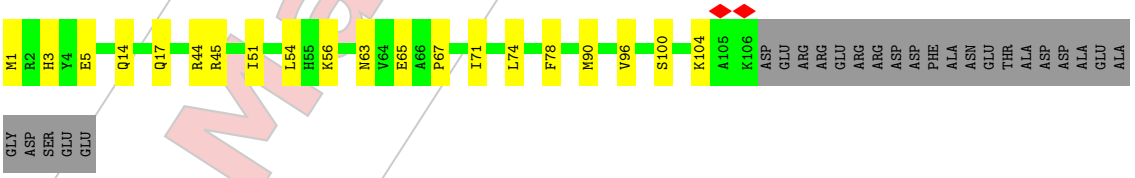
• Molecule 37: 30S ribosomal protein S5





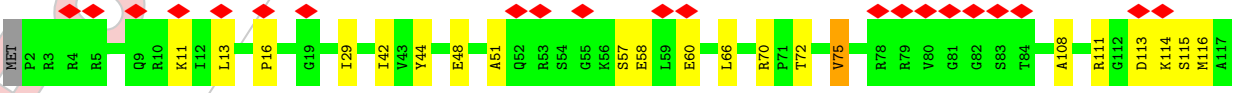
• Molecule 38: Small ribosomal subunit protein bS6, non-modified isoform





• Molecule 39: 30S ribosomal protein S7





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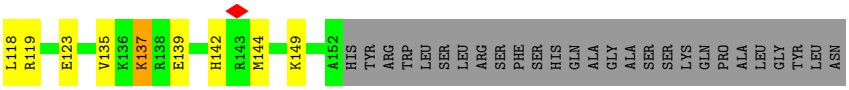


• Molecule 40: 30S ribosomal protein S8

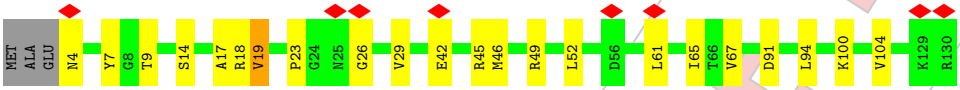
Chain l:



• Molecule 41: 30S ribosomal protein S9

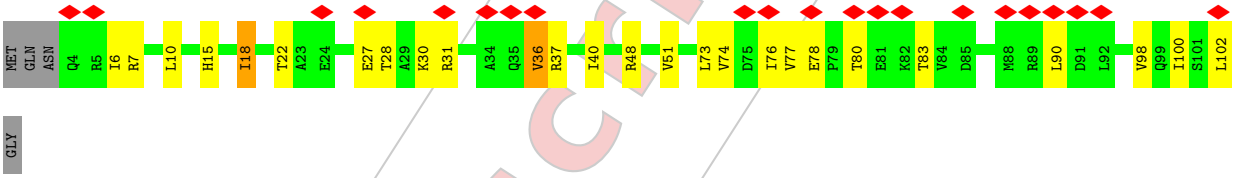
Chain m:





• Molecule 42: 30S ribosomal protein S10

Chain n:



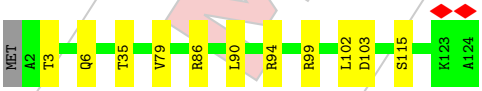
• Molecule 43: Small ribosomal subunit protein uS11

Chain o:



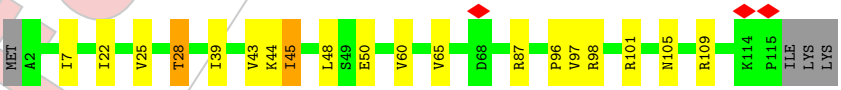
• Molecule 44: Small ribosomal subunit protein uS12

Chain p:



• Molecule 45: 30S ribosomal protein S13

Chain q:



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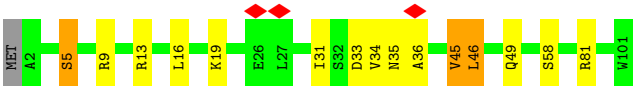
• Molecule 46: 30S ribosomal protein S14

Chain r:

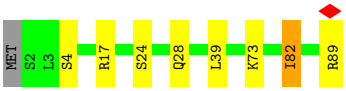




• Molecule 47: 30S ribosomal protein S15

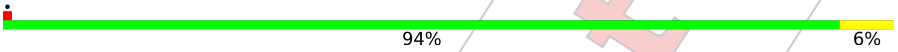
Chain s:

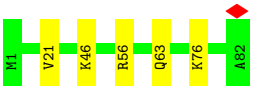




• Molecule 48: 30S ribosomal protein S16

Chain t:

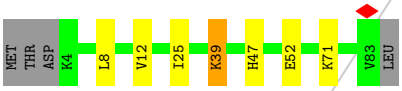




• Molecule 49: 30S ribosomal protein S17

Chain u:





• Molecule 50: 30S ribosomal protein S18

Chain v:

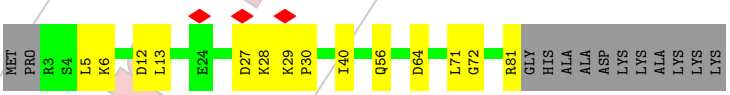




• Molecule 51: 30S ribosomal protein S19

Chain w:





• Molecule 52: 30S ribosomal protein S20

Chain x:



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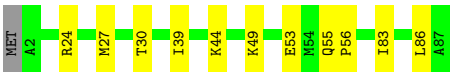
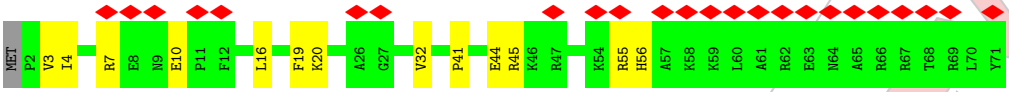


• Molecule 53: 30S ribosomal protein S21

Chain y:





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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76720	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.618	Depositor
Minimum map value	-0.190	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	465.6, 465.6, 465.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

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5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH

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	0.26	0/66069	0.35	0/103071
2	1	0.21	0/2869	0.29	0/4474
3	2	0.21	0/36546	0.34	0/57010
4	A	0.23	0/2121	0.37	0/2852
5	B	0.21	0/1580	0.35	0/2127
6	C	0.19	0/1571	0.36	0/2113
7	D	0.18	0/1434	0.38	0/1926
8	E	0.17	0/1315	0.35	0/1783
9	F	0.16	0/1122	0.43	0/1515
10	G	0.21	0/1152	0.32	0/1551
11	H	0.21	0/956	0.37	0/1279
12	I	0.21	0/1062	0.33	0/1413
13	J	0.23	0/1093	0.39	0/1460
14	K	0.22	0/958	0.37	0/1281
15	L	0.19	0/902	0.38	0/1209
16	M	0.21	0/929	0.32	0/1242
17	N	0.24	0/960	0.34	0/1278
18	O	0.20	0/829	0.35	0/1107
19	P	0.20	0/864	0.33	0/1156
20	Q	0.20	0/744	0.39	0/994
21	R	0.18	0/787	0.31	0/1051
22	S	0.21	0/766	0.43	0/1025
23	T	0.23	0/579	0.37	0/767
24	U	0.20	0/635	0.31	0/848
25	V	0.20	0/492	0.37	0/655
26	W	0.20	0/443	0.30	0/593
27	X	0.15	0/488	0.42	0/649
28	Y	0.20	0/1276	0.38	0/1732
28	Z	0.20	0/1219	0.38	0/1657
29	a	0.21	0/440	0.31	0/588
30	b	0.19	0/424	0.37	0/565
31	c	0.22	0/380	0.32	0/498

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Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	d	0.24	0/513	0.41	0/676
33	e	0.22	0/303	0.29	0/397
34	f	0.17	0/1784	0.42	0/2403
35	g	0.17	0/1651	0.36	0/2225
36	h	0.18	0/1665	0.34	0/2227
37	i	0.20	0/1157	0.38	0/1557
38	j	0.19	0/881	0.43	0/1189
39	k	0.14	0/1195	0.35	0/1602
40	l	0.20	0/989	0.36	0/1326
41	m	0.19	0/1034	0.45	0/1375
42	n	0.19	0/805	0.50	0/1089
43	o	0.21	0/893	0.42	0/1205
44	p	0.20	0/969	0.38	0/1300
45	q	0.15	0/892	0.33	0/1193
46	r	0.17	0/817	0.35	0/1088
47	s	0.20	0/722	0.38	0/964
48	t	0.19	0/659	0.35	0/884
49	u	0.19	0/657	0.41	0/881
50	v	0.18	0/553	0.33	0/742
51	w	0.17	0/652	0.42	0/877
52	x	0.23	0/676	0.37	0/895
53	y	0.16	0/598	0.33	0/792
All	All	0.23	0/153070	0.35	0/228356

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	0	58988	0	29672	113	0
2	1	2566	0	1302	6	0
3	2	32638	0	16425	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2082	0	2154	9	0
5	B	1559	0	1611	4	0
6	C	1552	0	1619	8	0
7	D	1410	0	1444	18	0
8	E	1295	0	1332	7	0
9	F	1111	0	1148	24	0
10	G	1129	0	1162	7	0
11	H	947	0	1023	7	0
12	I	1053	0	1129	7	0
13	J	1074	0	1157	3	0
14	K	945	0	989	6	0
15	L	892	0	923	8	0
16	M	917	0	962	5	0
17	N	947	0	1019	2	0
18	O	816	0	839	3	0
19	P	857	0	922	0	0
20	Q	738	0	807	7	0
21	R	779	0	831	2	0
22	S	753	0	780	5	0
23	T	572	0	593	3	0
24	U	625	0	652	0	0
25	V	491	0	523	4	0
26	W	439	0	482	1	0
27	X	480	0	482	7	0
28	Y	1245	0	1274	8	0
28	Z	1190	0	1223	11	0
29	a	434	0	445	2	0
30	b	417	0	451	0	0
31	c	377	0	418	2	0
32	d	504	0	572	2	0
33	e	302	0	343	4	0
34	f	1753	0	1780	24	0
35	g	1624	0	1696	11	0
36	h	1643	0	1707	5	0
37	i	1144	0	1185	5	0
38	j	862	0	864	10	0
39	k	1181	0	1238	19	0
40	l	979	0	1031	5	0
41	m	1022	0	1070	11	0
42	n	795	0	836	19	0
43	o	877	0	887	7	0
44	p	955	0	1016	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	q	883	0	941	14	0
46	r	805	0	844	12	0
47	s	714	0	734	6	0
48	t	649	0	666	3	0
49	u	648	0	691	3	0
50	v	544	0	565	1	0
51	w	637	0	665	15	0
52	x	670	0	719	6	0
53	y	590	0	629	9	0
54	Y	26	0	19	4	0
54	Z	26	0	19	2	0
All	All	141151	0	96510	577	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 (577) 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)
39:k:16:PRO:HA	41:m:46:MET:HE1	1.50	0.93
3:2:1013:G:H21	3:2:1219:A:H1'	1.45	0.81
3:2:688:G:H1	3:2:699:C:H5	1.29	0.80
54:Y:201:SAH:HB2	54:Y:201:SAH:H3'	1.63	0.79
1:0:2796:U:H3	1:0:2799:A:H61	1.31	0.78
7:D:105:THR:HG22	7:D:106:ILE:HG13	1.72	0.72
34:f:49:MET:HE3	34:f:49:MET:HA	1.70	0.72
3:2:1038:C:H2'	3:2:1039:G:H8	1.54	0.72
3:2:1303:C:H5	3:2:1334:G:H1	1.37	0.70
3:2:673:A:H2'	3:2:674:G:C8	2.25	0.70
28:Z:2:LYS:HG2	28:Z:32:PRO:HG2	1.74	0.70
1:0:2324:U:H3'	1:0:2325:G:H5"	1.72	0.70
9:F:8:LYS:HD2	9:F:14:SER:HB3	1.73	0.69
3:2:1182:G:H4'	3:2:1183:U:H5'	1.75	0.69
54:Z:201:SAH:H3'	54:Z:201:SAH:HN1	1.58	0.68
3:2:1158:C:H5	3:2:1181:G:H1	1.42	0.68
39:k:113:ASP:HB3	39:k:118:LEU:HD23	1.76	0.68
3:2:767:A:H8	3:2:1511:G:H21	1.42	0.67
46:r:46:LEU:HD23	51:w:13:LEU:HD13	1.75	0.67
3:2:1008:U:H3	3:2:1021:A:H2	1.40	0.66
3:2:1009:U:H3	3:2:1018:G:H22	1.40	0.66
9:F:3:VAL:HG21	9:F:36:ALA:HB1	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:w:29:LYS:HD3	51:w:30:PRO:HD2	1.78	0.66
54:Y:201:SAH:HB2	54:Y:201:SAH:C3'	2.27	0.65
42:n:40:ILE:HD13	42:n:73:LEU:HD23	1.78	0.65
1:0:284:U:H3	1:0:356:G:H1	1.44	0.64
3:2:1086:U:H3	3:2:1099:G:H22	1.46	0.64
3:2:1038:C:H2'	3:2:1039:G:C8	2.33	0.64
42:n:30:LYS:HB2	42:n:31:ARG:HH12	1.64	0.63
15:L:31:THR:HG23	15:L:33:ARG:H	1.63	0.63
3:2:1323:G:H2'	3:2:1324:A:C8	2.34	0.63
34:f:208:ARG:H	34:f:208:ARG:HD3	1.62	0.63
10:G:95:ARG:CZ	10:G:96:ARG:HH12	2.12	0.63
42:n:6:ILE:HD11	42:n:100:ILE:HG23	1.80	0.62
34:f:117:LEU:HB3	34:f:141:LEU:HD12	1.81	0.62
5:B:56:LYS:HD2	5:B:59:ARG:HG3	1.82	0.62
2:1:1:U:H2'	2:1:2:G:H8	1.62	0.62
47:s:73:LYS:HA	47:s:73:LYS:HE2	1.82	0.61
1:0:1869:G:H21	1:0:1872:A:H2	1.48	0.61
31:c:24:THR:HG22	31:c:26:ASN:H	1.64	0.61
35:g:72:ARG:HG3	35:g:72:ARG:HH11	1.65	0.61
34:f:148:LEU:HD12	34:f:151:ILE:HD11	1.81	0.61
1:0:981:A:H8	1:0:2027:G:H21	1.48	0.61
3:2:458:U:H2'	3:2:459:A:H8	1.65	0.61
20:Q:14:PRO:HD3	25:V:30:MET:HE2	1.83	0.61
1:0:1469:A:H2'	1:0:1470:A:C8	2.35	0.60
52:x:39:ILE:HD11	52:x:83:ILE:HG13	1.83	0.60
1:0:2102:G:O6	1:0:2187:U:O2	2.19	0.60
35:g:135:LYS:O	35:g:139:GLN:HG2	2.01	0.60
42:n:18:ILE:O	42:n:22:THR:HG23	2.02	0.60
1:0:856:G:H2'	1:0:857:G:C8	2.37	0.59
3:2:946:A:H2'	3:2:947:G:C8	2.37	0.59
1:0:1802:A:H2'	1:0:1803:A:C8	2.37	0.59
35:g:108:LYS:HD3	35:g:111:LEU:HD12	1.83	0.59
3:2:459:A:H2'	3:2:460:A:H8	1.67	0.59
5:B:55:LYS:HD3	5:B:60:VAL:HG22	1.85	0.59
3:2:337:G:H2'	3:2:338:A:C8	2.38	0.59
3:2:1040:U:H2'	3:2:1041:G:C8	2.38	0.59
21:R:26:LYS:HD2	21:R:37:GLU:HG3	1.85	0.58
9:F:58:LEU:HD23	9:F:62:LEU:HD23	1.86	0.58
28:Z:80:ASP:OD1	28:Z:83:GLN:HG3	2.03	0.58
3:2:492:C:H2'	3:2:493:A:C8	2.37	0.58
3:2:746:A:H2'	3:2:747:A:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1144:G:N2	3:2:1146:A:H62	2.02	0.58
8:E:44:LYS:HB2	8:E:51:THR:HG22	1.86	0.58
37:i:108:GLY:O	37:i:112:ARG:HG3	2.04	0.58
1:0:45:G:H5'	1:0:46:G:OP1	2.04	0.57
3:2:1040:U:H2'	3:2:1041:G:H8	1.69	0.57
44:p:102:LEU:HD23	44:p:102:LEU:H	1.68	0.57
3:2:946:A:H2'	3:2:947:G:H8	1.68	0.57
3:2:1356:G:H2'	3:2:1357:A:C8	2.40	0.57
3:2:458:U:H2'	3:2:459:A:C8	2.39	0.57
53:y:20:LYS:NZ	53:y:20:LYS:HB3	2.20	0.57
10:G:62:VAL:HG11	10:G:101:ILE:HD11	1.87	0.57
15:L:88:LYS:HD2	15:L:116:GLN:HG3	1.86	0.57
1:0:2521:C:O2'	1:0:2564:A:H8	1.87	0.57
3:2:714:G:H2'	3:2:715:A:C8	2.40	0.57
45:q:87:ARG:HG3	45:q:97:VAL:HG11	1.85	0.57
51:w:28:LYS:N	51:w:28:LYS:HE2	2.19	0.57
3:2:1218:C:H2'	3:2:1219:A:C8	2.39	0.56
28:Z:29:LYS:HE2	28:Z:29:LYS:N	2.21	0.56
51:w:40:ILE:HD11	51:w:71:LEU:HD13	1.86	0.56
1:0:2328:A:H2'	1:0:2329:U:C6	2.40	0.56
3:2:1137:C:H1'	3:2:1138:G:C2	2.41	0.56
1:0:2071:A:H2'	1:0:2072:C:C6	2.41	0.56
3:2:1305:G:H22	3:2:1331:G:H2'	1.71	0.55
41:m:19:VAL:HG13	41:m:65:ILE:HG12	1.87	0.55
9:F:3:VAL:CG2	9:F:36:ALA:HB1	2.36	0.55
28:Y:122:LEU:H	54:Y:201:SAH:C2	2.19	0.55
43:o:83:GLU:HG2	43:o:109:ASN:HB2	1.89	0.55
43:o:87:LYS:HB2	43:o:113:VAL:HG13	1.87	0.55
45:q:43:VAL:HG12	45:q:45:ILE:H	1.71	0.55
3:2:5:U:H4'	3:2:6:G:O5'	2.06	0.55
3:2:147:G:H2'	3:2:148:G:C8	2.41	0.55
9:F:4:ILE:HG23	9:F:39:ALA:HB2	1.89	0.55
13:J:60:GLN:HG3	13:J:60:GLN:O	2.07	0.55
16:M:33:VAL:HG22	16:M:38:LYS:HG2	1.88	0.55
27:X:63:ARG:HH12	51:w:5:LEU:HD22	1.72	0.55
3:2:713:G:H2'	3:2:714:G:C8	2.42	0.54
1:0:1590:A:H2'	1:0:1591:A:H8	1.71	0.54
1:0:2554:U:H2'	1:0:2555:U:O2	2.07	0.54
1:0:639:U:H2'	1:0:640:C:C6	2.42	0.54
3:2:1071:C:H2'	3:2:1072:G:H8	1.72	0.54
46:r:31:ILE:HG12	46:r:45:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1306:A:H61	3:2:1331:G:H1'	1.73	0.54
33:e:12:ARG:HB3	33:e:12:ARG:NH1	2.23	0.54
28:Z:28:PRO:HG2	28:Z:144:TRP:CZ2	2.43	0.54
25:V:30:MET:HE3	25:V:30:MET:HA	1.88	0.54
7:D:43:ALA:HB2	7:D:50:LEU:HD21	1.90	0.54
38:j:45:ARG:O	38:j:56:LYS:HA	2.08	0.54
12:I:112:LEU:HD12	12:I:130:GLY:HA3	1.89	0.54
3:2:1412:C:H2'	3:2:1413:A:C8	2.43	0.53
34:f:134:ALA:O	34:f:138:THR:HG23	2.07	0.53
42:n:27:GLU:O	42:n:31:ARG:HG2	2.08	0.53
42:n:51:VAL:HG13	46:r:81:ARG:HB2	1.90	0.53
9:F:68:ARG:O	9:F:72:ILE:HG22	2.09	0.53
42:n:78:GLU:HG2	42:n:78:GLU:O	2.09	0.53
3:2:1144:G:H21	3:2:1146:A:H62	1.55	0.53
38:j:3:HIS:HD2	38:j:65:GLU:HG2	1.73	0.53
1:0:1728:C:H4'	1:0:1729:U:H5	1.74	0.53
3:2:664:G:H22	3:2:741:G:H1	1.57	0.53
42:n:15:HIS:O	42:n:18:ILE:HG13	2.09	0.53
54:Z:201:SAH:H8	54:Z:201:SAH:H5'1	1.92	0.52
20:Q:67:VAL:HG22	20:Q:76:ARG:HG3	1.92	0.52
34:f:147:SER:HB3	34:f:148:LEU:HD22	1.92	0.52
4:A:199:GLU:CD	4:A:199:GLU:H	2.17	0.52
3:2:459:A:H2'	3:2:460:A:C8	2.44	0.52
3:2:820:U:H5	3:2:873:A:N7	2.07	0.52
7:D:40:VAL:HG21	7:D:50:LEU:HD21	1.91	0.52
1:0:5:A:H2'	1:0:6:A:C8	2.45	0.52
4:A:8:PRO:HB3	4:A:14:ARG:HG3	1.92	0.52
7:D:35:THR:HG23	7:D:155:THR:HB	1.91	0.52
47:s:17:ARG:HG3	47:s:17:ARG:HH11	1.75	0.52
1:0:2305:U:H5"	7:D:131:GLY:HA3	1.91	0.52
1:0:272:A:H2'	1:0:273:G:H8	1.75	0.51
27:X:63:ARG:HH22	51:w:5:LEU:HD22	1.74	0.51
28:Z:50:LYS:NZ	28:Z:50:LYS:HB3	2.26	0.51
42:n:40:ILE:HD12	42:n:40:ILE:H	1.74	0.51
45:q:22:ILE:HB	45:q:25:VAL:HG22	1.92	0.51
51:w:5:LEU:O	51:w:6:LYS:HD2	2.10	0.51
1:0:281:C:H2'	1:0:282:A:H8	1.75	0.51
53:y:41:PRO:HA	53:y:44:GLU:HG2	1.91	0.51
3:2:744:C:H2'	3:2:745:G:H8	1.75	0.51
3:2:1305:G:H1'	3:2:1332:A:N6	2.25	0.51
40:l:11:LEU:HD22	40:l:75:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1141:U:H4'	1:0:1142:A:O4'	2.10	0.51
3:2:949:A:H2	45:q:105:ASN:HD21	1.58	0.51
1:0:479:A:N3	1:0:481:G:H5"	2.25	0.51
34:f:213:TYR:O	34:f:217:VAL:HG22	2.10	0.51
45:q:45:ILE:HA	45:q:48:LEU:HG	1.93	0.51
3:2:841:C:H3'	3:2:842:U:H4'	1.92	0.51
34:f:115:LYS:O	34:f:119:THR:HG23	2.10	0.51
1:0:947:A:H2'	1:0:948:C:C6	2.46	0.51
3:2:728:A:H2'	3:2:729:A:C8	2.46	0.51
3:2:1287:A:H2'	3:2:1288:A:C8	2.46	0.51
52:x:24:ARG:HH21	52:x:27:MET:HE2	1.76	0.51
1:0:191:A:H2'	1:0:192:C:C6	2.46	0.50
1:0:281:C:H2'	1:0:282:A:C8	2.46	0.50
1:0:1746:A:H2'	1:0:1747:U:C6	2.46	0.50
8:E:52:PHE:CE1	8:E:72:LEU:HD12	2.46	0.50
9:F:50:ARG:NE	9:F:51:ARG:HB2	2.26	0.50
3:2:524:G:H2'	3:2:525:C:C6	2.46	0.50
3:2:413:G:H4'	3:2:414:A:H5"	1.94	0.50
46:r:33:ASP:HB3	46:r:36:ALA:HB2	1.92	0.50
1:0:593:U:H2'	1:0:594:U:C6	2.46	0.50
1:0:1433:A:O2'	1:0:1434:A:H5'	2.11	0.50
6:C:123:LYS:NZ	6:C:123:LYS:HB3	2.26	0.50
41:m:42:GLU:H	41:m:42:GLU:CD	2.19	0.50
1:0:2291:U:H2'	1:0:2292:U:C6	2.47	0.50
7:D:8:TYR:HA	7:D:12:VAL:HG12	1.94	0.50
22:S:55:GLU:O	22:S:59:GLU:HG3	2.12	0.50
43:o:89:PRO:HG3	53:y:32:VAL:HG11	1.93	0.50
53:y:55:ARG:HG3	53:y:56:HIS:N	2.25	0.50
9:F:51:ARG:HH11	9:F:55:GLU:HG2	1.77	0.50
1:0:2246:G:H2'	1:0:2247:A:C8	2.47	0.50
3:2:337:G:H2'	3:2:338:A:H8	1.76	0.50
7:D:114:PHE:HE2	27:X:44:PHE:HE1	1.59	0.50
38:j:5:GLU:HG3	38:j:63:ASN:ND2	2.26	0.50
1:0:2327:A:H2'	1:0:2328:A:C8	2.47	0.50
3:2:950:U:H5"	45:q:101:ARG:HH21	1.77	0.50
9:F:6:LEU:HD11	9:F:37:VAL:HG23	1.92	0.50
10:G:37:ARG:HA	10:G:118:MET:HE3	1.94	0.50
14:K:37:THR:HG22	14:K:39:PRO:HD2	1.92	0.50
16:M:63:LYS:HE2	16:M:65:SER:HB2	1.94	0.50
42:n:6:ILE:HD12	42:n:7:ARG:H	1.77	0.50
1:0:275:C:H2'	1:0:276:U:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:411:A:C4	3:2:413:G:H1'	2.47	0.49
6:C:1:MET:HG3	6:C:14:VAL:HG23	1.93	0.49
12:I:108:ALA:HB3	12:I:125:LEU:HD22	1.93	0.49
41:m:46:MET:HA	41:m:49:ARG:HG2	1.93	0.49
4:A:29:PRO:HG2	4:A:34:LEU:HD11	1.94	0.49
39:k:51:ALA:HB2	39:k:58:GLU:HG3	1.94	0.49
50:v:16:GLU:HG2	50:v:18:VAL:HG22	1.93	0.49
1:0:272:A:H2'	1:0:273:G:C8	2.47	0.49
1:0:639:U:H2'	1:0:640:C:H6	1.76	0.49
39:k:72:THR:HG22	39:k:142:HIS:NE2	2.27	0.49
6:C:145:ASP:HB3	6:C:184:ASP:HB2	1.94	0.49
15:L:77:ALA:O	15:L:81:ARG:HG3	2.11	0.49
1:0:1590:A:H2'	1:0:1591:A:C8	2.48	0.49
9:F:125:THR:HA	9:F:146:VAL:HG13	1.94	0.49
38:j:67:PRO:O	38:j:71:ILE:HG12	2.13	0.49
20:Q:69:ARG:HH12	20:Q:74:ILE:HD11	1.76	0.49
34:f:45:LYS:HB3	34:f:50:PHE:CE1	2.47	0.49
35:g:131:ARG:O	35:g:135:LYS:HG2	2.13	0.49
38:j:1:MET:HE1	38:j:67:PRO:HD3	1.93	0.49
3:2:1201:A:H4'	3:2:1202:U:H5'	1.95	0.49
49:u:8:LEU:HD21	49:u:25:ILE:HG21	1.95	0.49
28:Z:23:TYR:CE1	28:Z:138:GLU:HG2	2.48	0.48
3:2:17:U:H2'	3:2:18:C:C6	2.48	0.48
3:2:992:U:H4'	3:2:993:G:O5'	2.13	0.48
3:2:1218:C:H2'	3:2:1219:A:H8	1.77	0.48
3:2:745:G:H2'	3:2:746:A:C8	2.48	0.48
39:k:57:SER:HB3	39:k:60:GLU:HG2	1.95	0.48
44:p:79:VAL:O	44:p:103:ASP:HB2	2.13	0.48
46:r:9:ARG:O	46:r:13:ARG:HG3	2.13	0.48
8:E:54:PRO:HB3	8:E:61:GLY:HA3	1.95	0.48
1:0:2228:G:H2'	1:0:2229:U:C6	2.48	0.48
35:g:130:PHE:HD2	35:g:134:MET:HE2	1.79	0.48
28:Y:70:VAL:HB	28:Y:100:LEU:HD23	1.96	0.48
52:x:49:LYS:O	52:x:53:GLU:HG2	2.13	0.48
1:0:280:U:H2'	1:0:281:C:C6	2.49	0.48
2:1:1:U:H2'	2:1:2:G:C8	2.45	0.48
4:A:161:TYR:HB3	4:A:194:GLU:HB3	1.96	0.48
14:K:24:MET:HG2	14:K:44:LEU:HD13	1.95	0.48
28:Z:2:LYS:NZ	28:Z:2:LYS:HB3	2.28	0.48
1:0:2788:C:H2'	1:0:2789:C:C6	2.48	0.48
3:2:382:A:H2'	3:2:383:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2336:A:H61	23:T:43:THR:HG21	1.79	0.48
1:0:1000:A:H2'	1:0:1001:A:C8	2.49	0.47
3:2:745:G:H2'	3:2:746:A:H8	1.79	0.47
1:0:1952:A:C6	11:H:22:ILE:HD12	2.50	0.47
3:2:208:U:H2'	3:2:210:C:H5	1.79	0.47
3:2:539:A:H2'	3:2:540:G:C8	2.50	0.47
3:2:1268:G:H2'	3:2:1269:A:C8	2.49	0.47
42:n:77:VAL:HG23	42:n:78:GLU:H	1.79	0.47
2:1:66:A:H61	2:1:107:G:H2'	1.79	0.47
25:V:5:GLU:H	25:V:5:GLU:CD	2.22	0.47
42:n:36:VAL:HG23	42:n:76:ILE:HG13	1.96	0.47
23:T:41:ARG:HA	23:T:41:ARG:HD3	1.69	0.47
37:i:54:ARG:HG3	37:i:54:ARG:HH11	1.78	0.47
1:0:1589:U:H2'	1:0:1590:A:H8	1.80	0.47
1:0:3:U:H2'	1:0:4:U:C6	2.50	0.47
1:0:581:C:H2'	1:0:582:A:C8	2.49	0.47
1:0:1506:U:H2'	1:0:1507:C:H6	1.78	0.47
3:2:780:A:H5"	43:o:125:LYS:HD3	1.96	0.47
4:A:118:SER:HB2	4:A:129:THR:HB	1.96	0.47
20:Q:89:GLU:CD	20:Q:89:GLU:H	2.23	0.47
40:l:50:LYS:HD2	40:l:52:GLU:OE2	2.14	0.47
29:a:54:VAL:HG23	29:a:55:ILE:HG12	1.97	0.47
39:k:135:VAL:O	39:k:139:GLU:HG2	2.15	0.47
1:0:608:A:H2'	1:0:609:A:C8	2.49	0.47
1:0:2547:A:H2'	1:0:2548:U:C6	2.49	0.47
12:I:109:LYS:HG2	12:I:126:ARG:HB2	1.97	0.47
1:0:2102:G:O6	1:0:2187:U:C2	2.68	0.47
6:C:190:ALA:O	6:C:194:LYS:HG2	2.15	0.47
15:L:16:ARG:NH1	15:L:16:ARG:HG2	2.30	0.46
3:2:1530:G:H2'	3:2:1531:A:C8	2.50	0.46
12:I:132:ARG:HG3	12:I:142:ILE:HD13	1.95	0.46
37:i:151:GLU:OE1	37:i:151:GLU:N	2.47	0.46
14:K:103:ARG:HD2	14:K:106:ASP:OD1	2.15	0.46
20:Q:24:MET:O	20:Q:24:MET:HE3	2.15	0.46
23:T:11:ARG:HD3	23:T:11:ARG:HA	1.72	0.46
53:y:4:ILE:HG13	53:y:19:PHE:HA	1.96	0.46
3:2:299:G:H2'	3:2:300:A:C8	2.50	0.46
3:2:575:G:H4'	3:2:576:C:O5'	2.15	0.46
39:k:44:TYR:O	39:k:48:GLU:HG2	2.16	0.46
46:r:49:GLN:HE22	51:w:12:ASP:CB	2.28	0.46
3:2:160:A:H2'	3:2:161:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:26:ASP:C	18:O:27:ILE:HD13	2.40	0.46
22:S:30:ILE:HG12	22:S:91:PHE:HB2	1.97	0.46
27:X:63:ARG:HH12	51:w:5:LEU:CD2	2.28	0.46
39:k:75:VAL:HG11	39:k:144:MET:HE1	1.97	0.46
1:0:2243:U:H2'	1:0:2244:U:C6	2.51	0.46
28:Y:50:LYS:HE2	28:Y:50:LYS:HB2	1.64	0.46
36:h:87:GLY:HA3	36:h:197:GLU:HG3	1.98	0.46
1:0:1353:A:H2'	1:0:1354:A:C8	2.51	0.46
42:n:48:ARG:HG2	42:n:48:ARG:HH11	1.81	0.46
1:0:851:C:H2'	1:0:852:U:H6	1.81	0.46
3:2:722:G:H2'	3:2:722:G:N3	2.30	0.46
3:2:1134:G:H2'	3:2:1135:U:O4'	2.16	0.46
43:o:67:ALA:HB2	43:o:96:THR:HG23	1.97	0.46
1:0:2228:G:H2'	1:0:2229:U:H6	1.81	0.46
3:2:131:A:H2'	3:2:132:C:C6	2.51	0.45
35:g:175:LEU:HD23	35:g:182:ILE:HD13	1.98	0.45
3:2:662:U:H2'	3:2:663:A:C8	2.52	0.45
45:q:87:ARG:HG3	45:q:97:VAL:CG1	2.46	0.45
45:q:96:PRO:HA	45:q:109:ARG:HD3	1.98	0.45
1:0:2478:A:H5'	33:e:32:LYS:HE2	1.98	0.45
12:I:36:LYS:H	12:I:36:LYS:HG3	1.57	0.45
1:0:1469:A:H2'	1:0:1470:A:H8	1.78	0.45
26:W:56:LYS:HE2	26:W:56:LYS:HB3	1.55	0.45
1:0:848:C:H2'	1:0:849:A:C8	2.51	0.45
1:0:1539:U:H2'	1:0:1540:G:H8	1.81	0.45
3:2:1272:G:H2'	3:2:1273:C:C6	2.51	0.45
11:H:20:MET:HE3	11:H:44:LYS:HE3	1.97	0.45
52:x:27:MET:O	52:x:30:THR:HG22	2.17	0.45
3:2:1306:A:H3'	3:2:1307:U:O2	2.16	0.45
10:G:98:GLU:O	10:G:102:GLU:HG3	2.17	0.45
16:M:24:ASP:HB2	16:M:88:ARG:O	2.17	0.45
28:Y:90:ARG:NH1	28:Y:90:ARG:HB3	2.32	0.45
40:l:89:LYS:HD3	40:l:120:GLY:HA2	1.99	0.45
8:E:52:PHE:HE1	8:E:72:LEU:HD12	1.82	0.45
15:L:16:ARG:HG2	15:L:16:ARG:HH11	1.80	0.45
16:M:112:GLU:HG2	16:M:114:LEU:HG	1.98	0.45
41:m:23:PRO:HA	41:m:61:LEU:HD13	1.98	0.45
41:m:26:GLY:HA2	41:m:61:LEU:O	2.16	0.45
3:2:676:A:H2'	3:2:677:U:H6	1.82	0.45
3:2:1360:A:C8	46:r:58:SER:HB2	2.52	0.45
51:w:71:LEU:H	51:w:71:LEU:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:64:A:H2'	1:0:65:U:C6	2.52	0.45
1:0:581:C:H2'	1:0:582:A:H8	1.82	0.45
1:0:1847:A:O2'	1:0:1848:A:C8	2.70	0.45
1:0:2557:G:H2'	1:0:2558:C:C6	2.51	0.45
3:2:178:C:H2'	3:2:179:A:H5"	1.99	0.45
42:n:10:LEU:HD12	42:n:22:THR:HG22	1.99	0.45
1:0:849:A:H2'	1:0:850:U:C6	2.52	0.45
1:0:2674:G:H4'	11:H:30:ARG:HD2	1.98	0.45
3:2:592:G:H2'	3:2:593:U:C6	2.52	0.45
3:2:1391:U:H2'	3:2:1392:G:C8	2.52	0.45
20:Q:54:GLU:HB3	20:Q:88:LYS:HG3	1.98	0.45
48:t:56:ARG:HA	48:t:56:ARG:HD2	1.59	0.45
3:2:81:A:N6	3:2:88:U:H3	2.16	0.44
3:2:1238:A:H2	3:2:1241:G:N3	2.15	0.44
1:0:2064:C:H2'	1:0:2065:C:C6	2.52	0.44
7:D:78:LYS:HD2	7:D:78:LYS:N	2.32	0.44
9:F:50:ARG:CZ	9:F:51:ARG:HB2	2.46	0.44
53:y:44:GLU:HG3	53:y:45:ARG:N	2.31	0.44
1:0:150:U:H2'	1:0:151:C:C6	2.52	0.44
1:0:1548:A:H2'	1:0:1549:A:C8	2.53	0.44
1:0:2812:G:H2'	1:0:2813:A:C8	2.52	0.44
3:2:407:U:O2'	36:h:113:GLU:HG2	2.16	0.44
3:2:1477:U:H2'	3:2:1478:U:C6	2.52	0.44
34:f:114:LEU:HD13	34:f:144:LEU:HB3	1.99	0.44
34:f:139:ARG:CZ	34:f:139:ARG:HA	2.47	0.44
46:r:5:SER:O	46:r:9:ARG:HG3	2.17	0.44
1:0:634:C:H2'	1:0:635:C:C6	2.51	0.44
1:0:2030:A:C2	1:0:2499:C:H5"	2.53	0.44
5:B:32:ASN:N	5:B:32:ASN:HD22	2.15	0.44
9:F:58:LEU:O	9:F:61:VAL:HG12	2.18	0.44
15:L:24:THR:HG22	15:L:42:PRO:HD3	1.98	0.44
28:Y:80:ASP:OD1	28:Y:82:PRO:HD2	2.18	0.44
1:0:2740:A:H2'	1:0:2741:A:C8	2.52	0.44
39:k:108:ALA:HA	39:k:123:GLU:HG3	2.00	0.44
40:l:47:GLU:HG2	40:l:64:LYS:HG2	1.99	0.44
3:2:1131:G:H2'	3:2:1131:G:N3	2.32	0.44
1:0:274:C:C5	1:0:275:C:N3	2.86	0.44
1:0:2074:U:H2'	1:0:2075:U:C6	2.52	0.44
32:d:14:PHE:O	32:d:15:LYS:HD3	2.18	0.44
39:k:111:ARG:HB2	39:k:119:ARG:HG2	2.00	0.44
44:p:3:THR:OG1	44:p:6:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:60:VAL:HG13	45:q:65:VAL:HG21	1.99	0.44
1:0:1149:G:H2'	1:0:1150:C:C6	2.52	0.44
6:C:6:LYS:HE3	6:C:6:LYS:HB2	1.85	0.44
11:H:7:MET:SD	11:H:20:MET:HG3	2.57	0.44
1:0:554:U:H2'	1:0:555:G:O4'	2.18	0.44
1:0:645:C:H2'	1:0:647:G:N7	2.33	0.44
6:C:12:LEU:HD12	6:C:13:THR:N	2.32	0.44
9:F:62:LEU:HA	9:F:62:LEU:HD13	1.77	0.44
36:h:124:MET:HE3	36:h:124:MET:HB3	1.78	0.44
39:k:11:LYS:HZ1	39:k:13:LEU:HA	1.83	0.44
39:k:116:MET:HA	39:k:119:ARG:HE	1.83	0.44
39:k:137:LYS:HE3	39:k:137:LYS:HB3	1.85	0.44
43:o:72:ASP:OD1	43:o:72:ASP:C	2.60	0.44
1:0:1005:C:O2'	10:G:30:THR:HG21	2.18	0.43
1:0:2246:G:H2'	1:0:2247:A:H8	1.82	0.43
35:g:24:ALA:HB1	35:g:28:GLU:HG2	1.99	0.43
1:0:782:A:N1	4:A:225:MET:HE2	2.33	0.43
1:0:1496:A:H2'	1:0:1498:C:C5	2.53	0.43
1:0:2809:A:H2'	1:0:2810:A:C8	2.53	0.43
9:F:147:VAL:HG13	9:F:148:ALA:O	2.18	0.43
13:J:30:SER:HA	13:J:133:LYS:HE3	1.99	0.43
15:L:31:THR:HG22	15:L:34:HIS:H	1.83	0.43
38:j:90:MET:HE2	38:j:90:MET:HB3	1.74	0.43
39:k:114:LYS:HA	39:k:114:LYS:HD3	1.71	0.43
3:2:1071:C:H2'	3:2:1072:G:C8	2.53	0.43
9:F:8:LYS:HA	9:F:14:SER:HA	2.00	0.43
34:f:60:ILE:N	34:f:60:ILE:HD13	2.33	0.43
35:g:27:LYS:HB2	35:g:27:LYS:HE3	1.72	0.43
12:I:74:THR:HG23	12:I:107:PHE:HB2	2.01	0.43
3:2:703:G:H8	3:2:703:G:OP2	2.02	0.43
7:D:79:ILE:HD12	7:D:79:ILE:O	2.19	0.43
34:f:59:LYS:HG2	34:f:63:ARG:NE	2.33	0.43
34:f:130:THR:HB	34:f:133:GLU:HG3	2.00	0.43
41:m:100:LYS:HB2	41:m:100:LYS:NZ	2.33	0.43
42:n:102:LEU:HD22	42:n:102:LEU:H	1.83	0.43
49:u:47:HIS:HB2	49:u:71:LYS:HE3	1.99	0.43
3:2:555:U:H2'	3:2:556:C:C6	2.53	0.43
3:2:1062:U:H2'	3:2:1063:C:C6	2.54	0.43
8:E:99:LYS:C	8:E:99:LYS:HD2	2.43	0.43
9:F:57:LYS:HG3	9:F:58:LEU:N	2.34	0.43
3:2:502:A:OP1	44:p:115:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:695:A:H2'	3:2:696:A:C8	2.53	0.43
25:V:13:GLU:H	25:V:13:GLU:CD	2.26	0.43
37:i:39:VAL:HG23	37:i:71:MET:HE2	2.00	0.43
53:y:16:LEU:HD12	53:y:16:LEU:HA	1.86	0.43
1:0:645:C:O2'	1:0:646:U:H5"	2.19	0.43
1:0:742:A:H2'	1:0:743:A:C8	2.53	0.43
3:2:384:G:H2'	3:2:385:C:C6	2.53	0.43
4:A:76:ALA:O	4:A:115:GLN:HA	2.19	0.43
20:Q:88:LYS:HB2	20:Q:91:GLN:HG2	2.01	0.43
36:h:124:MET:HG3	36:h:146:ARG:HG2	1.99	0.43
42:n:28:THR:HG21	42:n:90:LEU:HD22	2.01	0.43
1:0:851:C:H2'	1:0:852:U:C6	2.53	0.43
3:2:748:G:H2'	3:2:749:A:H8	1.84	0.43
7:D:85:ILE:HD13	7:D:85:ILE:HA	1.89	0.43
41:m:91:ASP:OD2	41:m:94:LEU:HG	2.19	0.43
42:n:30:LYS:HD3	42:n:36:VAL:HG12	2.00	0.43
46:r:49:GLN:HE22	51:w:12:ASP:HB3	1.84	0.43
1:0:2537:U:H2'	1:0:2538:C:C6	2.53	0.43
3:2:1273:C:H2'	3:2:1274:A:O4'	2.19	0.43
28:Y:49:ILE:H	28:Y:49:ILE:HG12	1.56	0.43
38:j:51:ILE:O	38:j:54:LEU:HB2	2.18	0.43
1:0:280:U:H2'	1:0:281:C:H6	1.84	0.42
3:2:399:G:H2'	3:2:400:C:C6	2.54	0.42
3:2:678:U:H2'	3:2:679:C:H6	1.84	0.42
34:f:165:ASP:OD2	34:f:168:HIS:HB2	2.19	0.42
40:l:106:THR:HG22	40:l:107:SER:H	1.83	0.42
52:x:55:GLN:HB3	52:x:56:PRO:HD3	2.00	0.42
1:0:644:A:H2'	1:0:645:C:O4'	2.20	0.42
3:2:744:C:H2'	3:2:745:G:C8	2.54	0.42
7:D:79:ILE:HG22	7:D:83:TYR:HD2	1.83	0.42
11:H:40:LYS:HE3	11:H:57:VAL:HG12	2.01	0.42
14:K:8:ARG:HD2	14:K:43:GLU:HG2	2.01	0.42
34:f:7:ARG:HD2	34:f:7:ARG:N	2.34	0.42
48:t:76:LYS:HE3	48:t:76:LYS:HB2	1.79	0.42
1:0:546:U:O3'	1:0:547:A:H8	2.02	0.42
3:2:1053:G:H4'	3:2:1054:C:O5'	2.19	0.42
7:D:96:MET:HE2	7:D:96:MET:HB3	1.85	0.42
8:E:160:LYS:H	8:E:160:LYS:HG2	1.64	0.42
13:J:95:LEU:HD23	13:J:95:LEU:HA	1.88	0.42
35:g:93:ASP:C	35:g:93:ASP:OD1	2.62	0.42
53:y:20:LYS:HB3	53:y:20:LYS:HZ3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:576:C:H3'	3:2:577:G:H5"	2.02	0.42
3:2:997:U:H2'	3:2:998:C:O4'	2.20	0.42
10:G:95:ARG:NE	10:G:96:ARG:HH12	2.18	0.42
22:S:40:ILE:HD12	22:S:42:LEU:HD21	2.00	0.42
3:2:767:A:H2'	3:2:768:A:O4'	2.18	0.42
1:0:5:A:H2'	1:0:6:A:H8	1.83	0.42
3:2:390:U:H2'	3:2:391:G:C8	2.55	0.42
3:2:1003:G:N2	3:2:1004:A:H1'	2.34	0.42
3:2:1320:C:C2	51:w:72:GLY:HA3	2.55	0.42
31:c:42:LEU:HD12	31:c:42:LEU:HA	1.90	0.42
43:o:36:ASP:OD1	43:o:36:ASP:C	2.62	0.42
1:0:1856:U:H2'	1:0:1857:G:O4'	2.20	0.42
2:1:28:C:OP1	15:L:31:THR:HG21	2.20	0.42
3:2:89:U:H4'	3:2:90:C:O5'	2.20	0.42
6:C:105:LEU:HD23	6:C:105:LEU:HA	1.90	0.42
46:r:19:LYS:HB2	46:r:19:LYS:HE2	1.86	0.42
47:s:24:SER:O	47:s:28:GLN:HG3	2.20	0.42
51:w:29:LYS:HD3	51:w:30:PRO:CD	2.48	0.42
51:w:64:ASP:C	51:w:64:ASP:OD1	2.63	0.42
1:0:1735:A:H2'	1:0:1736:U:C6	2.55	0.42
1:0:832:U:H2'	1:0:833:A:H8	1.83	0.42
4:A:78:VAL:HG21	4:A:110:LEU:HD21	2.01	0.42
28:Z:42:LYS:HE2	28:Z:42:LYS:HB2	1.62	0.42
29:a:12:LYS:HA	29:a:12:LYS:HD2	1.85	0.42
33:e:16:ILE:HD13	33:e:25:VAL:HG22	2.02	0.42
44:p:99:ARG:HA	44:p:99:ARG:HD2	1.81	0.42
46:r:16:LEU:HD23	46:r:16:LEU:HA	1.88	0.42
2:1:42:C:C5	7:D:66:LEU:HD22	2.54	0.42
3:2:1330:U:H2'	3:2:1331:G:O4'	2.20	0.42
7:D:40:VAL:HG21	7:D:50:LEU:CD2	2.49	0.42
7:D:161:LYS:HE2	7:D:161:LYS:HB2	1.86	0.42
11:H:71:ARG:HD3	11:H:71:ARG:HA	1.89	0.42
36:h:177:LYS:H	36:h:177:LYS:HG2	1.57	0.42
39:k:42:ILE:HD13	39:k:116:MET:HG2	2.02	0.42
45:q:44:LYS:O	45:q:45:ILE:HG22	2.20	0.42
1:0:995:C:N4	10:G:2:LYS:HD2	2.35	0.41
1:0:2461:A:H2'	1:0:2462:C:C6	2.55	0.41
3:2:978:A:C4	3:2:1319:A:C2	3.07	0.41
3:2:1157:A:C2	3:2:1181:G:C4	3.08	0.41
4:A:132:MET:HA	4:A:135:ILE:HD12	2.01	0.41
38:j:14:GLN:HB3	38:j:17:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:k:149:LYS:HB2	39:k:149:LYS:HE3	1.59	0.41
52:x:86:LEU:HD23	52:x:86:LEU:HA	1.90	0.41
1:0:351:C:H2'	1:0:352:A:H8	1.85	0.41
3:2:766:A:N7	3:2:813:U:H5	2.18	0.41
41:m:42:GLU:HA	41:m:45:ARG:HD2	2.03	0.41
44:p:90:LEU:HD23	44:p:90:LEU:HA	1.91	0.41
1:0:969:G:H2'	1:0:970:U:C6	2.55	0.41
7:D:38:MET:SD	7:D:53:ALA:HB1	2.59	0.41
17:N:117:LEU:HD23	17:N:117:LEU:HA	1.93	0.41
54:Y:201:SAH:H5'2	54:Y:201:SAH:HB1	1.31	0.41
34:f:45:LYS:HB3	34:f:50:PHE:CD1	2.55	0.41
41:m:7:TYR:HE1	41:m:18:ARG:HB3	1.85	0.41
1:0:265:A:H4'	1:0:266:G:OP1	2.21	0.41
1:0:276:U:H2'	1:0:277:G:C5	2.56	0.41
3:2:1323:G:H2'	3:2:1324:A:H8	1.79	0.41
9:F:30:LEU:HB3	9:F:36:ALA:HB3	2.03	0.41
12:I:62:PRO:HG2	32:d:25:LYS:HG2	2.02	0.41
18:O:73:LYS:HE2	18:O:73:LYS:HB3	1.43	0.41
22:S:69:GLU:OE2	22:S:69:GLU:N	2.53	0.41
27:X:35:ASP:OD1	27:X:36:VAL:HG12	2.20	0.41
34:f:56:GLU:OE2	34:f:60:ILE:HD11	2.21	0.41
1:0:714:U:OP2	47:s:89:ARG:HB3	2.19	0.41
1:0:857:G:H2'	1:0:858:G:O4'	2.21	0.41
6:C:155:GLU:H	6:C:155:GLU:HG3	1.61	0.41
28:Z:144:TRP:O	28:Z:147:THR:HG22	2.19	0.41
42:n:40:ILE:HD12	42:n:40:ILE:N	2.34	0.41
47:s:82:ILE:HD13	47:s:82:ILE:HA	1.80	0.41
1:0:1794:A:H2'	1:0:1795:C:C6	2.56	0.41
1:0:2070:A:H2'	1:0:2071:A:C8	2.56	0.41
2:1:106:G:H2'	2:1:107:G:O4'	2.20	0.41
5:B:17:GLU:H	5:B:17:GLU:CD	2.29	0.41
16:M:24:ASP:HB2	16:M:89:ARG:HA	2.01	0.41
28:Y:0:MET:HE3	28:Y:92:LYS:HD2	2.03	0.41
34:f:5:SER:OG	34:f:8:ASP:HB2	2.21	0.41
3:2:1435:G:H2'	3:2:1436:U:C6	2.55	0.41
7:D:164:GLU:H	7:D:164:GLU:CD	2.28	0.41
11:H:63:VAL:HG12	11:H:107:LEU:HD11	2.02	0.41
17:N:15:LYS:HB3	17:N:15:LYS:HE3	1.80	0.41
34:f:139:ARG:NH2	34:f:142:GLU:HB3	2.36	0.41
1:0:286:U:H2'	1:0:287:G:H8	1.86	0.41
1:0:880:G:C2	1:0:881:G:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:76:G:H1	3:2:93:U:H3	1.68	0.41
14:K:45:ARG:O	14:K:49:GLU:HG3	2.21	0.41
28:Z:10:THR:C	28:Z:11:LYS:HG2	2.46	0.41
34:f:117:LEU:O	34:f:120:GLN:HG3	2.21	0.41
37:i:45:ARG:HD2	37:i:73:ASN:OD1	2.20	0.41
39:k:115:SER:O	39:k:119:ARG:HD3	2.21	0.41
1:0:2795:C:H2'	1:0:2796:U:C6	2.55	0.41
1:0:2799:A:O2'	1:0:2800:A:H5"	2.20	0.41
3:2:440:C:C2	3:2:441:A:C8	3.09	0.41
3:2:501:C:H2'	3:2:502:A:C8	2.56	0.41
3:2:736:C:H2'	3:2:737:C:H6	1.86	0.41
3:2:1306:A:H2	3:2:1331:G:H21	1.65	0.41
18:O:37:GLU:O	18:O:37:GLU:HG2	2.20	0.41
34:f:15:HIS:HB3	34:f:43:LEU:HD11	2.02	0.41
35:g:156:ARG:HG3	35:g:160:ALA:O	2.21	0.41
38:j:100:SER:O	38:j:104:LYS:HG3	2.20	0.41
45:q:97:VAL:HG12	45:q:98:ARG:H	1.86	0.41
53:y:7:ARG:O	53:y:10:GLU:HB3	2.20	0.41
1:0:1506:U:H2'	1:0:1507:C:C6	2.56	0.41
1:0:1796:U:H2'	1:0:1797:G:H8	1.86	0.41
7:D:63:GLN:HB2	27:X:6:HIS:CE1	2.56	0.41
22:S:1:MET:HE3	22:S:1:MET:O	2.21	0.41
27:X:56:ARG:NH2	27:X:59:ARG:HH21	2.19	0.41
38:j:74:LEU:HD11	38:j:78:PHE:CZ	2.56	0.41
39:k:57:SER:O	39:k:60:GLU:HG3	2.20	0.41
45:q:7:ILE:HD11	45:q:22:ILE:HD13	2.02	0.41
48:t:46:LYS:HA	48:t:46:LYS:HD3	1.89	0.41
1:0:39:G:H2'	1:0:40:U:C6	2.56	0.40
1:0:1357:C:H2'	1:0:1358:G:O4'	2.22	0.40
1:0:1432:G:H2'	1:0:1433:A:C8	2.56	0.40
3:2:1328:C:OP1	45:q:28:THR:HG21	2.21	0.40
14:K:38:LEU:HB3	14:K:39:PRO:HD3	2.03	0.40
3:2:1149:C:H2'	3:2:1150:A:C8	2.56	0.40
9:F:51:ARG:HH22	9:F:58:LEU:HD12	1.86	0.40
9:F:80:ILE:HD12	9:F:81:ALA:H	1.85	0.40
35:g:169:ARG:HG3	35:g:170:GLU:N	2.34	0.40
1:0:832:U:H2'	1:0:833:A:C8	2.56	0.40
9:F:51:ARG:CZ	9:F:54:LEU:HG	2.51	0.40
33:e:12:ARG:HB3	33:e:12:ARG:HH11	1.85	0.40
42:n:80:THR:H	42:n:83:THR:CG2	2.34	0.40
3:2:868:C:H2'	3:2:869:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:1149:C:H2'	3:2:1150:A:H8	1.85	0.40
9:F:8:LYS:HE3	9:F:9:VAL:O	2.21	0.40
9:F:110:VAL:HG11	9:F:132:PHE:HE2	1.86	0.40
9:F:135:HIS:H	9:F:138:VAL:HG22	1.87	0.40
21:R:79:LYS:HB2	21:R:79:LYS:HE3	1.97	0.40
39:k:66:LEU:HB3	39:k:70:ARG:HH21	1.86	0.40
41:m:17:ALA:HB2	41:m:67:VAL:HG23	2.02	0.40
45:q:50:GLU:HA	45:q:50:GLU:OE1	2.22	0.40
1:0:1585:C:H2'	1:0:1586:A:O4'	2.22	0.40
1:0:2567:G:H2'	1:0:2568:U:C6	2.57	0.40
3:2:864:A:H2'	3:2:865:A:C8	2.57	0.40
8:E:72:LEU:HD23	8:E:72:LEU:HA	1.77	0.40
9:F:40:THR:O	9:F:44:ILE:HD12	2.22	0.40
28:Y:129:HIS:CG	28:Y:130:PRO:HD3	2.56	0.40
28:Z:61:LEU:HD23	28:Z:61:LEU:HA	1.96	0.40
34:f:42:ASN:O	34:f:43:LEU:HB2	2.20	0.40
34:f:49:MET:HA	34:f:49:MET:CE	2.44	0.40
44:p:86:ARG:HA	44:p:94:ARG:HA	2.03	0.40
46:r:34:VAL:HG23	46:r:35:ASN:OD1	2.21	0.40
47:s:39:LEU:HD23	47:s:39:LEU:HA	1.94	0.40
49:u:39:LYS:HE3	49:u:39:LYS:HB2	1.97	0.40
51:w:27:ASP:C	51:w:28:LYS:HE2	2.47	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	
4	A	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
5	B	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
6	C	199/201 (99%)	193 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	D	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
8	E	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
9	F	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
10	G	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
11	H	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
12	I	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
13	J	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
14	K	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
15	L	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
16	M	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
17	N	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
18	O	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
19	P	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
20	Q	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
21	R	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
22	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
23	T	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
24	U	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	V	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
26	W	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
27	X	56/70 (80%)	54 (96%)	2 (4%)	0	100	100
28	Y	156/178 (88%)	151 (97%)	5 (3%)	0	100	100
28	Z	150/178 (84%)	146 (97%)	4 (3%)	0	100	100
29	a	53/57 (93%)	53 (100%)	0	0	100	100
30	b	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
31	c	44/46 (96%)	44 (100%)	0	0	100	100
32	d	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
33	e	36/38 (95%)	36 (100%)	0	0	100	100
34	f	222/241 (92%)	202 (91%)	20 (9%)	0	100	100
35	g	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
36	h	203/206 (98%)	202 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	i	153/167 (92%)	149 (97%)	4 (3%)	0	100	100
38	j	104/131 (79%)	100 (96%)	4 (4%)	0	100	100
39	k	149/179 (83%)	145 (97%)	4 (3%)	0	100	100
40	l	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
41	m	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
42	n	97/103 (94%)	94 (97%)	3 (3%)	0	100	100
43	o	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
44	p	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
45	q	112/118 (95%)	101 (90%)	10 (9%)	1 (1%)	14	14
46	r	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
47	s	86/89 (97%)	86 (100%)	0	0	100	100
48	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
49	u	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
50	v	64/75 (85%)	64 (100%)	0	0	100	100
51	w	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
52	x	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
53	y	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	5887/6265 (94%)	5679 (96%)	207 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
45	q	45	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	
4	A	216/218 (99%)	211 (98%)	5 (2%)	44	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	164/164 (100%)	161 (98%)	3 (2%)	51	68
6	C	165/165 (100%)	164 (99%)	1 (1%)	78	89
7	D	148/150 (99%)	141 (95%)	7 (5%)	23	31
8	E	134/138 (97%)	130 (97%)	4 (3%)	36	49
9	F	114/114 (100%)	105 (92%)	9 (8%)	11	13
10	G	116/116 (100%)	114 (98%)	2 (2%)	53	69
11	H	104/104 (100%)	103 (99%)	1 (1%)	68	81
12	I	103/103 (100%)	103 (100%)	0	100	100
13	J	109/109 (100%)	105 (96%)	4 (4%)	30	41
14	K	98/103 (95%)	96 (98%)	2 (2%)	48	64
15	L	86/87 (99%)	83 (96%)	3 (4%)	32	43
16	M	99/100 (99%)	98 (99%)	1 (1%)	68	81
17	N	89/90 (99%)	89 (100%)	0	100	100
18	O	84/84 (100%)	83 (99%)	1 (1%)	63	78
19	P	93/93 (100%)	92 (99%)	1 (1%)	65	79
20	Q	80/84 (95%)	79 (99%)	1 (1%)	61	76
21	R	83/85 (98%)	81 (98%)	2 (2%)	43	58
22	S	78/78 (100%)	77 (99%)	1 (1%)	61	76
23	T	57/63 (90%)	56 (98%)	1 (2%)	51	68
24	U	67/68 (98%)	67 (100%)	0	100	100
25	V	54/55 (98%)	52 (96%)	2 (4%)	30	41
26	W	47/49 (96%)	47 (100%)	0	100	100
27	X	55/62 (89%)	53 (96%)	2 (4%)	31	42
28	Y	132/150 (88%)	130 (98%)	2 (2%)	57	73
28	Z	126/150 (84%)	123 (98%)	3 (2%)	43	58
29	a	46/48 (96%)	45 (98%)	1 (2%)	45	61
30	b	46/49 (94%)	46 (100%)	0	100	100
31	c	38/38 (100%)	37 (97%)	1 (3%)	40	55
32	d	51/52 (98%)	50 (98%)	1 (2%)	48	64
33	e	34/34 (100%)	32 (94%)	2 (6%)	18	22
34	f	186/199 (94%)	179 (96%)	7 (4%)	29	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	g	170/190 (90%)	164 (96%)	6 (4%)	32	43
36	h	172/173 (99%)	162 (94%)	10 (6%)	18	22
37	i	118/126 (94%)	117 (99%)	1 (1%)	73	85
38	j	92/112 (82%)	90 (98%)	2 (2%)	45	61
39	k	124/147 (84%)	121 (98%)	3 (2%)	43	58
40	l	104/105 (99%)	103 (99%)	1 (1%)	68	81
41	m	105/107 (98%)	98 (93%)	7 (7%)	15	17
42	n	87/90 (97%)	82 (94%)	5 (6%)	18	23
43	o	90/99 (91%)	87 (97%)	3 (3%)	33	45
44	p	103/104 (99%)	102 (99%)	1 (1%)	68	81
45	q	92/96 (96%)	90 (98%)	2 (2%)	45	61
46	r	83/84 (99%)	80 (96%)	3 (4%)	31	42
47	s	76/77 (99%)	74 (97%)	2 (3%)	40	55
48	t	65/65 (100%)	63 (97%)	2 (3%)	35	48
49	u	74/78 (95%)	71 (96%)	3 (4%)	27	37
50	v	57/65 (88%)	51 (90%)	6 (10%)	6	6
51	w	70/79 (89%)	68 (97%)	2 (3%)	37	51
52	x	65/66 (98%)	64 (98%)	1 (2%)	57	73
53	y	60/61 (98%)	59 (98%)	1 (2%)	53	69
All	All	4909/5126 (96%)	4778 (97%)	131 (3%)	40	53

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	50	THR
4	A	114	ASP
4	A	140	THR
4	A	194	GLU
4	A	219	THR
5	B	100	LEU
5	B	107	VAL
5	B	129	THR
6	C	21	ARG
7	D	18	THR
7	D	35	THR

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Mol	Chain	Res	Type
7	D	40	VAL
7	D	44	ILE
7	D	50	LEU
7	D	144	ASP
7	D	152	LEU
8	E	32	GLU
8	E	107	LEU
8	E	160	LYS
8	E	162	VAL
9	F	4	ILE
9	F	14	SER
9	F	15	LEU
9	F	62	LEU
9	F	101	ASP
9	F	108	VAL
9	F	114	GLU
9	F	115	VAL
9	F	143	ILE
10	G	14	ASP
10	G	64	VAL
11	H	76	VAL
13	J	1	MET
13	J	95	LEU
13	J	115	GLU
13	J	135	VAL
14	K	14	SER
14	K	95	THR
15	L	12	THR
15	L	19	GLN
15	L	28	VAL
16	M	28	VAL
18	O	37	GLU
19	P	53	SER
20	Q	74	ILE
21	R	15	THR
21	R	54	GLN
22	S	65	VAL
23	T	62	LYS
25	V	30	MET
25	V	34	SER
27	X	4	ASP
27	X	12	ILE

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Mol	Chain	Res	Type
28	Y	-3	PHE
28	Y	50	LYS
28	Z	34	GLU
28	Z	147	THR
28	Z	150	HIS
29	a	25	VAL
31	c	4	THR
32	d	16	LYS
33	e	8	LYS
33	e	36	ARG
34	f	14	VAL
34	f	110	SER
34	f	122	GLN
34	f	141	LEU
34	f	161	LEU
34	f	163	VAL
34	f	227	GLN
35	g	52	VAL
35	g	63	SER
35	g	84	VAL
35	g	151	VAL
35	g	169	ARG
35	g	207	ILE
36	h	28	ILE
36	h	29	ASP
36	h	47	ARG
36	h	50	ASP
36	h	73	ARG
36	h	125	VAL
36	h	128	ARG
36	h	151	LYS
36	h	172	GLU
36	h	177	LYS
37	i	32	SER
38	j	44	ARG
38	j	96	VAL
39	k	29	ILE
39	k	75	VAL
39	k	137	LYS
40	l	114	ARG
41	m	4	ASN
41	m	9	THR

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Mol	Chain	Res	Type
41	m	14	SER
41	m	19	VAL
41	m	29	VAL
41	m	52	LEU
41	m	104	VAL
42	n	18	ILE
42	n	36	VAL
42	n	37	ARG
42	n	74	VAL
42	n	98	VAL
43	o	30	THR
43	o	35	THR
43	o	58	SER
44	p	35	THR
45	q	28	THR
45	q	39	ILE
46	r	5	SER
46	r	45	VAL
46	r	46	LEU
47	s	4	SER
47	s	82	ILE
48	t	21	VAL
48	t	63	GLN
49	u	12	VAL
49	u	39	LYS
49	u	52	GLU
50	v	18	VAL
50	v	42	SER
50	v	48	ARG
50	v	63	ARG
50	v	71	THR
50	v	73	ARG
51	w	56	GLN
51	w	81	ARG
52	x	44	LYS
53	y	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	25	HIS
5	B	94	GLN

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Mol	Chain	Res	Type
5	B	130	GLN
5	B	140	HIS
6	C	9	GLN
6	C	165	HIS
6	C	195	GLN
8	E	22	GLN
8	E	38	ASN
10	G	76	HIS
11	H	3	GLN
12	I	104	GLN
13	J	45	GLN
18	O	18	GLN
21	R	46	GLN
22	S	49	ASN
23	T	46	HIS
24	U	36	HIS
25	V	39	GLN
28	Z	67	ASN
30	b	19	HIS
32	d	24	HIS
32	d	26	HIS
34	f	18	HIS
36	h	164	GLN
38	j	14	GLN
38	j	63	ASN
40	l	38	ASN
41	m	5	GLN
41	m	110	GLN
42	n	64	GLN
43	o	118	HIS
46	r	62	ASN
48	t	59	HIS
49	u	50	ASN
50	v	31	ASN
52	x	3	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2744/2904 (94%)	310 (11%)	8 (0%)
2	1	119/120 (99%)	10 (8%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	1519/1542 (98%)	219 (14%)	32 (2%)
All	All	4382/4566 (95%)	539 (12%)	40 (0%)

All (539) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	2	G
1	0	10	A
1	0	34	U
1	0	46	G
1	0	51	G
1	0	60	G
1	0	63	A
1	0	71	A
1	0	74	A
1	0	75	G
1	0	84	A
1	0	92	U
1	0	99	U
1	0	101	A
1	0	102	U
1	0	118	A
1	0	119	A
1	0	120	U
1	0	139	U
1	0	140	C
1	0	160	A
1	0	163	C
1	0	181	A
1	0	196	A
1	0	199	A
1	0	216	A
1	0	221	A
1	0	222	A
1	0	230	G
1	0	233	A
1	0	248	G
1	0	266	G
1	0	275	C
1	0	277	G
1	0	278	A
1	0	280	U

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Mol	Chain	Res	Type
1	0	302	C
1	0	311	A
1	0	323	C
1	0	329	G
1	0	330	A
1	0	338	G
1	0	359	G
1	0	361	G
1	0	362	A
1	0	367	G
1	0	372	G
1	0	386	G
1	0	396	G
1	0	404	A
1	0	405	U
1	0	411	G
1	0	412	A
1	0	413	C
1	0	467	G
1	0	481	G
1	0	490	C
1	0	491	G
1	0	494	G
1	0	505	A
1	0	509	C
1	0	530	G
1	0	531	C
1	0	532	A
1	0	538	A
1	0	546	U
1	0	547	A
1	0	548	G
1	0	549	G
1	0	563	A
1	0	573	U
1	0	575	A
1	0	586	A
1	0	603	A
1	0	613	A
1	0	614	A
1	0	615	U
1	0	637	A

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Mol	Chain	Res	Type
1	0	645	C
1	0	647	G
1	0	655	A
1	0	686	U
1	0	711	G
1	0	716	A
1	0	717	C
1	0	730	A
1	0	747	U
1	0	764	A
1	0	775	G
1	0	776	G
1	0	782	A
1	0	784	G
1	0	785	G
1	0	792	A
1	0	805	G
1	0	812	C
1	0	827	U
1	0	828	U
1	0	845	A
1	0	846	U
1	0	847	U
1	0	858	G
1	0	859	G
1	0	877	A
1	0	878	A
1	0	879	G
1	0	881	G
1	0	910	A
1	0	914	G
1	0	915	C
1	0	931	U
1	0	946	C
1	0	961	C
1	0	974	G
1	0	983	A
1	0	996	A
1	0	1009	A
1	0	1012	U
1	0	1013	C
1	0	1026	G

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Mol	Chain	Res	Type
1	0	1027	A
1	0	1033	U
1	0	1046	A
1	0	1047	G
1	0	1050	A
1	0	1051	G
1	0	1110	G
1	0	1111	A
1	0	1112	G
1	0	1132	U
1	0	1135	C
1	0	1136	G
1	0	1142	A
1	0	1173	U
1	0	1174	U
1	0	1175	A
1	0	1176	U
1	0	1177	G
1	0	1206	G
1	0	1212	G
1	0	1238	G
1	0	1250	G
1	0	1253	A
1	0	1256	G
1	0	1271	G
1	0	1272	A
1	0	1273	U
1	0	1283	G
1	0	1284	A
1	0	1300	G
1	0	1301	A
1	0	1345	C
1	0	1352	U
1	0	1365	A
1	0	1374	G
1	0	1379	U
1	0	1383	A
1	0	1387	A
1	0	1395	A
1	0	1416	G
1	0	1417	C
1	0	1420	A

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Mol	Chain	Res	Type
1	0	1428	C
1	0	1452	G
1	0	1453	A
1	0	1460	U
1	0	1482	G
1	0	1486	U
1	0	1488	C
1	0	1490	A
1	0	1493	C
1	0	1503	A
1	0	1509	A
1	0	1510	G
1	0	1515	A
1	0	1524	G
1	0	1534	U
1	0	1535	A
1	0	1536	C
1	0	1537	G
1	0	1542	U
1	0	1566	A
1	0	1569	A
1	0	1578	U
1	0	1584	U
1	0	1585	C
1	0	1607	C
1	0	1608	A
1	0	1647	U
1	0	1648	U
1	0	1674	G
1	0	1714	U
1	0	1729	U
1	0	1730	C
1	0	1731	G
1	0	1733	G
1	0	1738	G
1	0	1750	G
1	0	1764	C
1	0	1773	A
1	0	1780	A
1	0	1782	U
1	0	1800	C
1	0	1801	A

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Mol	Chain	Res	Type
1	0	1808	A
1	0	1811	G
1	0	1816	C
1	0	1829	A
1	0	1872	A
1	0	1876	A
1	0	1906	G
1	0	1913	A
1	0	1929	G
1	0	1930	G
1	0	1937	A
1	0	1955	U
1	0	1964	G
1	0	1967	C
1	0	1970	A
1	0	1971	U
1	0	1972	G
1	0	1975	G
1	0	1991	U
1	0	1993	U
1	0	1997	C
1	0	2023	C
1	0	2031	A
1	0	2033	A
1	0	2043	C
1	0	2055	C
1	0	2056	G
1	0	2060	A
1	0	2061	G
1	0	2069	G
1	0	2102	G
1	0	2198	A
1	0	2204	G
1	0	2211	A
1	0	2225	A
1	0	2238	G
1	0	2239	G
1	0	2268	A
1	0	2283	C
1	0	2287	A
1	0	2288	A
1	0	2297	A

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Mol	Chain	Res	Type
1	0	2305	U
1	0	2308	G
1	0	2309	A
1	0	2312	U
1	0	2322	A
1	0	2325	G
1	0	2333	A
1	0	2347	C
1	0	2361	G
1	0	2383	G
1	0	2385	C
1	0	2396	G
1	0	2402	U
1	0	2406	A
1	0	2410	G
1	0	2423	U
1	0	2425	A
1	0	2429	G
1	0	2430	A
1	0	2435	A
1	0	2441	U
1	0	2448	A
1	0	2474	U
1	0	2476	A
1	0	2491	U
1	0	2502	G
1	0	2505	G
1	0	2506	U
1	0	2507	C
1	0	2518	A
1	0	2520	C
1	0	2529	G
1	0	2547	A
1	0	2566	A
1	0	2567	G
1	0	2573	C
1	0	2582	G
1	0	2602	A
1	0	2603	G
1	0	2609	U
1	0	2613	U
1	0	2615	U

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Mol	Chain	Res	Type
1	0	2629	U
1	0	2636	C
1	0	2663	G
1	0	2689	U
1	0	2690	U
1	0	2714	G
1	0	2726	A
1	0	2733	A
1	0	2744	G
1	0	2748	A
1	0	2749	A
1	0	2765	A
1	0	2778	A
1	0	2820	A
1	0	2821	A
1	0	2835	A
1	0	2867	G
1	0	2873	A
1	0	2880	C
1	0	2884	U
1	0	2886	A
1	0	2899	A
2	1	25	U
2	1	35	C
2	1	42	C
2	1	45	A
2	1	56	G
2	1	66	A
2	1	89	U
2	1	90	C
2	1	105	G
2	1	109	A
3	2	6	G
3	2	7	A
3	2	9	G
3	2	22	G
3	2	32	A
3	2	39	G
3	2	47	C
3	2	48	C
3	2	51	A
3	2	66	A

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Mol	Chain	Res	Type
3	2	71	A
3	2	78	A
3	2	80	A
3	2	81	A
3	2	83	C
3	2	84	U
3	2	85	U
3	2	86	G
3	2	88	U
3	2	89	U
3	2	90	C
3	2	92	U
3	2	94	G
3	2	121	U
3	2	122	G
3	2	130	A
3	2	131	A
3	2	179	A
3	2	180	U
3	2	183	C
3	2	184	G
3	2	197	A
3	2	205	A
3	2	209	U
3	2	210	C
3	2	211	G
3	2	212	G
3	2	220	G
3	2	240	G
3	2	245	U
3	2	247	G
3	2	251	G
3	2	266	G
3	2	267	C
3	2	280	C
3	2	282	A
3	2	289	G
3	2	316	C
3	2	321	A
3	2	328	C
3	2	332	G
3	2	346	G

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Mol	Chain	Res	Type
3	2	352	C
3	2	354	G
3	2	365	U
3	2	367	U
3	2	372	C
3	2	373	A
3	2	376	G
3	2	397	A
3	2	406	G
3	2	413	G
3	2	414	A
3	2	421	U
3	2	422	C
3	2	423	G
3	2	429	U
3	2	448	A
3	2	468	A
3	2	474	G
3	2	481	G
3	2	482	A
3	2	484	G
3	2	496	A
3	2	499	A
3	2	509	A
3	2	511	C
3	2	513	C
3	2	518	C
3	2	524	G
3	2	531	U
3	2	532	A
3	2	535	A
3	2	547	A
3	2	548	G
3	2	559	A
3	2	560	A
3	2	564	C
3	2	572	A
3	2	573	A
3	2	576	C
3	2	577	G
3	2	623	C
3	2	633	G

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Mol	Chain	Res	Type
3	2	653	U
3	2	665	A
3	2	687	A
3	2	703	G
3	2	704	A
3	2	718	A
3	2	721	G
3	2	722	G
3	2	724	G
3	2	734	G
3	2	755	G
3	2	758	C
3	2	777	A
3	2	793	U
3	2	794	A
3	2	815	A
3	2	817	C
3	2	821	G
3	2	840	C
3	2	841	C
3	2	842	U
3	2	844	G
3	2	845	A
3	2	872	A
3	2	890	G
3	2	891	U
3	2	914	A
3	2	922	G
3	2	926	G
3	2	927	G
3	2	934	C
3	2	935	A
3	2	960	U
3	2	966	G
3	2	969	A
3	2	971	G
3	2	975	A
3	2	976	G
3	2	977	A
3	2	983	A
3	2	989	U
3	2	990	C

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Mol	Chain	Res	Type
3	2	991	U
3	2	992	U
3	2	993	G
3	2	998	C
3	2	1001	C
3	2	1006	G
3	2	1007	U
3	2	1012	A
3	2	1022	A
3	2	1023	U
3	2	1041	G
3	2	1046	A
3	2	1053	G
3	2	1054	C
3	2	1094	G
3	2	1095	U
3	2	1101	A
3	2	1102	A
3	2	1117	A
3	2	1118	U
3	2	1124	G
3	2	1125	U
3	2	1126	U
3	2	1131	G
3	2	1136	C
3	2	1138	G
3	2	1139	G
3	2	1140	C
3	2	1158	C
3	2	1159	U
3	2	1168	U
3	2	1171	A
3	2	1180	A
3	2	1183	U
3	2	1184	G
3	2	1191	A
3	2	1196	A
3	2	1197	A
3	2	1202	U
3	2	1212	U
3	2	1214	C
3	2	1227	A

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Mol	Chain	Res	Type
3	2	1233	G
3	2	1236	A
3	2	1238	A
3	2	1245	C
3	2	1248	A
3	2	1257	A
3	2	1258	G
3	2	1268	G
3	2	1280	A
3	2	1286	U
3	2	1287	A
3	2	1300	G
3	2	1301	U
3	2	1302	C
3	2	1306	A
3	2	1317	C
3	2	1320	C
3	2	1323	G
3	2	1336	C
3	2	1338	G
3	2	1345	U
3	2	1347	G
3	2	1348	U
3	2	1363	A
3	2	1364	U
3	2	1374	A
3	2	1398	A
3	2	1400	C
3	2	1419	G
3	2	1446	A
3	2	1487	G
3	2	1492	A
3	2	1497	G
3	2	1503	A
3	2	1504	G
3	2	1506	U
3	2	1517	G
3	2	1520	C
3	2	1529	G
3	2	1530	G
3	2	1534	A

All (40) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
1	0	1	G
1	0	274	C
1	0	279	A
1	0	546	U
1	0	547	A
1	0	613	A
1	0	1026	G
1	0	1583	A
3	2	5	U
3	2	79	G
3	2	89	U
3	2	183	C
3	2	210	C
3	2	281	G
3	2	315	A
3	2	345	C
3	2	365	U
3	2	422	C
3	2	428	G
3	2	467	U
3	2	495	A
3	2	559	A
3	2	575	G
3	2	703	G
3	2	792	A
3	2	890	G
3	2	982	U
3	2	992	U
3	2	1040	U
3	2	1053	G
3	2	1117	A
3	2	1137	C
3	2	1179	A
3	2	1182	G
3	2	1190	G
3	2	1201	A
3	2	1267	C
3	2	1305	G
3	2	1347	G
3	2	1399	C

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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

2 ligands 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	$\#\|Z\| > 2$
54	SAH	Z	201	-	27,28,28	0.70	0	38,40,40	0.66	1 (2%)
54	SAH	Y	201	-	27,28,28	1.39	4 (14%)	38,40,40	2.09	10 (26%)

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
54	SAH	Z	201	-	-	5/15/31/31	0/3/3/3
54	SAH	Y	201	-	-	9/15/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Y	201	SAH	C5-C4	3.80	1.46	1.39
54	Y	201	SAH	C4-N9	-2.44	1.32	1.37
54	Y	201	SAH	C5-C6	2.32	1.47	1.41
54	Y	201	SAH	C5-N7	-2.21	1.34	1.39

All (11) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	Y	201	SAH	C5-C4-N3	-5.15	120.03	126.75
54	Y	201	SAH	N3-C4-N9	4.38	134.30	127.08
54	Y	201	SAH	CB-CG-SD	-3.83	104.72	113.31
54	Y	201	SAH	C4-N9-C8	3.76	109.80	105.73
54	Y	201	SAH	C2-N3-C4	3.73	120.56	111.75
54	Y	201	SAH	N3-C2-N1	-3.50	123.12	128.60
54	Y	201	SAH	C4-C5-N7	-3.29	106.61	110.62
54	Y	201	SAH	C5-N7-C8	2.97	107.73	103.51
54	Y	201	SAH	C6-C5-N7	2.76	137.16	132.02
54	Y	201	SAH	N9-C8-N7	-2.72	110.20	113.91
54	Z	201	SAH	CB-CG-SD	-2.11	108.58	113.31

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	Y	201	SAH	CB-CG-SD-C5'
54	Y	201	SAH	O4'-C4'-C5'-SD
54	Y	201	SAH	C3'-C4'-C5'-SD
54	Y	201	SAH	OXT-C-CA-CB
54	Y	201	SAH	OXT-C-CA-N
54	Y	201	SAH	O-C-CA-CB
54	Y	201	SAH	C-CA-CB-CG
54	Y	201	SAH	O-C-CA-N
54	Y	201	SAH	N-CA-CB-CG
54	Z	201	SAH	C3'-C4'-C5'-SD
54	Z	201	SAH	O4'-C4'-C5'-SD
54	Z	201	SAH	OXT-C-CA-CB
54	Z	201	SAH	O-C-CA-CB
54	Z	201	SAH	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	Z	201	SAH	2	0
54	Y	201	SAH	4	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

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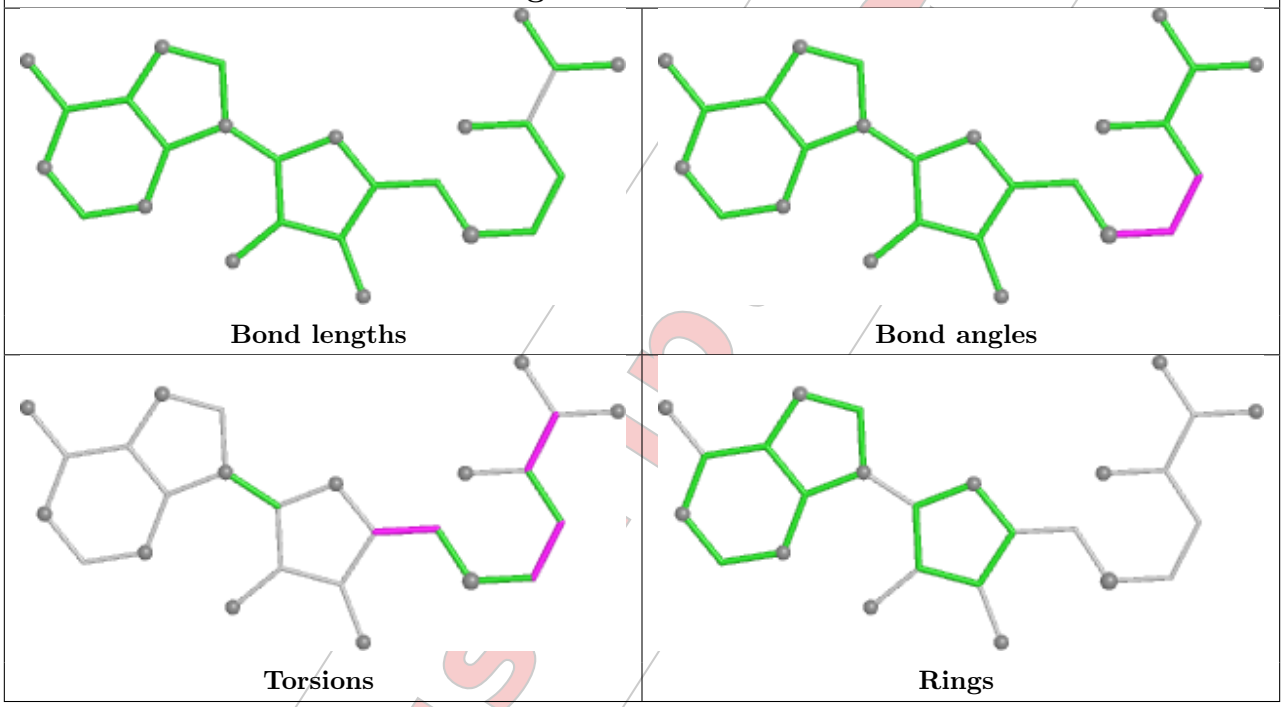
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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 SAH Z 201



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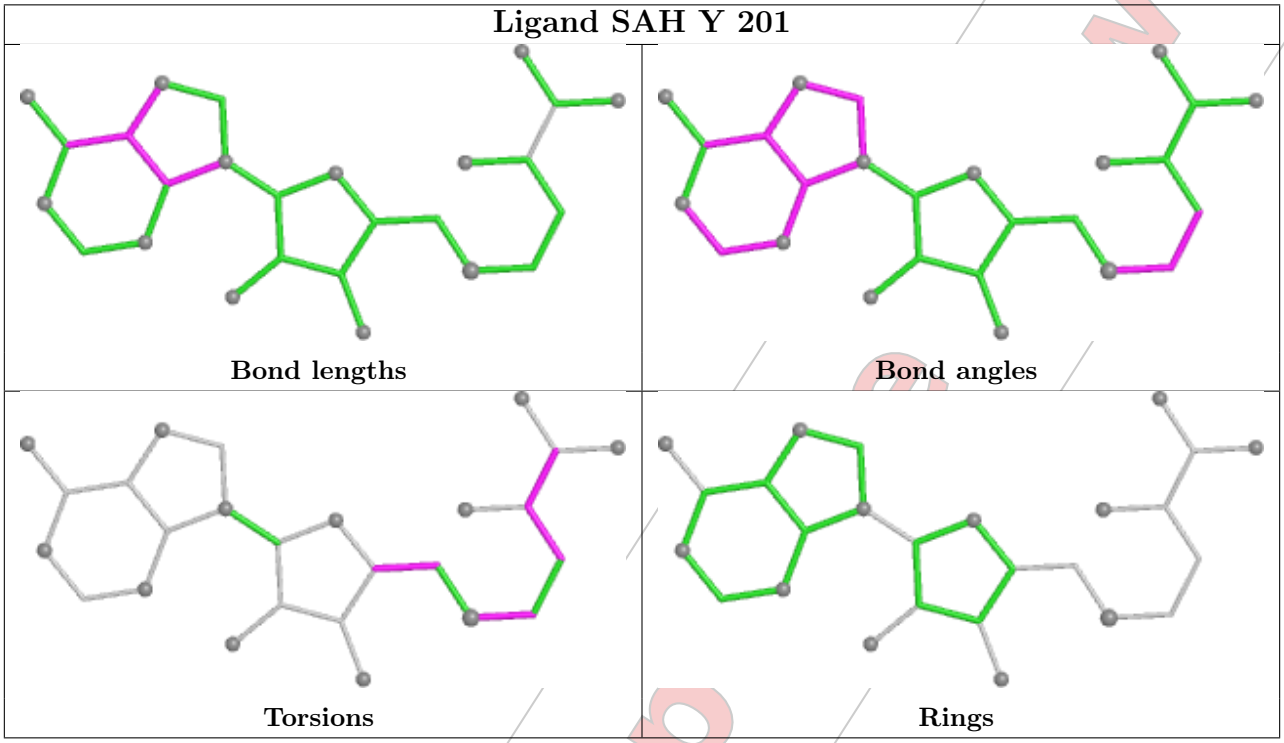

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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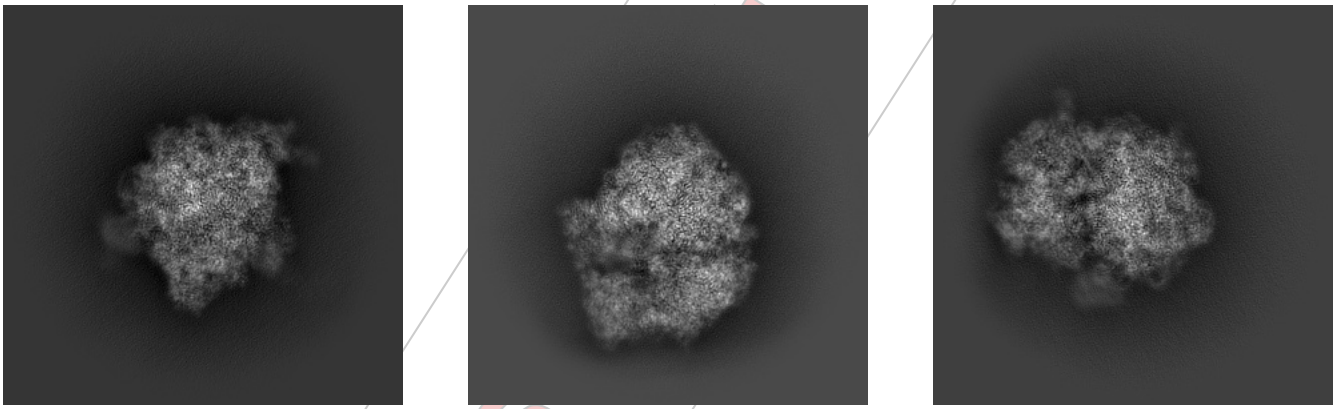
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-82546. 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.

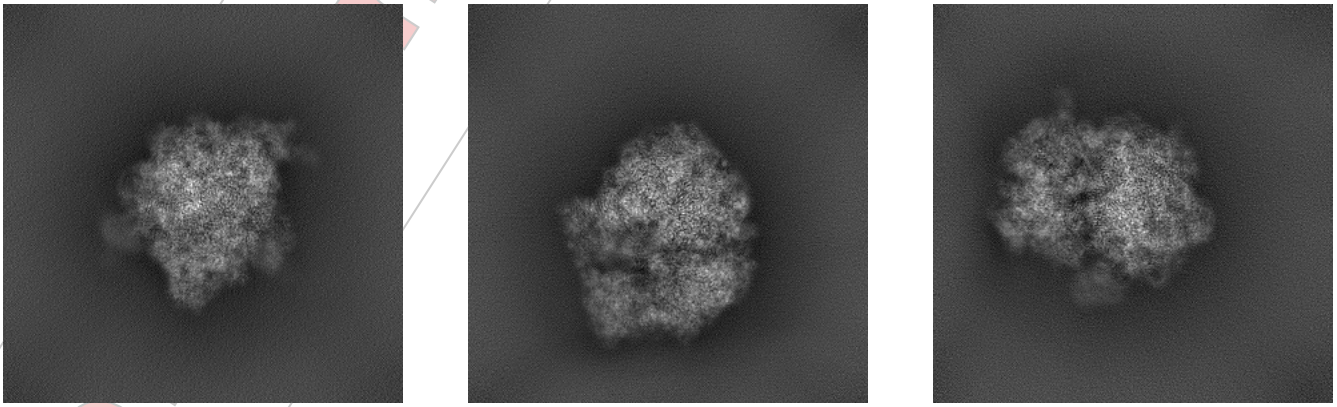
6.1 Orthogonal projections

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.

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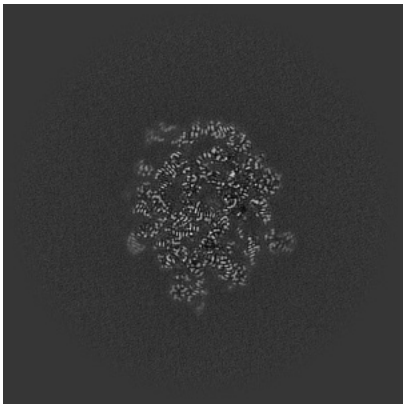
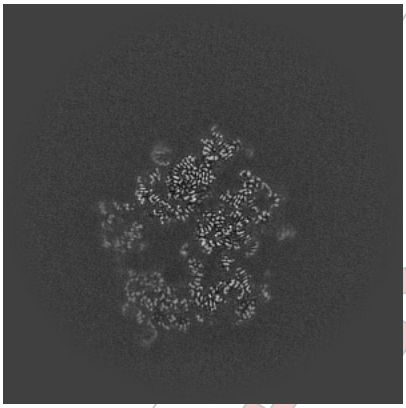
6.2 Central slices (i)

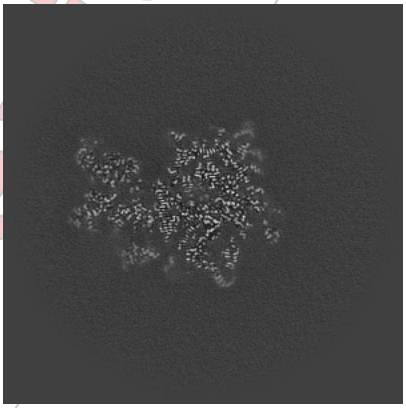
6.2.1 Primary map



X Index: 240

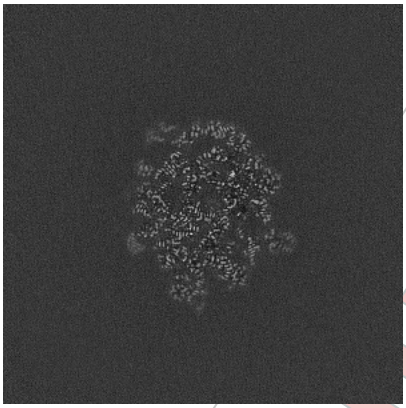


Y Index: 240

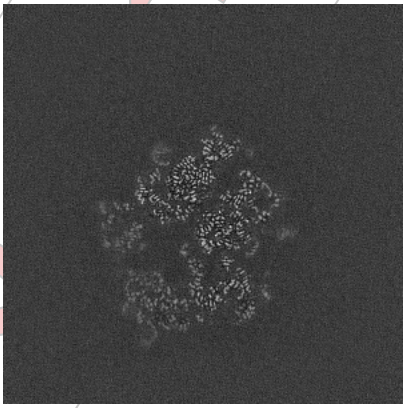


Z Index: 240

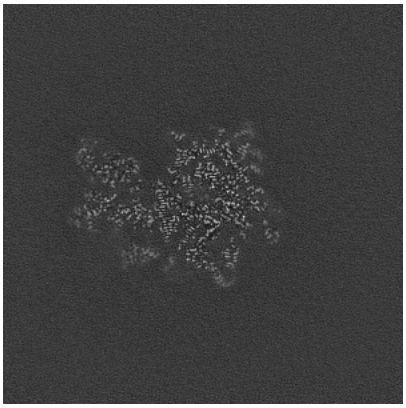
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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

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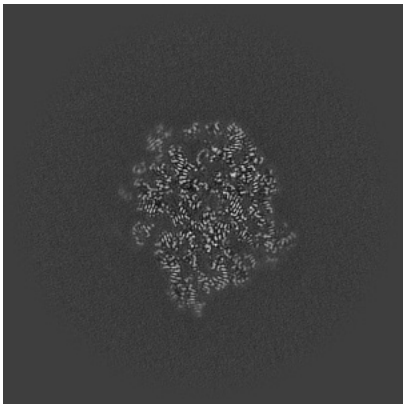
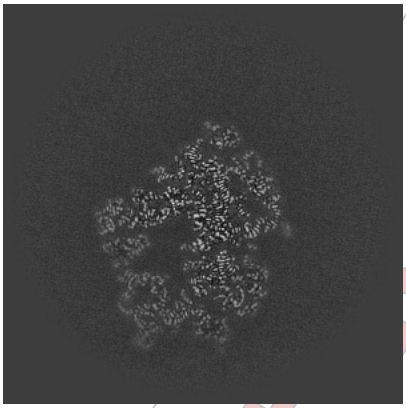
6.3 Largest variance slices (i)

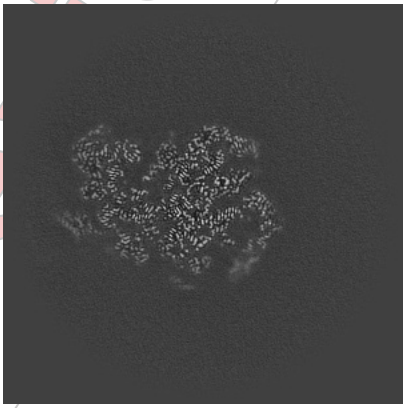
6.3.1 Primary map



X Index: 233

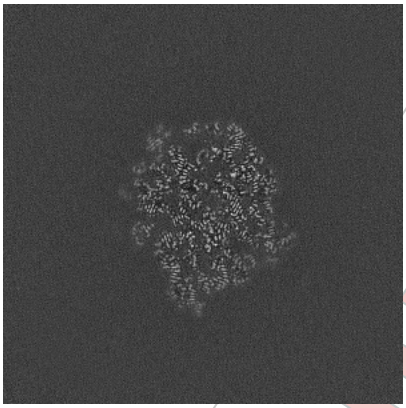


Y Index: 225

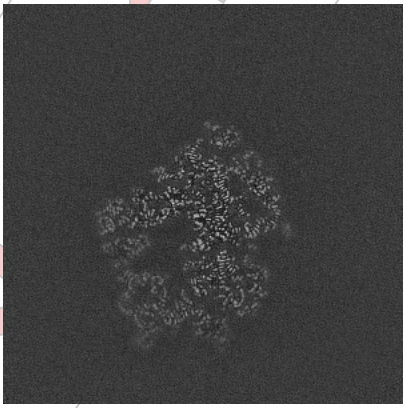


Z Index: 263

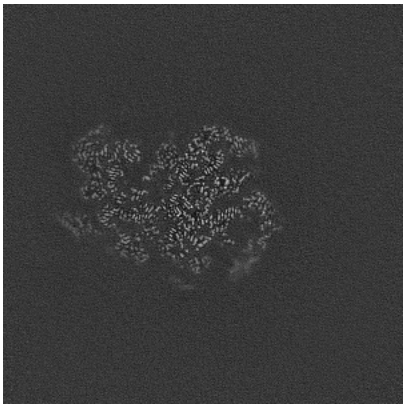
6.3.2 Raw map



X Index: 233



Y Index: 225



Z Index: 263

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

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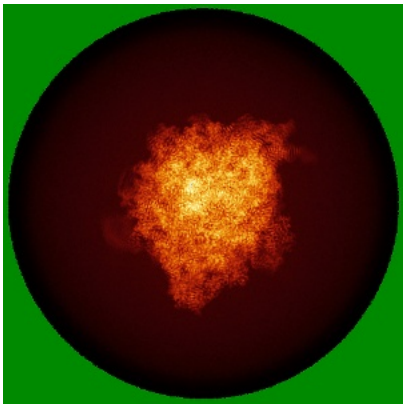
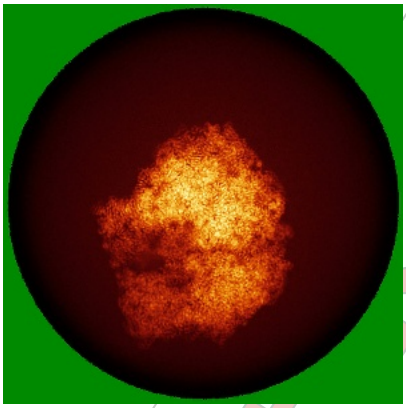
6.4 Orthogonal standard-deviation projections (False-color)

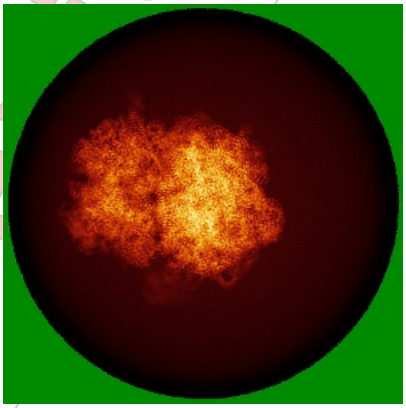
6.4.1 Primary map



X

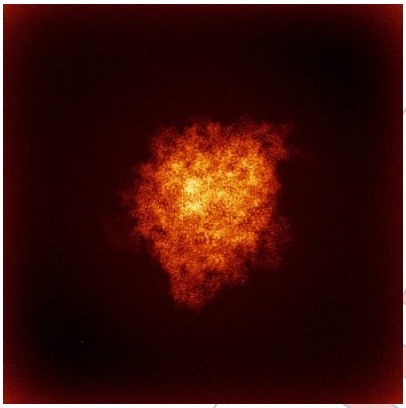


Y

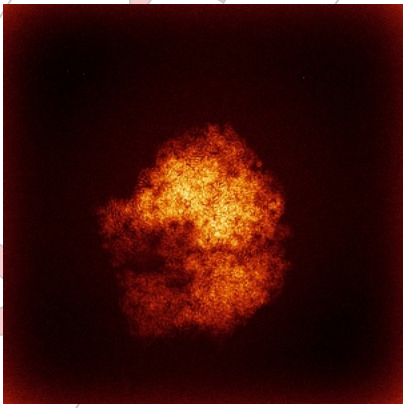


Z

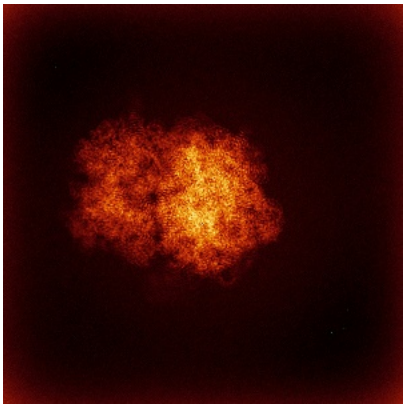
6.4.2 Raw map



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.

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6.5 Orthogonal surface views (i)

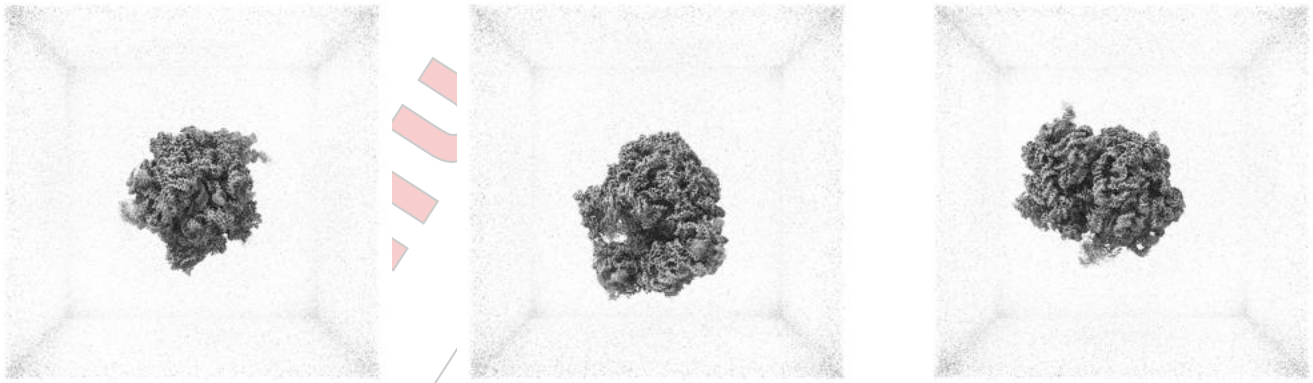
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

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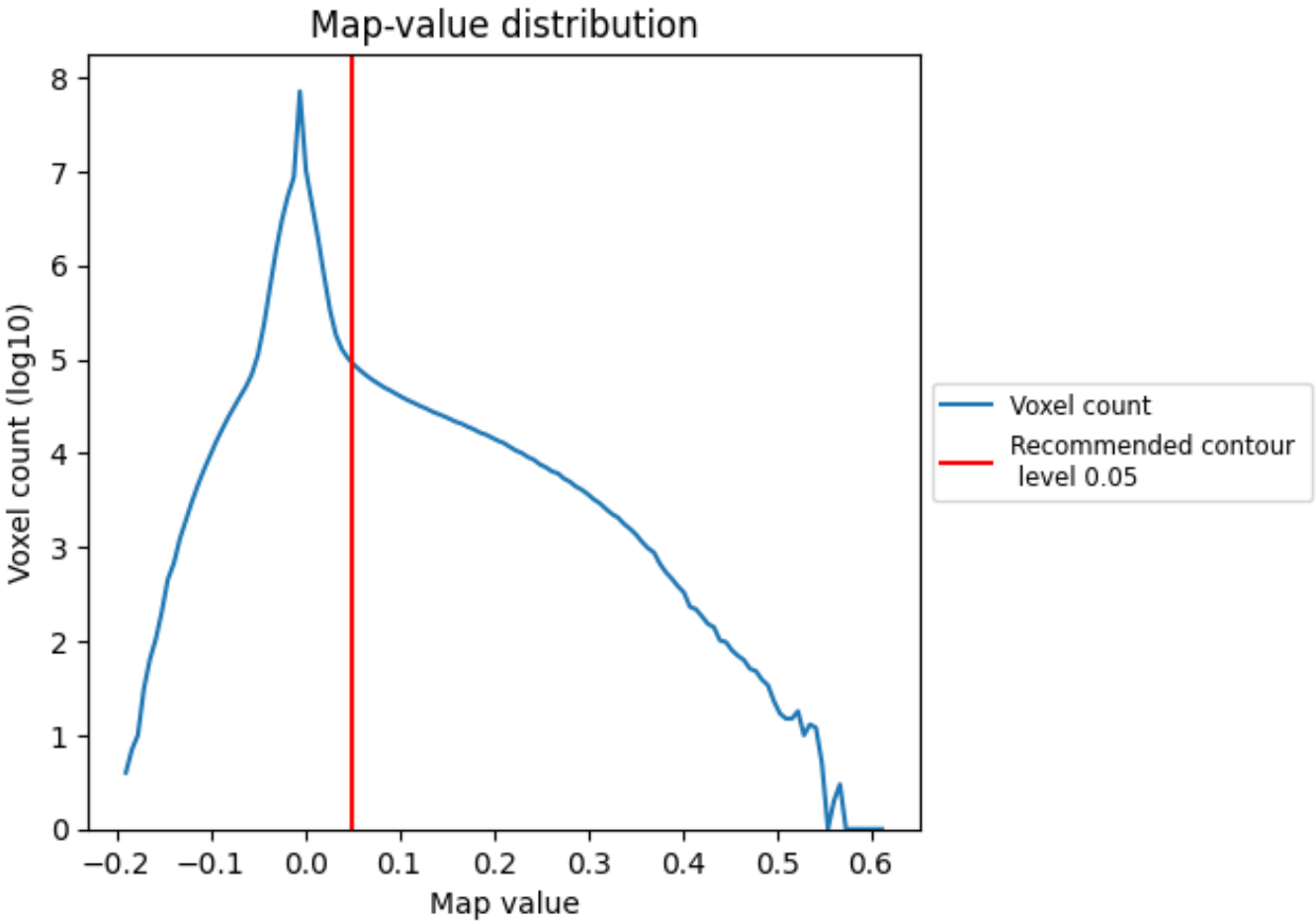
7 Map analysis

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.

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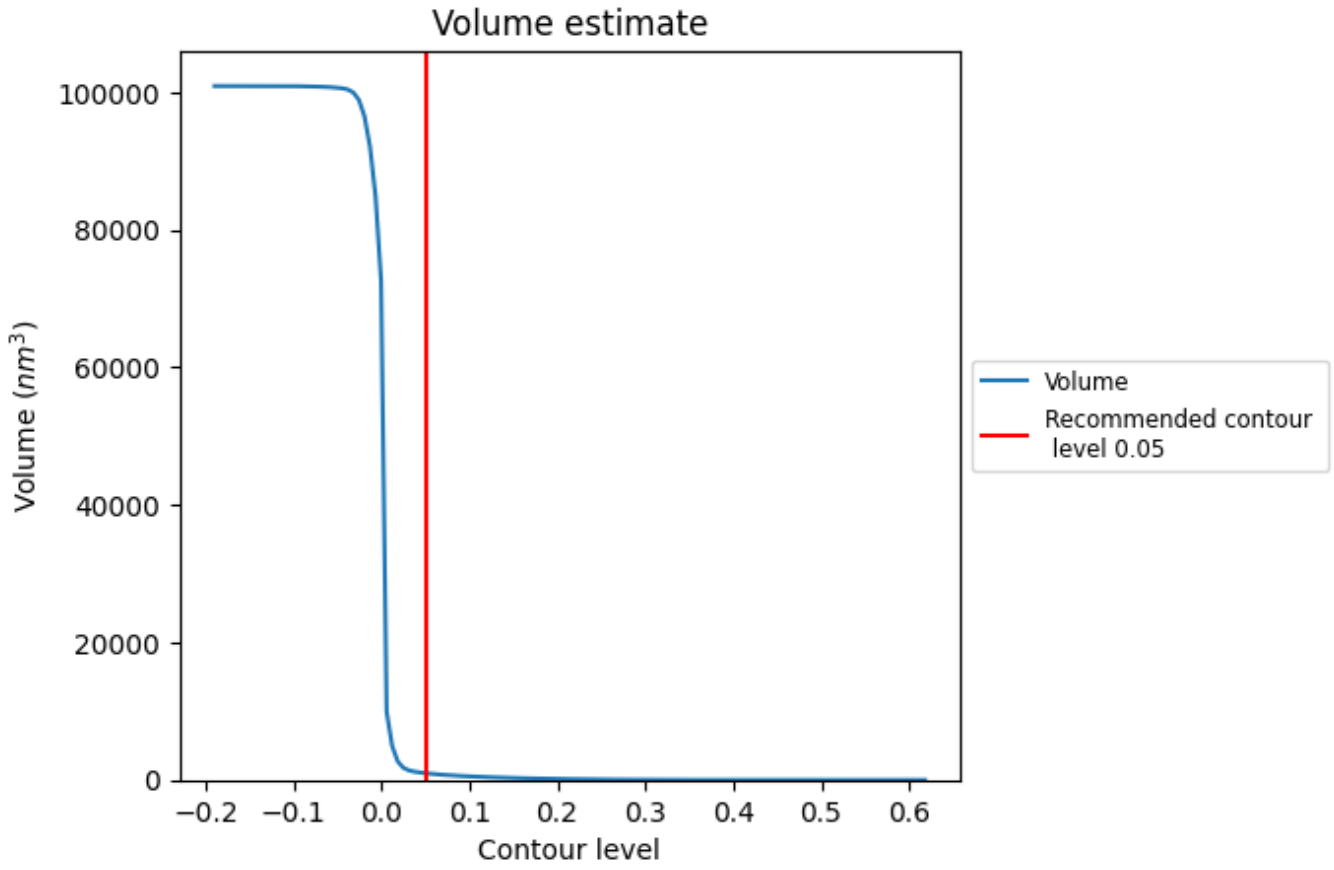
7.2 Volume estimate (i)



The volume at the recommended contour level is 980 nm^3; this corresponds to an approximate mass of 885 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.

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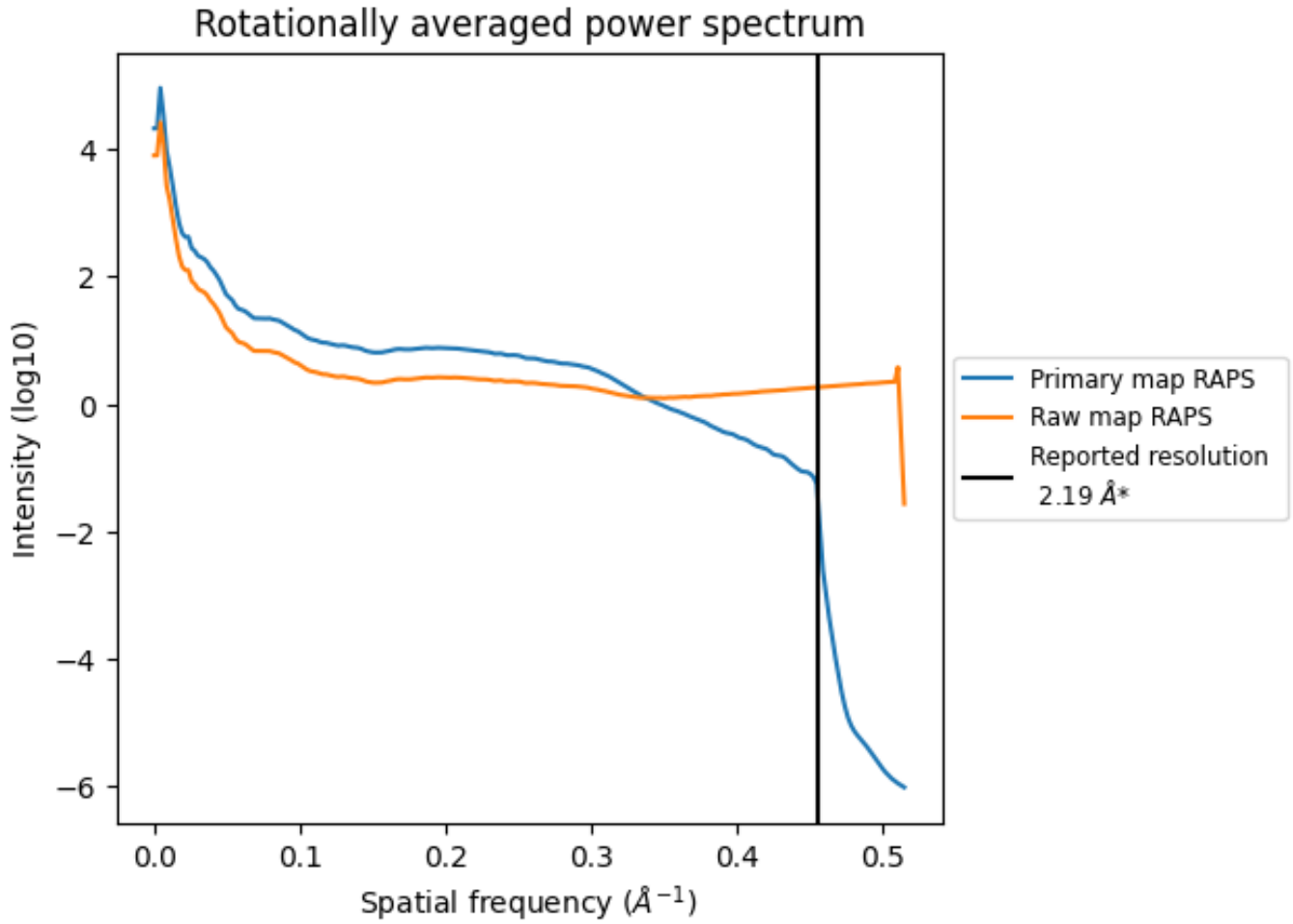
7.3 Rotationally averaged power spectrum (i)



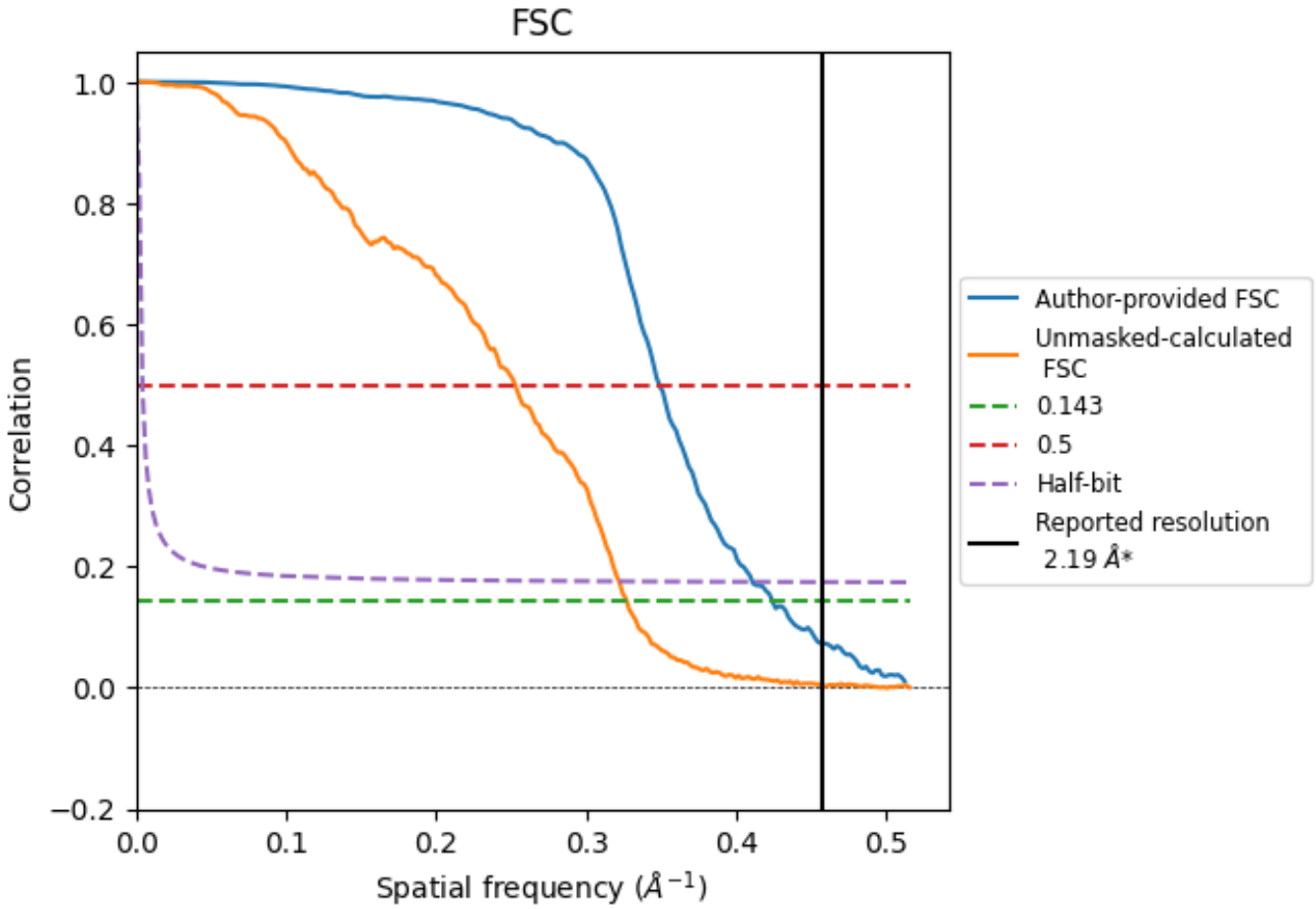
*Reported resolution corresponds to spatial frequency of 0.457 Å^{-1}

For Manu

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 0.457 Å^{-1}

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8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	2.36	2.87	2.43
Unmasked-calculated*	3.06	3.96	3.11

*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 3.06 differs from the reported value 2.19 by more than 10 %

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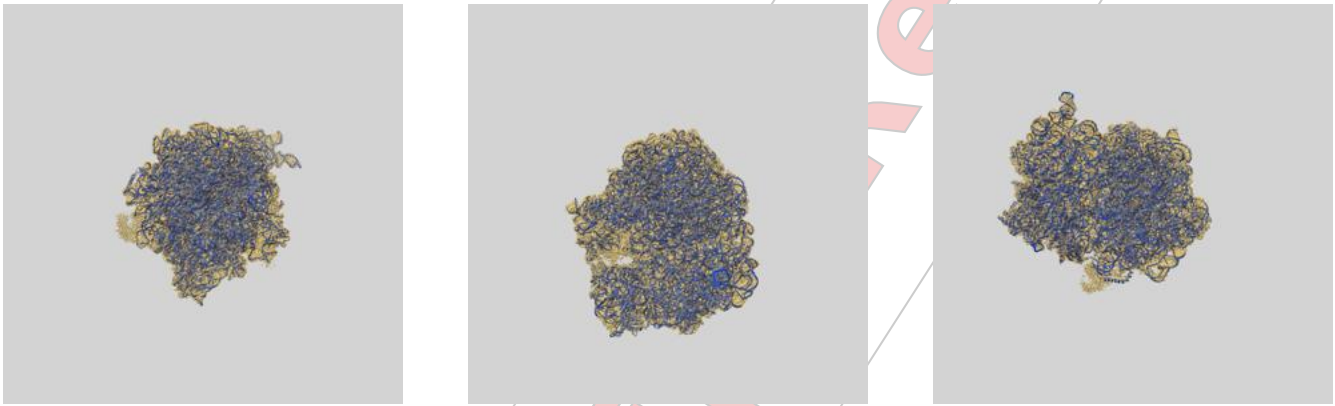
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-82546 and PDB model 44EW. 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 0.05 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.

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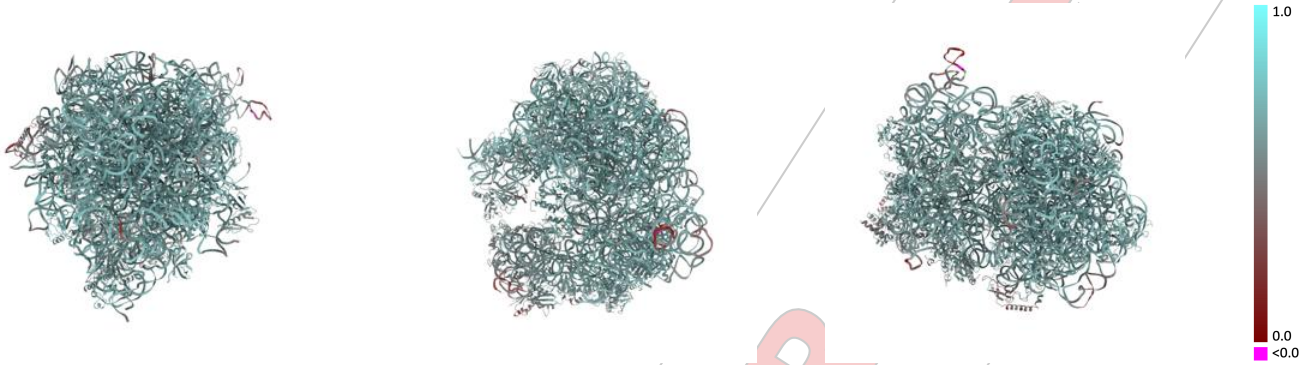
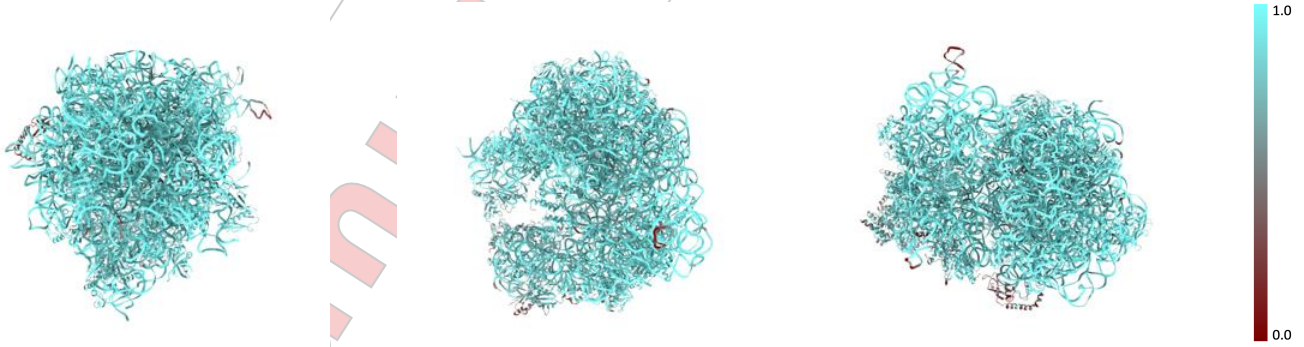
9.2 Q-score mapped to coordinate model



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 (0.05).

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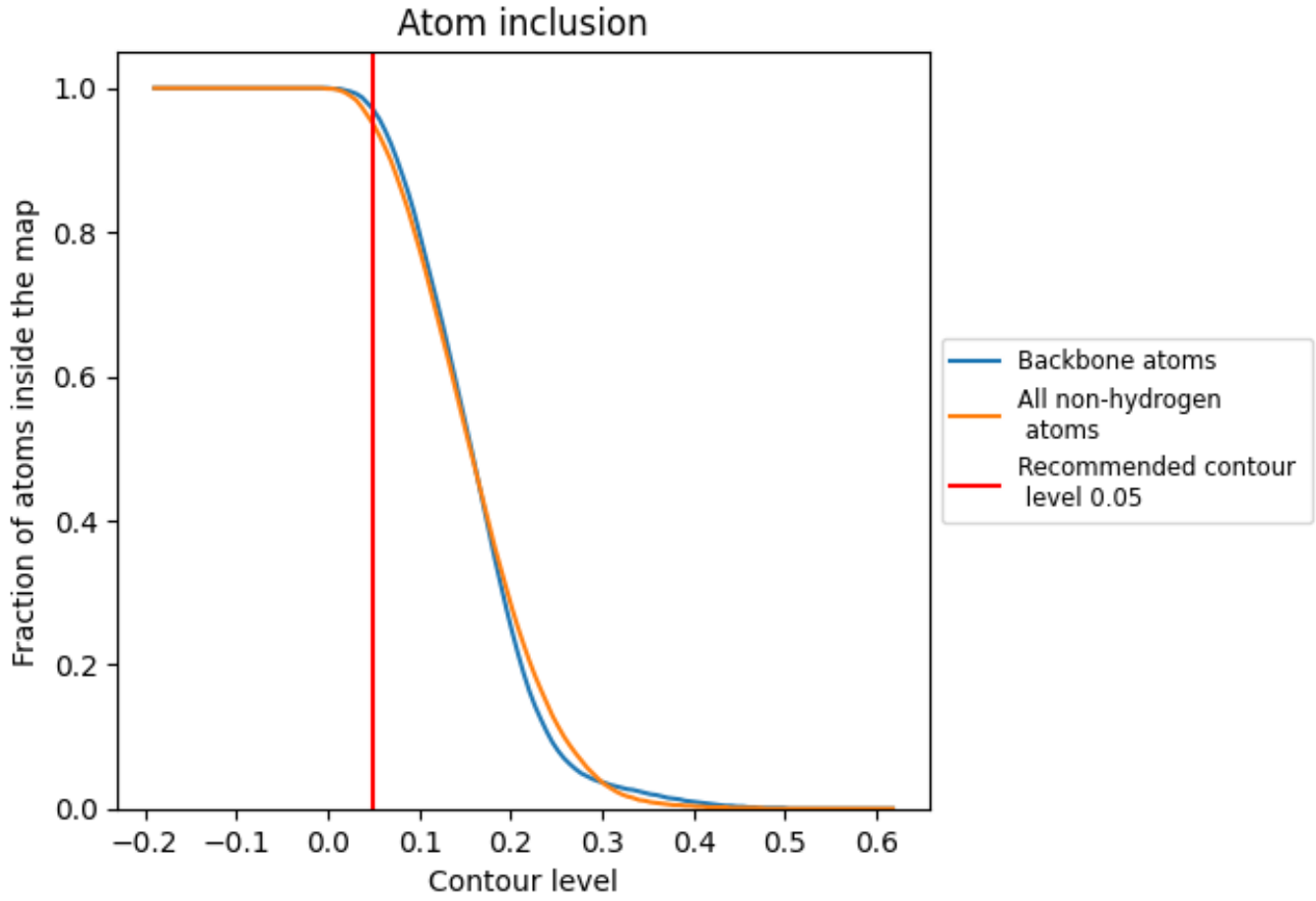
9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

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9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9490	0.6320
0	0.9890	0.6530
1	0.9870	0.6340
2	0.9680	0.6140
A	0.9730	0.6760
B	0.9670	0.6700
C	0.9320	0.6400
D	0.8420	0.5700
E	0.9040	0.5940
F	0.4640	0.4690
G	0.9600	0.6640
H	0.9650	0.6690
I	0.9600	0.6630
J	0.9590	0.6550
K	0.9860	0.6790
L	0.9340	0.6310
M	0.9430	0.6620
N	0.9800	0.6780
O	0.9490	0.6560
P	0.9470	0.6570
Q	0.9240	0.6370
R	0.9310	0.6250
S	0.9210	0.6330
T	0.9590	0.6740
U	0.9600	0.6620
V	0.9250	0.6120
W	0.9560	0.6630
X	0.7470	0.5290
Y	0.8930	0.6210
Z	0.9230	0.6370
a	0.9760	0.6690
b	0.9460	0.6480
c	0.9750	0.6820
d	0.9780	0.6840
e	0.9660	0.6670



Continued on next page...

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Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.7040	0.5380
g	0.8530	0.5900
h	0.9240	0.6230
i	0.9430	0.6370
j	0.8600	0.5710
k	0.6380	0.5370
l	0.9420	0.6410
m	0.7700	0.5350
n	0.6660	0.5080
o	0.8930	0.5910
p	0.9300	0.6490
q	0.7800	0.5590
r	0.8630	0.5760
s	0.9260	0.6160
t	0.9440	0.6270
u	0.9050	0.6210
v	0.8740	0.5980
w	0.7660	0.5490
x	0.9370	0.6210
y	0.5070	0.5080

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