



Full wwPDB EM Validation Report ⓘ

Jul 22, 2022 – 12:46 PM JST

PDB ID : 7YI4
EMDB ID : EMD-33851
Title : Cryo-EM structure of Rpd3S complex bound to H3K36me3 nucleosome in close state
Deposited on : 2022-07-14
Resolution : 3.96 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:

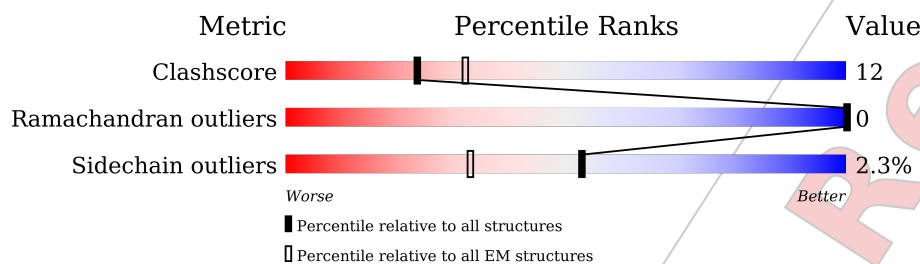
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	?? (??), CSD ??CSD?? (???)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.96 Å.

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



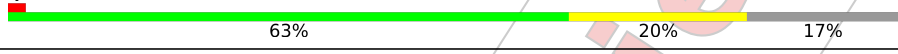
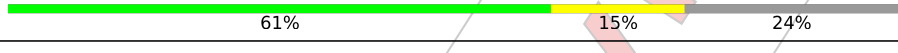
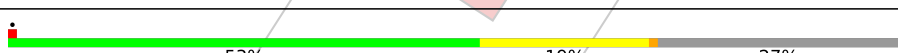
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1536	12% 25% 8% 67%
2	B	433	61% 22% 15%
3	C	401	21% 47% 23% 29%
3	E	401	24% 18% 7% 74%
4	D	684	14% 30% 16% 54%
4	F	684	97%
5	H	102	57% 21% 23%
5	L	102	66% 13% 21%

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Mol	Chain	Length	Quality of chain
6	I	129	
6	M	129	
7	J	122	
7	N	122	
8	O	167	
9	P	167	
10	G	135	
10	K	135	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 25351 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 protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	506	Total	C	N	O	S	0	0
			4258	2737	712	796	13		

- Molecule 2 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	368	Total	C	N	O	S	0	0
			2923	1858	495	545	25		

- Molecule 3 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	286	Total	C	N	O	S	0	0
			2326	1495	379	438	14		
3	E	104	Total	C	N	O	S	0	0
			853	551	142	155	5		

- Molecule 4 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	316	Total	C	N	O	S	0	0
			2588	1644	445	481	18		
4	F	20	Total	C	N	O	S	0	0
			178	117	30	30	1		

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	79	Total	C	N	O	S	0	0
			633	399	124	109	1		
5	L	81	Total	C	N	O	S	0	0
			646	407	126	112	1		

- Molecule 6 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	107	Total	C	N	O	0	0
			823	519	161	143		
6	M	107	Total	C	N	O	0	0
			823	519	161	143		

- Molecule 7 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	93	Total	C	N	O	0	0
			726	457	130	137		
7	N	93	Total	C	N	O	0	0
			726	457	130	137		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	29	THR	SER	engineered mutation	UNP P02281
N	29	THR	SER	engineered mutation	UNP P02281

- Molecule 8 is a DNA chain called Wisdom 601 DNA (167-MER).

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	151	Total	C	N	O	0	0
			3076	1462	554	909		

- Molecule 9 is a DNA chain called Wisdom 601 DNA (167-MER).

Mol	Chain	Residues	Atoms				AltConf	Trace
9	P	151	Total	C	N	O	0	0
			3115	1474	587	903		

- Molecule 10 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	G	100	Total	C	N	O	0	0
			830	526	160	141		
10	K	99	Total	C	N	O	0	0
			822	521	159	140		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

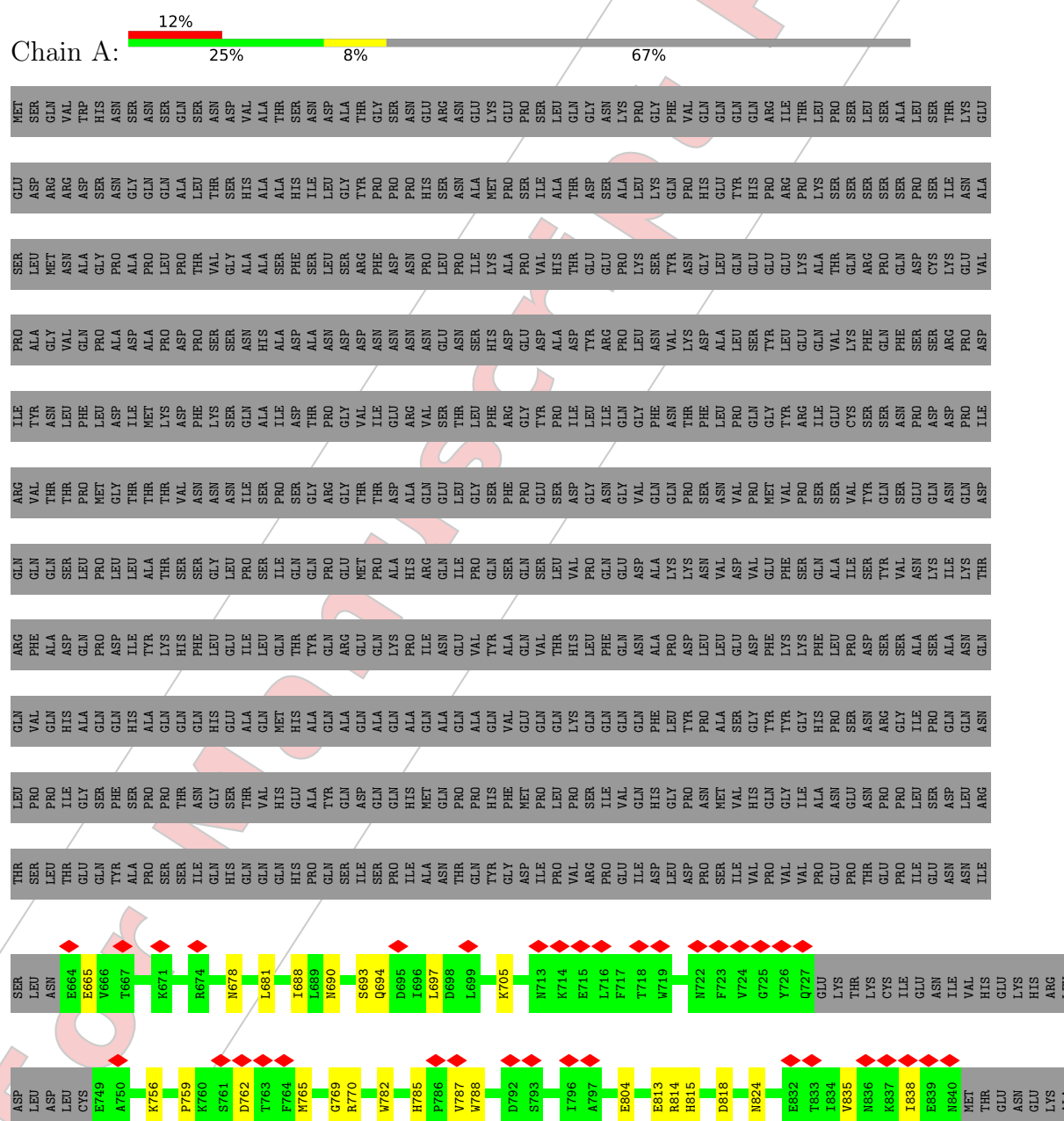
Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total 1	Zn 1	0
11	D	4	Total 4	Zn 4	0

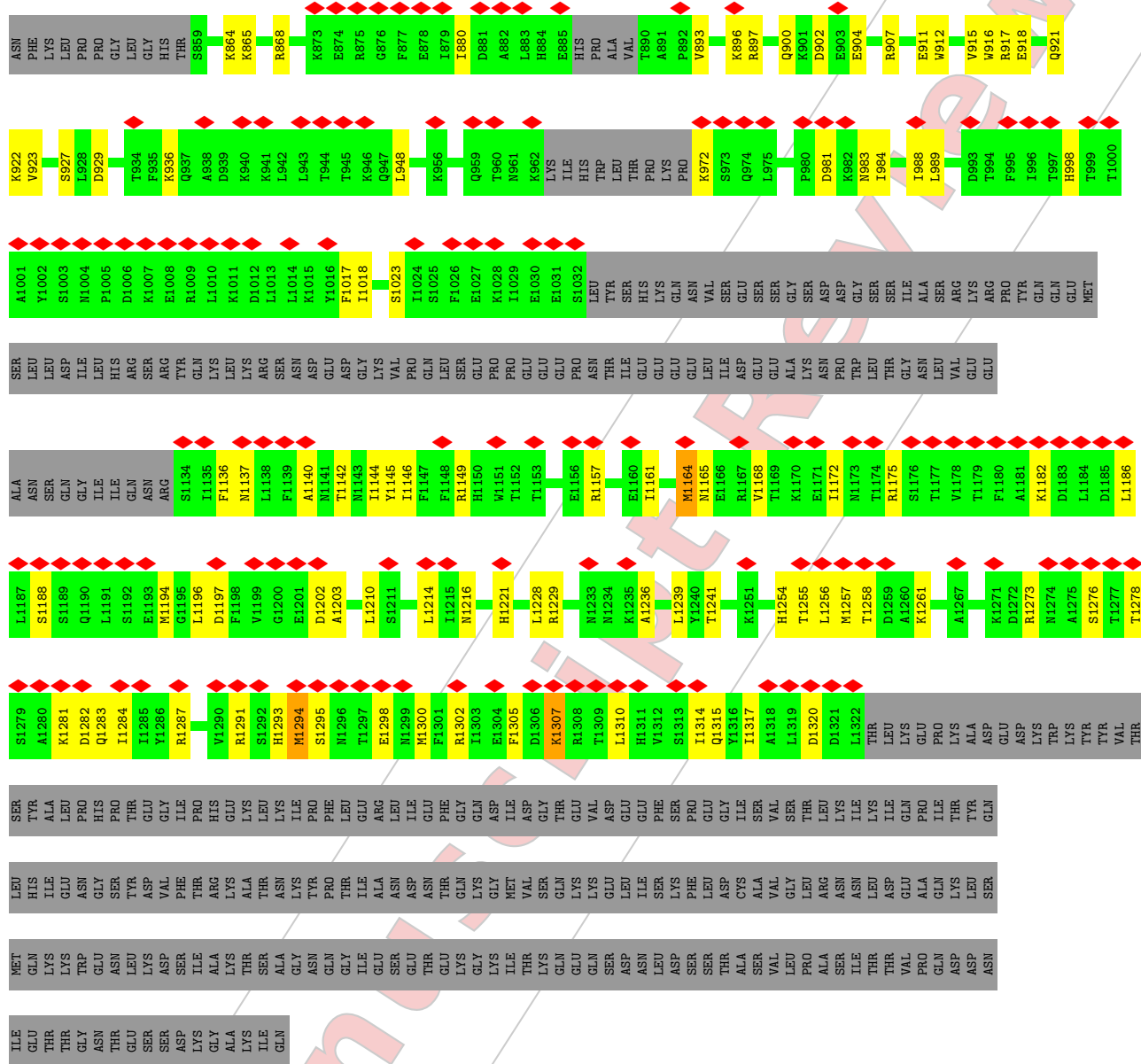
For Manuscript Review

3 Residue-property plots

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.

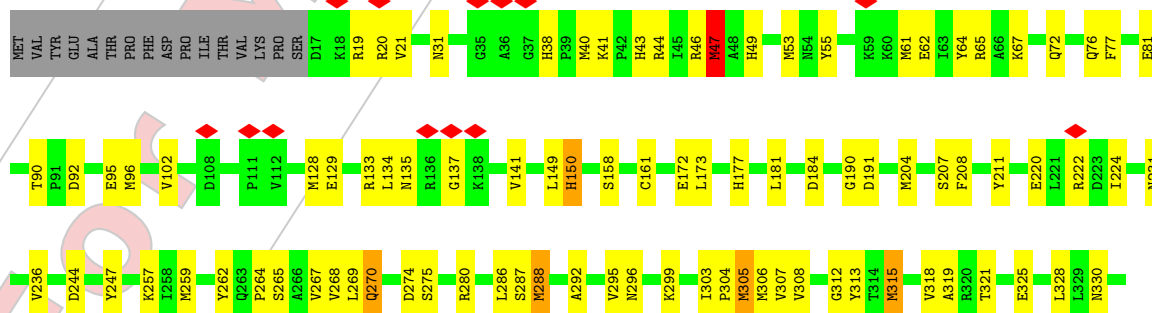
- Molecule 1: Transcriptional regulatory protein SIN3

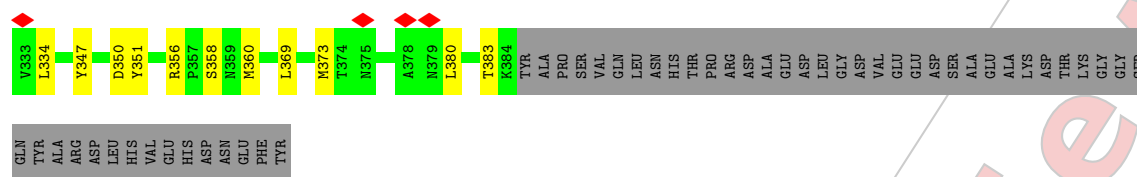




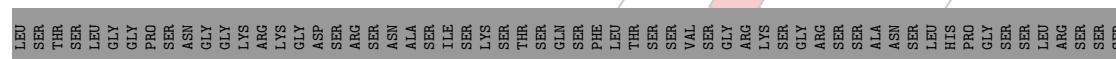
● Molecule 2: Histone deacetylase RPD3

Chain B: 61% 22% 15%

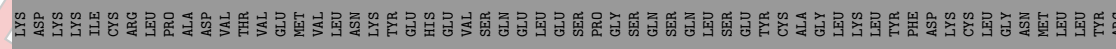
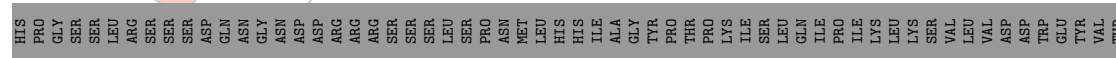
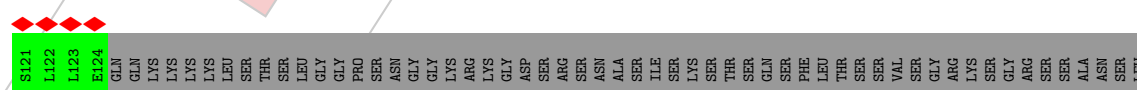
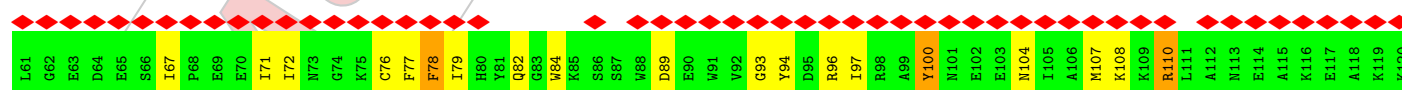
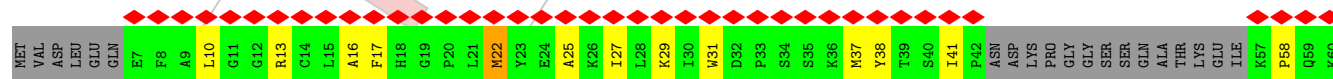




• Molecule 3: Chromatin modification-related protein EAF3



• Molecule 3: Chromatin modification-related protein EAF3



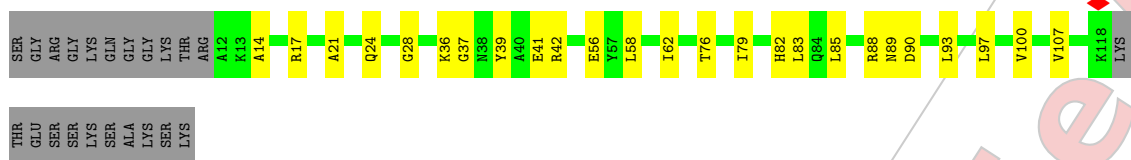
Chain D:  14% 30% 16% 40%

Chain D:



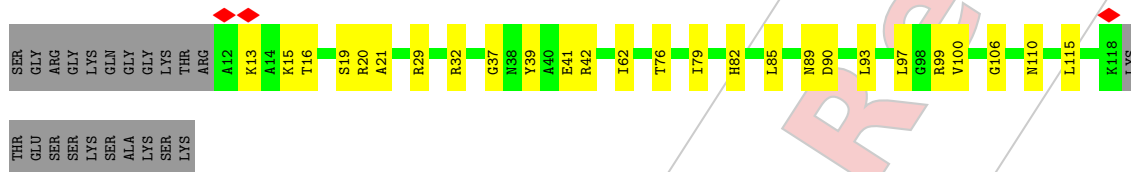
Chain F:

97%



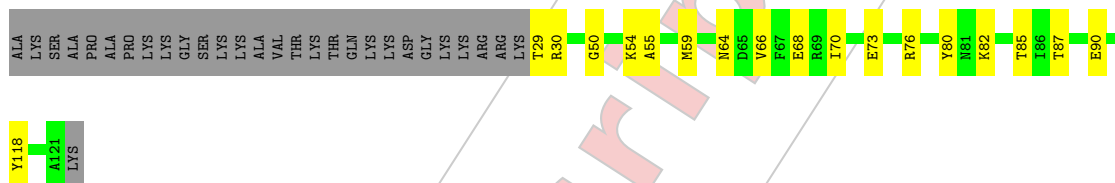
Molecule 6: Histone H2A

Chain M: 63% 20% 17%



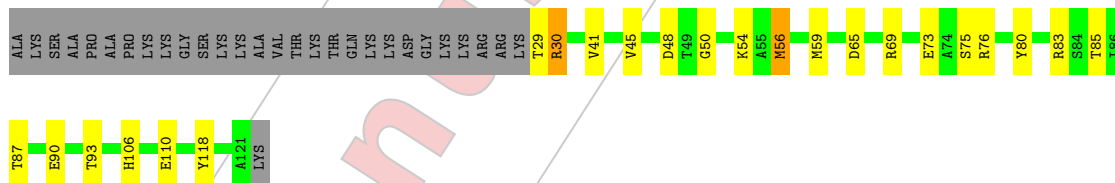
Molecule 7: Histone H2B 1.1

Chain J: 61% 15% 24%



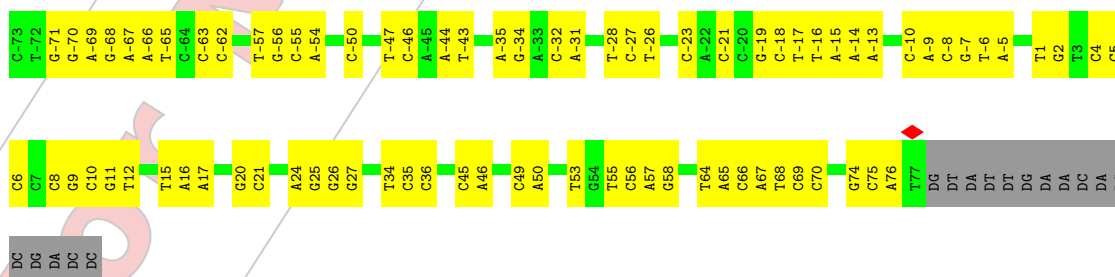
Molecule 7: Histone H2B 1.1

Chain N: 57% 17% 24%



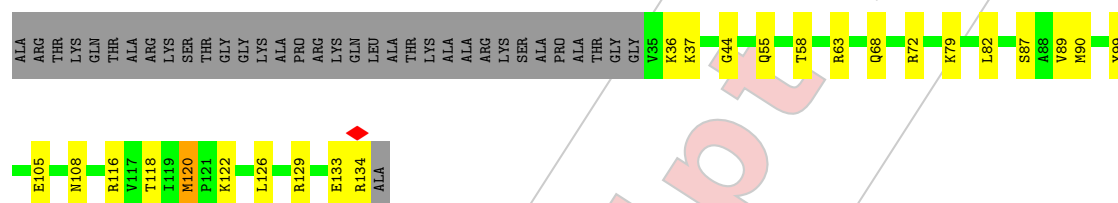
Molecule 8: Wisdom 601 DNA (167-MER)

Chain O: 42% 49% 10%



Molecule 9: Wisdom 601 DNA (167-MER)

- Molecule 10: Histone H3



- Molecule 10: Histone H3



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87742	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	324.75, 324.75, 324.75	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M3L

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/4346	0.48	1/5848 (0.0%)
2	B	0.26	0/2997	0.52	1/4051 (0.0%)
3	C	0.26	0/2374	0.48	0/3202
3	E	0.26	0/875	0.52	0/1174
4	D	0.25	0/2649	0.44	0/3566
4	F	0.24	0/181	0.38	0/237
5	H	0.28	0/640	0.56	0/857
5	L	0.27	0/653	0.65	1/873 (0.1%)
6	I	0.26	0/833	0.50	0/1124
6	M	0.26	0/833	0.50	0/1124
7	J	0.27	0/737	0.48	0/993
7	N	0.27	0/737	0.52	0/993
8	O	0.58	0/3445	0.92	0/5310
9	P	0.56	0/3499	0.89	0/5403
10	G	0.27	0/830	0.55	0/1114
10	K	0.27	0/823	0.58	0/1106
All	All	0.37	0/26452	0.65	3/36975 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	49	LEU	CA-CB-CG	7.94	133.57	115.30
1	A	1164	MET	CA-CB-CG	6.99	125.18	113.30
2	B	47	MET	CA-CB-CG	6.57	124.47	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4258	0	4211	87	0
2	B	2923	0	2805	73	0
3	C	2326	0	2337	85	0
3	E	853	0	840	23	0
4	D	2588	0	2534	88	0
4	F	178	0	185	5	0
5	H	633	0	673	14	0
5	L	646	0	687	15	0
6	I	823	0	882	18	0
6	M	823	0	882	19	0
7	J	726	0	747	13	0
7	N	726	0	747	17	0
8	O	3076	0	1697	74	0
9	P	3115	0	1694	95	0
10	G	830	0	881	22	0
10	K	822	0	871	26	0
11	B	1	0	0	0	0
11	D	4	0	0	0	0
All	All	25351	0	22673	583	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 12.

All (583) 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)
8:O:-50:DC:N3	9:P:50:DG:N1	2.23	0.86
4:D:420:CYS:SG	4:D:448:HIS:CE1	2.70	0.84
3:C:347:MET:SD	3:C:351:SER:OG	2.38	0.82
8:O:66:DC:H2'	8:O:67:DA:C8	2.15	0.81
9:P:61:DC:H2'	9:P:62:DG:C8	2.16	0.81
2:B:128:MET:HB3	4:D:182:ARG:HD2	1.60	0.80
8:O:70:DC:N3	9:P:-70:DG:N1	2.27	0.79
4:D:417:CYS:HB3	4:D:420:CYS:SG	2.22	0.79
8:O:-50:DC:O2	9:P:50:DG:N2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:66:DC:H42	9:P:-66:DG:H1	1.30	0.78
10:K:107:THR:HG22	10:K:119:ILE:HD12	1.64	0.77
8:O:70:DC:O2	9:P:-70:DG:N2	2.11	0.77
3:C:323:ILE:O	3:C:324:ARG:NH1	2.19	0.76
3:C:99:ALA:O	3:C:104:ASN:ND2	2.20	0.74
8:O:-21:DC:O2	9:P:21:DG:N2	2.13	0.74
3:E:76:CYS:HA	3:E:93:GLY:HA2	1.70	0.73
8:O:-21:DC:N3	9:P:21:DG:N1	2.27	0.73
3:C:313:SER:OG	3:C:318:LYS:O	2.06	0.73
1:A:1023:SER:OG	1:A:1273:ARG:NH2	2.21	0.72
5:H:31:LYS:HG2	5:H:32:PRO:HD3	1.72	0.72
6:I:42:ARG:NH2	7:J:85:THR:OG1	2.23	0.71
2:B:19:ARG:NH2	2:B:299:LYS:O	2.24	0.71
6:M:41:GLU:HG3	6:M:42:ARG:HG3	1.71	0.71
4:D:265:ALA:HB3	4:D:286:CYS:HB3	1.71	0.71
9:P:17:DA:H4'	10:G:63:ARG:HD3	1.72	0.71
3:C:253:THR:HA	3:C:327:GLY:HA3	1.73	0.70
9:P:-74:DC:H2'	9:P:-73:DA:H8	1.56	0.70
6:M:42:ARG:NH1	7:N:85:THR:OG1	2.26	0.69
3:C:76:CYS:HA	3:C:93:GLY:HA2	1.75	0.68
3:C:300:ARG:NH2	3:C:401:MET:O	2.26	0.68
6:M:90:ASP:HB3	6:M:93:LEU:HB2	1.76	0.68
10:G:129:ARG:NH2	10:K:105:GLU:OE1	2.27	0.68
5:H:42:GLY:O	10:G:108:ASN:ND2	2.27	0.67
3:C:297:LEU:O	3:C:333:ARG:NH1	2.26	0.67
2:B:44:ARG:HA	2:B:47:MET:SD	2.35	0.67
2:B:274:ASP:OD1	2:B:312:GLY:N	2.27	0.66
5:H:39:ARG:NH1	5:H:43:VAL:O	2.28	0.66
5:H:59:LYS:O	5:H:63:GLU:HG2	1.95	0.66
3:C:293:LEU:HD23	3:C:322:PRO:HB2	1.76	0.66
5:H:65:VAL:HA	5:H:93:GLN:HE22	1.62	0.65
4:D:120:SER:O	4:D:123:ILE:N	2.26	0.65
3:E:100:TYR:HA	3:E:104:ASN:HD22	1.61	0.64
6:M:15:LYS:O	6:M:20:ARG:NH1	2.31	0.64
1:A:1300:MET:SD	1:A:1300:MET:N	2.71	0.64
2:B:53:MET:HG2	4:D:169:THR:HA	1.80	0.64
7:N:29:THR:OG1	7:N:30:ARG:N	2.31	0.64
4:D:503:GLN:NE2	4:D:504:LEU:O	2.31	0.63
2:B:259:MET:HE2	2:B:264:PRO:HD2	1.81	0.63
2:B:149:LEU:HB3	2:B:161:CYS:HB3	1.80	0.63
3:E:17:PHE:O	3:E:96:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:106:SER:HB2	4:D:114:PRO:HB3	1.81	0.62
8:O:64:DT:H2"	8:O:65:DA:C8	2.34	0.62
1:A:921:GLN:HE22	1:A:1188:SER:HB2	1.64	0.62
3:C:22:MET:SD	3:C:22:MET:N	2.72	0.62
1:A:765:MET:HE2	2:B:81:GLU:HG2	1.80	0.62
3:C:234:ASP:OD1	4:D:496:ARG:NH1	2.33	0.62
1:A:688:ILE:HD13	1:A:705:LYS:HG2	1.81	0.62
9:P:-6:DG:H2"	9:P:-5:DG:C8	2.35	0.62
2:B:133:ARG:HG2	4:D:181:ILE:HD11	1.82	0.61
10:G:105:GLU:OE1	10:K:129:ARG:NH2	2.33	0.61
7:N:106:HIS:O	7:N:110:GLU:HG2	2.00	0.61
9:P:62:DG:H2"	9:P:63:DG:C8	2.36	0.61
6:M:85:LEU:O	6:M:89:ASN:ND2	2.33	0.61
4:D:113:LEU:HD11	4:D:120:SER:HB2	1.82	0.61
9:P:71:DC:H2"	9:P:72:DA:C8	2.36	0.61
8:O:-71:DG:H2"	8:O:-70:DG:H5"	1.82	0.60
3:C:376:ASP:HB3	4:D:491:VAL:HB	1.82	0.60
4:D:266:CYS:HB3	4:D:286:CYS:SG	2.41	0.60
6:M:39:TYR:HB3	7:N:75:SER:HB2	1.83	0.60
8:O:17:DA:OP2	10:K:69:ARG:NH1	2.31	0.60
1:A:1137:ASN:OD1	1:A:1302:ARG:NH1	2.33	0.60
2:B:208:PHE:HA	2:B:236:VAL:HB	1.83	0.60
7:J:87:THR:OG1	7:J:90:GLU:OE1	2.18	0.60
5:L:39:ARG:NH1	5:L:43:VAL:O	2.33	0.60
4:D:548:LYS:HE3	4:F:548:LYS:HE3	1.84	0.60
3:C:290:ASP:HA	3:C:322:PRO:HG2	1.83	0.59
3:C:255:GLU:HB2	3:C:324:ARG:NH1	2.17	0.59
8:O:-7:DG:H2"	8:O:-6:DT:H71	1.84	0.59
4:D:263:CYS:HB2	4:D:283:HIS:ND1	2.17	0.59
3:C:88:TRP:HE3	10:G:36:M3L:HM13	1.66	0.59
8:O:-47:DT:H2"	8:O:-46:DC:C5	2.37	0.59
9:P:-74:DC:H2'	9:P:-73:DA:C8	2.37	0.59
1:A:1161:ILE:HG13	1:A:1239:LEU:HD11	1.84	0.59
2:B:184:ASP:HB3	2:B:207:SER:HA	1.84	0.59
3:C:256:MET:HE2	3:C:324:ARG:HH22	1.67	0.59
7:J:29:THR:OG1	7:J:30:ARG:N	2.35	0.59
8:O:35:DC:H2"	8:O:36:DC:C5	2.38	0.59
2:B:129:GLU:OE2	4:D:181:ILE:N	2.36	0.59
4:D:510:GLN:HG2	4:D:512:ILE:H	1.66	0.58
3:C:15:LEU:HD11	3:C:22:MET:HG2	1.85	0.58
1:A:972:LYS:HA	1:A:1315:GLN:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:87:THR:OG1	7:N:90:GLU:OE1	2.20	0.58
8:O:-8:DC:H2''	8:O:-7:DG:C8	2.38	0.58
3:C:78:PHE:HB2	3:C:91:TRP:CE2	2.38	0.58
2:B:38:HIS:CE1	2:B:40:MET:HG2	2.39	0.58
7:J:66:VAL:O	7:J:70:ILE:HG12	2.03	0.58
6:M:76:THR:O	7:N:50:GLY:N	2.35	0.58
9:P:-38:DA:H2''	9:P:-37:DG:C8	2.37	0.58
2:B:244:ASP:OD2	2:B:287:SER:OG	2.20	0.58
3:C:378:ASP:N	4:D:489:TYR:OH	2.35	0.58
3:C:27:ILE:HA	3:C:79:ILE:HG22	1.85	0.58
8:O:9:DG:N3	10:K:40:ARG:NH2	2.52	0.58
1:A:678:ASN:HD22	1:A:681:LEU:HG	1.69	0.58
8:O:15:DT:H2''	8:O:16:DA:C8	2.39	0.57
7:J:59:MET:SD	7:J:59:MET:N	2.77	0.57
7:N:83:ARG:NH2	9:P:-33:DG:OP2	2.36	0.57
8:O:-7:DG:H2''	8:O:-6:DT:C7	2.34	0.57
3:C:108:LYS:HG3	3:C:109:LYS:HE2	1.86	0.57
8:O:67:DA:H2''	8:O:68:DT:H5''	1.86	0.57
4:D:262:PHE:O	4:D:281:SER:OG	2.22	0.57
8:O:8:DC:H2''	8:O:9:DG:C8	2.39	0.57
9:P:-39:DT:H2''	9:P:-38:DA:C8	2.39	0.57
4:D:365:LYS:HG2	4:D:373:SER:HB2	1.86	0.57
9:P:-69:DG:H1'	9:P:-68:DA:H5'	1.87	0.57
8:O:45:DC:H2''	8:O:46:DA:N7	2.20	0.57
9:P:61:DC:H2''	9:P:62:DG:H5'	1.86	0.57
3:E:31:TRP:HE3	3:E:38:TYR:HB3	1.70	0.57
4:D:277:THR:OG1	4:D:306:CYS:SG	2.63	0.57
1:A:922:LYS:HG3	1:A:923:VAL:HG23	1.86	0.56
5:L:52:GLU:N	5:L:52:GLU:OE1	2.38	0.56
7:N:76:ARG:HG2	7:N:80:TYR:CZ	2.40	0.56
4:D:476:LYS:HG3	4:D:490:LYS:HB2	1.87	0.56
10:G:129:ARG:HB2	10:G:134:ARG:HD3	1.87	0.56
2:B:95:GLU:HG2	2:B:96:MET:SD	2.46	0.56
9:P:3:DC:H2''	9:P:4:DG:N7	2.19	0.56
3:C:236:TRP:O	3:C:240:THR:OG1	2.22	0.56
3:C:324:ARG:CZ	3:C:324:ARG:HA	2.35	0.56
3:E:107:MET:HB2	3:E:110:ARG:NH2	2.20	0.56
10:K:108:ASN:HA	10:K:119:ILE:HD11	1.87	0.56
1:A:1196:LEU:HD22	1:A:1210:LEU:HD21	1.88	0.56
6:I:85:LEU:O	6:I:89:ASN:ND2	2.36	0.56
1:A:1194:MET:SD	1:A:1196:LEU:HG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ARG:NH2	2:B:77:PHE:O	2.38	0.55
3:C:323:ILE:HG13	3:C:324:ARG:HD2	1.88	0.55
9:P:-28:DC:H2''	9:P:-27:DC:C5	2.42	0.55
3:C:330:HIS:HA	3:C:333:ARG:HG2	1.88	0.55
6:I:42:ARG:CZ	8:O:-35:DA:H4'	2.37	0.55
1:A:694:GLN:OE1	4:D:516:ASN:ND2	2.40	0.55
3:C:289:PHE:CE2	3:C:293:LEU:HD22	2.42	0.55
3:C:22:MET:SD	3:C:108:LYS:HA	2.46	0.55
4:D:520:ILE:HB	4:D:542:ILE:HB	1.88	0.55
5:L:37:LEU:HD22	10:K:61:LEU:HD12	1.89	0.55
3:C:113:ASN:O	3:C:117:GLU:HG2	2.07	0.54
4:D:437:ILE:HD11	4:D:446:PRO:HB2	1.89	0.54
1:A:1282:ASP:OD1	1:A:1283:GLN:N	2.40	0.54
8:O:4:DC:H2''	8:O:5:DC:C5	2.42	0.54
10:G:99:TYR:OH	10:G:133:GLU:OE1	2.24	0.54
10:G:116:ARG:NH1	10:G:118:THR:O	2.41	0.54
3:C:342:ILE:O	3:C:345:THR:OG1	2.25	0.54
3:E:67:ILE:HB	3:E:72:ILE:HD13	1.90	0.54
1:A:1294:MET:SD	1:A:1298:GLU:HG3	2.48	0.54
6:I:58:LEU:O	6:I:62:ILE:HG22	2.08	0.54
7:N:48:ASP:OD1	7:N:48:ASP:N	2.39	0.54
9:P:-7:DG:H2''	9:P:-6:DG:N7	2.23	0.54
3:C:289:PHE:HD2	3:C:323:ILE:HG22	1.73	0.54
9:P:-4:DG:H2''	9:P:-3:DA:C8	2.43	0.54
2:B:275:SER:HB3	2:B:286:LEU:HD12	1.90	0.54
9:P:8:DG:H2'	9:P:9:DT:H71	1.90	0.54
3:E:67:ILE:HG22	3:E:71:ILE:HG13	1.90	0.53
1:A:814:ARG:HG2	1:A:916:TRP:CE3	2.44	0.53
9:P:-44:DG:H2''	9:P:-43:DA:H8	1.73	0.53
10:G:129:ARG:HA	10:G:134:ARG:HB2	1.90	0.53
4:D:278:CYS:HB2	4:D:306:CYS:SG	2.48	0.53
5:L:37:LEU:HB3	10:K:104:PHE:HE2	1.74	0.53
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.89	0.53
1:A:1294:MET:SD	1:A:1295:SER:N	2.81	0.53
3:C:70:GLU:HG2	3:C:71:ILE:HG23	1.91	0.53
9:P:-72:DC:H2''	9:P:-71:DA:C8	2.44	0.53
1:A:981:ASP:HB3	1:A:984:ILE:HD12	1.91	0.52
3:C:31:TRP:NE1	3:C:72:ILE:O	2.36	0.52
3:C:107:MET:HB3	3:C:110:ARG:HH21	1.73	0.52
3:C:256:MET:CE	3:C:324:ARG:HH22	2.22	0.52
1:A:824:ASN:OD1	1:A:902:ASP:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ASN:HB2	2:B:328:LEU:HD13	1.91	0.52
4:F:555:ILE:O	4:F:559:LYS:HG3	2.10	0.52
4:D:312:ILE:HD11	4:D:321:LYS:HD3	1.92	0.52
7:J:64:ASN:O	7:J:68:GLU:HG2	2.10	0.52
3:E:104:ASN:HA	3:E:107:MET:HG3	1.91	0.52
2:B:43:HIS:CE1	2:B:46:ARG:HE	2.27	0.52
9:P:50:DG:H2''	9:P:51:DG:H8	1.74	0.52
9:P:63:DG:H2''	9:P:64:DG:C8	2.45	0.52
3:C:271:SER:HB2	3:C:274:SER:HB2	1.92	0.52
8:O:70:DC:N4	9:P:-70:DG:O6	2.30	0.52
2:B:90:THR:HG22	2:B:92:ASP:H	1.75	0.52
3:C:8:PHE:HE1	3:C:97:ILE:HG22	1.74	0.52
4:D:378:LYS:HB2	4:D:463:LYS:HG3	1.91	0.52
1:A:864:LYS:HG2	1:A:880:ILE:HD13	1.90	0.52
5:H:50:ILE:O	5:H:54:THR:HG23	2.10	0.52
7:N:65:ASP:OD2	7:N:69:ARG:NH2	2.39	0.52
2:B:61:MET:SD	2:B:330:ASN:ND2	2.81	0.51
4:D:125:ARG:NH2	4:D:130:ASN:O	2.42	0.51
6:I:76:THR:O	7:J:50:GLY:N	2.32	0.51
2:B:270:GLN:HA	2:B:308:VAL:HG23	1.93	0.51
4:D:312:ILE:HG12	4:D:312:ILE:O	2.11	0.51
8:O:15:DT:H2''	8:O:16:DA:N7	2.26	0.51
1:A:915:VAL:HA	1:A:918:GLU:OE1	2.10	0.51
1:A:1165:ASN:ND2	1:A:1202:ASP:OD1	2.44	0.51
3:C:17:PHE:O	3:C:96:ARG:NH1	2.44	0.51
4:F:561:VAL:HA	4:F:564:ARG:HG2	1.93	0.51
5:H:29:ILE:O	5:H:55:ARG:NH2	2.43	0.51
9:P:12:DG:H1'	9:P:13:DT:H5'	1.92	0.51
7:J:73:GLU:OE1	7:J:76:ARG:NH1	2.44	0.51
5:L:49:LEU:O	5:L:49:LEU:HD23	2.11	0.51
9:P:49:DC:H2''	9:P:50:DG:H8	1.73	0.51
4:D:307:LYS:HA	4:D:310:ILE:HG22	1.92	0.51
8:O:-23:DC:OP2	10:G:72:ARG:NH2	2.42	0.51
9:P:3:DC:H2''	9:P:4:DG:C8	2.46	0.51
1:A:1284:ILE:HG13	1:A:1287:ARG:HH21	1.75	0.50
8:O:20:DG:H2''	8:O:21:DC:O5'	2.11	0.50
3:E:78:PHE:CE1	3:E:89:ASP:HB2	2.46	0.50
8:O:11:DG:H2'	8:O:12:DT:H71	1.92	0.50
3:C:17:PHE:HE1	3:C:98:ARG:HD2	1.77	0.50
5:H:38:ALA:HB1	5:H:43:VAL:HB	1.94	0.50
8:O:-6:DT:H2''	8:O:-5:DA:N7	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:16:THR:O	6:M:19:SER:OG	2.25	0.50
8:O:-26:DT:H5'	8:O:-26:DT:C6	2.46	0.50
8:O:56:DC:H1'	8:O:57:DA:C5	2.47	0.50
9:P:37:DC:H2''	9:P:38:DG:C8	2.46	0.50
10:G:120:MET:SD	10:G:120:MET:N	2.84	0.50
10:K:86:SER:O	10:K:90:MET:HE3	2.11	0.50
1:A:1136:PHE:HE1	1:A:1276:SER:HA	1.77	0.50
4:D:500:LYS:HD3	4:D:503:GLN:HB3	1.94	0.50
8:O:-44:DA:H2'	8:O:-43:DT:H71	1.94	0.50
3:E:89:ASP:OD1	3:E:89:ASP:N	2.43	0.50
2:B:96:MET:SD	2:B:96:MET:N	2.85	0.50
9:P:8:DG:H2''	9:P:9:DT:H5'	1.93	0.50
1:A:693:SER:HA	4:D:554:LYS:HD3	1.94	0.49
2:B:380:LEU:O	2:B:383:THR:OG1	2.29	0.49
3:C:29:LYS:HB2	3:C:78:PHE:HB3	1.94	0.49
3:C:31:TRP:HE3	3:C:38:TYR:HB3	1.77	0.49
8:O:24:DA:H2''	8:O:25:DG:C8	2.47	0.49
9:P:-43:DA:H2''	9:P:-42:DG:H8	1.76	0.49
1:A:912:TRP:HA	1:A:915:VAL:HG12	1.94	0.49
4:F:556:TYR:O	4:F:560:MET:HG2	2.13	0.49
6:I:79:ILE:HG12	6:I:82:HIS:CE1	2.47	0.49
3:E:25:ALA:HB3	3:E:79:ILE:HD12	1.94	0.49
4:D:332:ASN:OD1	4:D:332:ASN:N	2.45	0.49
5:L:58:LEU:HD12	10:K:100:LEU:HD11	1.94	0.49
6:M:110:ASN:N	10:G:55:GLN:OE1	2.44	0.49
2:B:134:LEU:HD22	2:B:304:PRO:HB3	1.94	0.49
5:L:39:ARG:HD2	10:K:50:GLU:HG3	1.94	0.49
1:A:813:GLU:HG2	4:D:111:THR:HG22	1.95	0.49
2:B:181:LEU:HB2	2:B:264:PRO:HG3	1.94	0.49
3:C:252:VAL:HG13	3:C:256:MET:HG3	1.94	0.49
3:C:347:MET:HG3	3:C:352:CYS:SG	2.52	0.49
4:D:424:ARG:HG3	4:D:448:HIS:CE1	2.47	0.49
5:L:84:MET:SD	5:L:88:TYR:CZ	3.06	0.49
1:A:818:ASP:OD1	2:B:43:HIS:NE2	2.44	0.49
3:C:247:ARG:NH2	3:C:384:ASP:O	2.45	0.49
3:C:321:VAL:HG12	3:C:323:ILE:HG12	1.95	0.49
4:D:272:PHE:HB3	4:D:281:SER:HB2	1.94	0.49
6:I:21:ALA:HB2	7:J:118:TYR:HB2	1.94	0.49
9:P:-32:DT:H2''	9:P:-31:DA:H8	1.78	0.49
4:D:424:ARG:HG3	4:D:448:HIS:HE1	1.78	0.49
1:A:1164:MET:SD	1:A:1168:VAL:HG13	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:VAL:O	2:B:305:MET:HA	2.13	0.49
4:D:264:SER:N	4:D:281:SER:O	2.45	0.49
8:O:-57:DT:H2''	8:O:-56:DG:N7	2.28	0.49
1:A:815:HIS:CG	2:B:41:LYS:HD3	2.48	0.48
3:C:103:GLU:O	3:C:107:MET:HG3	2.13	0.48
4:D:498:ILE:HD11	4:D:537:PHE:HD2	1.78	0.48
6:I:90:ASP:HB3	6:I:93:LEU:HB2	1.94	0.48
8:O:58:DG:N2	9:P:-57:DT:O2	2.46	0.48
9:P:56:DC:H2''	9:P:57:DA:N7	2.27	0.48
4:D:317:ALA:HA	4:D:320:LYS:HG2	1.96	0.48
4:D:374:ASP:N	4:D:374:ASP:OD1	2.44	0.48
6:I:37:GLY:HA3	6:I:39:TYR:CE2	2.49	0.48
6:M:21:ALA:HB2	7:N:118:TYR:HB2	1.95	0.48
1:A:912:TRP:HZ2	4:D:113:LEU:HD12	1.79	0.48
5:L:37:LEU:HB3	10:K:104:PHE:CE2	2.48	0.48
3:E:16:ALA:HB2	3:E:97:ILE:HG12	1.94	0.48
3:E:37:MET:SD	3:E:58:PRO:HA	2.53	0.48
2:B:62:GLU:OE1	2:B:64:TYR:OH	2.23	0.48
1:A:835:VAL:HA	1:A:838:ILE:HG22	1.94	0.48
2:B:358:SER:OG	2:B:360:MET:HG3	2.13	0.48
1:A:665:GLU:HB3	4:D:552:PHE:CE2	2.49	0.48
2:B:41:LYS:O	2:B:44:ARG:HG2	2.13	0.48
3:C:83:GLY:HA2	9:P:11:DC:H4'	1.95	0.48
3:C:292:CYS:HB2	3:C:296:MET:SD	2.54	0.48
3:C:337:VAL:HG12	4:D:354:PRO:HB3	1.95	0.48
8:O:-66:DA:H2'	8:O:-65:DT:H71	1.94	0.48
8:O:49:DC:H2''	8:O:50:DA:C8	2.48	0.48
9:P:9:DT:OP1	10:G:44:GLY:N	2.39	0.48
3:C:225:PRO:HD2	3:C:228:LEU:HD12	1.93	0.48
6:M:29:ARG:HG3	6:M:32:ARG:NH2	2.28	0.48
7:N:56:MET:HA	7:N:59:MET:HB2	1.96	0.48
9:P:43:DA:H1'	9:P:44:DT:H5'	1.96	0.48
3:C:224:ILE:HD12	4:D:357:ILE:HD11	1.95	0.48
4:D:408:ASP:HA	4:D:415:LEU:HD21	1.96	0.48
5:L:22:LEU:HB3	10:K:73:GLU:HB2	1.95	0.48
3:E:84:TRP:CE2	10:K:36:M3L:HM12	2.49	0.48
3:C:293:LEU:HD12	3:C:297:LEU:HB2	1.96	0.47
4:D:424:ARG:HD3	4:D:435:ARG:HG3	1.95	0.47
8:O:-54:DA:C8	8:O:-54:DA:H5'	2.49	0.47
2:B:128:MET:HE3	2:B:172:GLU:HB2	1.96	0.47
9:P:-27:DC:H4'	9:P:-26:DC:H5'	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:49:DC:H2''	9:P:50:DG:C8	2.47	0.47
9:P:17:DA:H2''	9:P:18:DG:H8	1.78	0.47
1:A:989:LEU:HD21	1:A:1018:ILE:HD13	1.97	0.47
1:A:1305:PHE:HZ	1:A:1310:LEU:HD23	1.78	0.47
2:B:141:VAL:HG22	2:B:305:MET:CE	2.43	0.47
3:C:250:ALA:HB3	3:C:253:THR:HG22	1.96	0.47
9:P:-24:DT:OP1	10:K:85:GLN:HG2	2.14	0.47
9:P:19:DC:H2''	9:P:20:DG:H8	1.79	0.47
2:B:135:ASN:ND2	2:B:172:GLU:HG3	2.29	0.47
1:A:1228:LEU:HD11	1:A:1239:LEU:HB2	1.96	0.47
1:A:1317:ILE:HG23	1:A:1320:ASP:HB3	1.97	0.47
3:C:253:THR:OG1	3:C:324:ARG:NH1	2.47	0.47
4:D:404:ASP:OD1	4:D:404:ASP:N	2.45	0.47
4:D:438:MET:HG3	4:D:447:TRP:O	2.15	0.47
8:O:20:DG:H4'	8:O:21:DC:OP1	2.15	0.47
1:A:804:GLU:HG3	1:A:927:SER:HB2	1.96	0.47
4:D:353:LEU:HB2	4:D:358:LYS:HE3	1.97	0.47
4:D:419:LYS:HD3	4:D:451:CYS:HB3	1.95	0.47
2:B:268:VAL:HA	2:B:306:MET:HB2	1.97	0.47
9:P:-48:DC:H2''	9:P:-47:DC:C6	2.50	0.47
9:P:15:DT:H2''	9:P:16:DA:C8	2.50	0.47
1:A:690:ASN:O	1:A:694:GLN:HG2	2.15	0.46
1:A:936:LYS:HG2	1:A:1241:THR:HG22	1.97	0.46
1:A:1182:LYS:HB3	1:A:1182:LYS:HE3	1.63	0.46
2:B:20:ARG:NH2	2:B:137:GLY:O	2.47	0.46
10:K:99:TYR:OH	10:K:133:GLU:OE1	2.32	0.46
1:A:697:LEU:HD23	1:A:697:LEU:HA	1.83	0.46
9:P:-1:DA:H2''	9:P:0:DG:H8	1.79	0.46
9:P:7:DC:H2'	9:P:8:DG:C8	2.50	0.46
2:B:280:ARG:HB2	2:B:313:TYR:HB2	1.98	0.46
3:C:293:LEU:CD2	3:C:322:PRO:HB2	2.44	0.46
2:B:292:ALA:HB1	2:B:328:LEU:HD12	1.98	0.46
4:D:556:TYR:O	4:D:560:MET:HG2	2.15	0.46
6:M:79:ILE:HG12	6:M:82:HIS:CE1	2.51	0.46
3:C:22:MET:HE3	3:C:111:LEU:HD12	1.97	0.46
3:C:37:MET:HB3	3:C:60:LYS:HD3	1.97	0.46
4:D:283:HIS:HB2	4:D:286:CYS:HB2	1.98	0.46
4:D:318:THR:O	4:D:322:ILE:HG13	2.15	0.46
9:P:-7:DG:H2''	9:P:-6:DG:C8	2.51	0.46
1:A:1145:TYR:HE1	1:A:1314:ILE:HD13	1.81	0.46
9:P:-28:DC:H2''	9:P:-27:DC:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:-24:DT:H2'	9:P:-23:DT:H71	1.97	0.46
1:A:813:GLU:HB3	1:A:916:TRP:CZ2	2.51	0.46
1:A:917:ARG:HD2	1:A:1186:LEU:HD13	1.98	0.46
1:A:1278:THR:OG1	1:A:1282:ASP:OD2	2.32	0.46
4:D:420:CYS:HB3	4:D:451:CYS:SG	2.56	0.46
9:P:35:DT:H2''	9:P:36:DA:C8	2.50	0.46
3:E:29:LYS:HB2	3:E:78:PHE:HB2	1.98	0.46
1:A:911:GLU:HB3	4:D:119:PRO:HG3	1.98	0.46
1:A:948:LEU:HD22	1:A:1149:ARG:HG3	1.98	0.46
3:C:111:LEU:HA	3:C:114:GLU:HB3	1.98	0.46
4:D:419:LYS:HB2	4:D:447:TRP:CZ3	2.51	0.46
4:D:266:CYS:SG	4:D:268:GLN:HB2	2.56	0.45
6:M:37:GLY:HA3	6:M:39:TYR:CE2	2.51	0.45
8:O:-35:DA:H2''	8:O:-34:DG:C8	2.52	0.45
1:A:1214:LEU:HD11	1:A:1221:HIS:CE1	2.51	0.45
3:C:92:VAL:HB	3:C:97:ILE:HD11	1.97	0.45
6:M:97:LEU:HB3	6:M:100:VAL:HB	1.98	0.45
10:G:68:GLN:HG3	10:G:89:VAL:HG11	1.98	0.45
1:A:1278:THR:HB	1:A:1282:ASP:HB3	1.99	0.45
2:B:369:LEU:O	2:B:373:MET:HG3	2.15	0.45
4:D:500:LYS:HD3	4:D:500:LYS:HA	1.76	0.45
9:P:39:DA:H2''	9:P:40:DC:H5'	1.97	0.45
9:P:58:DG:H2''	9:P:59:DA:H8	1.81	0.45
3:E:13:ARG:HH12	3:E:82:GLN:HG3	1.82	0.45
1:A:865:LYS:NZ	2:B:31:ASN:O	2.45	0.45
3:C:300:ARG:HG3	4:D:286:CYS:SG	2.56	0.45
5:H:91:LYS:NZ	7:J:80:TYR:OH	2.48	0.45
10:G:116:ARG:NH1	10:G:120:MET:SD	2.90	0.45
1:A:1172:ILE:HG12	1:A:1175:ARG:HH21	1.82	0.45
2:B:177:HIS:HB3	2:B:265:SER:HB2	1.98	0.45
3:C:348:ASP:OD1	3:C:348:ASP:N	2.49	0.45
4:D:172:THR:O	4:D:176:THR:HG23	2.17	0.45
8:O:16:DA:H1'	8:O:17:DA:C8	2.52	0.45
8:O:24:DA:H2''	8:O:25:DG:H8	1.80	0.45
3:E:22:MET:CE	3:E:108:LYS:HA	2.47	0.45
10:K:129:ARG:HA	10:K:134:ARG:HB2	1.97	0.45
3:C:33:PRO:HB3	3:C:73:ASN:HA	1.98	0.45
3:C:67:ILE:HG22	3:C:71:ILE:HG13	1.99	0.45
6:I:41:GLU:CD	6:I:41:GLU:H	2.20	0.45
9:P:58:DG:H2''	9:P:59:DA:C8	2.52	0.45
3:E:31:TRP:CE3	3:E:38:TYR:HB3	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:THR:O	1:A:1146:ILE:HG12	2.17	0.45
4:D:260:GLU:HG3	4:D:262:PHE:H	1.82	0.45
2:B:21:VAL:HG13	2:B:141:VAL:HG12	1.99	0.45
9:P:-52:DC:H2"	9:P:-51:DG:H8	1.82	0.45
9:P:41:DC:H2"	9:P:42:DA:C8	2.52	0.45
1:A:984:ILE:O	1:A:988:ILE:HG13	2.17	0.45
1:A:1254:HIS:HA	1:A:1257:MET:HE2	1.99	0.45
8:O:-71:DG:H2"	8:O:-70:DG:C8	2.52	0.45
8:O:-28:DT:H2"	8:O:-27:DC:C6	2.52	0.45
3:E:29:LYS:HD2	3:E:78:PHE:HD2	1.81	0.45
3:C:15:LEU:O	3:C:97:ILE:HA	2.17	0.44
9:P:60:DC:C2	9:P:61:DC:C5	3.05	0.44
2:B:55:TYR:CE2	2:B:334:LEU:HB3	2.51	0.44
6:I:97:LEU:HD22	6:I:100:VAL:HG21	1.99	0.44
8:O:-8:DC:H2"	8:O:-7:DG:H8	1.82	0.44
9:P:7:DC:N4	9:P:8:DG:O6	2.51	0.44
10:G:79:LYS:HD3	10:G:82:LEU:HD21	1.99	0.44
1:A:922:LYS:NZ	4:D:128:LEU:O	2.38	0.44
1:A:1164:MET:SD	1:A:1164:MET:O	2.75	0.44
1:A:1255:THR:HA	1:A:1258:THR:HG22	1.99	0.44
2:B:269:LEU:HD21	2:B:295:VAL:HG22	1.99	0.44
4:D:318:THR:HA	4:D:321:LYS:HD2	1.98	0.44
4:D:466:CYS:SG	4:D:469:HIS:HD2	2.20	0.44
9:P:-48:DC:H2"	9:P:-47:DC:C5	2.52	0.44
9:P:4:DG:H1'	9:P:5:DT:C2	2.51	0.44
2:B:38:HIS:HE1	2:B:40:MET:HG2	1.81	0.44
2:B:350:ASP:OD2	2:B:356:ARG:NH2	2.34	0.44
6:M:32:ARG:NE	9:P:-44:DG:OP1	2.35	0.44
3:E:22:MET:SD	3:E:22:MET:N	2.90	0.44
2:B:65:ARG:HB3	4:D:178:GLU:HG2	2.00	0.44
3:C:110:ARG:CZ	3:C:111:LEU:HG	2.48	0.44
9:P:-23:DT:C2	9:P:-22:DG:C8	3.05	0.44
9:P:38:DG:H2"	9:P:39:DA:C8	2.52	0.44
4:D:542:ILE:O	4:D:546:SER:OG	2.34	0.44
8:O:-56:DG:H2"	8:O:-55:DC:C5	2.52	0.44
1:A:1307:LYS:HB3	1:A:1307:LYS:HE3	1.69	0.44
2:B:67:LYS:O	4:D:182:ARG:NH1	2.50	0.44
3:C:111:LEU:HA	3:C:111:LEU:HD23	1.81	0.44
8:O:26:DG:H2"	8:O:27:DG:C8	2.53	0.44
9:P:24:DC:H2"	9:P:25:DT:C6	2.53	0.44
3:C:252:VAL:HG13	3:C:256:MET:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:8:DG:C2'	9:P:9:DT:H71	2.48	0.44
8:O:66:DC:N4	9:P:-66:DG:H1	2.08	0.43
10:G:126:LEU:HD22	10:K:113:HIS:CG	2.53	0.43
1:A:785:HIS:O	1:A:787:VAL:N	2.51	0.43
1:A:1291:ARG:HA	1:A:1294:MET:HB3	1.99	0.43
2:B:150:HIS:CD2	2:B:190:GLY:HA2	2.53	0.43
2:B:315:MET:HA	2:B:318:VAL:HG12	2.01	0.43
1:A:756:LYS:HE3	3:C:389:ASN:HB3	1.99	0.43
4:D:416:ILE:O	4:D:446:PRO:HG2	2.19	0.43
8:O:34:DT:H2''	8:O:35:DC:C6	2.53	0.43
10:K:106:ASP:OD2	10:K:131:ARG:NH2	2.47	0.43
1:A:665:GLU:HB3	4:D:552:PHE:CZ	2.52	0.43
8:O:-50:DC:N4	9:P:50:DG:O6	2.27	0.43
9:P:50:DG:H2''	9:P:51:DG:C8	2.53	0.43
4:D:304:ASN:HB2	4:D:347:ASN:HA	2.00	0.43
4:D:310:ILE:HG23	4:D:311:PHE:HD1	1.84	0.43
7:N:73:GLU:OE1	7:N:76:ARG:NH1	2.51	0.43
8:O:75:DC:H2''	8:O:76:DA:C8	2.52	0.43
9:P:-72:DC:H2''	9:P:-71:DA:H8	1.82	0.43
10:K:81:ASP:CG	10:K:81:ASP:O	2.57	0.43
3:C:289:PHE:CD2	3:C:323:ILE:HG22	2.52	0.43
3:C:293:LEU:HD23	3:C:322:PRO:CB	2.46	0.43
3:C:390:THR:HB	3:C:394:TYR:CD1	2.54	0.43
9:P:-52:DC:H2''	9:P:-51:DG:C8	2.53	0.43
9:P:-26:DC:H2''	9:P:-25:DC:C6	2.53	0.43
1:A:785:HIS:HB3	1:A:788:TRP:CD2	2.53	0.43
2:B:222:ARG:HE	2:B:222:ARG:HB2	1.54	0.43
2:B:321:THR:HG22	2:B:325:GLU:OE1	2.19	0.43
3:C:109:LYS:HA	3:C:109:LYS:HD3	1.65	0.43
3:C:266:SER:O	3:C:275:GLN:NE2	2.52	0.43
8:O:-70:DG:H2''	8:O:-69:DA:H8	1.83	0.43
8:O:5:DC:H2''	8:O:6:DC:C5	2.53	0.43
1:A:929:ASP:HB2	1:A:1229:ARG:HD3	2.01	0.43
3:C:107:MET:HB3	3:C:110:ARG:NH2	2.34	0.43
3:C:255:GLU:HB2	3:C:324:ARG:CZ	2.49	0.43
4:D:440:CYS:O	4:D:444:GLN:HA	2.19	0.43
3:E:10:LEU:HD13	3:E:41:ILE:HG23	2.00	0.43
3:E:27:ILE:HG23	3:E:77:PHE:HB3	2.00	0.43
1:A:815:HIS:CE1	2:B:41:LYS:HB3	2.54	0.43
1:A:868:ARG:HE	1:A:868:ARG:HB2	1.55	0.43
1:A:813:GLU:HB3	1:A:916:TRP:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:551:PHE:O	4:F:554:LYS:HG3	2.19	0.43
9:P:9:DT:C2	9:P:10:DG:C5	3.06	0.43
2:B:191:ASP:N	2:B:191:ASP:OD1	2.52	0.42
7:N:41:VAL:O	7:N:45:VAL:HG22	2.19	0.42
10:G:122:LYS:HG3	10:K:113:HIS:HE1	1.83	0.42
9:P:0:DG:C4	9:P:1:DC:C5	3.08	0.42
2:B:102:VAL:HG21	3:C:401:MET:SD	2.59	0.42
2:B:267:VAL:HB	2:B:303:ILE:HD11	2.00	0.42
2:B:380:LEU:HD23	2:B:383:THR:HG21	1.99	0.42
5:L:50:ILE:HD12	10:K:124:ILE:HD11	2.01	0.42
2:B:305:MET:SD	2:B:307:VAL:HG23	2.59	0.42
4:D:114:PRO:HD2	4:D:117:LYS:HG2	2.01	0.42
9:P:-16:DT:H2''	9:P:-15:DA:N7	2.34	0.42
1:A:759:PRO:HG2	1:A:762:ASP:HB2	2.01	0.42
2:B:247:TYR:CD2	2:B:286:LEU:HD11	2.54	0.42
3:C:260:LYS:NZ	3:C:372:GLU:OE2	2.52	0.42
3:C:307:ASP:HB2	4:D:290:PRO:HG2	2.02	0.42
9:P:-25:DC:C6	9:P:-24:DT:H72	2.54	0.42
9:P:29:DG:C4	9:P:30:DC:C5	3.07	0.42
1:A:1294:MET:CE	1:A:1298:GLU:HG3	2.50	0.42
8:O:-10:DC:H2''	8:O:-9:DA:C8	2.53	0.42
8:O:57:DA:H1'	8:O:58:DG:O4'	2.19	0.42
9:P:-40:DC:H2''	9:P:-39:DT:H71	2.01	0.42
1:A:998:HIS:NE2	1:A:1216:ASN:O	2.53	0.42
3:C:291:LYS:HA	3:C:291:LYS:HD3	1.75	0.42
3:C:324:ARG:HA	3:C:324:ARG:NE	2.34	0.42
4:D:276:ASP:OD1	4:D:276:ASP:N	2.53	0.42
5:L:90:LEU:HB3	5:L:95:ARG:O	2.19	0.42
8:O:-14:DA:H2''	8:O:-13:DA:C8	2.54	0.42
9:P:-14:DA:H2''	9:P:-13:DA:H8	1.84	0.42
1:A:756:LYS:O	1:A:782:TRP:HA	2.20	0.42
6:I:17:ARG:NH2	6:I:28:GLY:HA2	2.35	0.42
6:I:83:LEU:HD11	7:J:55:ALA:HB1	2.02	0.42
6:I:88:ARG:HA	6:I:88:ARG:HD3	1.87	0.42
5:L:62:LEU:HD23	5:L:62:LEU:HA	1.88	0.42
8:O:74:DG:H2''	8:O:75:DC:C6	2.54	0.42
9:P:-54:DC:H2''	9:P:-53:DA:C8	2.54	0.42
9:P:-32:DT:H2''	9:P:-31:DA:C8	2.55	0.42
2:B:43:HIS:CD2	2:B:47:MET:HE1	2.55	0.42
2:B:347:TYR:HB2	2:B:351:TYR:CD1	2.55	0.42
1:A:893:VAL:O	1:A:896:LYS:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:436:LEU:HD13	4:D:449:LEU:HD12	2.02	0.41
7:J:30:ARG:HA	9:P:50:DG:OP1	2.19	0.41
5:L:50:ILE:HD13	10:K:121:PRO:HG3	2.02	0.41
7:N:54:LYS:HD3	7:N:54:LYS:N	2.34	0.41
8:O:53:DT:H6	8:O:53:DT:H5'	1.85	0.41
9:P:-36:DG:H2''	9:P:-35:DG:N7	2.35	0.41
9:P:-4:DG:H2''	9:P:-3:DA:H8	1.84	0.41
1:A:1144:ILE:HG12	1:A:1256:LEU:HD12	2.02	0.41
2:B:204:MET:HG2	2:B:262:TYR:CE2	2.54	0.41
3:C:338:LEU:HD23	3:C:338:LEU:HA	1.81	0.41
4:D:335:ILE:HG13	4:D:336:PHE:CD2	2.55	0.41
8:O:16:DA:H1'	8:O:17:DA:N7	2.35	0.41
1:A:1157:ARG:O	1:A:1161:ILE:HG12	2.20	0.41
5:L:75:HIS:HB2	7:N:93:THR:HG21	2.02	0.41
6:M:62:ILE:HD11	7:N:59:MET:SD	2.61	0.41
8:O:-32:DC:H2''	8:O:-31:DA:C8	2.54	0.41
8:O:-19:DG:H2''	8:O:-18:DC:H5''	2.02	0.41
9:P:-62:DA:H2'	9:P:-61:DT:H71	2.02	0.41
2:B:288:MET:SD	2:B:321:THR:HA	2.60	0.41
5:H:95:ARG:CZ	6:M:99:ARG:HH12	2.33	0.41
1:A:1136:PHE:CD1	1:A:1273:ARG:HD2	2.56	0.41
1:A:1261:LYS:NZ	1:A:1293:HIS:O	2.43	0.41
2:B:224:ILE:HD12	2:B:231:ASN:OD1	2.20	0.41
6:I:36:LYS:HA	6:I:36:LYS:HD3	1.82	0.41
10:G:87:SER:HA	10:G:90:MET:HG2	2.01	0.41
4:D:329:GLN:HB2	4:D:337:ALA:HB2	2.01	0.41
5:H:50:ILE:HD13	5:H:50:ILE:HA	1.91	0.41
8:O:-63:DC:H2''	8:O:-62:DC:C6	2.55	0.41
2:B:49:HIS:NE2	4:D:172:THR:HG21	2.36	0.41
2:B:173:LEU:HD23	2:B:173:LEU:HA	1.90	0.41
3:C:331:LEU:O	3:C:335:ILE:HG12	2.21	0.41
5:H:36:ARG:NH2	8:O:-13:DA:OP1	2.45	0.41
8:O:-70:DG:H2''	8:O:-69:DA:C8	2.55	0.41
2:B:47:MET:HG2	2:B:319:ALA:CB	2.51	0.41
6:I:107:VAL:HG11	10:K:101:VAL:HG11	2.03	0.41
7:J:54:LYS:HD2	7:J:54:LYS:HA	1.90	0.41
6:M:106:GLY:HA3	10:G:58:THR:HG22	2.02	0.41
8:O:-68:DG:H2''	8:O:-67:DA:C8	2.56	0.41
8:O:25:DG:H2''	8:O:26:DG:N7	2.36	0.41
8:O:55:DT:H2''	8:O:56:DC:C6	2.55	0.41
9:P:-20:DC:H2''	9:P:-19:DG:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:1:DC:H2''	9:P:2:DG:C8	2.56	0.41
1:A:1172:ILE:HG12	1:A:1175:ARG:NH2	2.36	0.41
2:B:347:TYR:HB2	2:B:351:TYR:HD1	1.86	0.41
4:D:441:ASP:OD1	4:D:441:ASP:N	2.54	0.41
5:H:44:LYS:HB2	6:M:115:LEU:HD13	2.03	0.41
5:H:100:PHE:HE2	10:G:90:MET:HG3	1.85	0.41
8:O:68:DT:H2''	8:O:69:DC:C6	2.56	0.41
9:P:-19:DG:H2''	9:P:-18:DG:C8	2.56	0.41
9:P:53:DC:H2''	9:P:54:DT:C6	2.55	0.41
1:A:900:GLN:NE2	1:A:904:GLU:OE2	2.55	0.40
4:D:320:LYS:O	4:D:323:GLU:HG3	2.21	0.40
8:O:-18:DC:C6	8:O:-17:DT:H72	2.56	0.40
3:E:13:ARG:NH2	3:E:25:ALA:O	2.54	0.40
1:A:769:GLY:O	2:B:76:GLN:HG2	2.21	0.40
3:C:378:ASP:HB3	3:C:381:ARG:HG3	2.04	0.40
9:P:-37:DG:H2''	9:P:-36:DG:C8	2.55	0.40
9:P:31:DT:H2''	9:P:32:DG:C8	2.56	0.40
1:A:1228:LEU:HD22	1:A:1236:ALA:HB3	2.02	0.40
1:A:1298:GLU:H	1:A:1298:GLU:HG2	1.70	0.40
3:C:336:SER:O	4:D:354:PRO:HG3	2.20	0.40
3:C:337:VAL:O	3:C:341:LEU:N	2.53	0.40
4:D:322:ILE:HG12	4:D:341:PHE:CE2	2.56	0.40
9:P:-71:DA:C8	9:P:-71:DA:H5'	2.56	0.40
1:A:1197:ASP:O	1:A:1197:ASP:OD1	2.38	0.40
1:A:1294:MET:HE2	1:A:1300:MET:HG3	2.03	0.40
2:B:67:LYS:HD3	4:D:185:ILE:HD11	2.03	0.40
2:B:280:ARG:HE	2:B:280:ARG:HB3	1.66	0.40
3:C:85:LYS:HE3	3:C:85:LYS:HB2	1.89	0.40
8:O:-23:DC:P	10:G:72:ARG:HH22	2.44	0.40
8:O:-16:DT:H2''	8:O:-15:DA:N7	2.36	0.40
10:K:38:PRO:HB2	10:K:40:ARG:HG3	2.04	0.40
1:A:1165:ASN:OD1	1:A:1203:ALA:HB3	2.22	0.40
2:B:211:TYR:CE2	2:B:220:GLU:HG3	2.56	0.40
4:D:121:GLU:O	4:D:124:LYS:HB2	2.22	0.40
4:D:303:CYS:HB2	4:D:306:CYS:H	1.86	0.40
6:I:14:ALA:HB1	8:O:-43:DT:H4'	2.03	0.40
6:I:24:GLN:N	6:I:56:GLU:OE1	2.43	0.40
8:O:1:DT:H2''	8:O:2:DG:C8	2.57	0.40
8:O:10:DC:H2''	8:O:11:DG:C8	2.56	0.40
9:P:-51:DG:C2'	9:P:-50:DT:H71	2.50	0.40
10:K:124:ILE:H	10:K:124:ILE:HG13	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/1536 (32%)	474 (96%)	20 (4%)	0	100	100
2	B	366/433 (84%)	353 (96%)	13 (4%)	0	100	100
3	C	280/401 (70%)	270 (96%)	10 (4%)	0	100	100
3	E	100/401 (25%)	97 (97%)	3 (3%)	0	100	100
4	D	304/684 (44%)	278 (91%)	26 (9%)	0	100	100
4	F	18/684 (3%)	18 (100%)	0	0	100	100
5	H	77/102 (76%)	77 (100%)	0	0	100	100
5	L	79/102 (78%)	76 (96%)	3 (4%)	0	100	100
6	I	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
6	M	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
7	J	91/122 (75%)	88 (97%)	3 (3%)	0	100	100
7	N	91/122 (75%)	90 (99%)	1 (1%)	0	100	100
10	G	97/135 (72%)	94 (97%)	3 (3%)	0	100	100
10	K	97/135 (72%)	96 (99%)	1 (1%)	0	100	100
All	All	2304/5115 (45%)	2215 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	472/1391 (34%)	465 (98%)	7 (2%)	65	79
2	B	311/367 (85%)	302 (97%)	9 (3%)	42	64
3	C	260/359 (72%)	253 (97%)	7 (3%)	44	66
3	E	89/359 (25%)	84 (94%)	5 (6%)	21	49
4	D	299/653 (46%)	290 (97%)	9 (3%)	41	64
4	F	20/653 (3%)	18 (90%)	2 (10%)	7	29
5	H	65/78 (83%)	63 (97%)	2 (3%)	40	63
5	L	66/78 (85%)	66 (100%)	0	100	100
6	I	84/101 (83%)	84 (100%)	0	100	100
6	M	84/101 (83%)	83 (99%)	1 (1%)	71	83
7	J	79/102 (78%)	78 (99%)	1 (1%)	69	81
7	N	79/102 (78%)	77 (98%)	2 (2%)	47	68
10	G	87/109 (80%)	85 (98%)	2 (2%)	50	70
10	K	85/109 (78%)	84 (99%)	1 (1%)	71	83
All	All	2080/4562 (46%)	2032 (98%)	48 (2%)	53	70

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	897	ARG
1	A	907	ARG
1	A	983	ASN
1	A	1017	PHE
1	A	1281	LYS
1	A	1294	MET
1	A	1307	LYS
2	B	47	MET
2	B	72	GLN
2	B	150	HIS
2	B	158	SER
2	B	257	LYS
2	B	270	GLN
2	B	288	MET
2	B	305	MET
2	B	315	MET
3	C	37	MET
3	C	76	CYS
3	C	94	TYR

Continued on next page...

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Mol	Chain	Res	Type
3	C	256	MET
3	C	296	MET
3	C	333	ARG
3	C	350	GLN
4	D	116	ASN
4	D	274	CYS
4	D	278	CYS
4	D	326	PHE
4	D	334	LYS
4	D	410	ASN
4	D	441	ASP
4	D	507	GLU
4	D	514	TYR
4	F	554	LYS
4	F	556	TYR
5	H	77	LYS
5	H	92	ARG
7	J	82	LYS
6	M	13	LYS
7	N	30	ARG
7	N	56	MET
3	E	22	MET
3	E	78	PHE
3	E	94	TYR
3	E	100	TYR
3	E	110	ARG
10	G	37	LYS
10	G	120	MET
10	K	81	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	815	HIS
4	D	503	GLN
4	D	516	ASN
3	E	104	ASN
10	K	39	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

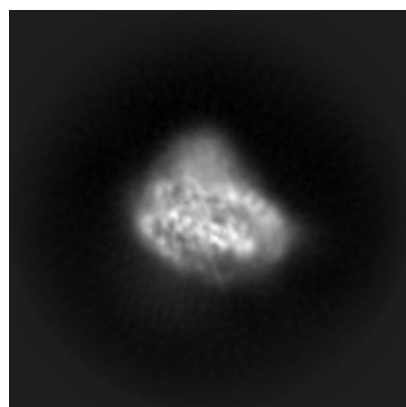
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33851. These allow visual inspection of the internal detail of the map and identification of artifacts.

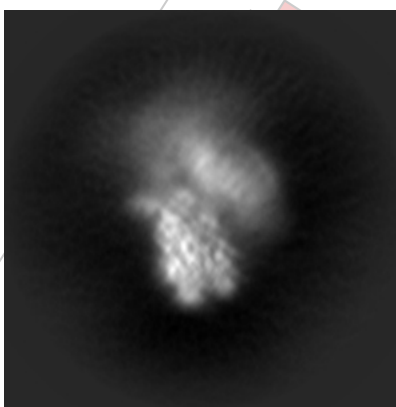
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

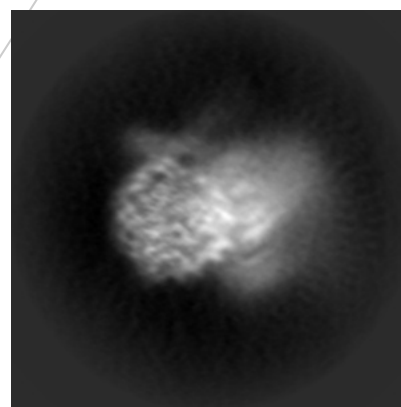
6.1.1 Primary map



X

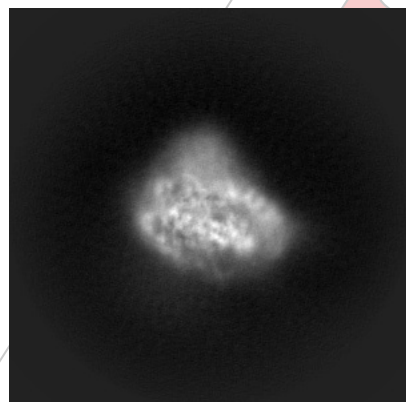


Y

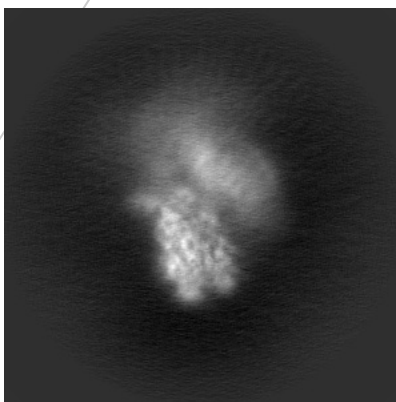


Z

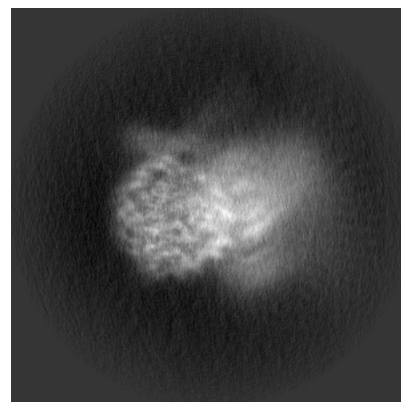
6.1.2 Raw map



X



Y

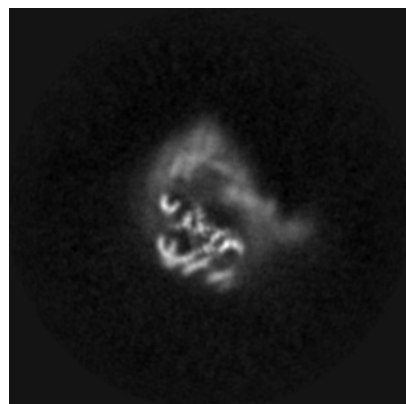


Z

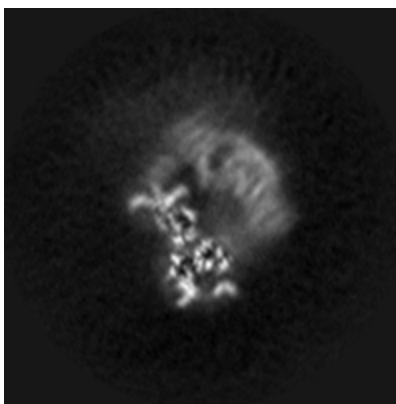
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

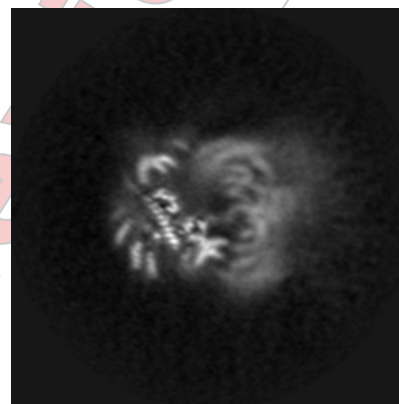
6.2.1 Primary map



X Index: 150

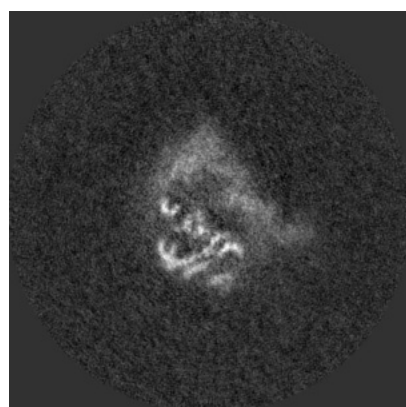


Y Index: 150

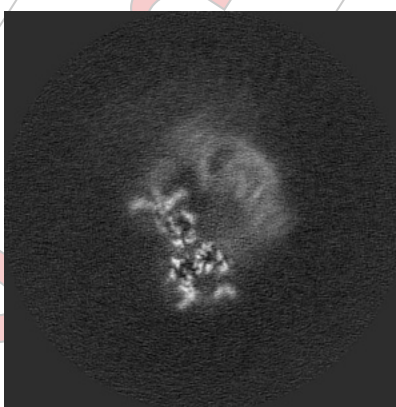


Z Index: 150

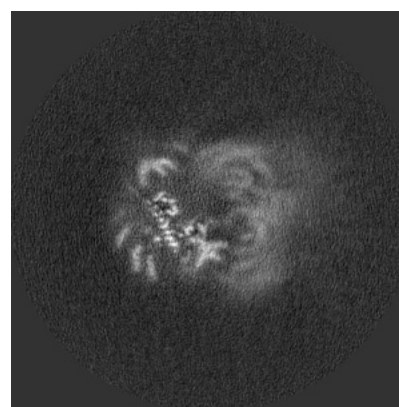
6.2.2 Raw map



X Index: 150



Y Index: 150

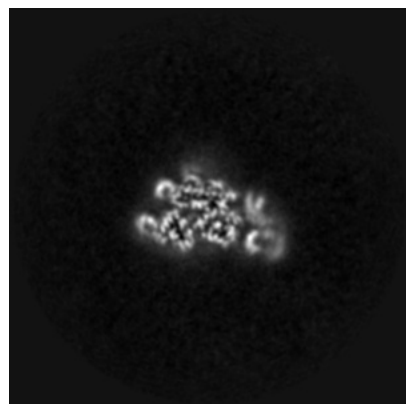


Z Index: 150

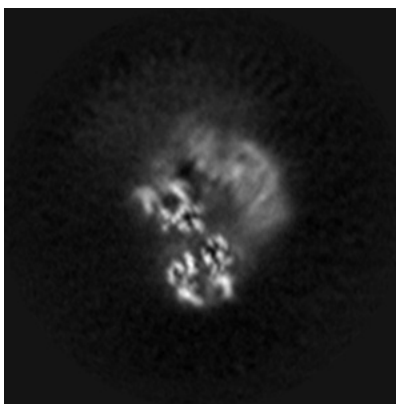
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

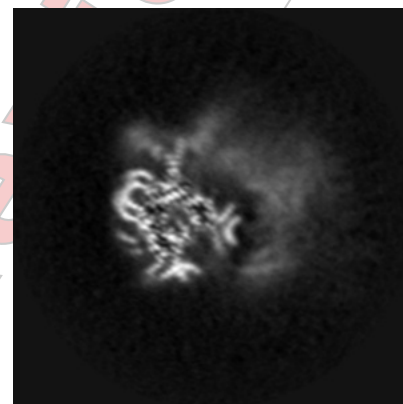
6.3.1 Primary map



X Index: 112

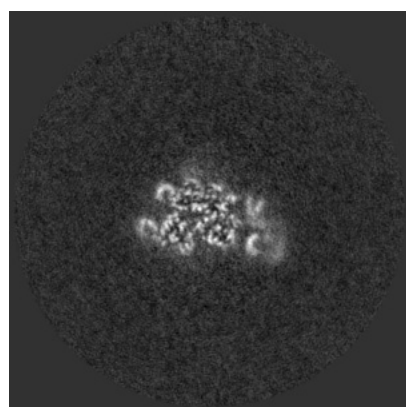


Y Index: 143

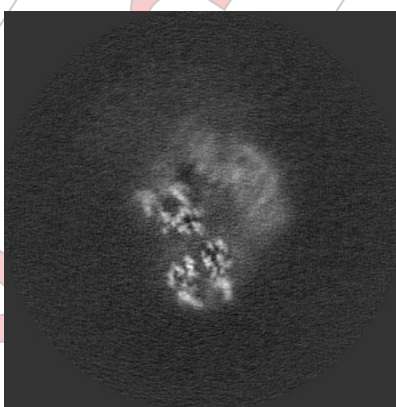


Z Index: 135

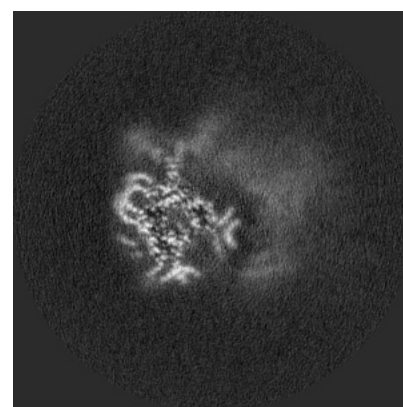
6.3.2 Raw map



X Index: 112



Y Index: 143

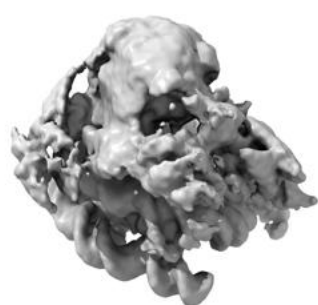


Z Index: 135

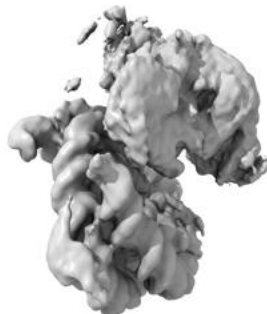
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

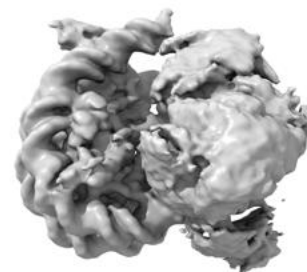
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

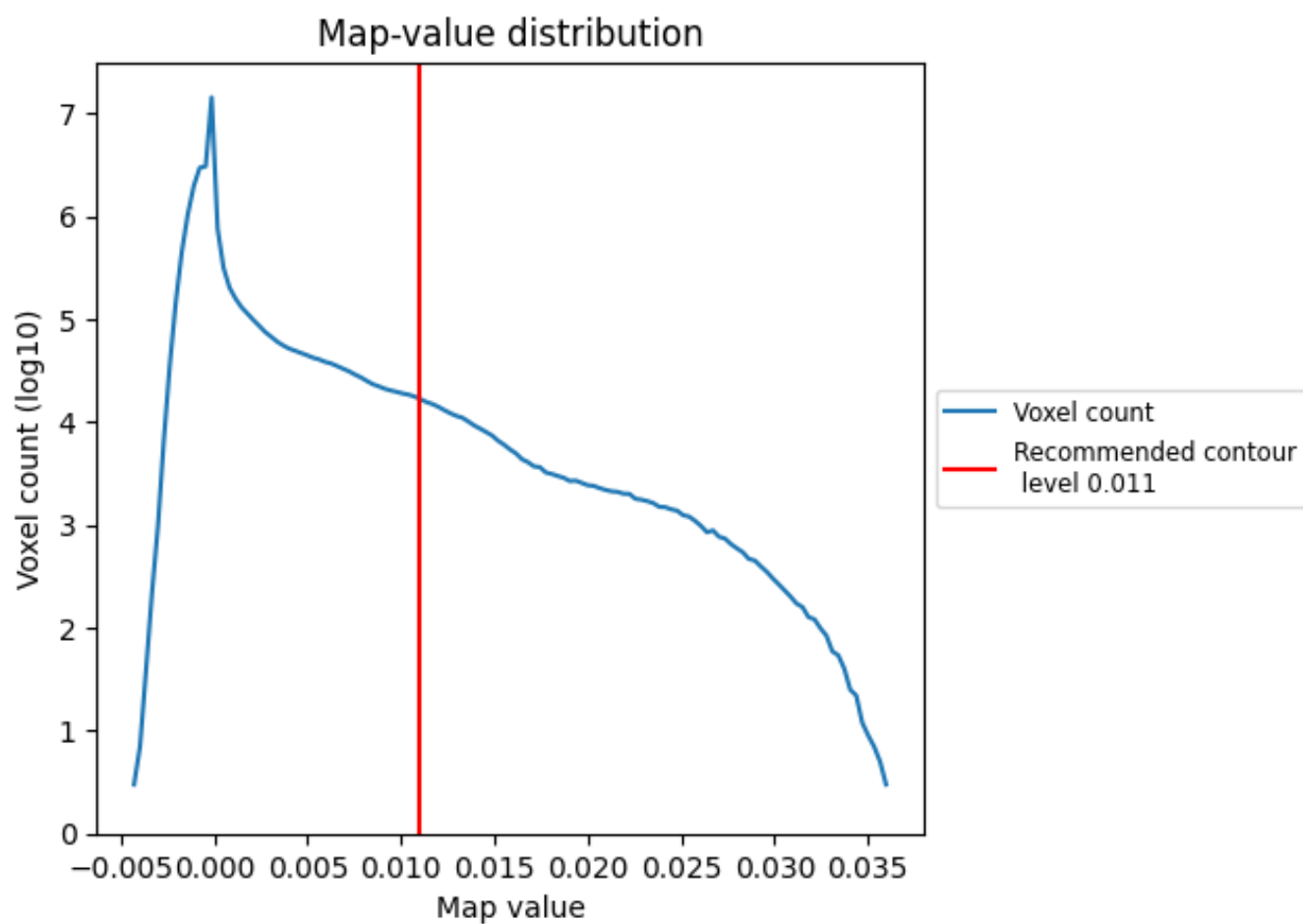
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

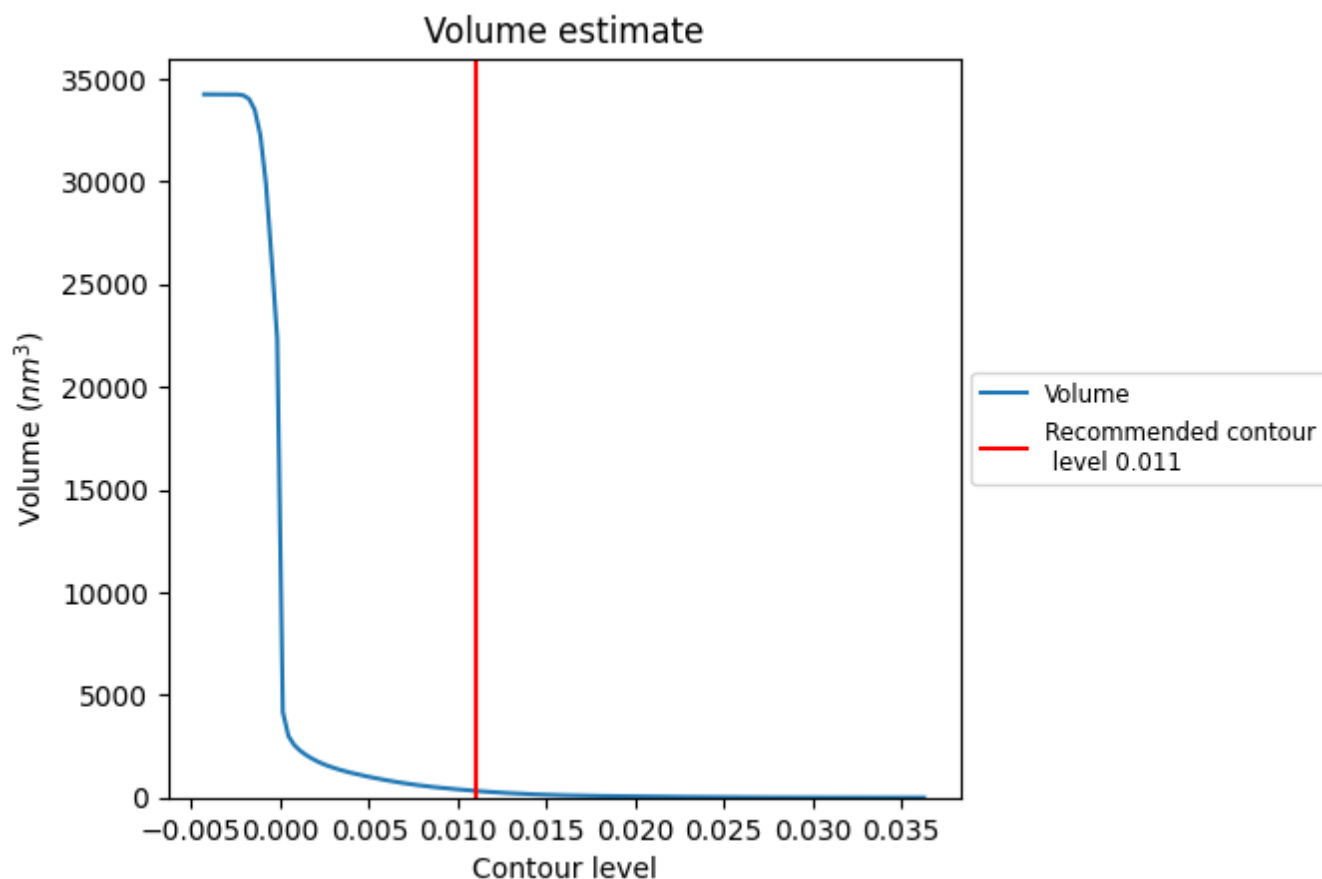
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

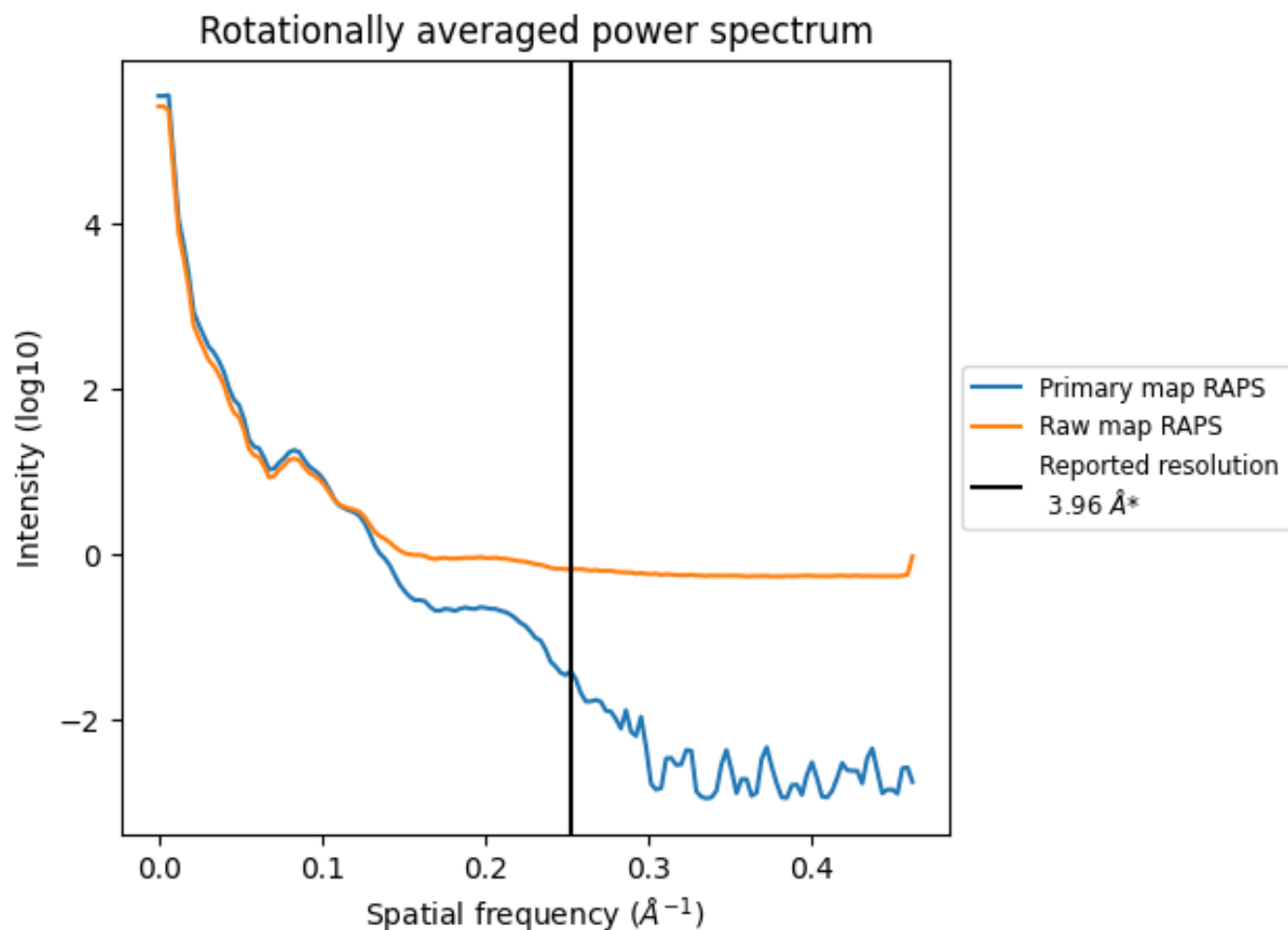
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326 nm³; this corresponds to an approximate mass of 295 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

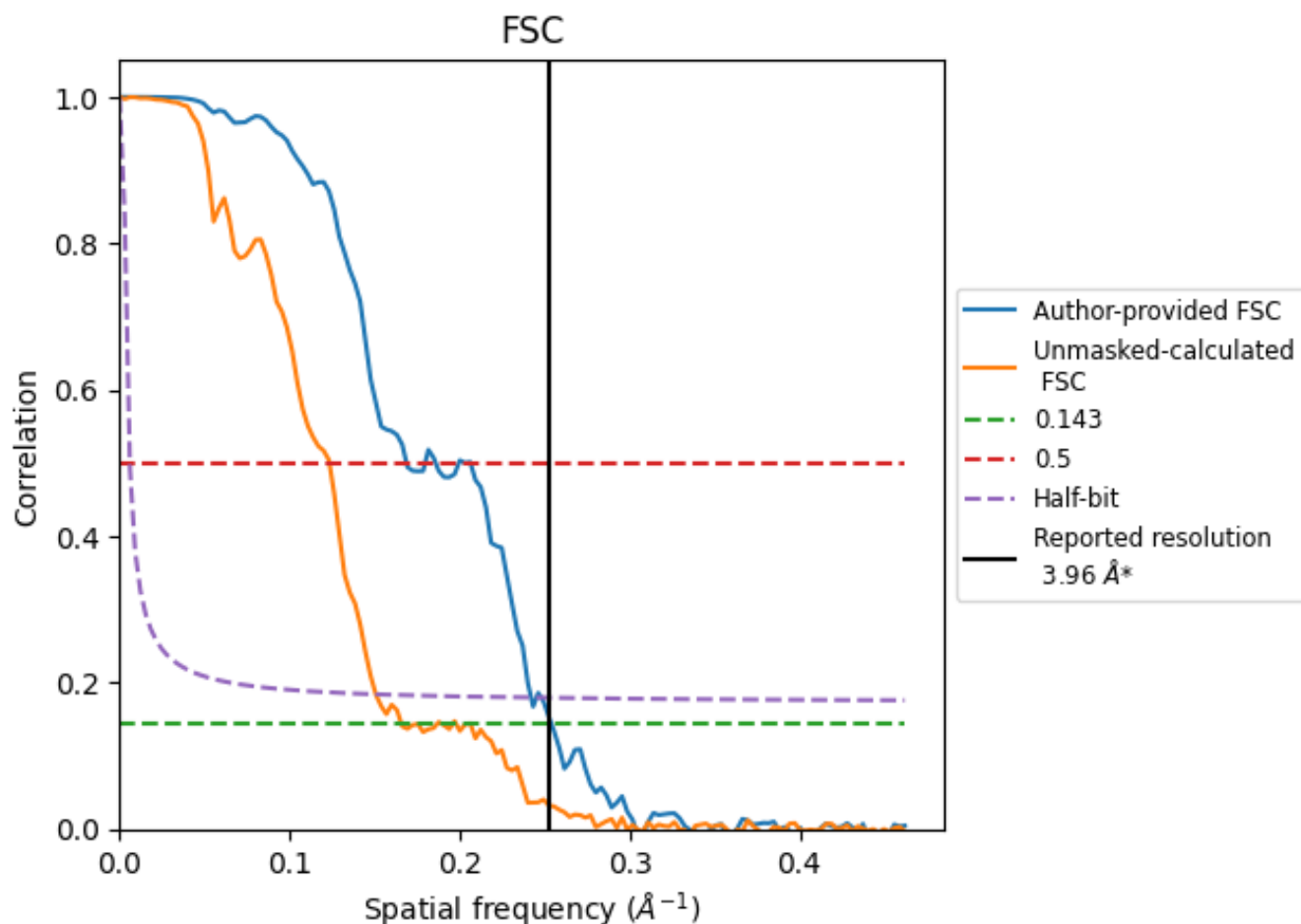


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

8.2 Resolution estimates [i](#)

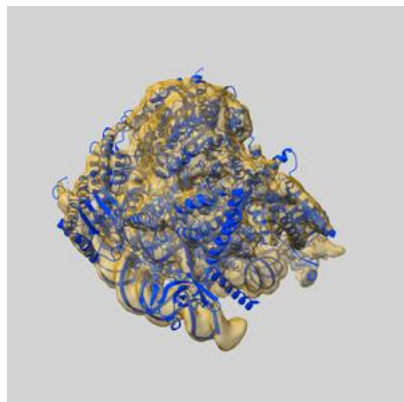
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	3.94	5.92	4.13
Unmasked-calculated*	6.03	8.10	6.63

*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 6.03 differs from the reported value 3.96 by more than 10 %

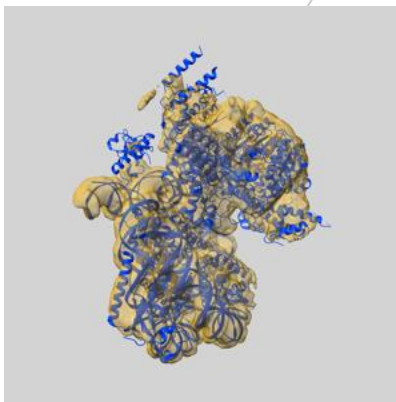
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-33851 and PDB model 7YI4. Per-residue inclusion information can be found in section 3 on page 7.

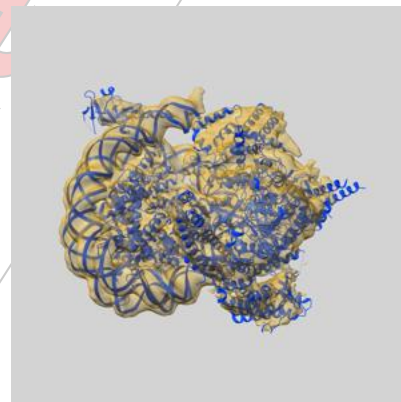
9.1 Map-model overlay ⓘ



X



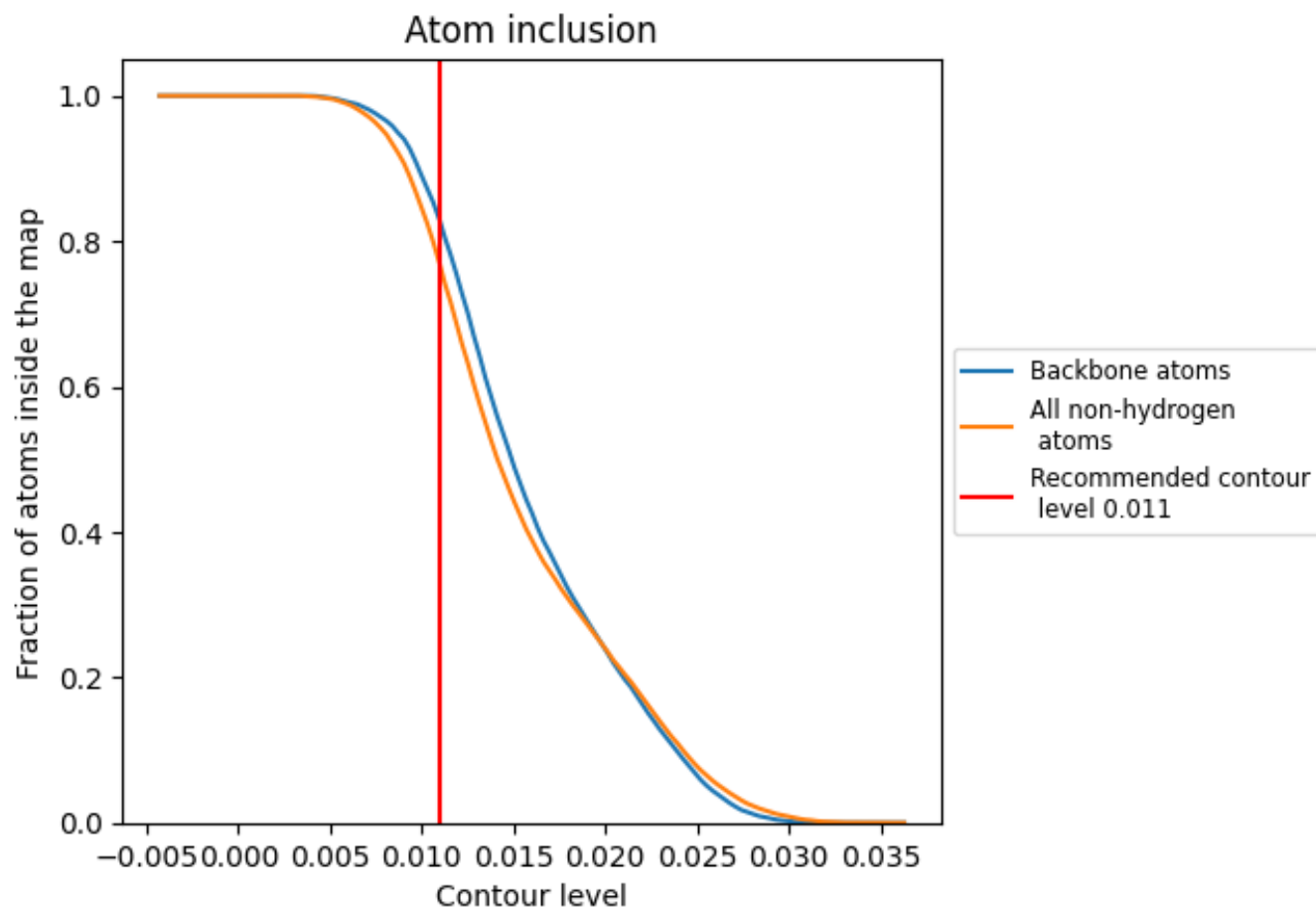
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.