



Full wwPDB EM Validation Report ⓘ

Sep 25, 2024 – 12:04 pm BST

PDB ID : 9FPZ
EMDB ID : EMD-50641
Title : Human NatA-MAP2 80S ribosome complex
Authors : Klein, M.A.; Wild, K.; Sinning, I.
Deposited on : 2024-06-14
Resolution : 2.69 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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.dev112
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

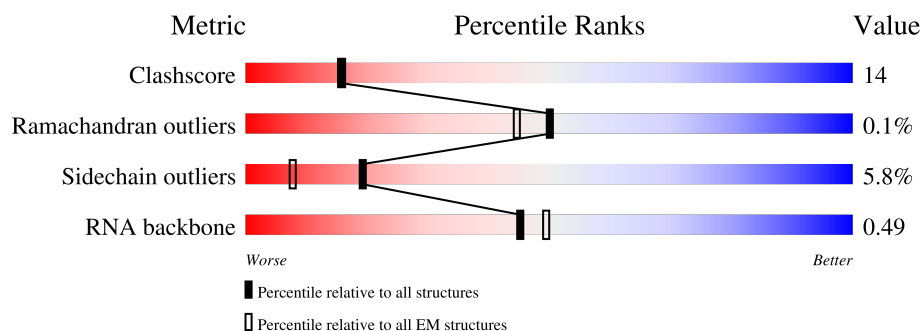
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 Å.

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



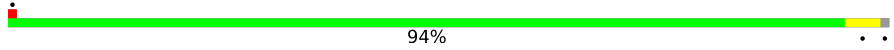

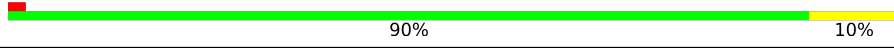
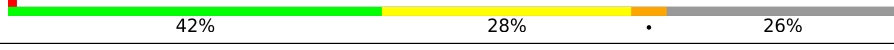


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2	171	
2	8	58	
3	A	484	
4	B	840	
5	1	5070	
6	LC	427	
7	LE	288	

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Mol	Chain	Length	Quality of chain
8	Lk	70	
9	LY	144	
10	Lh	122	
11	LX	156	
12	LR	196	
13	Lr	137	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29394 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 N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	169	Total	C	N	O	S	0	0
			1388	869	253	256	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	0	MET	-	initiating methionine	UNP P41227
2	1	GLY	-	expression tag	UNP P41227

- Molecule 2 is a RNA chain called 5.8S rRNA (58-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	8	58	Total	C	N	O	P	0	0
			1237	554	224	401	58		

- Molecule 3 is a protein called Methionine aminopeptidase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	370	Total	C	N	O	S	0	0
			2901	1823	499	556	23		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P50579
A	-4	PRO	-	expression tag	UNP P50579
A	-3	GLY	-	expression tag	UNP P50579
A	-2	SER	-	expression tag	UNP P50579
A	-1	GLY	-	expression tag	UNP P50579
A	0	SER	-	expression tag	UNP P50579

- Molecule 4 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	834	Total	C	N	O	S	0	0
			6881	4379	1189	1272	41		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP Q9BXJ9

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	300	Total	C	N	O	P	0	0
			6425	2859	1169	2097	300		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	365	Total	C	N	O	S	0	0
			2908	1829	580	486	13		

- Molecule 7 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LE	214	Total	C	N	O	S	0	0
			1724	1111	327	282	4		

- Molecule 8 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 9 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LY	129	Total	C	N	O	S	0	0
			1075	675	218	179	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LY	?	-	LYS	deletion	UNP P61254

- Molecule 10 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 11 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LX	116	Total	C	N	O	S	0	0
			950	606	178	165	1		

- Molecule 12 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LR	153	Total	C	N	O	S	0	0
			1281	799	276	197	9		

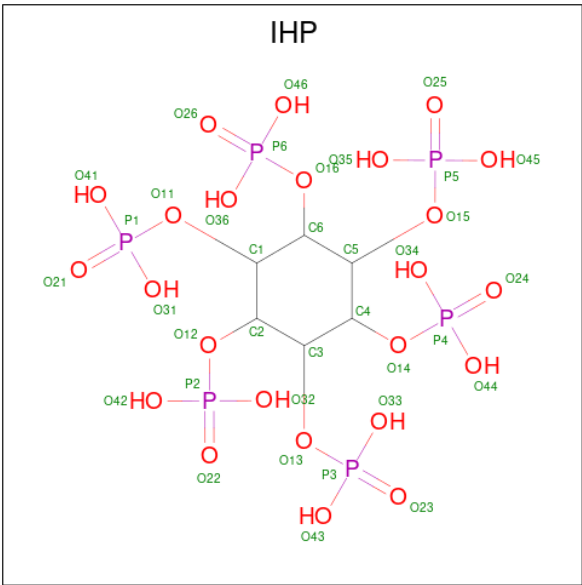
- Molecule 13 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

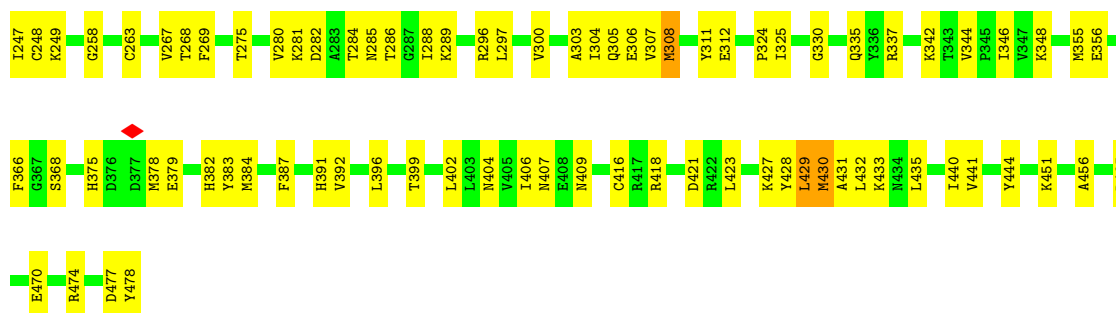
- Molecule 14 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		AltConf
14	A	2	Total	Co	0
			2	2	

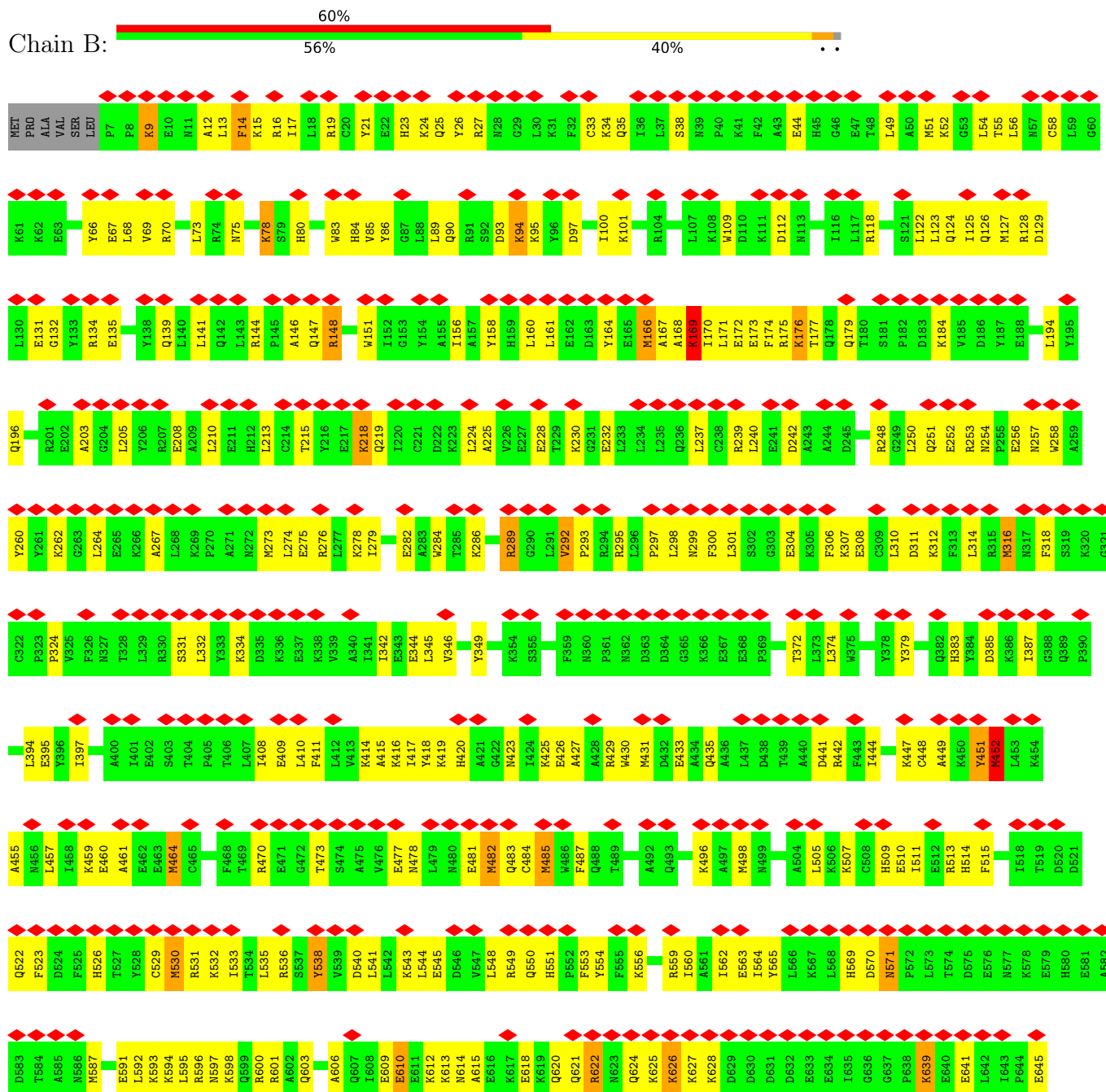
- Molecule 15 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).

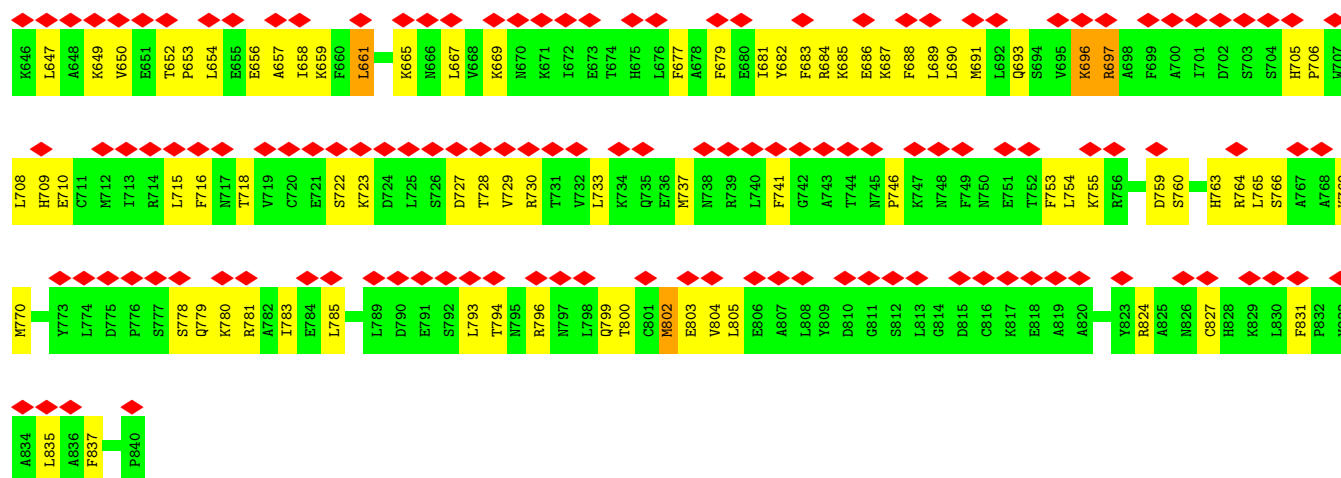


Mol	Chain	Residues	Atoms				AltConf
15	B	1	Total	C	O	P	0
			36	6	24	6	



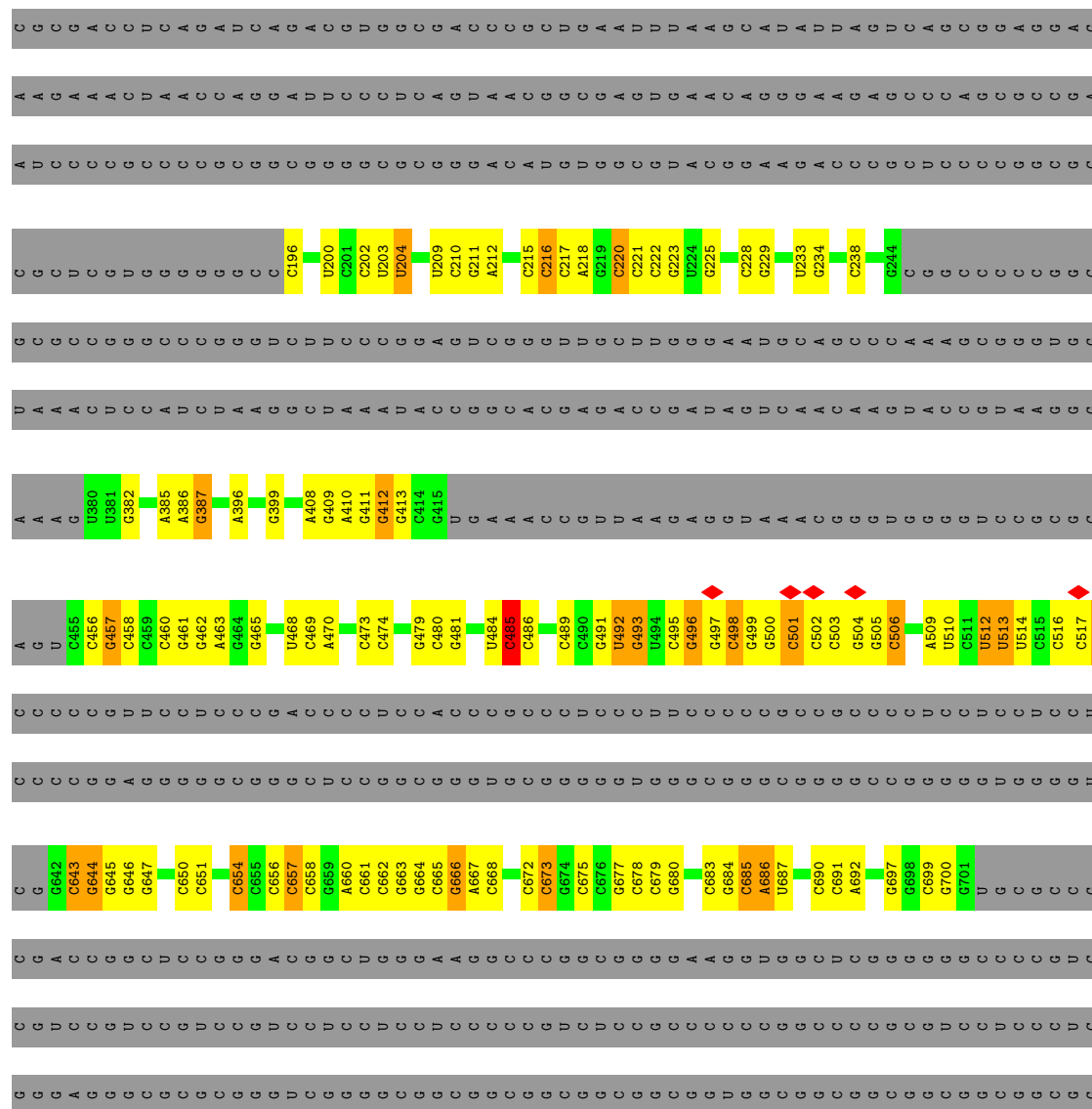
• Molecule 4: N-alpha-acetyltransferase 15, NatA auxiliary subunit





• Molecule 5: 28S rRNA

Chain 1: 94%








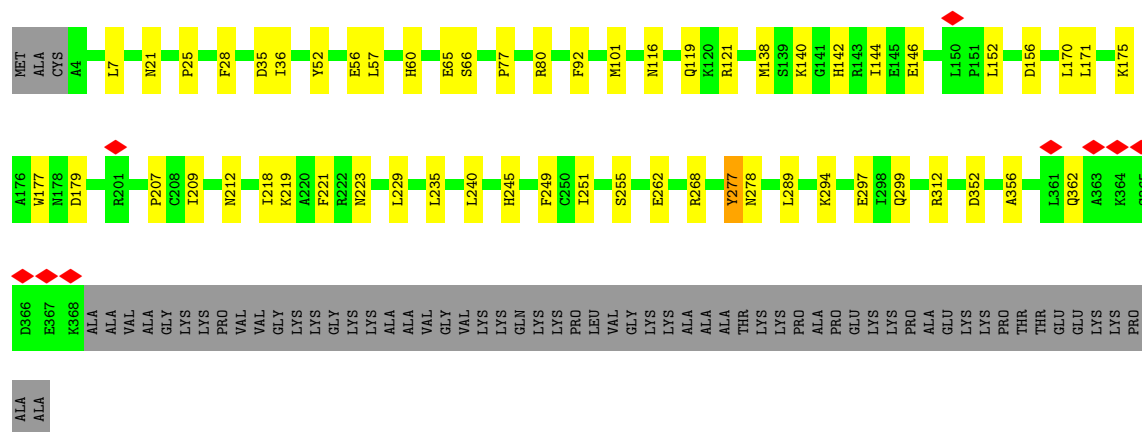
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A A U G C C U C G G U C A U C U U A A U U A G U G A C G C G C A A U G G A U G A A U C C C A C C U G U C C C C
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C U C G C C C G U C C G A C C C A C G U C C G U G G A A G A A C C D G G C C U A A C C C A U U G U A A C G G A C
C U G C C U C U G G G U G G G G U C U A C G U A A G C A A A G C C C C U G C C G A U C C U A U U G A A
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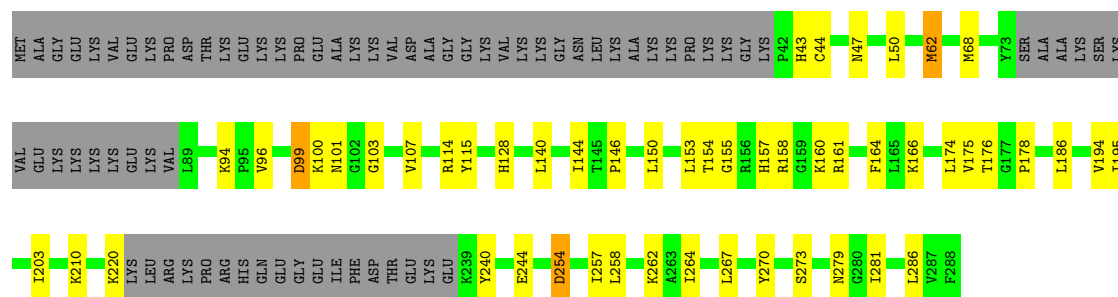
- Molecule 6: 60S ribosomal protein L4

Chain LC:  72% 13% 15%



• Molecule 7: Large ribosomal subunit protein eL6

Chain LE:



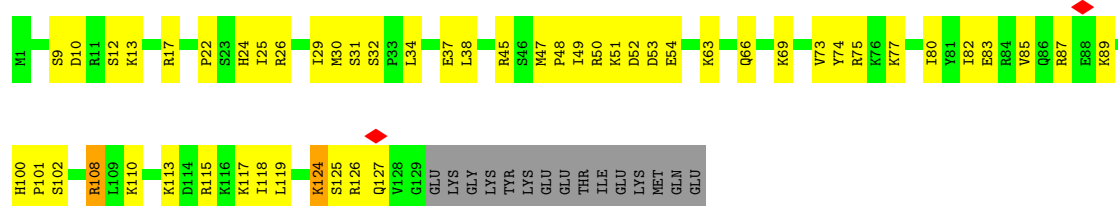
• Molecule 8: 60S ribosomal protein L38

Chain Lk:



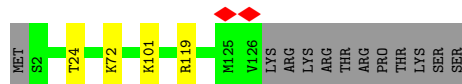
• Molecule 9: Large ribosomal subunit protein uL24

Chain LY:



• Molecule 10: 60S ribosomal protein L35

Chain Lh:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25404	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 ($e^-/\text{\AA}^2$)	41.28	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.457	Depositor
Minimum map value	-0.166	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	604.8, 604.8, 604.8	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84, 0.84, 0.84	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2	0.27	0/1418	0.64	1/1909 (0.1%)
2	8	0.23	0/1384	0.75	0/2154
3	A	0.27	0/2964	0.56	1/4014 (0.0%)
4	B	0.27	0/7019	0.55	4/9441 (0.0%)
5	1	0.22	0/7175	0.82	8/11173 (0.1%)
6	LC	0.25	0/2962	0.56	0/3977
7	LE	0.26	0/1758	0.59	0/2359
8	Lk	0.29	0/575	0.65	0/761
9	LY	0.29	0/1092	0.65	0/1454
10	Lh	0.28	0/1023	0.61	0/1351
11	LX	0.28	0/967	0.64	1/1301 (0.1%)
12	LR	0.26	0/1297	0.61	0/1716
13	Lr	0.25	0/1017	0.62	0/1364
All	All	0.26	0/30651	0.66	15/42974 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	485	C	C2-N1-C1'	8.96	128.66	118.80
5	1	3598	C	C5-C6-N1	8.96	125.48	121.00
4	B	661	LEU	CA-CB-CG	8.01	133.72	115.30
5	1	3598	C	C6-N1-C2	-7.04	117.48	120.30
3	A	430	MET	CB-CG-SD	-6.97	91.49	112.40
5	1	485	C	C6-N1-C1'	-6.70	112.76	120.80
5	1	485	C	N1-C2-O2	6.21	122.62	118.90
4	B	452	MET	CA-CB-CG	5.87	123.27	113.30
5	1	3598	C	C2-N1-C1'	5.71	125.08	118.80
5	1	209	U	C2-N1-C1'	5.67	124.50	117.70
5	1	220	C	C2-N1-C1'	5.29	124.62	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	169	LYS	CA-CB-CG	5.16	124.75	113.40
4	B	595	LEU	CA-CB-CG	5.16	127.16	115.30
1	2	91	MET	CB-CG-SD	5.14	127.81	112.40
11	LX	81	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1388	0	1356	90	0
2	8	1237	0	625	18	0
3	A	2901	0	2848	75	0
4	B	6881	0	6924	303	0
5	1	6425	0	3260	122	0
6	LC	2908	0	3082	33	0
7	LE	1724	0	1874	30	0
8	Lk	569	0	637	0	0
9	LY	1075	0	1157	45	0
10	Lh	1015	0	1148	0	0
11	LX	950	0	1016	45	0
12	LR	1281	0	1418	30	0
13	Lr	1002	0	1068	0	0
14	A	2	0	0	0	0
15	B	36	0	6	1	0
All	All	29394	0	26419	733	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 14.

All (733) 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)
4:B:93:ASP:HB2	4:B:95:LYS:HE2	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:166:MET:HB2	4:B:169:LYS:HE3	1.51	0.89
5:1:3597:G:HO2'	5:1:3598:C:H6	0.96	0.88
5:1:196:C:O2'	9:LY:126:ARG:NH2	2.07	0.86
4:B:496:LYS:HD2	4:B:560:ILE:HG23	1.58	0.84
4:B:27:ARG:HH12	5:1:204:U:H5''	1.41	0.83
4:B:682:TYR:HB3	4:B:687:LYS:HB2	1.61	0.83
4:B:452:MET:HB2	4:B:457:LEU:HB2	1.63	0.79
5:1:493:G:O6	5:1:660:A:N1	2.16	0.78
4:B:210:LEU:HG	4:B:230:LYS:HZ3	1.49	0.78
5:1:512:U:H3	5:1:647:G:H1	1.33	0.76
4:B:778:SER:HB3	4:B:781:ARG:HE	1.50	0.75
12:LR:28:GLU:OE1	12:LR:28:GLU:N	4.30	0.75
1:2:82:ARG:NH2	4:B:441:ASP:OD2	2.21	0.74
4:B:431:MET:SD	4:B:431:MET:N	2.58	0.74
5:1:493:G:H1	5:1:660:A:H2	1.36	0.74
4:B:429:ARG:NH1	4:B:433:GLU:OE2	2.22	0.73
12:LR:31:GLU:OE2	12:LR:31:GLU:N	2.20	0.72
11:LX:89:LYS:HG2	11:LX:95:THR:HB	1.70	0.72
4:B:49:LEU:HD22	4:B:68:LEU:HD11	1.72	0.72
4:B:284:TRP:HB3	4:B:293:PRO:HB2	1.72	0.72
5:1:664:G:N2	5:1:666:G:O6	2.22	0.72
4:B:131:GLU:HG3	4:B:134:ARG:HH22	1.55	0.71
4:B:770:MET:SD	4:B:770:MET:N	2.62	0.71
5:1:662:C:H2'	5:1:663:G:H8	1.54	0.71
6:LC:146:GLU:N	6:LC:146:GLU:OE1	2.22	0.71
4:B:624:GLN:HE22	5:1:216:C:H4'	1.55	0.71
5:1:496:G:H2'	5:1:498:C:H5''	1.73	0.70
1:2:100:GLU:OE1	4:B:253:ARG:NH2	2.25	0.70
3:A:151:THR:OG1	3:A:153:GLU:OE1	2.09	0.70
1:2:7:ARG:NH2	1:2:9:GLU:OE2	2.20	0.70
3:A:465:ARG:HH21	3:A:470:GLU:HB3	1.56	0.70
12:LR:142:ILE:HD12	12:LR:142:ILE:H	1.57	0.70
4:B:66:TYR:OH	4:B:95:LYS:NZ	2.20	0.69
4:B:612:LYS:HG3	4:B:613:LYS:HD2	1.74	0.69
4:B:254:ASN:HB3	4:B:260:TYR:HE2	1.58	0.69
3:A:247:ILE:HG22	3:A:268:THR:HG22	1.74	0.69
4:B:34:LYS:O	4:B:34:LYS:NZ	2.24	0.69
4:B:416:LYS:HD3	4:B:419:LYS:HD3	1.76	0.68
4:B:657:ALA:O	4:B:661:LEU:HD12	1.94	0.68
5:1:3597:G:OP1	12:LR:143:HIS:NE2	2.27	0.67
4:B:126:GLN:OE1	4:B:526:HIS:NE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:559:ARG:HA	4:B:562:ILE:HG22	1.77	0.67
4:B:427:ALA:O	4:B:431:MET:HG2	1.95	0.67
6:LC:212:ASN:HD22	6:LC:255:SER:HB3	1.60	0.67
4:B:9:LYS:H	4:B:9:LYS:HD3	1.58	0.66
4:B:194:LEU:HB3	4:B:536:ARG:HD3	1.76	0.66
7:LE:210:LYS:N	7:LE:210:LYS:HE2	2.10	0.66
1:2:109:LEU:HG	1:2:147:MET:HB3	1.77	0.66
4:B:529:CYS:O	4:B:533:ILE:N	2.29	0.66
4:B:759:ASP:O	4:B:794:THR:N	2.27	0.66
5:1:386:A:OP2	9:LY:89:LYS:NZ	2.27	0.66
4:B:448:CYS:HA	4:B:451:TYR:CD2	2.31	0.66
3:A:474:ARG:NH1	3:A:478:TYR:O	2.29	0.66
11:LX:76:ILE:HG22	11:LX:77:ILE:HD13	1.77	0.66
1:2:77:VAL:O	1:2:82:ARG:NH1	2.30	0.65
5:1:512:U:O4	5:1:647:G:O6	2.15	0.65
4:B:556:LYS:HA	4:B:559:ARG:HG2	1.78	0.65
4:B:123:LEU:O	4:B:127:MET:HE1	1.97	0.65
7:LE:96:VAL:HG12	7:LE:103:GLY:HA2	1.79	0.65
4:B:128:ARG:HH12	4:B:522:GLN:HE22	1.44	0.64
4:B:307:LYS:NZ	4:B:344:GLU:OE2	2.31	0.64
6:LC:140:LYS:HE3	6:LC:245:HIS:HB2	1.78	0.64
4:B:523:PHE:HA	4:B:526:HIS:CD2	2.32	0.64
4:B:213:LEU:HD22	4:B:230:LYS:HE3	1.79	0.64
5:1:513:U:N3	5:1:516:C:OP2	2.29	0.64
12:LR:142:ILE:HG22	12:LR:146:LYS:HG3	1.80	0.64
7:LE:164:PHE:HA	7:LE:175:VAL:HG23	1.78	0.64
1:2:22:LEU:O	4:B:442:ARG:NH2	2.31	0.63
1:2:30:TYR:HA	1:2:33:TYR:HB3	1.79	0.63
3:A:136:GLU:OE1	3:A:137:TYR:N	2.31	0.63
6:LC:218:ILE:HD12	6:LC:219:LYS:H	1.63	0.63
7:LE:128:HIS:O	7:LE:128:HIS:ND1	2.30	0.63
4:B:505:LEU:O	4:B:509:HIS:ND1	2.30	0.63
4:B:224:LEU:HG	4:B:253:ARG:HE	1.63	0.62
2:8:67:U:H2'	2:8:68:G:H8	1.65	0.62
4:B:716:PHE:HD2	4:B:746:PRO:HG3	1.64	0.62
6:LC:156:ASP:OD2	6:LC:255:SER:OG	2.15	0.62
4:B:13:LEU:HD22	4:B:16:ARG:HH21	1.64	0.62
4:B:545:GLU:HA	4:B:548:LEU:HB2	1.82	0.62
5:1:2527:A:OP1	12:LR:38:ARG:NH2	2.32	0.62
3:A:427:LYS:NZ	11:LX:151:ASN:OD1	2.25	0.62
4:B:665:LYS:NZ	4:B:682:TYR:OH	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:342:ILE:O	4:B:346:VAL:HG12	1.99	0.62
4:B:693:GLN:O	4:B:697:ARG:HD3	1.98	0.62
6:LC:235:LEU:HD12	6:LC:240:LEU:HD11	1.82	0.62
1:2:26:TYR:OH	1:2:29:LYS:HB2	2.00	0.62
4:B:94:LYS:N	4:B:94:LYS:HE2	2.13	0.62
4:B:550:GLN:HG3	4:B:667:LEU:HD23	1.82	0.61
5:1:2902:G:N2	5:1:3597:G:N7	2.47	0.61
3:A:399:THR:HA	3:A:431:ALA:HB1	1.82	0.61
4:B:69:VAL:HG11	4:B:89:LEU:HD22	1.82	0.61
4:B:562:ILE:HD13	4:B:677:PHE:HB3	1.83	0.61
6:LC:294:LYS:HA	6:LC:299:GLN:HE21	1.65	0.61
1:2:57:LEU:O	1:2:73:THR:N	2.32	0.61
4:B:256:GLU:HA	4:B:292:VAL:HG21	1.83	0.61
6:LC:56:GLU:HG2	6:LC:57:LEU:HD23	1.83	0.61
4:B:27:ARG:NH1	5:1:204:U:H5'	2.14	0.60
6:LC:35:ASP:OD2	6:LC:36:ILE:N	2.34	0.60
1:2:127:ASN:O	1:2:149:ARG:NH1	2.34	0.60
4:B:683:PHE:HE1	4:B:718:THR:HG21	1.65	0.60
1:2:26:TYR:HE2	1:2:30:TYR:H	1.50	0.60
3:A:137:TYR:OH	3:A:465:ARG:O	2.20	0.60
9:LY:22:PRO:HG2	9:LY:25:ILE:HG12	1.84	0.60
4:B:650:VAL:HG13	4:B:653:PRO:HG3	1.83	0.60
4:B:169:LYS:HA	4:B:172:GLU:HG3	1.82	0.60
4:B:318:PHE:HB3	4:B:372:THR:HG23	1.84	0.60
4:B:470:ARG:HH21	4:B:473:THR:HG21	1.66	0.60
1:2:97:ALA:O	1:2:101:ASN:ND2	2.34	0.60
4:B:112:ASP:OD1	4:B:112:ASP:N	2.34	0.60
5:1:2520:C:H2'	5:1:2521:G:H8	1.65	0.60
6:LC:146:GLU:HG2	6:LC:175:LYS:HB3	1.82	0.60
1:2:112:ARG:HD3	1:2:113:LYS:N	2.16	0.59
4:B:54:LEU:HB2	4:B:85:VAL:HG13	1.84	0.59
4:B:496:LYS:NZ	4:B:563:GLU:HB2	2.17	0.59
1:2:112:ARG:HD3	1:2:114:SER:H	1.66	0.59
4:B:310:LEU:HD21	4:B:342:ILE:HG22	1.82	0.59
5:1:223:G:N3	6:LC:223:ASN:ND2	2.50	0.59
11:LX:67:ARG:H	11:LX:67:ARG:HD3	1.67	0.59
2:8:47:C:H1'	2:8:61:A:H2'	1.83	0.59
3:A:384:MET:HB3	3:A:444:TYR:HE1	1.68	0.59
4:B:148:ARG:HB2	4:B:174:PHE:HE1	1.67	0.59
5:1:662:C:H2'	5:1:663:G:C8	2.37	0.59
9:LY:26:ARG:NH1	9:LY:75:ARG:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:210:LEU:HD13	4:B:237:LEU:HD12	1.83	0.59
9:LY:29:ILE:HD12	9:LY:29:ILE:H	1.67	0.59
3:A:193:MET:SD	3:A:193:MET:N	2.69	0.59
3:A:202:ASP:OD1	3:A:203:CYS:N	2.35	0.59
11:LX:143:ASP:OD2	11:LX:144:TYR:N	2.36	0.59
11:LX:52:LEU:HD23	11:LX:52:LEU:H	1.67	0.59
3:A:421:ASP:OD1	3:A:428:TYR:OH	2.19	0.59
4:B:215:THR:O	4:B:218:LYS:NZ	2.29	0.58
4:B:416:LYS:HD2	4:B:420:HIS:CE1	2.38	0.58
4:B:430:TRP:HD1	4:B:431:MET:HE1	1.67	0.58
9:LY:66:GLN:OE1	9:LY:66:GLN:N	2.18	0.58
5:1:684:G:H5''	7:LE:100:LYS:HE2	1.85	0.58
4:B:452:MET:HA	4:B:455:ALA:HB3	1.86	0.58
4:B:415:ALA:HB2	4:B:431:MET:HE3	1.86	0.58
3:A:167:ASN:O	3:A:171:GLU:HG2	2.03	0.58
1:2:26:TYR:CG	1:2:27:GLN:N	2.72	0.58
3:A:280:VAL:HG21	3:A:456:ALA:HB3	1.85	0.58
4:B:541:LEU:HD12	4:B:544:LEU:HD23	1.84	0.58
5:1:661:C:H2'	5:1:662:C:C6	2.39	0.58
4:B:496:LYS:NZ	4:B:560:ILE:O	2.37	0.58
7:LE:157:HIS:HB3	7:LE:160:LYS:HG3	1.85	0.58
3:A:281:LYS:O	3:A:285:ASN:ND2	2.37	0.57
11:LX:148:ASP:N	11:LX:148:ASP:OD1	2.33	0.57
1:2:128:PHE:HB3	1:2:147:MET:SD	2.44	0.57
4:B:553:PHE:HD1	4:B:556:LYS:HD3	1.70	0.57
4:B:166:MET:HA	4:B:169:LYS:HG3	1.85	0.57
4:B:570:ASP:OD1	4:B:571:ASN:N	2.37	0.57
5:1:2896:G:H5'	5:1:2897:G:OP2	2.04	0.57
3:A:356:GLU:N	3:A:356:GLU:OE2	2.38	0.57
4:B:426:GLU:OE2	4:B:429:ARG:NH2	2.33	0.57
11:LX:120:ASP:OD1	11:LX:121:VAL:N	2.38	0.57
6:LC:218:ILE:HD12	6:LC:219:LYS:N	2.19	0.56
1:2:7:ARG:NH2	4:B:540:ASP:O	2.37	0.56
1:2:28:MET:HG2	1:2:32:PHE:CZ	2.40	0.56
4:B:594:LYS:NZ	5:1:685:C:H3'	2.20	0.56
4:B:654:LEU:HD22	4:B:681:ILE:HG12	1.87	0.56
4:B:661:LEU:O	4:B:665:LYS:N	2.29	0.56
4:B:682:TYR:HA	4:B:685:LYS:HB2	1.87	0.56
11:LX:81:LEU:HB3	11:LX:97:VAL:HG23	1.86	0.56
9:LY:69:LYS:HB3	9:LY:83:GLU:OE1	2.05	0.56
12:LR:32:ILE:HD12	12:LR:32:ILE:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:224:SER:HB2	3:A:249:LYS:HE2	1.85	0.56
4:B:722:SER:O	4:B:730:ARG:NH2	2.36	0.56
9:LY:54:GLU:HG2	9:LY:108:ARG:HB3	1.87	0.56
7:LE:176:THR:HB	7:LE:186:LEU:HD23	1.88	0.56
3:A:247:ILE:HD12	3:A:247:ILE:O	2.06	0.56
3:A:435:LEU:HB3	3:A:441:VAL:HG12	1.88	0.56
4:B:122:LEU:HD22	4:B:526:HIS:HB3	1.87	0.55
1:2:12:MET:SD	1:2:16:HIS:NE2	2.79	0.55
6:LC:65:GLU:OE1	6:LC:80:ARG:HB3	2.06	0.55
6:LC:209:ILE:HB	6:LC:229:LEU:HD13	1.89	0.55
1:2:3:ILE:HD12	1:2:93:GLN:HG3	1.88	0.55
4:B:148:ARG:HH22	4:B:531:ARG:HA	1.71	0.55
5:1:215:C:H2'	5:1:220:C:O4'	2.06	0.55
5:1:458:C:OP2	7:LE:114:ARG:NH1	2.38	0.55
5:1:2532:C:O2'	11:LX:93:ASN:ND2	2.40	0.55
4:B:171:LEU:HD13	4:B:196:GLN:HA	1.87	0.55
5:1:481:G:H1	5:1:673:C:H42	1.53	0.55
5:1:2533:C:OP1	11:LX:139:ARG:NH1	2.40	0.55
6:LC:218:ILE:HG22	6:LC:229:LEU:HG	1.87	0.55
1:2:28:MET:HG2	1:2:32:PHE:CE2	2.42	0.55
1:2:77:VAL:HG13	1:2:82:ARG:HG2	1.89	0.55
3:A:174:GLU:OE1	3:A:177:ARG:NH1	2.39	0.55
4:B:473:THR:OG1	4:B:477:GLU:OE1	2.19	0.55
1:2:3:ILE:HG12	4:B:256:GLU:HB2	1.89	0.55
4:B:737:MET:HA	4:B:741:PHE:HD1	1.72	0.54
4:B:513:ARG:HH11	4:B:639:LYS:HD3	1.73	0.54
4:B:9:LYS:O	4:B:13:LEU:HG	2.08	0.54
4:B:310:LEU:O	4:B:314:LEU:HG	2.07	0.54
11:LX:151:ASN:N	11:LX:156:ILE:HG22	2.23	0.54
4:B:652:THR:O	4:B:656:GLU:HG2	2.07	0.54
4:B:765:LEU:HD22	4:B:804:VAL:HG22	1.89	0.54
11:LX:121:VAL:HG13	11:LX:138:VAL:HG23	1.90	0.54
4:B:141:LEU:HD11	4:B:151:TRP:CE2	2.42	0.54
4:B:70:ARG:HB2	4:B:70:ARG:NH1	2.23	0.54
5:1:499:G:H2'	5:1:504:G:N2	2.22	0.54
9:LY:115:ARG:O	9:LY:119:LEU:HD22	2.08	0.54
5:1:2701:U:H3	5:1:2715:G:H1	1.56	0.54
12:LR:141:HIS:HA	12:LR:144:LYS:HE2	1.90	0.54
3:A:227:ASN:HD22	3:A:451:LYS:HA	1.74	0.53
3:A:429:LEU:HA	3:A:432:LEU:HB3	1.90	0.53
4:B:148:ARG:HB2	4:B:174:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:691:C:H2'	5:1:692:A:C8	2.44	0.53
1:2:30:TYR:O	1:2:34:HIS:ND1	2.30	0.53
4:B:21:TYR:CE2	4:B:54:LEU:HD23	2.44	0.53
6:LC:352:ASP:O	6:LC:356:ALA:N	2.36	0.53
11:LX:153:ILE:H	11:LX:153:ILE:HD12	1.73	0.53
2:8:75:G:OP2	9:LY:74:TYR:OH	2.23	0.53
4:B:205:LEU:HG	4:B:208:GLU:HB2	1.91	0.53
4:B:240:LEU:HD12	4:B:267:ALA:HA	1.91	0.53
5:1:679:C:H2'	5:1:680:G:H8	1.73	0.53
3:A:303:ALA:O	3:A:307:VAL:HG12	2.09	0.53
4:B:295:ARG:NH1	4:B:299:ASN:OD1	2.41	0.53
4:B:485:MET:SD	4:B:553:PHE:HB3	2.48	0.53
4:B:754:LEU:HB3	4:B:755:LYS:HZ2	1.73	0.53
5:1:493:G:C6	5:1:660:A:N1	2.77	0.53
2:8:82:A:H3'	2:8:83:C:H5'	1.90	0.53
5:1:3599:A:H2'	5:1:3600:G:C8	2.43	0.53
6:LC:60:HIS:HA	6:LC:92:PHE:HE1	1.74	0.53
1:2:7:ARG:O	1:2:9:GLU:N	2.41	0.52
3:A:120:ILE:HG13	3:A:175:ALA:HB2	1.91	0.52
4:B:169:LYS:HD2	4:B:170:ILE:N	2.24	0.52
4:B:478:ASN:O	4:B:482:MET:HE2	2.08	0.52
4:B:541:LEU:O	4:B:544:LEU:HB3	2.09	0.52
5:1:3596:A:C5	12:LR:143:HIS:HB3	2.44	0.52
1:2:63:ASP:HB3	1:2:66:ASP:HB3	1.91	0.52
4:B:158:TYR:HA	4:B:161:LEU:HD12	1.92	0.52
4:B:416:LYS:NZ	15:B:901:IHP:O45	2.33	0.52
5:1:2521:G:H2'	5:1:2522:G:H8	1.74	0.52
7:LE:150:LEU:HD13	7:LE:194:VAL:HG11	1.91	0.52
11:LX:73:HIS:HB3	11:LX:115:LYS:HE3	1.92	0.52
3:A:430:MET:HA	3:A:433:LYS:HE3	1.91	0.52
4:B:312:LYS:O	4:B:316:MET:HG3	2.10	0.52
1:2:138:TYR:CE2	1:2:144:ALA:HB2	2.44	0.52
11:LX:87:MET:HE2	11:LX:87:MET:HA	1.92	0.52
1:2:112:ARG:HG3	1:2:115:ASN:H	1.75	0.52
4:B:90:GLN:HA	4:B:95:LYS:HE3	1.90	0.52
5:1:2693:G:H2'	5:1:2694:G:N2	2.25	0.52
3:A:399:THR:HG23	3:A:435:LEU:HD22	1.91	0.52
4:B:620:GLN:OE1	4:B:624:GLN:NE2	2.43	0.52
1:2:43:TYR:HE1	1:2:93:GLN:HB3	1.74	0.52
3:A:189:PRO:HG3	3:A:269:PHE:CD2	2.44	0.52
4:B:80:HIS:HB3	4:B:109:TRP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LE:161:ARG:NH1	7:LE:273:SER:OG	2.42	0.52
1:2:72:ILE:O	1:2:72:ILE:HD12	2.09	0.51
4:B:540:ASP:HA	4:B:543:LYS:HG2	1.91	0.51
5:1:382:G:N1	5:1:385:A:OP2	2.38	0.51
5:1:462:G:H2'	5:1:463:A:C8	2.45	0.51
6:LC:297:GLU:OE1	6:LC:297:GLU:N	2.26	0.51
9:LY:100:HIS:ND1	9:LY:102:SER:OG	2.39	0.51
11:LX:87:MET:HE3	11:LX:90:ILE:HD13	1.92	0.51
3:A:286:THR:HA	3:A:289:LYS:HE3	1.92	0.51
4:B:12:ALA:O	4:B:16:ARG:HG3	2.09	0.51
6:LC:362:GLN:N	6:LC:362:GLN:OE1	2.42	0.51
4:B:800:THR:O	4:B:803:GLU:HG3	2.10	0.51
7:LE:99:ASP:O	7:LE:100:LYS:HG2	2.10	0.51
7:LE:140:LEU:HD11	7:LE:144:ILE:HG21	1.92	0.51
3:A:325:ILE:HD13	3:A:366:PHE:HB3	1.93	0.51
9:LY:10:ASP:OD2	9:LY:12:SER:N	2.43	0.51
1:2:14:MET:HG2	1:2:31:TYR:HE2	1.76	0.51
2:8:83:C:H5	9:LY:50:ARG:HH21	1.59	0.51
3:A:391:HIS:ND1	12:LR:34:ASN:OD1	2.44	0.51
6:LC:277:TYR:HD1	6:LC:278:ASN:N	2.09	0.51
2:8:67:U:H2'	2:8:68:G:C8	2.44	0.50
11:LX:90:ILE:H	11:LX:90:ILE:HD12	1.76	0.50
11:LX:150:ALA:HA	11:LX:153:ILE:CD1	2.40	0.50
1:2:95:SER:O	1:2:99:ILE:HG12	2.11	0.50
2:8:83:C:H41	9:LY:50:ARG:HE	1.58	0.50
4:B:706:PRO:O	4:B:710:GLU:HG3	2.11	0.50
3:A:193:MET:HA	3:A:196:ILE:HB	1.93	0.50
4:B:27:ARG:HH22	5:1:204:U:H5''	1.76	0.50
4:B:258:TRP:HZ3	4:B:292:VAL:HG13	1.76	0.50
1:2:81:HIS:CD2	4:B:324:PRO:HB3	2.46	0.50
5:1:2519:U:O2'	5:1:2530:U:O2	2.28	0.50
12:LR:98:ARG:NH2	12:LR:130:ASN:OD1	2.27	0.50
4:B:218:LYS:HE2	4:B:219:GLN:HG2	1.94	0.50
5:1:2526:C:H2'	5:1:2527:A:C8	2.46	0.50
5:1:2900:U:H2'	5:1:2901:G:C8	2.46	0.50
4:B:44:GLU:O	4:B:75:ASN:ND2	2.45	0.50
4:B:452:MET:HG2	4:B:461:ALA:HB2	1.93	0.50
5:1:3596:A:C6	12:LR:143:HIS:HB3	2.47	0.50
4:B:144:ARG:HH12	4:B:146:ALA:HB3	1.75	0.50
4:B:496:LYS:HZ1	4:B:563:GLU:HB2	1.76	0.50
4:B:570:ASP:HB3	4:B:684:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LC:7:LEU:HG	6:LC:21:ASN:HB3	1.93	0.50
6:LC:25:PRO:HG2	6:LC:28:PHE:CD2	2.47	0.50
5:1:196:C:H4'	9:LY:126:ARG:NH1	2.27	0.50
4:B:16:ARG:HB3	4:B:19:ARG:NH2	2.27	0.49
6:LC:152:LEU:HD23	6:LC:251:ILE:HG12	1.93	0.49
6:LC:138:MET:SD	6:LC:144:ILE:HD12	2.52	0.49
7:LE:43:HIS:CD2	7:LE:44:CYS:H	2.30	0.49
12:LR:45:ILE:HD12	12:LR:46:LYS:N	2.27	0.49
4:B:34:LYS:NZ	4:B:38:SER:HB3	2.28	0.49
11:LX:153:ILE:HB	11:LX:155:ILE:HG22	1.93	0.49
3:A:176:HIS:CE1	3:A:263:CYS:HB3	2.47	0.49
9:LY:82:ILE:HG22	9:LY:83:GLU:OE2	2.12	0.49
1:2:36:LEU:HB3	4:B:529:CYS:SG	2.52	0.49
4:B:540:ASP:HA	4:B:543:LYS:HE3	1.94	0.49
5:1:2897:G:H2'	5:1:2898:G:H8	1.77	0.49
3:A:248:CYS:HB3	3:A:267:VAL:HG22	1.94	0.49
3:A:383:TYR:CZ	3:A:432:LEU:HD21	2.48	0.49
3:A:409:ASN:HD22	3:A:423:LEU:HD13	1.77	0.49
1:2:25:ASN:CG	4:B:442:ARG:HH22	2.15	0.49
1:2:133:VAL:HG22	1:2:145:TYR:HD1	1.77	0.49
3:A:392:VAL:HB	3:A:440:ILE:HD11	1.94	0.49
4:B:483:GLN:HG2	4:B:514:HIS:CD2	2.48	0.49
5:1:679:C:H2'	5:1:680:G:C8	2.47	0.49
5:1:2705:G:H1'	5:1:2712:G:N2	2.28	0.49
3:A:184:MET:HE3	3:A:187:ILE:HG21	1.95	0.49
4:B:156:ILE:O	4:B:160:LEU:HG	2.13	0.49
5:1:2525:U:P	12:LR:42:ARG:HH22	2.36	0.49
4:B:408:ILE:HD12	4:B:409:GLU:N	2.28	0.48
4:B:606:ALA:O	4:B:610:GLU:HG3	2.13	0.48
5:1:690:C:H2'	5:1:691:C:C6	2.48	0.48
1:2:7:ARG:HH11	1:2:8:PRO:HD2	1.78	0.48
4:B:592:LEU:HD22	4:B:596:ARG:HH21	1.77	0.48
5:1:485:C:H2'	5:1:485:C:O2	2.13	0.48
4:B:73:LEU:HD11	4:B:83:TRP:CE2	2.49	0.48
4:B:127:MET:SD	4:B:127:MET:N	2.87	0.48
4:B:289:ARG:H	4:B:289:ARG:HE	1.61	0.48
4:B:416:LYS:HD3	4:B:416:LYS:HA	1.69	0.48
4:B:827:CYS:O	4:B:831:PHE:N	2.40	0.48
5:1:685:C:H5''	5:1:686:A:OP1	2.12	0.48
1:2:7:ARG:NH1	4:B:540:ASP:OD1	2.46	0.48
3:A:383:TYR:CD2	3:A:432:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:122:LEU:O	4:B:125:ILE:HG13	2.13	0.48
4:B:592:LEU:HB3	4:B:596:ARG:HH21	1.78	0.48
4:B:824:ARG:NH1	4:B:837:PHE:O	2.47	0.48
5:1:2520:C:H2'	5:1:2521:G:C8	2.47	0.48
7:LE:99:ASP:O	7:LE:101:ASN:ND2	2.46	0.48
9:LY:50:ARG:HG2	9:LY:51:LYS:H	1.78	0.48
4:B:132:GLY:O	4:B:135:GLU:HG3	2.13	0.48
4:B:176:LYS:HA	4:B:179:GLN:HG2	1.96	0.48
4:B:526:HIS:HA	4:B:538:TYR:OH	2.13	0.48
9:LY:124:LYS:HG2	9:LY:127:GLN:HE21	1.79	0.48
2:8:90:C:O2'	9:LY:24:HIS:ND1	2.38	0.48
3:A:379:GLU:OE1	3:A:379:GLU:N	2.44	0.48
4:B:124:GLN:O	4:B:129:ASP:N	2.43	0.48
4:B:754:LEU:HB3	4:B:755:LYS:NZ	2.27	0.48
3:A:304:ILE:HD13	3:A:346:ILE:HG22	1.95	0.48
4:B:248:ARG:O	4:B:252:GLU:HG2	2.14	0.48
4:B:654:LEU:HD11	4:B:684:ARG:HB2	1.94	0.48
12:LR:78:ILE:HD12	12:LR:79:GLY:N	2.28	0.48
4:B:12:ALA:HA	4:B:15:LYS:HE2	1.96	0.48
4:B:21:TYR:OH	4:B:58:CYS:SG	2.65	0.48
5:1:3597:G:O2'	5:1:3598:C:O5'	2.32	0.48
11:LX:55:ARG:NE	11:LX:56:ARG:H	2.11	0.48
4:B:21:TYR:CZ	4:B:26:TYR:HE2	2.32	0.48
4:B:515:PHE:CE2	4:B:554:TYR:HB2	2.49	0.48
5:1:3599:A:H2'	5:1:3600:G:H8	1.77	0.48
4:B:134:ARG:NH1	4:B:161:LEU:HD11	2.28	0.48
4:B:529:CYS:HA	4:B:532:LYS:HB2	1.96	0.48
4:B:691:MET:HG3	4:B:715:LEU:HD23	1.96	0.48
7:LE:281:ILE:HD12	7:LE:281:ILE:O	2.14	0.48
12:LR:140:GLU:HA	12:LR:143:HIS:CD2	2.48	0.48
1:2:69:HIS:HA	1:2:104:ALA:HB1	1.96	0.47
2:8:66:A:H2'	2:8:67:U:C6	2.49	0.47
4:B:97:ASP:HA	4:B:100:ILE:HD12	1.96	0.47
5:1:2386:U:H2'	5:1:2387:G:H8	1.79	0.47
11:LX:105:ASN:O	11:LX:109:ILE:HG13	2.13	0.47
4:B:166:MET:CB	4:B:169:LYS:HE3	2.34	0.47
4:B:274:LEU:O	4:B:278:LYS:HG2	2.14	0.47
4:B:449:ALA:HA	4:B:452:MET:SD	2.54	0.47
7:LE:281:ILE:HB	7:LE:286:LEU:HD21	1.96	0.47
4:B:27:ARG:NH1	5:1:204:U:OP2	2.47	0.47
4:B:780:LYS:HA	4:B:783:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:64:U:C2	2:8:65:A:C8	3.02	0.47
2:8:79:G:C2	2:8:80:A:H1'	2.49	0.47
4:B:587:MET:HG3	4:B:592:LEU:HG	1.97	0.47
12:LR:67:THR:O	12:LR:71:ARG:N	2.47	0.47
3:A:308:MET:HG2	3:A:324:PRO:HG3	1.97	0.47
4:B:509:HIS:CE1	4:B:647:LEU:HD11	2.49	0.47
4:B:598:LYS:HA	4:B:601:ARG:HD3	1.95	0.47
4:B:765:LEU:HG	4:B:769:LYS:HE3	1.96	0.47
9:LY:34:LEU:HD21	9:LY:47:MET:HB2	1.97	0.47
11:LX:110:LYS:HG3	11:LX:121:VAL:HB	1.96	0.47
1:2:71:HIS:HA	1:2:108:SER:O	2.14	0.47
3:A:141:GLN:HB3	3:A:144:ARG:NH2	2.29	0.47
4:B:435:GLN:HG2	4:B:444:ILE:HG23	1.96	0.47
4:B:553:PHE:O	4:B:556:LYS:HG2	2.15	0.47
5:1:2521:G:H2'	5:1:2522:G:C8	2.49	0.47
9:LY:32:SER:OG	9:LY:101:PRO:O	2.25	0.47
11:LX:92:ASP:OD1	11:LX:92:ASP:N	2.48	0.47
12:LR:34:ASN:O	12:LR:34:ASN:ND2	2.48	0.47
4:B:14:PHE:HE1	4:B:51:MET:HG3	1.79	0.47
4:B:654:LEU:HB3	4:B:681:ILE:HG23	1.97	0.47
4:B:686:GLU:N	4:B:686:GLU:OE1	2.48	0.47
5:1:677:G:H2'	5:1:678:C:C6	2.50	0.47
3:A:297:LEU:O	3:A:300:VAL:HG22	2.15	0.47
5:1:678:C:H2'	5:1:679:C:C6	2.50	0.47
4:B:251:GLN:HG3	4:B:264:LEU:HD11	1.97	0.46
4:B:301:LEU:HB3	4:B:306:PHE:HB2	1.97	0.46
1:2:10:ASP:HA	1:2:13:ASN:OD1	2.15	0.46
3:A:477:ASP:N	3:A:477:ASP:OD1	2.48	0.46
4:B:250:LEU:HD22	4:B:260:TYR:CZ	2.50	0.46
4:B:706:PRO:HG3	4:B:763:HIS:CE1	2.51	0.46
11:LX:96:LEU:HB2	11:LX:138:VAL:HG13	1.97	0.46
3:A:141:GLN:HB3	3:A:144:ARG:HH21	1.79	0.46
3:A:384:MET:HB3	3:A:444:TYR:CE1	2.50	0.46
4:B:13:LEU:HD23	4:B:16:ARG:HE	1.80	0.46
6:LC:171:LEU:HD11	6:LC:177:TRP:HE3	1.79	0.46
11:LX:81:LEU:CD2	11:LX:83:THR:H	2.28	0.46
1:2:154:MET:HA	1:2:157:GLU:OE1	2.15	0.46
3:A:305:GLN:OE1	3:A:348:LYS:N	2.44	0.46
5:1:457:G:H2'	5:1:458:C:H6	1.81	0.46
9:LY:49:ILE:HD12	9:LY:49:ILE:HA	1.83	0.46
9:LY:74:TYR:CD2	9:LY:77:LYS:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:492:U:H3'	5:1:493:G:H8	1.80	0.46
6:LC:140:LYS:HB3	6:LC:142:HIS:HD2	1.80	0.46
11:LX:73:HIS:HD2	11:LX:116:LEU:HD21	1.80	0.46
6:LC:116:ASN:HB2	6:LC:119:GLN:HG3	1.97	0.46
4:B:374:LEU:HD11	4:B:410:LEU:HD11	1.98	0.46
9:LY:52:ASP:O	9:LY:110:LYS:HB2	2.15	0.46
5:1:501:C:H42	5:1:506:C:N4	2.14	0.46
1:2:2:ASN:HB2	4:B:258:TRP:CZ2	2.51	0.46
1:2:7:ARG:HD2	1:2:8:PRO:HD2	1.97	0.46
1:2:27:GLN:NE2	4:B:481:GLU:OE2	2.49	0.46
3:A:193:MET:HG2	3:A:234:PRO:HG3	1.98	0.46
4:B:52:LYS:O	4:B:56:LEU:HD22	2.16	0.46
4:B:297:PRO:HA	4:B:300:PHE:CE2	2.51	0.46
11:LX:109:ILE:O	11:LX:113:VAL:HG12	2.16	0.46
1:2:2:ASN:HD21	4:B:257:ASN:HA	1.80	0.45
1:2:46:GLU:OE2	4:B:258:TRP:NE1	2.46	0.45
1:2:112:ARG:CD	1:2:114:SER:H	2.29	0.45
4:B:496:LYS:NZ	4:B:564:ILE:HG13	2.31	0.45
4:B:625:LYS:HA	4:B:628:LYS:HD2	1.98	0.45
4:B:173:GLU:O	4:B:177:THR:HG23	2.16	0.45
4:B:460:GLU:O	4:B:464:MET:HG3	2.16	0.45
4:B:622:ARG:HA	4:B:625:LYS:HG2	1.98	0.45
5:1:2376:A:H2'	5:1:2377:C:C6	2.51	0.45
7:LE:94:LYS:HE2	7:LE:107:VAL:HG21	1.98	0.45
9:LY:125:SER:HB2	9:LY:126:ARG:HH12	1.81	0.45
1:2:16:HIS:HE1	4:B:551:HIS:CE1	2.34	0.45
4:B:24:LYS:HG3	4:B:26:TYR:CE1	2.52	0.45
4:B:411:PHE:O	4:B:414:LYS:N	2.49	0.45
5:1:691:C:H2'	5:1:692:A:H8	1.82	0.45
5:1:2694:G:H5'	5:1:2695:A:C2	2.52	0.45
9:LY:73:VAL:HA	9:LY:80:ILE:HG22	1.97	0.45
11:LX:73:HIS:CD2	11:LX:116:LEU:HD21	2.50	0.45
3:A:430:MET:CE	11:LX:156:ILE:HG12	2.47	0.45
4:B:224:LEU:H	4:B:224:LEU:HD12	1.80	0.45
4:B:530:MET:SD	4:B:531:ARG:N	2.90	0.45
7:LE:258:LEU:O	7:LE:262:LYS:HG2	2.16	0.45
12:LR:23:TRP:HB3	12:LR:51:ILE:HD12	1.98	0.45
1:2:2:ASN:ND2	4:B:257:ASN:HA	2.31	0.45
1:2:14:MET:HE3	1:2:14:MET:H	1.82	0.45
1:2:28:MET:O	1:2:31:TYR:HB2	2.17	0.45
1:2:52:ILE:HD11	1:2:55:TYR:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:118:ARG:O	4:B:122:LEU:HG	2.16	0.45
4:B:275:GLU:O	4:B:279:ILE:HG13	2.17	0.45
4:B:304:GLU:O	4:B:308:GLU:HG2	2.17	0.45
12:LR:74:ARG:HD3	12:LR:74:ARG:HA	1.78	0.45
4:B:35:GLN:O	4:B:38:SER:OG	2.27	0.45
7:LE:50:LEU:HD23	7:LE:50:LEU:H	1.82	0.45
9:LY:30:MET:SD	9:LY:101:PRO:HG2	2.56	0.45
1:2:26:TYR:CD1	1:2:27:GLN:N	2.84	0.45
4:B:553:PHE:CD1	4:B:556:LYS:HD3	2.51	0.45
4:B:609:GLU:O	4:B:613:LYS:HG2	2.17	0.45
9:LY:50:ARG:HB2	9:LY:115:ARG:NH2	2.32	0.45
9:LY:31:SER:HA	9:LY:48:PRO:HA	1.99	0.45
1:2:25:ASN:OD1	4:B:442:ARG:NH2	2.46	0.45
3:A:131:LYS:NZ	3:A:131:LYS:HB2	2.32	0.45
3:A:163:GLU:HA	3:A:166:TRP:CD1	2.51	0.45
4:B:13:LEU:O	4:B:17:ILE:HG13	2.16	0.45
4:B:14:PHE:CE1	4:B:51:MET:HG3	2.51	0.45
4:B:239:ARG:NE	4:B:242:ASP:OD2	2.50	0.45
4:B:515:PHE:CD1	4:B:549:ARG:HG2	2.52	0.45
4:B:705:HIS:HB3	4:B:708:LEU:HB3	1.98	0.45
11:LX:145:ASP:OD1	11:LX:146:ALA:N	2.50	0.45
3:A:209:LYS:HG3	3:A:209:LYS:O	2.17	0.45
4:B:67:GLU:HA	4:B:70:ARG:NH2	2.32	0.45
5:1:196:C:HO2'	9:LY:126:ARG:NH2	2.11	0.45
5:1:654:C:H5'	6:LC:268:ARG:HE	1.82	0.45
5:1:699:C:H2'	5:1:700:G:C8	2.52	0.45
1:2:91:MET:HG3	1:2:126:LEU:HD13	1.99	0.44
4:B:164:TYR:O	4:B:168:ALA:HB2	2.17	0.44
4:B:478:ASN:ND2	4:B:482:MET:HE1	2.31	0.44
5:1:2717:G:H2'	5:1:2718:U:C6	2.52	0.44
9:LY:118:ILE:HD13	9:LY:118:ILE:HA	1.83	0.44
9:LY:126:ARG:CZ	9:LY:126:ARG:HA	2.47	0.44
3:A:312:GLU:HA	3:A:312:GLU:OE1	2.16	0.44
4:B:13:LEU:CD2	4:B:16:ARG:HE	2.30	0.44
4:B:66:TYR:O	4:B:70:ARG:HG3	2.17	0.44
4:B:570:ASP:HB3	4:B:684:ARG:NE	2.32	0.44
5:1:460:C:H2'	5:1:461:G:H8	1.82	0.44
1:2:112:ARG:HD3	1:2:113:LYS:H	1.82	0.44
3:A:112:GLN:HE21	3:A:123:LEU:HD11	1.83	0.44
4:B:535:LEU:HA	4:B:538:TYR:HB2	1.98	0.44
5:1:473:C:H2'	5:1:474:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LC:121:ARG:CB	6:LC:277:TYR:HE2	2.31	0.44
2:8:77:A:H5''	3:A:375:HIS:NE2	2.33	0.44
4:B:484:CYS:SG	4:B:487:PHE:HD2	2.40	0.44
4:B:688:PHE:HE1	4:B:729:VAL:HG11	1.83	0.44
2:8:93:C:O2'	2:8:94:G:H8	2.01	0.44
4:B:415:ALA:HB2	4:B:431:MET:CE	2.47	0.44
4:B:779:GLN:HB3	4:B:780:LYS:HE2	1.99	0.44
5:1:202:C:H2'	5:1:203:U:C6	2.53	0.44
7:LE:264:ILE:HD11	7:LE:267:LEU:HD13	2.00	0.44
12:LR:23:TRP:CZ2	12:LR:26:PRO:HD3	2.52	0.44
12:LR:101:ILE:HG22	12:LR:104:ARG:NH2	2.32	0.44
12:LR:142:ILE:O	12:LR:146:LYS:N	2.36	0.44
1:2:8:PRO:O	1:2:11:LEU:HG	2.18	0.44
1:2:111:VAL:HG13	1:2:145:TYR:HB2	2.00	0.44
4:B:123:LEU:O	4:B:126:GLN:N	2.50	0.44
5:1:386:A:O4'	9:LY:87:ARG:HD3	2.18	0.44
1:2:160:ARG:O	1:2:163:GLU:HG2	2.17	0.44
1:2:163:GLU:O	1:2:166:GLU:HG3	2.18	0.44
2:8:82:A:H3'	2:8:83:C:C5'	2.47	0.44
4:B:23:HIS:HB2	4:B:25:GLN:OE1	2.18	0.44
4:B:593:LYS:HA	4:B:596:ARG:HG2	2.00	0.44
5:1:457:G:H2'	5:1:458:C:C6	2.52	0.44
4:B:27:ARG:HH12	5:1:204:U:P	2.41	0.44
4:B:156:ILE:HG12	4:B:535:LEU:HD11	2.00	0.44
4:B:174:PHE:O	4:B:177:THR:OG1	2.19	0.44
4:B:733:LEU:O	4:B:737:MET:SD	2.75	0.44
5:1:479:G:H2'	5:1:480:C:C6	2.53	0.44
5:1:2691:U:H2'	5:1:2692:U:C6	2.52	0.44
1:2:26:TYR:CE2	1:2:30:TYR:CD2	3.06	0.44
4:B:78:LYS:HA	4:B:109:TRP:CD2	2.53	0.44
4:B:135:GLU:O	4:B:139:GLN:HG2	2.17	0.44
4:B:565:TYR:HD2	4:B:657:ALA:HB2	1.82	0.44
4:B:690:LEU:HA	4:B:693:GLN:HG3	2.00	0.44
4:B:793:LEU:HB2	4:B:796:ARG:HD3	2.00	0.44
5:1:2386:U:C2	5:1:2387:G:C8	3.05	0.44
1:2:121:LEU:O	1:2:125:THR:HB	2.18	0.43
1:2:162:LEU:O	1:2:165:LYS:HG3	2.17	0.43
2:8:60:G:O6	2:8:96:C:O2'	2.26	0.43
3:A:337:ARG:HD2	3:A:387:PHE:CG	2.53	0.43
5:1:238:C:OP2	9:LY:45:ARG:NH2	2.51	0.43
7:LE:155:GLY:O	7:LE:158:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LE:178:PRO:HB3	7:LE:258:LEU:HD21	1.99	0.43
11:LX:71:LEU:HD22	11:LX:103:LYS:HE3	1.99	0.43
3:A:406:ILE:HD12	3:A:407:ASN:N	2.33	0.43
5:1:408:A:H4'	5:1:409:G:H3'	1.99	0.43
5:1:460:C:H2'	5:1:461:G:C8	2.53	0.43
5:1:2899:C:OP1	12:LR:108:ARG:NH2	2.50	0.43
11:LX:96:LEU:HG	11:LX:140:LEU:HD21	1.99	0.43
12:LR:149:LYS:O	12:LR:153:LYS:HG2	2.18	0.43
4:B:134:ARG:HD2	4:B:158:TYR:CZ	2.53	0.43
4:B:307:LYS:HD2	4:B:345:LEU:HD11	2.00	0.43
4:B:665:LYS:HA	4:B:669:LYS:NZ	2.34	0.43
3:A:114:ASP:HB2	3:A:115:PRO:HD3	2.00	0.43
4:B:21:TYR:CE2	4:B:26:TYR:HE2	2.37	0.43
4:B:224:LEU:HG	4:B:253:ARG:NE	2.30	0.43
4:B:510:GLU:HG2	4:B:513:ARG:NH2	2.33	0.43
5:1:470:A:H61	5:1:684:G:H1'	1.84	0.43
5:1:3597:G:O2'	5:1:3598:C:H6	1.77	0.43
12:LR:101:ILE:HD12	12:LR:102:LEU:N	2.34	0.43
1:2:7:ARG:NH1	1:2:8:PRO:HB2	2.32	0.43
1:2:113:LYS:HG2	1:2:145:TYR:CE2	2.54	0.43
4:B:78:LYS:HE3	4:B:78:LYS:HB3	1.79	0.43
4:B:394:LEU:HG	4:B:417:ILE:HG21	1.99	0.43
4:B:626:LYS:NZ	5:1:215:C:H1'	2.34	0.43
4:B:658:ILE:HD13	4:B:661:LEU:HD13	2.00	0.43
5:1:211:G:C2	5:1:212:A:C8	3.07	0.43
6:LC:170:LEU:HD23	6:LC:221:PHE:HZ	1.82	0.43
12:LR:3:MET:HA	12:LR:3:MET:CE	2.49	0.43
1:2:12:MET:SD	1:2:16:HIS:CD2	3.12	0.43
1:2:36:LEU:HD11	4:B:541:LEU:HD22	2.01	0.43
3:A:188:LYS:H	3:A:191:MET:HE2	1.82	0.43
4:B:230:LYS:HE2	4:B:230:LYS:HA	2.01	0.43
7:LE:146:PRO:HB3	7:LE:203:ILE:HD11	2.01	0.43
9:LY:54:GLU:CG	9:LY:108:ARG:HB3	2.49	0.43
4:B:292:VAL:HB	4:B:293:PRO:HD3	2.01	0.43
4:B:334:LYS:HA	4:B:334:LYS:HD3	1.83	0.43
5:1:202:C:H2'	5:1:203:U:H6	1.84	0.43
5:1:499:G:N2	5:1:656:C:H1'	2.33	0.43
5:1:2897:G:H2'	5:1:2898:G:C8	2.53	0.43
6:LC:207:PRO:HB3	6:LC:249:PHE:CD2	2.54	0.43
9:LY:37:GLU:OE1	9:LY:38:LEU:N	2.51	0.43
11:LX:71:LEU:HD11	11:LX:76:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LR:78:ILE:H	12:LR:78:ILE:HG13	1.68	0.43
1:2:86:LEU:HD23	1:2:89:LYS:HD2	2.01	0.43
4:B:600:ARG:O	4:B:603:GLN:HG3	2.18	0.43
4:B:688:PHE:HA	4:B:691:MET:HB2	2.01	0.43
5:1:650:C:H2'	5:1:651:C:C6	2.54	0.43
6:LC:262:GLU:OE1	6:LC:262:GLU:N	2.50	0.43
1:2:4:ARG:HE	1:2:4:ARG:HB2	1.72	0.43
1:2:34:HIS:CD2	1:2:59:LYS:HB3	2.53	0.43
2:8:70:G:H1'	2:8:88:A:N6	2.34	0.43
4:B:383:HIS:O	4:B:387:ILE:HG12	2.19	0.43
5:1:518:G:H1'	5:1:644:G:C2	2.53	0.43
9:LY:63:LYS:HB3	9:LY:63:LYS:HE2	1.77	0.43
1:2:53:VAL:HG11	1:2:81:HIS:CE1	2.54	0.42
3:A:396:LEU:HD21	11:LX:84:GLU:HG3	2.01	0.42
4:B:164:TYR:HB2	4:B:203:ALA:HB2	2.01	0.42
4:B:397:ILE:HD12	4:B:397:ILE:HA	1.94	0.42
4:B:562:ILE:HG13	4:B:657:ALA:HB1	2.01	0.42
4:B:661:LEU:HD22	4:B:665:LYS:HE3	2.01	0.42
5:1:411:G:H4'	5:1:412:G:H5''	2.01	0.42
1:2:14:MET:HG2	1:2:31:TYR:CE2	2.54	0.42
3:A:284:THR:O	3:A:288:ILE:HG12	2.18	0.42
4:B:418:TYR:HB3	4:B:423:ASN:O	2.19	0.42
4:B:613:LYS:HE3	4:B:613:LYS:HA	1.99	0.42
7:LE:47:ASN:HB2	7:LE:62:MET:CE	2.50	0.42
1:2:7:ARG:NE	1:2:9:GLU:H	2.17	0.42
4:B:621:GLN:C	4:B:625:LYS:HZ2	2.23	0.42
4:B:683:PHE:CE1	4:B:718:THR:HG21	2.51	0.42
5:1:385:A:O2'	5:1:387:G:H5'	2.19	0.42
4:B:562:ILE:CD1	4:B:677:PHE:HB3	2.47	0.42
4:B:594:LYS:HZ3	5:1:685:C:H3'	1.84	0.42
12:LR:3:MET:HA	12:LR:3:MET:HE2	2.01	0.42
1:2:89:LYS:HA	1:2:92:ASP:OD1	2.20	0.42
3:A:153:GLU:HG2	3:A:155:LYS:H	1.84	0.42
4:B:213:LEU:HB3	4:B:230:LYS:NZ	2.34	0.42
4:B:311:ASP:OD1	4:B:349:TYR:OH	2.30	0.42
11:LX:86:ALA:O	11:LX:90:ILE:HD12	2.20	0.42
1:2:36:LEU:HD21	4:B:541:LEU:HD22	2.02	0.42
4:B:597:ASN:O	4:B:601:ARG:HG3	2.19	0.42
4:B:727:ASP:HA	4:B:730:ARG:HB2	2.02	0.42
4:B:799:GLN:HA	4:B:802:MET:HE2	2.02	0.42
5:1:223:G:H4'	5:1:225:G:N7	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:501:C:H42	5:1:506:C:H41	1.66	0.42
7:LE:153:LEU:HD11	7:LE:195:ILE:HG12	2.01	0.42
9:LY:13:LYS:O	9:LY:17:ARG:HG3	2.20	0.42
5:1:2898:G:H2'	5:1:2899:C:C6	2.54	0.42
11:LX:90:ILE:HG23	11:LX:146:ALA:HB1	2.01	0.42
1:2:153:GLN:HG2	1:2:154:MET:N	2.34	0.42
3:A:430:MET:SD	11:LX:156:ILE:HA	2.60	0.42
4:B:656:GLU:HA	4:B:659:LYS:NZ	2.35	0.42
5:1:518:G:H1	5:1:643:C:H2'	1.85	0.42
7:LE:254:ASP:N	7:LE:254:ASP:OD1	2.53	0.42
4:B:626:LYS:HD2	4:B:626:LYS:C	2.40	0.42
4:B:799:GLN:HA	4:B:802:MET:CE	2.50	0.42
5:1:2529:A:O2'	5:1:2531:C:OP2	2.37	0.42
6:LC:66:SER:HA	6:LC:77:PRO:HA	2.02	0.42
3:A:402:LEU:HD13	3:A:431:ALA:HB3	2.02	0.42
3:A:430:MET:HE2	3:A:430:MET:HB2	1.94	0.42
4:B:93:ASP:C	4:B:94:LYS:HE2	2.39	0.42
4:B:273:MET:CE	4:B:274:LEU:HD23	2.49	0.42
4:B:385:ASP:OD2	4:B:416:LYS:HB3	2.19	0.42
4:B:669:LYS:HE3	4:B:669:LYS:HA	2.02	0.42
4:B:766:SER:O	4:B:770:MET:HG2	2.20	0.42
7:LE:166:LYS:O	7:LE:174:LEU:HB3	2.20	0.42
11:LX:82:THR:HG23	11:LX:155:ILE:HD11	2.01	0.42
1:2:106:TYR:HA	1:2:151:LEU:HG	2.01	0.41
1:2:150:ASP:O	1:2:153:GLN:NE2	2.51	0.41
2:8:82:A:N3	2:8:83:C:H5'	2.35	0.41
4:B:166:MET:SD	4:B:167:ALA:N	2.93	0.41
4:B:626:LYS:HD2	4:B:627:LYS:N	2.35	0.41
4:B:696:LYS:HE3	4:B:696:LYS:HB3	1.92	0.41
4:B:733:LEU:HG	4:B:737:MET:SD	2.60	0.41
4:B:760:SER:O	4:B:764:ARG:HG3	2.20	0.41
5:1:3600:G:H2'	5:1:3601:C:C6	2.54	0.41
9:LY:37:GLU:OE1	9:LY:38:LEU:HD22	2.20	0.41
9:LY:124:LYS:HB3	9:LY:124:LYS:HE3	1.87	0.41
12:LR:139:MET:HE2	12:LR:139:MET:HB2	1.87	0.41
1:2:7:ARG:HH21	1:2:9:GLU:CD	2.14	0.41
1:2:11:LEU:HA	1:2:14:MET:SD	2.60	0.41
1:2:47:ASP:OD1	1:2:51:LYS:N	2.53	0.41
3:A:258:GLY:HA3	3:A:335:GLN:OE1	2.19	0.41
3:A:282:ASP:OD2	3:A:311:TYR:OH	2.25	0.41
4:B:597:ASN:OD1	4:B:600:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:755:LYS:HD3	4:B:755:LYS:N	2.34	0.41
5:1:2706:G:H2'	5:1:2707:U:C6	2.55	0.41
1:2:96:ARG:CZ	4:B:253:ARG:HG3	2.50	0.41
4:B:559:ARG:O	4:B:563:GLU:HG2	2.20	0.41
4:B:591:GLU:OE1	4:B:591:GLU:N	2.53	0.41
4:B:679:PHE:O	4:B:691:MET:HE1	2.19	0.41
4:B:781:ARG:O	4:B:785:LEU:HG	2.19	0.41
5:1:221:C:H2'	5:1:222:C:C6	2.54	0.41
1:2:116:ARG:HA	1:2:119:LEU:HD12	2.02	0.41
3:A:430:MET:HA	3:A:433:LYS:CE	2.51	0.41
4:B:101:LYS:HE3	4:B:101:LYS:HB3	1.78	0.41
5:1:657:C:H2'	5:1:658:C:O4'	2.20	0.41
4:B:21:TYR:HE2	4:B:55:THR:HA	1.84	0.41
5:1:3596:A:OP1	5:1:3597:G:H1'	2.20	0.41
1:2:133:VAL:HG22	1:2:145:TYR:CD1	2.54	0.41
3:A:177:ARG:O	3:A:181:LYS:HG3	2.21	0.41
3:A:404:ASN:HA	3:A:407:ASN:ND2	2.35	0.41
4:B:225:ALA:HA	4:B:228:GLU:HG3	2.01	0.41
4:B:276:ARG:HA	4:B:279:ILE:HD12	2.02	0.41
5:1:683:C:H2'	5:1:684:G:O4'	2.21	0.41
5:1:3598:C:H2'	5:1:3599:A:C8	2.55	0.41
3:A:342:LYS:NZ	3:A:356:GLU:OE2	2.54	0.41
4:B:144:ARG:NH2	4:B:147:GLN:HG3	2.36	0.41
5:1:2691:U:H2'	5:1:2692:U:H6	1.85	0.41
9:LY:85:VAL:HG23	9:LY:85:VAL:O	2.21	0.41
4:B:295:ARG:NH2	4:B:331:SER:OG	2.54	0.41
5:1:493:G:N1	5:1:660:A:C2	2.78	0.41
5:1:512:U:C4	5:1:647:G:O6	2.74	0.41
9:LY:113:LYS:HE2	9:LY:113:LYS:HB3	1.91	0.41
11:LX:147:LEU:HD13	11:LX:156:ILE:HD13	2.01	0.41
1:2:60:MET:SD	1:2:98:MET:HE1	2.61	0.41
4:B:100:ILE:HD11	4:B:127:MET:HE2	2.03	0.41
4:B:507:LYS:O	4:B:511:ILE:HG12	2.21	0.41
5:1:228:C:H2'	5:1:229:G:H8	1.86	0.41
5:1:499:G:H2'	5:1:504:G:H22	1.86	0.41
5:1:2385:U:H2'	5:1:2386:U:H6	1.85	0.41
5:1:2385:U:C2	5:1:2386:U:C5	3.09	0.41
11:LX:60:TYR:O	11:LX:62:ARG:NH1	2.54	0.41
3:A:192:THR:OG1	3:A:194:ILE:HG22	2.21	0.41
3:A:330:GLY:HA3	3:A:344:VAL:HG22	2.03	0.41
3:A:416:CYS:SG	3:A:418:ARG:HB2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:430:MET:HE1	11:LX:156:ILE:HG12	2.02	0.41
4:B:689:LEU:HD23	4:B:689:LEU:H	1.85	0.41
5:1:221:C:H2'	5:1:222:C:H6	1.86	0.41
7:LE:128:HIS:O	7:LE:128:HIS:CG	2.74	0.41
4:B:425:LYS:HE3	4:B:835:LEU:HG	2.02	0.40
5:1:473:C:H2'	5:1:474:C:H6	1.86	0.40
11:LX:91:GLU:HB2	11:LX:92:ASP:OD1	2.22	0.40
11:LX:116:LEU:HB3	11:LX:117:TYR:CE1	2.56	0.40
1:2:28:MET:H	1:2:28:MET:CE	2.34	0.40
1:2:43:TYR:CE1	1:2:93:GLN:HB3	2.55	0.40
1:2:148:LYS:HG2	1:2:149:ARG:N	2.36	0.40
4:B:100:ILE:HD11	4:B:127:MET:CE	2.51	0.40
4:B:430:TRP:O	4:B:433:GLU:HB2	2.21	0.40
4:B:615:ALA:O	4:B:618:GLU:HG3	2.21	0.40
5:1:491:G:H2'	5:1:492:U:O4'	2.21	0.40
9:LY:47:MET:HE3	9:LY:48:PRO:HD2	2.03	0.40
9:LY:117:LYS:HE2	9:LY:117:LYS:HB3	1.94	0.40
11:LX:67:ARG:HD3	11:LX:67:ARG:N	2.35	0.40
4:B:448:CYS:HA	4:B:451:TYR:CE2	2.55	0.40
4:B:513:ARG:NH1	4:B:639:LYS:HD3	2.35	0.40
4:B:709:HIS:CD2	4:B:753:PHE:CD2	3.09	0.40
5:1:644:G:C2	5:1:645:G:H1'	2.55	0.40
5:1:2377:C:H2'	5:1:2378:G:O4'	2.22	0.40
5:1:2700:G:C6	5:1:2717:G:C6	3.09	0.40
7:LE:254:ASP:HA	7:LE:257:ILE:HB	2.03	0.40
9:LY:69:LYS:HB2	9:LY:69:LYS:HE3	1.84	0.40
1:2:164:LEU:O	1:2:167:LYS:HG3	2.22	0.40
2:8:90:C:H2'	2:8:91:A:C8	2.57	0.40
4:B:298:LEU:HB3	4:B:332:LEU:HD11	2.04	0.40
4:B:452:MET:HB3	4:B:452:MET:HE2	1.70	0.40
4:B:569:HIS:CD2	4:B:654:LEU:HG	2.55	0.40
4:B:645:GLU:C	4:B:649:LYS:HZ2	2.24	0.40
4:B:737:MET:HA	4:B:741:PHE:CD1	2.55	0.40
4:B:805:LEU:HD22	4:B:837:PHE:CE1	2.56	0.40
5:1:685:C:P	7:LE:101:ASN:HD21	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2	167/171 (98%)	161 (96%)	5 (3%)	1 (1%)	22	45
3	A	368/484 (76%)	356 (97%)	12 (3%)	0	100	100
4	B	832/840 (99%)	808 (97%)	23 (3%)	1 (0%)	48	73
6	LC	363/427 (85%)	345 (95%)	18 (5%)	0	100	100
7	LE	208/288 (72%)	195 (94%)	13 (6%)	0	100	100
8	Lk	67/70 (96%)	67 (100%)	0	0	100	100
9	LY	127/144 (88%)	124 (98%)	3 (2%)	0	100	100
10	Lh	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
11	LX	114/156 (73%)	113 (99%)	1 (1%)	0	100	100
12	LR	151/196 (77%)	151 (100%)	0	0	100	100
13	Lr	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
All	All	2640/3035 (87%)	2554 (97%)	84 (3%)	2 (0%)	50	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	292	VAL
1	2	8	PRO

5.3.2 Protein sidechains

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	2	148/149 (99%)	127 (86%)	21 (14%)	2	7
3	A	318/402 (79%)	306 (96%)	12 (4%)	28	56
4	B	744/749 (99%)	700 (94%)	44 (6%)	16	38
6	LC	304/348 (87%)	298 (98%)	6 (2%)	50	78
7	LE	190/252 (75%)	179 (94%)	11 (6%)	17	39
8	Lk	64/65 (98%)	61 (95%)	3 (5%)	22	49
9	LY	120/134 (90%)	116 (97%)	4 (3%)	33	62
10	Lh	109/109 (100%)	97 (89%)	12 (11%)	5	12
11	LX	104/133 (78%)	96 (92%)	8 (8%)	10	26
12	LR	137/175 (78%)	125 (91%)	12 (9%)	8	20
13	Lr	109/121 (90%)	105 (96%)	4 (4%)	29	58
All	All	2347/2637 (89%)	2210 (94%)	137 (6%)	19	39

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	4	ARG
1	2	11	LEU
1	2	14	MET
1	2	17	CYS
1	2	28	MET
1	2	30	TYR
1	2	32	PHE
1	2	33	TYR
1	2	60	MET
1	2	65	ASP
1	2	91	MET
1	2	103	ASN
1	2	105	LYS
1	2	110	HIS
1	2	122	TYR
1	2	137	TYR
1	2	149	ARG
1	2	154	MET
1	2	160	ARG
1	2	165	LYS
1	2	167	LYS
3	A	178	GLN
3	A	191	MET

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Mol	Chain	Res	Type
3	A	193	MET
3	A	275	THR
3	A	296	ARG
3	A	306	GLU
3	A	308	MET
3	A	355	MET
3	A	368	SER
3	A	378	MET
3	A	382	HIS
3	A	429	LEU
4	B	9	LYS
4	B	14	PHE
4	B	33	CYS
4	B	78	LYS
4	B	84	HIS
4	B	86	TYR
4	B	94	LYS
4	B	148	ARG
4	B	166	MET
4	B	169	LYS
4	B	175	ARG
4	B	176	LYS
4	B	184	LYS
4	B	218	LYS
4	B	232	GLU
4	B	262	LYS
4	B	282	GLU
4	B	286	LYS
4	B	289	ARG
4	B	316	MET
4	B	379	TYR
4	B	395	GLU
4	B	447	LYS
4	B	451	TYR
4	B	452	MET
4	B	459	LYS
4	B	464	MET
4	B	482	MET
4	B	485	MET
4	B	498	MET
4	B	530	MET
4	B	538	TYR

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Mol	Chain	Res	Type
4	B	571	ASN
4	B	610	GLU
4	B	614	ASN
4	B	622	ARG
4	B	626	LYS
4	B	639	LYS
4	B	641	GLU
4	B	696	LYS
4	B	697	ARG
4	B	723	LYS
4	B	728	THR
4	B	802	MET
6	LC	52	TYR
6	LC	101	MET
6	LC	179	ASP
6	LC	277	TYR
6	LC	289	LEU
6	LC	312	ARG
7	LE	62	MET
7	LE	68	MET
7	LE	99	ASP
7	LE	115	TYR
7	LE	154	THR
7	LE	220	LYS
7	LE	240	TYR
7	LE	244	GLU
7	LE	254	ASP
7	LE	270	TYR
7	LE	279	ASN
8	Lk	18	LYS
8	Lk	30	ASP
8	Lk	40	ARG
9	LY	9	SER
9	LY	53	ASP
9	LY	108	ARG
9	LY	124	LYS
10	Lh	14	LYS
10	Lh	20	GLN
10	Lh	42	SER
10	Lh	43	LYS
10	Lh	45	SER
10	Lh	65	GLN

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Mol	Chain	Res	Type
10	Lh	68	ASN
10	Lh	96	ASN
10	Lh	100	GLU
10	Lh	107	GLN
10	Lh	111	GLU
10	Lh	118	LYS
11	LX	50	LYS
11	LX	55	ARG
11	LX	67	ARG
11	LX	78	LYS
11	LX	82	THR
11	LX	92	ASP
11	LX	116	LEU
11	LX	138	VAL
12	LR	16	ARG
12	LR	34	ASN
12	LR	47	ASP
12	LR	59	SER
12	LR	63	CYS
12	LR	89	MET
12	LR	96	MET
12	LR	99	MET
12	LR	119	MET
12	LR	139	MET
12	LR	140	GLU
12	LR	144	LYS
13	Lr	24	THR
13	Lr	72	LYS
13	Lr	101	LYS
13	Lr	119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	514	HIS
4	B	522	GLN
4	B	620	GLN
4	B	624	GLN
6	LC	299	GLN
11	LX	93	ASN
12	LR	34	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	8	57/58 (98%)	12 (21%)	0
5	1	291/5070 (5%)	76 (26%)	1 (0%)
All	All	348/5128 (6%)	88 (25%)	1 (0%)

All (88) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	8	52	A
2	8	59	A
2	8	62	A
2	8	63	U
2	8	80	A
2	8	82	A
2	8	83	C
2	8	84	A
2	8	85	U
2	8	86	U
2	8	87	G
2	8	94	G
5	1	200	U
5	1	204	U
5	1	210	C
5	1	216	C
5	1	217	C
5	1	218	A
5	1	233	U
5	1	234	G
5	1	387	G
5	1	396	A
5	1	399	G
5	1	410	A
5	1	412	G
5	1	413	G
5	1	456	C
5	1	457	G
5	1	465	G
5	1	468	U
5	1	469	C
5	1	484	U
5	1	485	C
5	1	486	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1	489	C
5	1	492	U
5	1	493	G
5	1	495	C
5	1	496	G
5	1	497	G
5	1	498	C
5	1	500	G
5	1	501	C
5	1	502	C
5	1	503	C
5	1	505	G
5	1	506	C
5	1	509	A
5	1	510	U
5	1	512	U
5	1	513	U
5	1	514	U
5	1	517	C
5	1	518	G
5	1	643	C
5	1	644	G
5	1	646	G
5	1	654	C
5	1	657	C
5	1	665	C
5	1	666	G
5	1	667	A
5	1	668	C
5	1	672	C
5	1	673	C
5	1	675	C
5	1	686	A
5	1	687	U
5	1	697	G
5	1	2523	G
5	1	2529	A
5	1	2537	A
5	1	2694	G
5	1	2695	A
5	1	2696	A
5	1	2701	U

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Mol	Chain	Res	Type
5	1	2708	U
5	1	2709	C
5	1	2710	C
5	1	2711	G
5	1	2712	G
5	1	2714	G
5	1	2897	G
5	1	3596	A
5	1	3597	G
5	1	3598	C
5	1	3604	A
5	1	3605	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	1	685	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	IHP	B	901	-	36,36,36	0.76	0	54,60,60	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	IHP	B	901	-	-	11/30/54/54	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	901	IHP	C4-C5-O15-P5
15	B	901	IHP	C6-C5-O15-P5
15	B	901	IHP	C5-O15-P5-O35
15	B	901	IHP	C4-C3-O13-P3
15	B	901	IHP	C3-O13-P3-O23
15	B	901	IHP	C1-C2-O12-P2
15	B	901	IHP	C2-C3-O13-P3
15	B	901	IHP	C1-O11-P1-O31
15	B	901	IHP	C3-O13-P3-O33
15	B	901	IHP	C3-O13-P3-O43
15	B	901	IHP	C5-O15-P5-O45

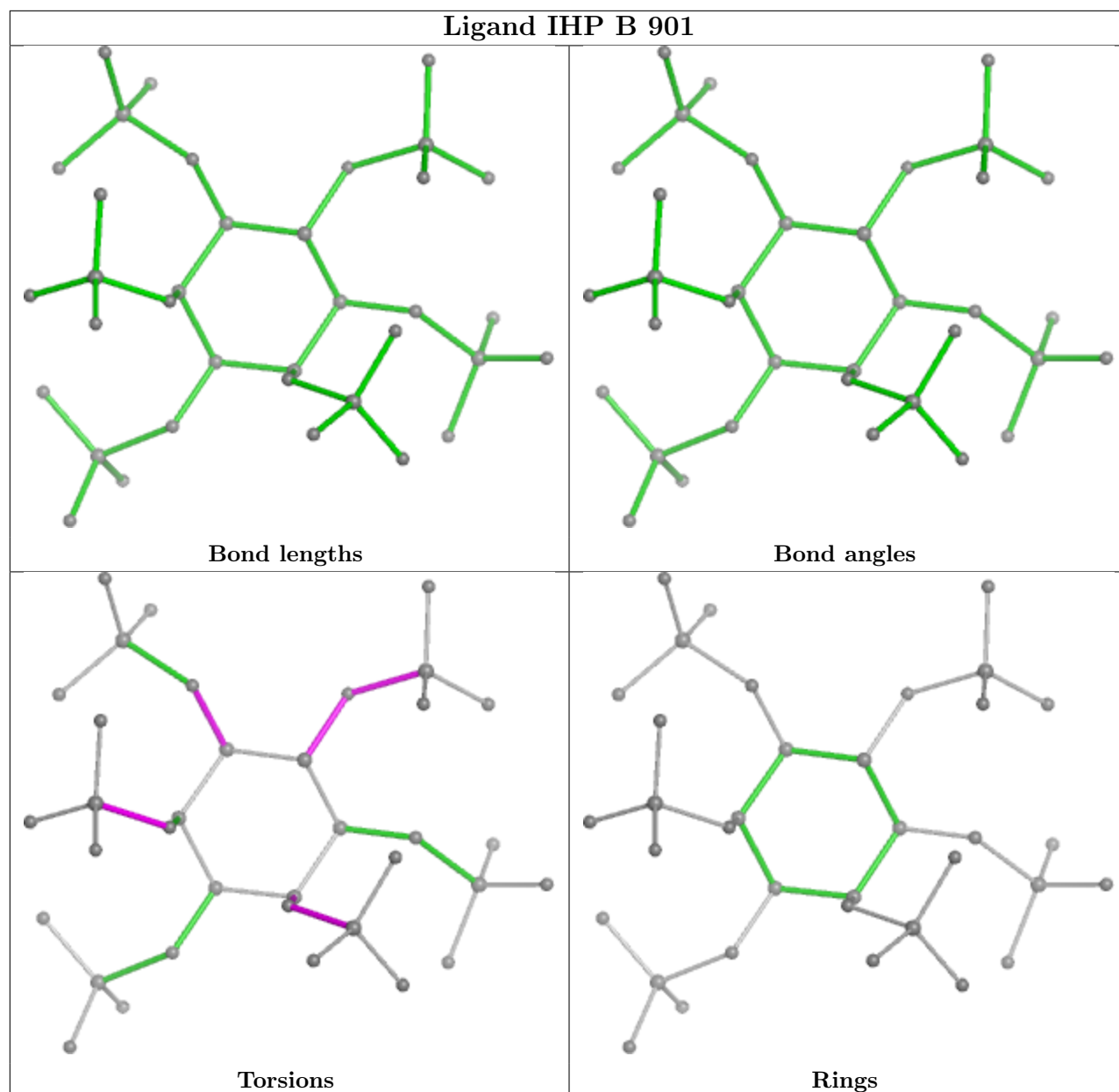
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	901	IHP	1	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

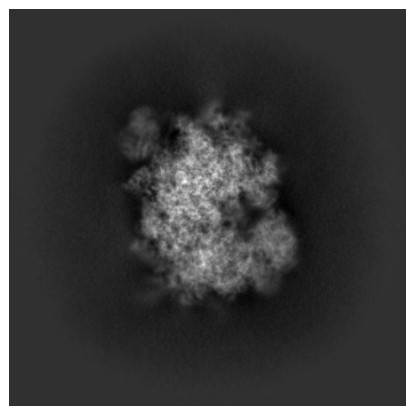
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50641. These allow visual inspection of the internal detail of the map and identification of artifacts.

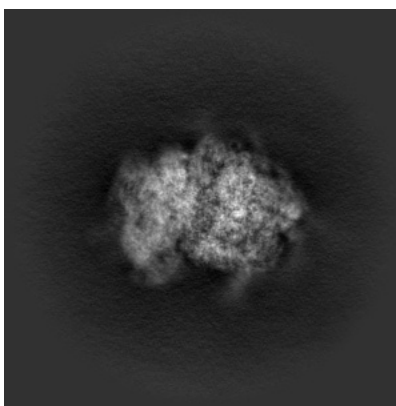
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

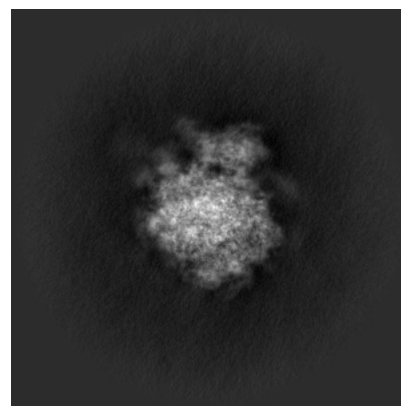
6.1.1 Primary map



X

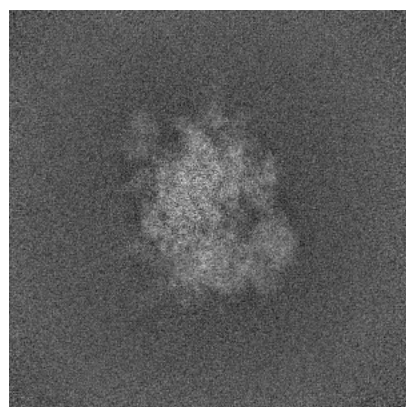


Y

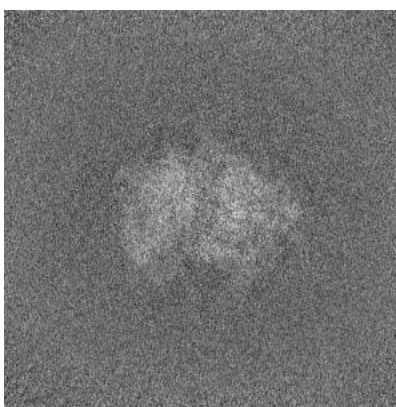


Z

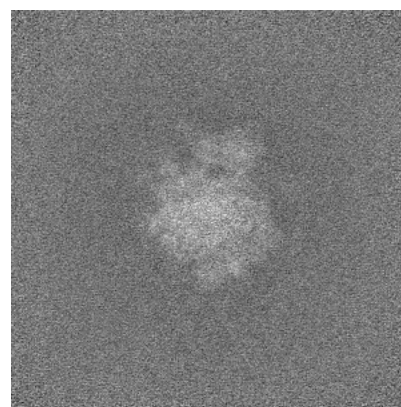
6.1.2 Raw map



X



Y

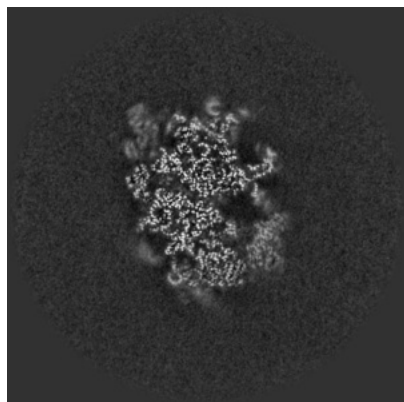


Z

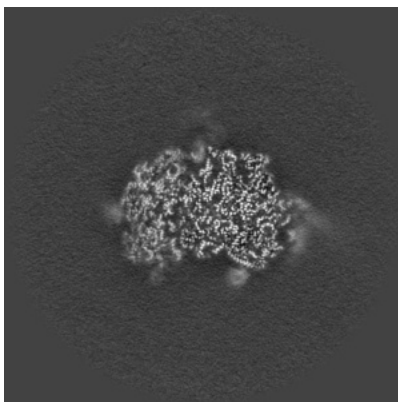
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

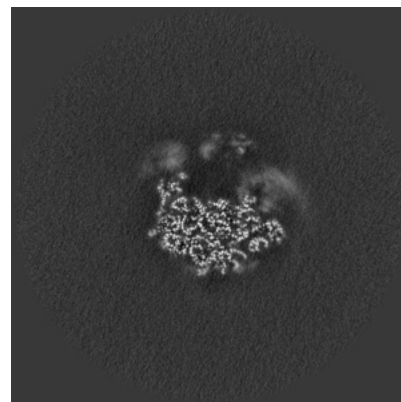
6.2.1 Primary map



X Index: 360

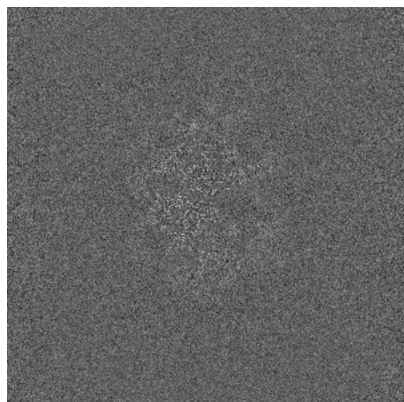


Y Index: 360

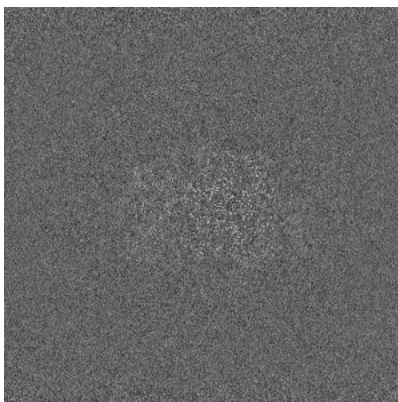


Z Index: 360

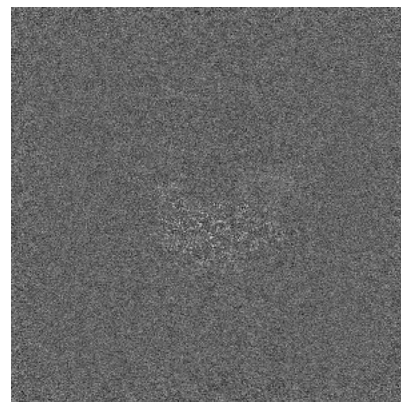
6.2.2 Raw map



X Index: 360



Y Index: 360

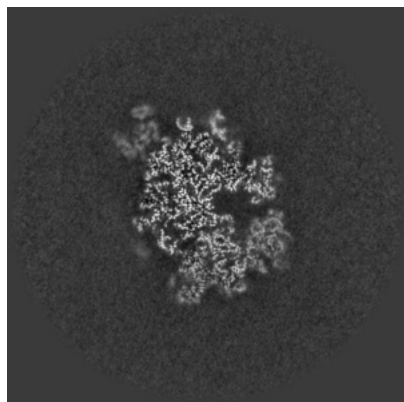


Z Index: 360

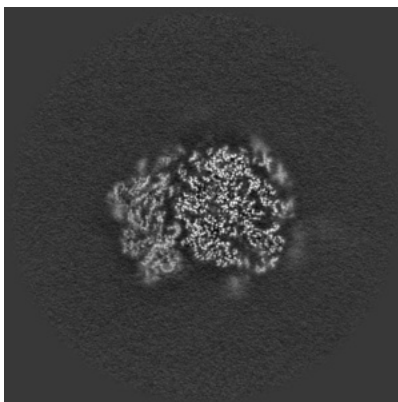
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

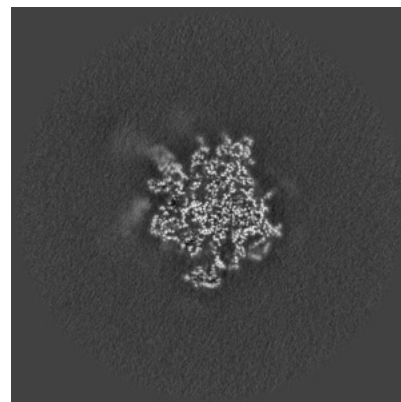
6.3.1 Primary map



X Index: 383

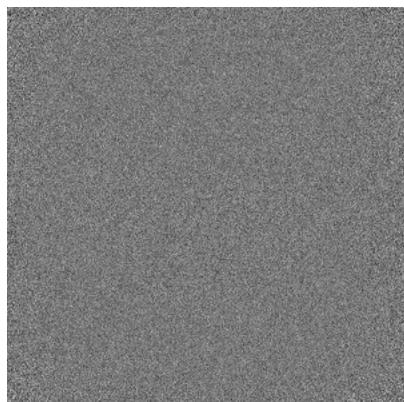


Y Index: 343

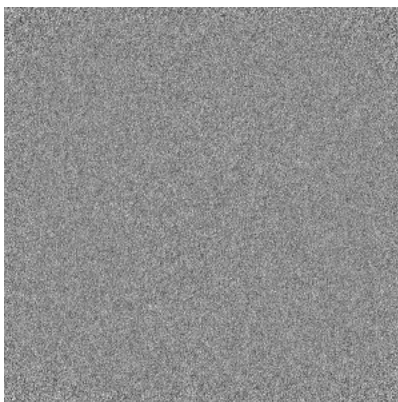


Z Index: 409

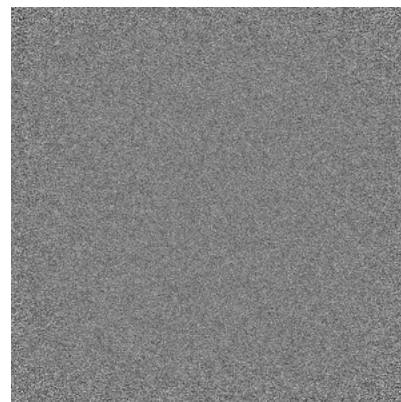
6.3.2 Raw map



X Index: 0



Y Index: 0

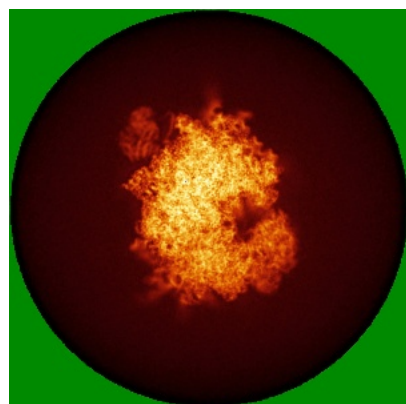


Z Index: 0

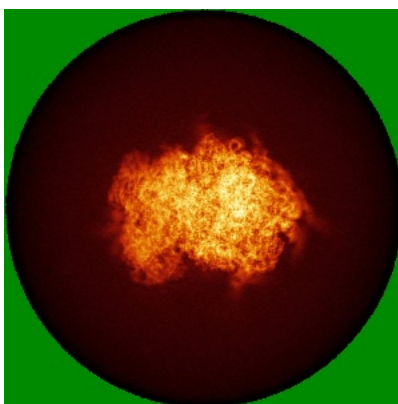
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

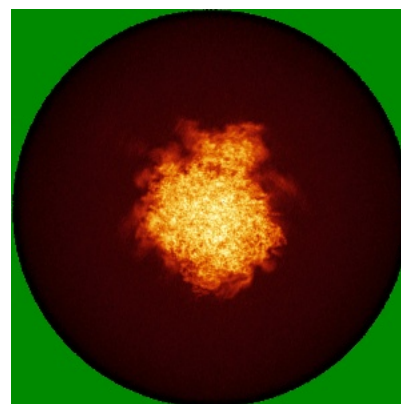
6.4.1 Primary map



X

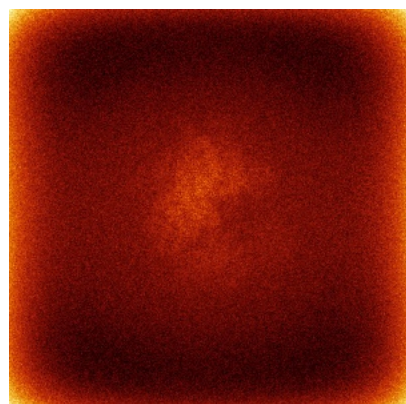


Y

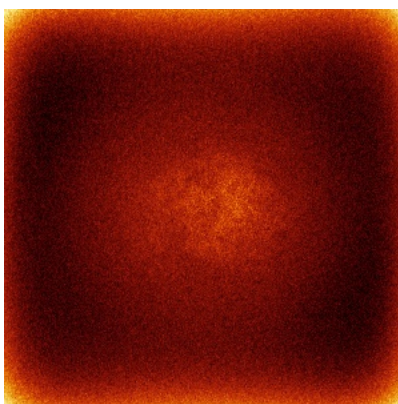


Z

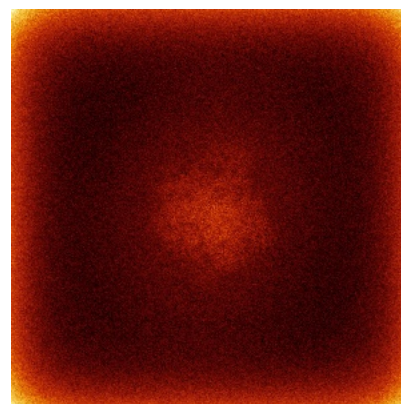
6.4.2 Raw map



X



Y

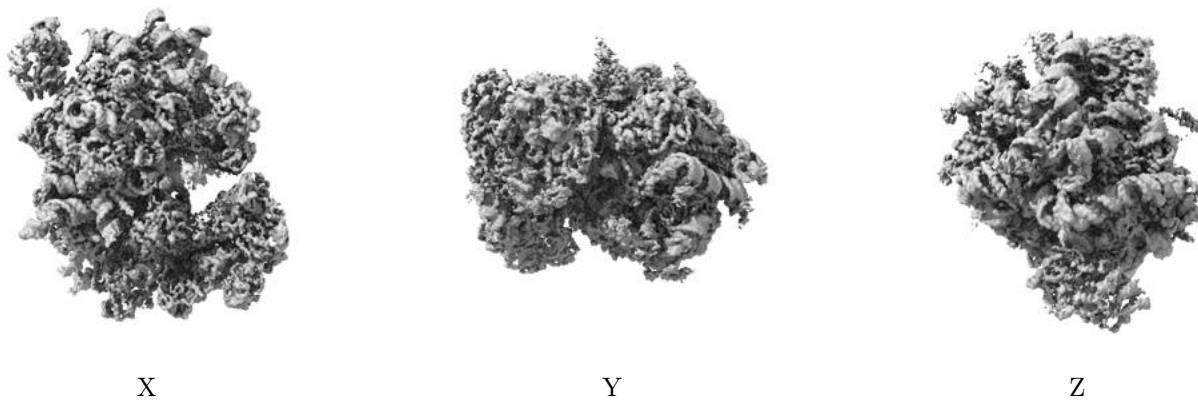


Z

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

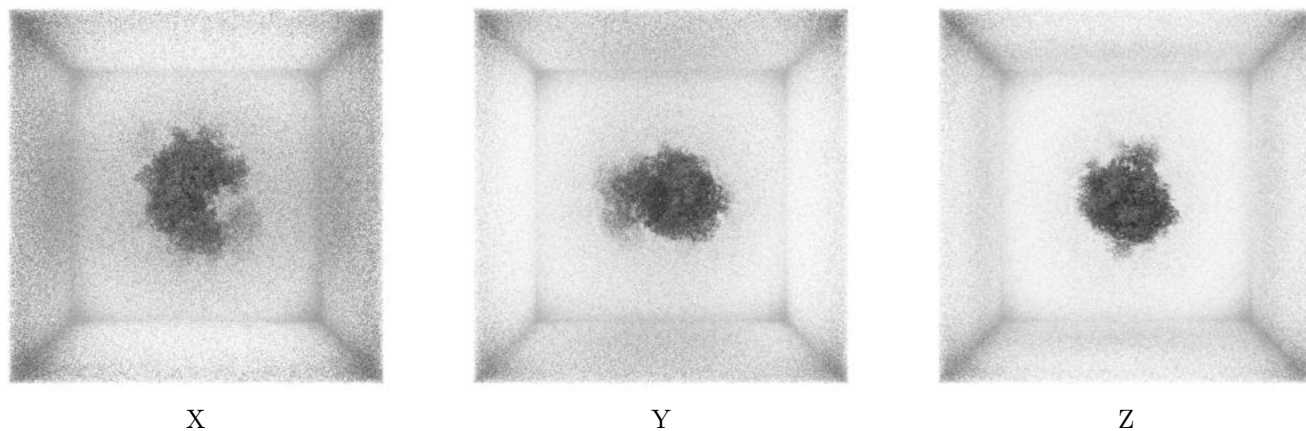
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



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

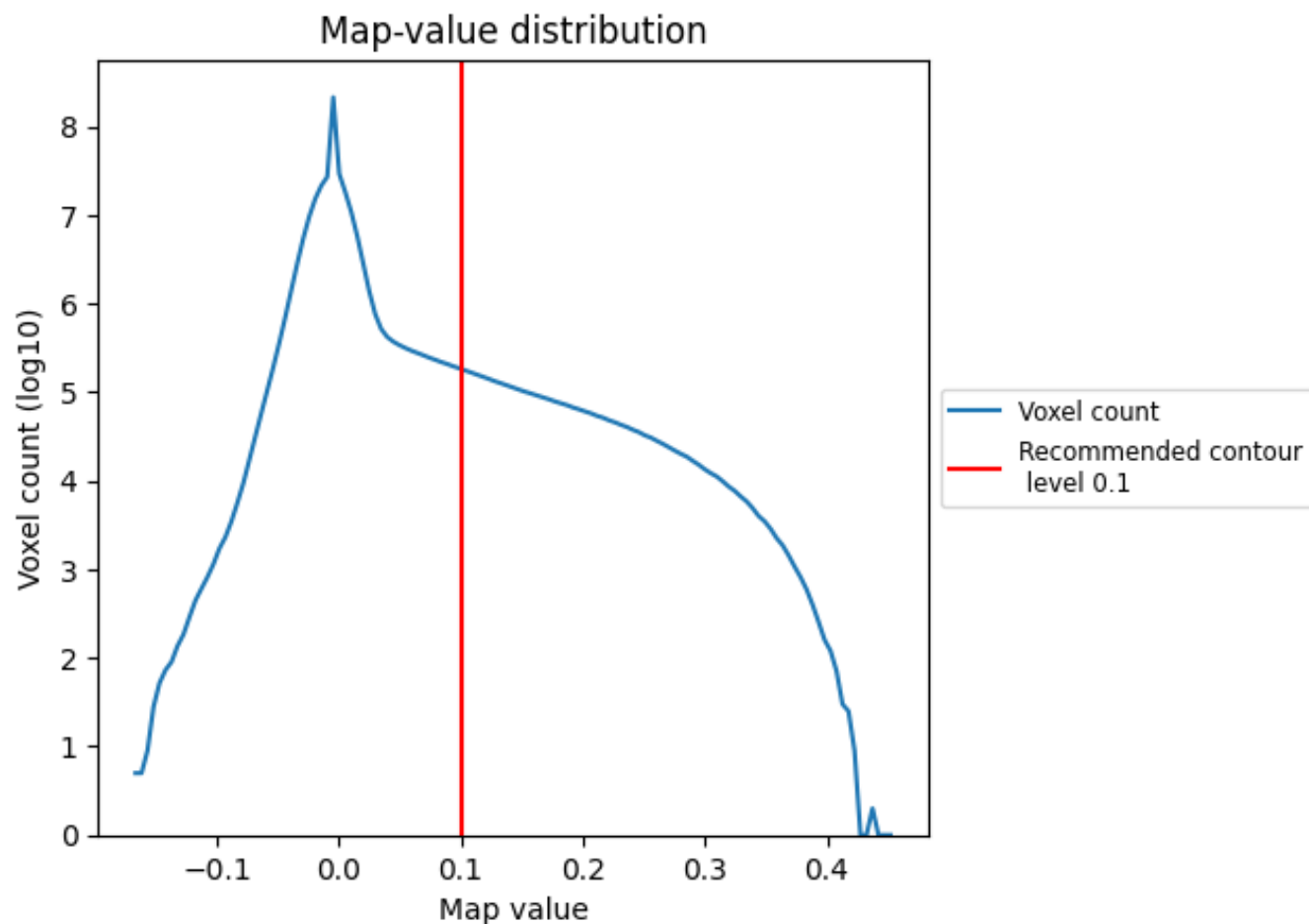
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

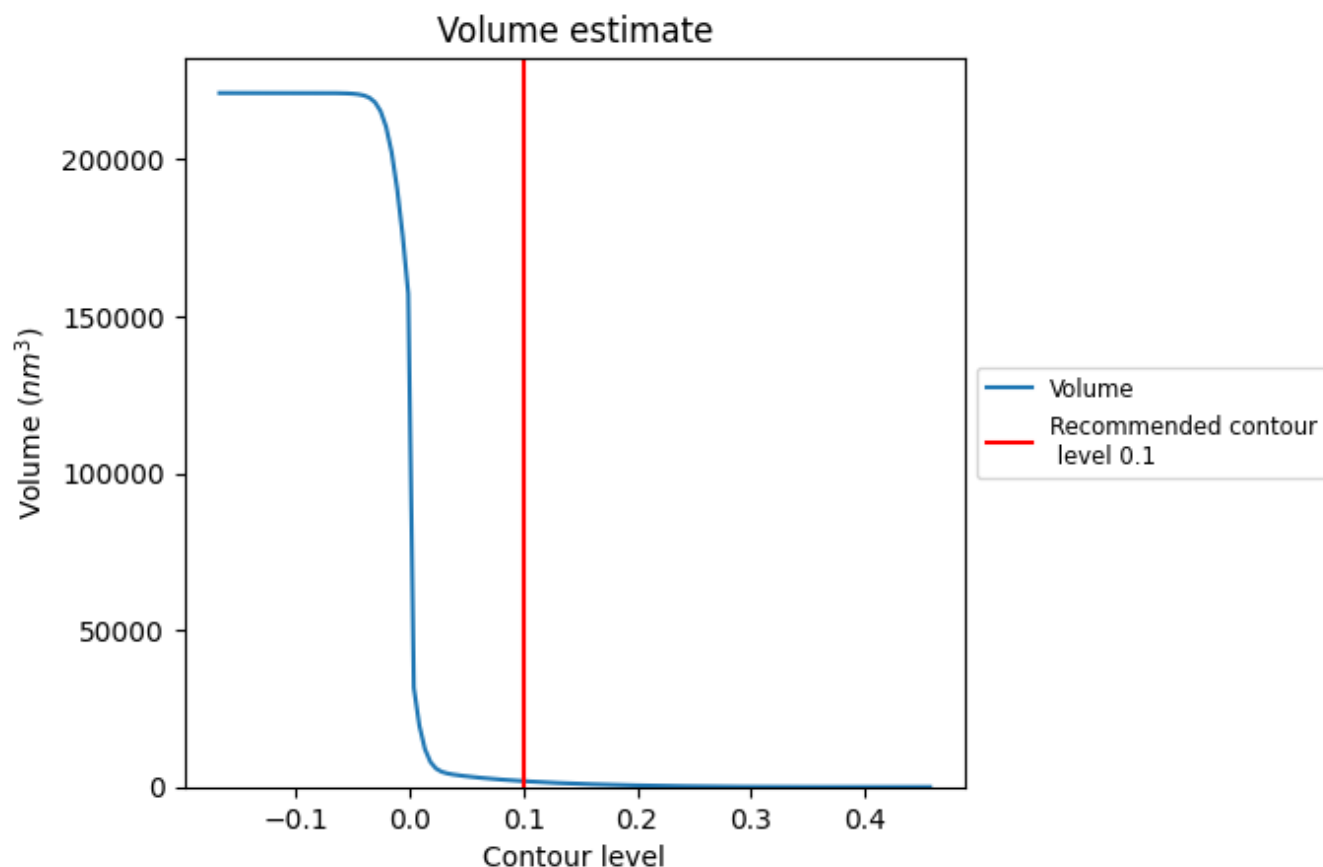
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

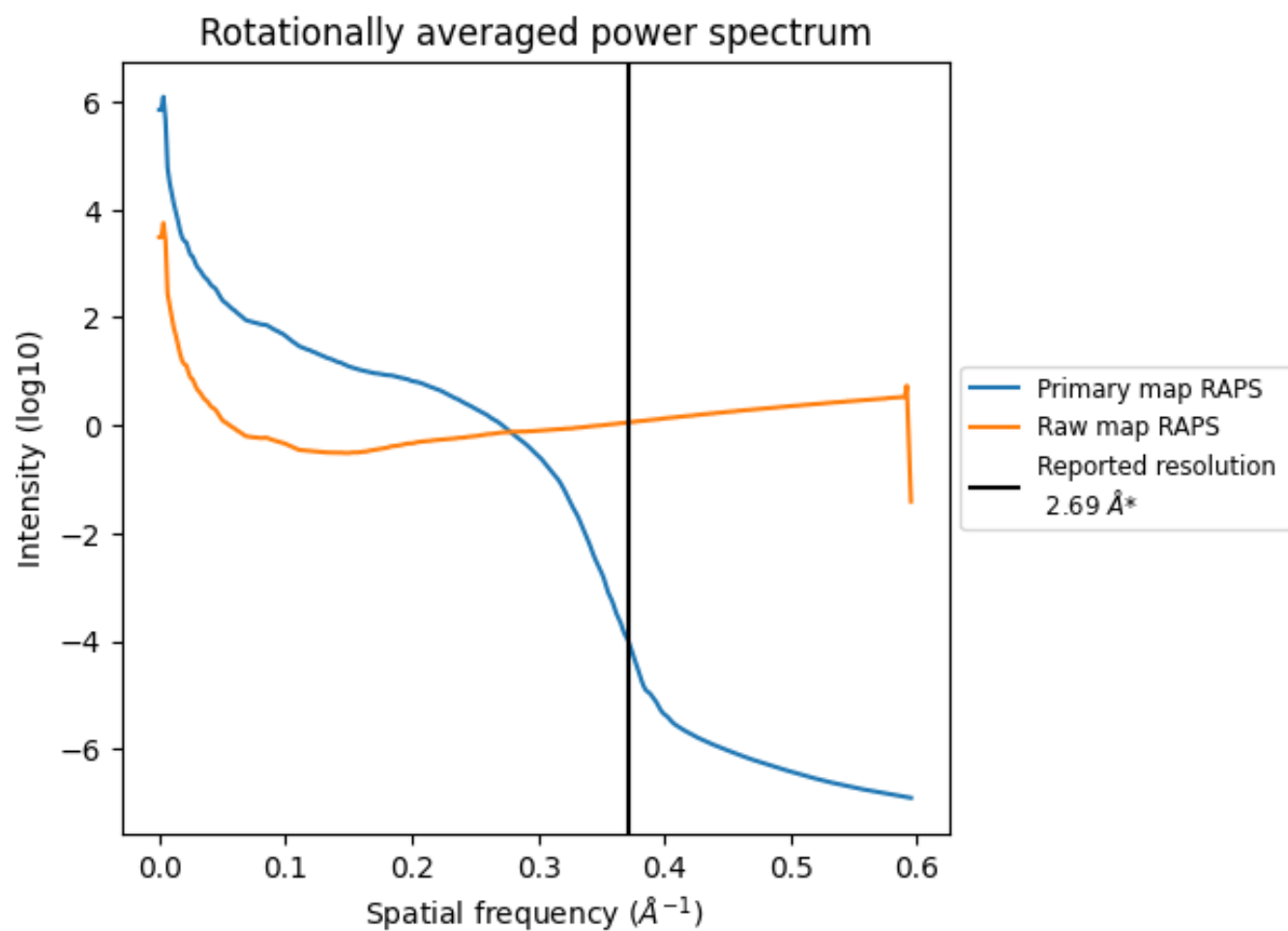
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1862 nm^3 ; this corresponds to an approximate mass of 1682 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 ⓘ

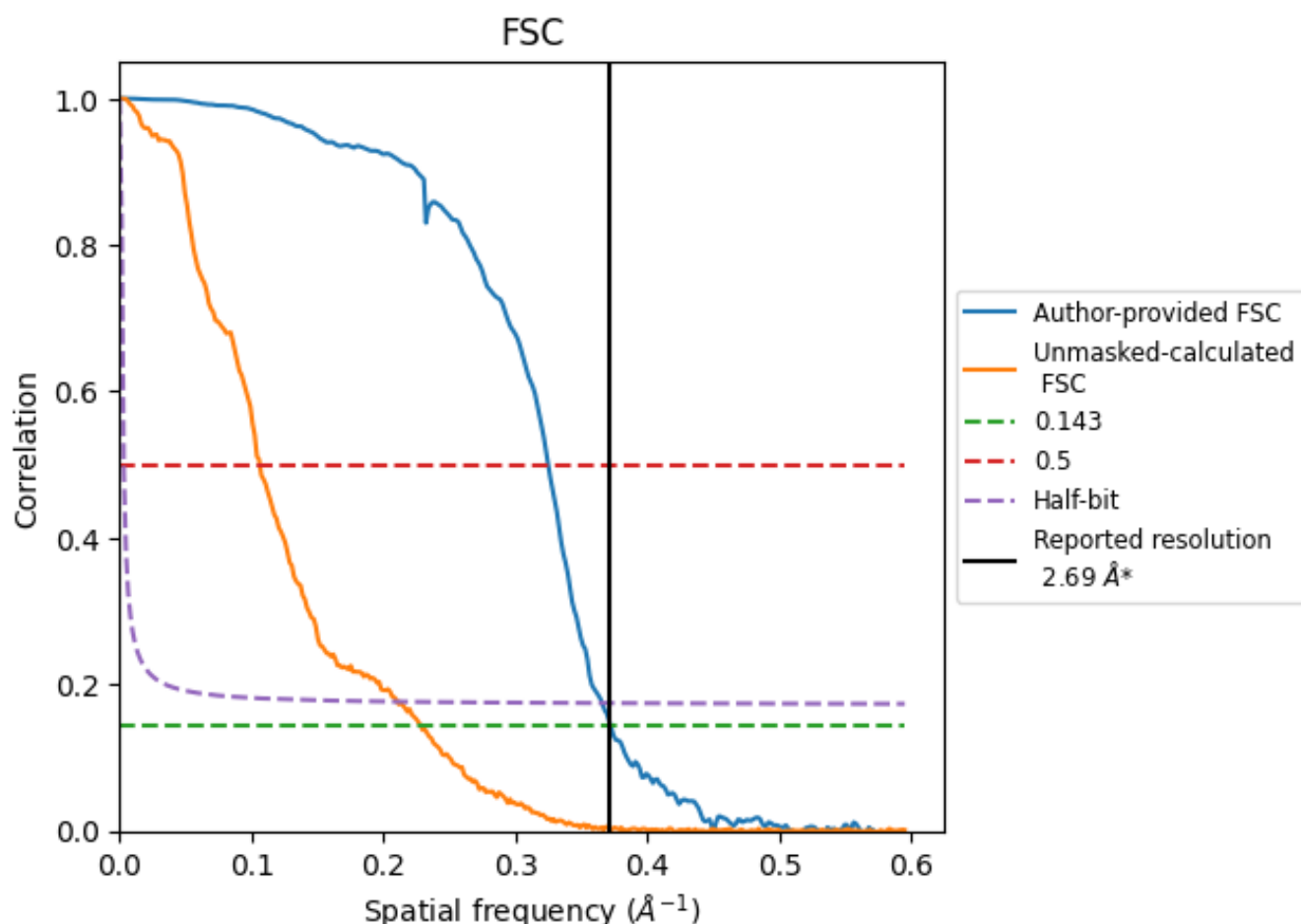


*Reported resolution corresponds to spatial frequency of 0.372 \AA^{-1}

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 0.372 Å⁻¹

8.2 Resolution estimates [i](#)

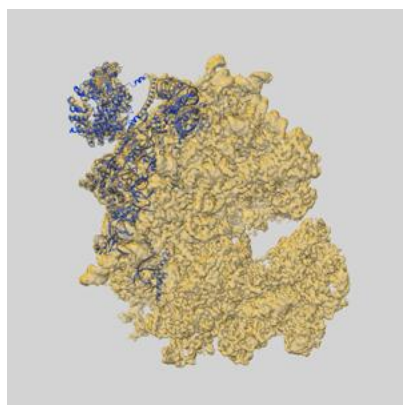
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	3.08	2.73
Unmasked-calculated*	4.38	9.40	4.75

*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 4.38 differs from the reported value 2.69 by more than 10 %

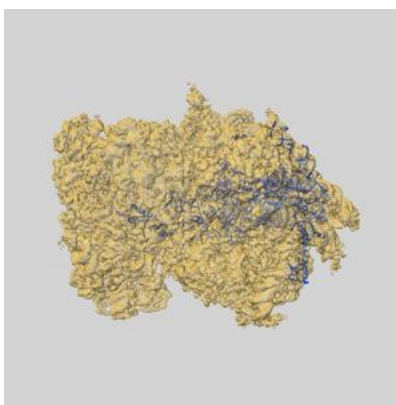
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50641 and PDB model 9FPZ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

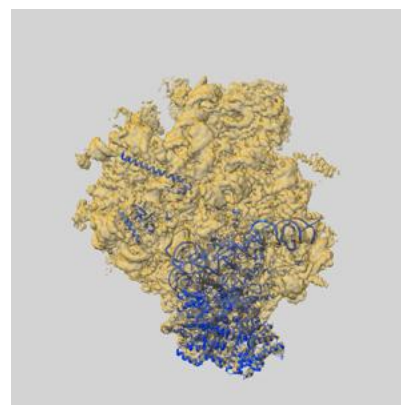
9.1 Map-model overlay [i](#)



X



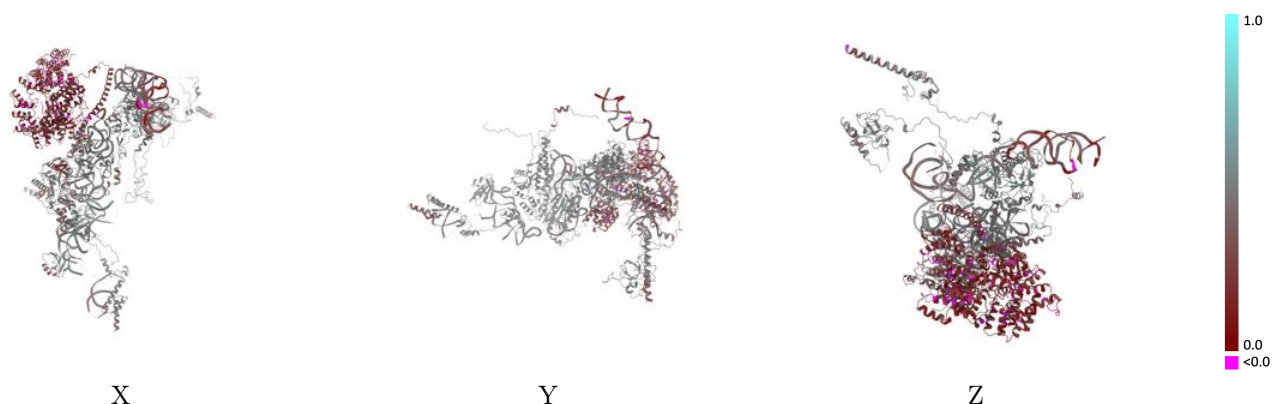
Y



Z

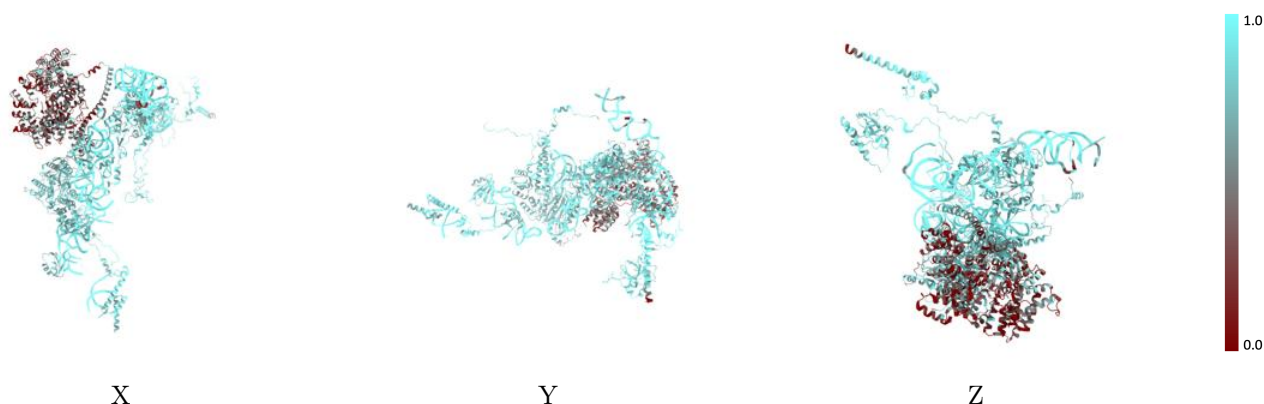
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



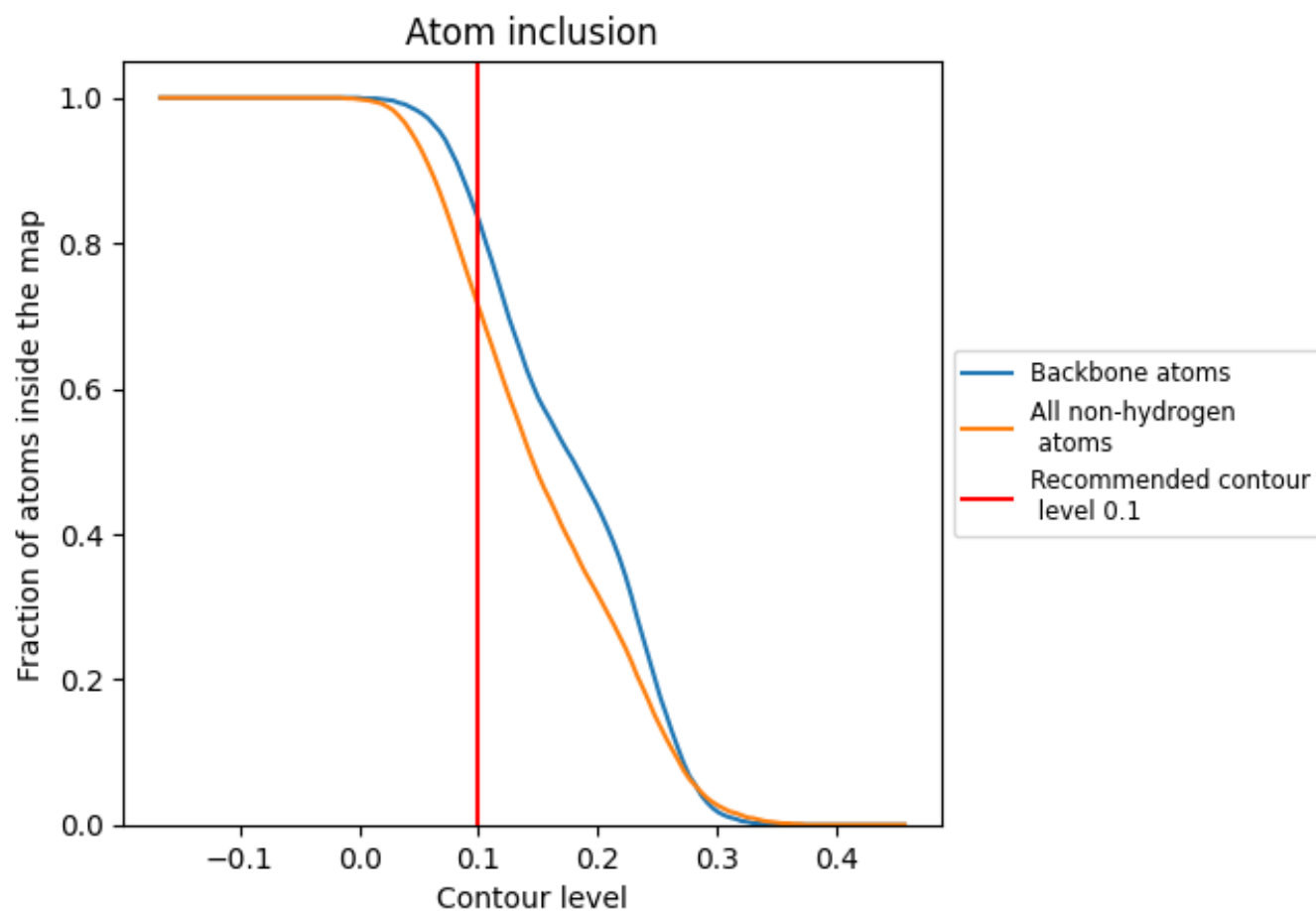
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.1).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.3740
1	 0.9420	 0.4200
2	 0.3260	 0.1820
8	 0.9600	 0.4630
A	 0.7950	 0.4330
B	 0.3280	 0.1690
LC	 0.8240	 0.4960
LE	 0.8550	 0.4700
LR	 0.8320	 0.4790
LX	 0.8030	 0.4750
LY	 0.8110	 0.4800
Lh	 0.7950	 0.4510
Lk	 0.7470	 0.4380
Lr	 0.8410	 0.4970

