



Full wwPDB EM Validation Report ⓘ

Apr 9, 2026 – 12:03 AM UTC

PDB ID : 9XTE / pdb_00009xte
EMDB ID : EMD-67203
Title : E.coli delta lepA 30S ribosomal subunit class A, body domain
Authors : Kravchenko, O.V.; Maksimova, E.M.; Baymukhametov, T.N.; Stolboushkina, E.A.
Deposited on : 2025-11-22
Resolution : 2.24 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

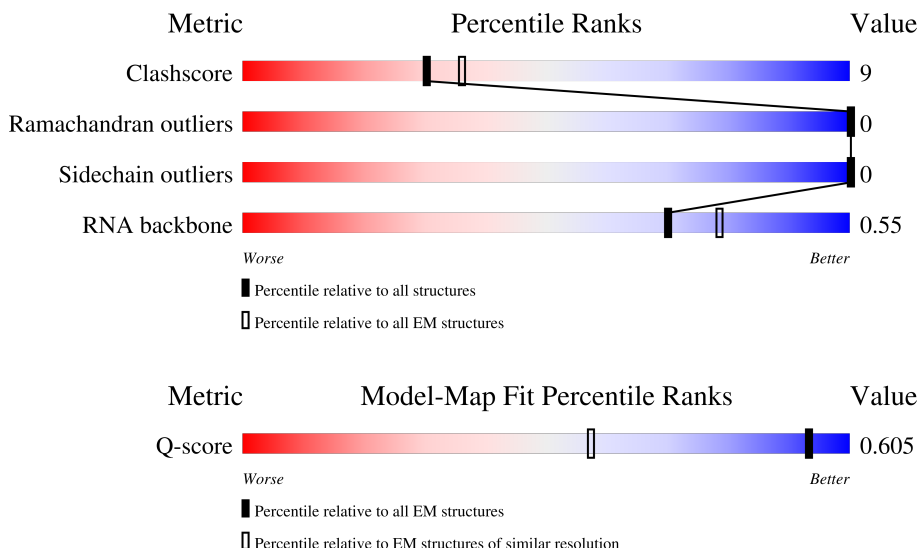
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.24 Å.

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






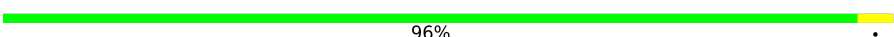






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3381 (1.75 - 2.74)

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	D	206	
2	E	167	
3	F	135	

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Mol	Chain	Length	Quality of chain
4	H	130	
5	L	124	
6	O	89	
7	P	81	
8	Q	84	
9	R	75	
10	T	87	
11	A	1542	
12	B	241	
13	K	129	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 35512 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 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	204	Total	C	N	O	S	0	0
			1633	1020	313	296	4		

- Molecule 2 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	155	Total	C	N	O	S	0	0
			1143	712	216	209	6		

- Molecule 3 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 4 is a protein called 30S ribosomal protein S8.

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

- Molecule 5 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 6 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	87	Total	C	N	O	S	0	0
			702	433	140	128	1		

- Molecule 7 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 8 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 9 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	52	Total	C	N	O	0	0
			426	272	78	76		

- Molecule 10 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

- Molecule 11 is a RNA chain called RNA (1026-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1026	Total	C	N	O	P	0	0
			22039	9826	4057	7130	1026		

- Molecule 12 is a protein called 30S ribosomal protein S2.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	115	Total	C	N	O	S	0	0
			858	529	169	157	3		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	A	34	Total 34	Mg 34	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	D	35	Total 35	O 35	0
15	E	5	Total 5	O 5	0
15	H	34	Total 34	O 34	0
15	L	48	Total 48	O 48	0
15	O	6	Total 6	O 6	0
15	P	56	Total 56	O 56	0
15	Q	25	Total 25	O 25	0
15	T	26	Total 26	O 26	0
15	A	1996	Total 1996	O 1996	0

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: 30S ribosomal protein S4

Chain D: 



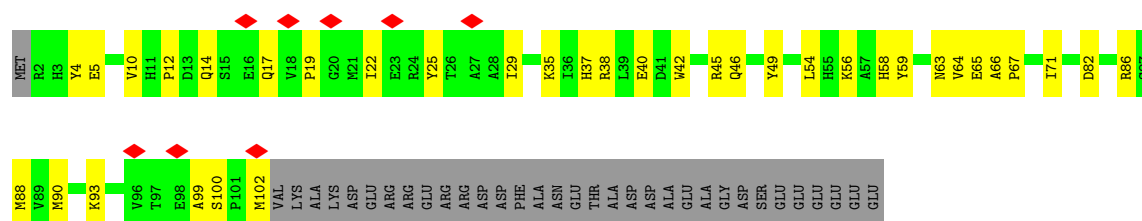
- Molecule 2: 30S ribosomal protein S5

Chain E: 




- Molecule 3: 30S ribosomal protein S6, fully modified isoform

Chain F: 




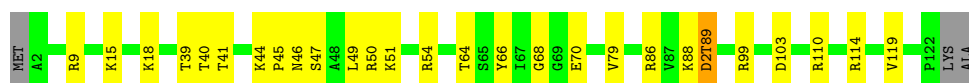
- Molecule 4: 30S ribosomal protein S8

Chain H: 



- Molecule 5: 30S ribosomal protein S12

Chain L:  76% 21% ..



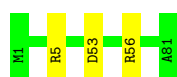
- Molecule 6: 30S ribosomal protein S15

Chain O:  91% 7% .




- Molecule 7: Small ribosomal subunit protein bS16

Chain P:  96% .



- Molecule 8: 30S ribosomal protein S17

Chain Q:  81% 13% 6%




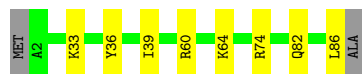
- Molecule 9: 30S ribosomal protein S18

Chain R:  56% 13% 31%



- Molecule 10: 30S ribosomal protein S20

Chain T:  89% 9% .

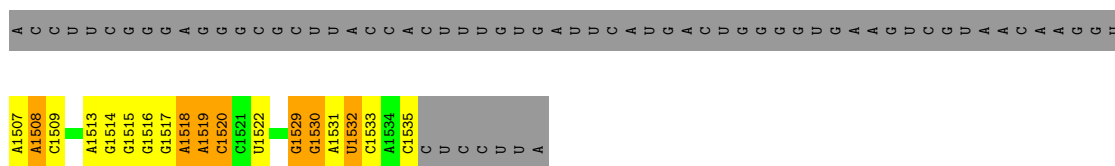


- Molecule 11: RNA (1026-MER)

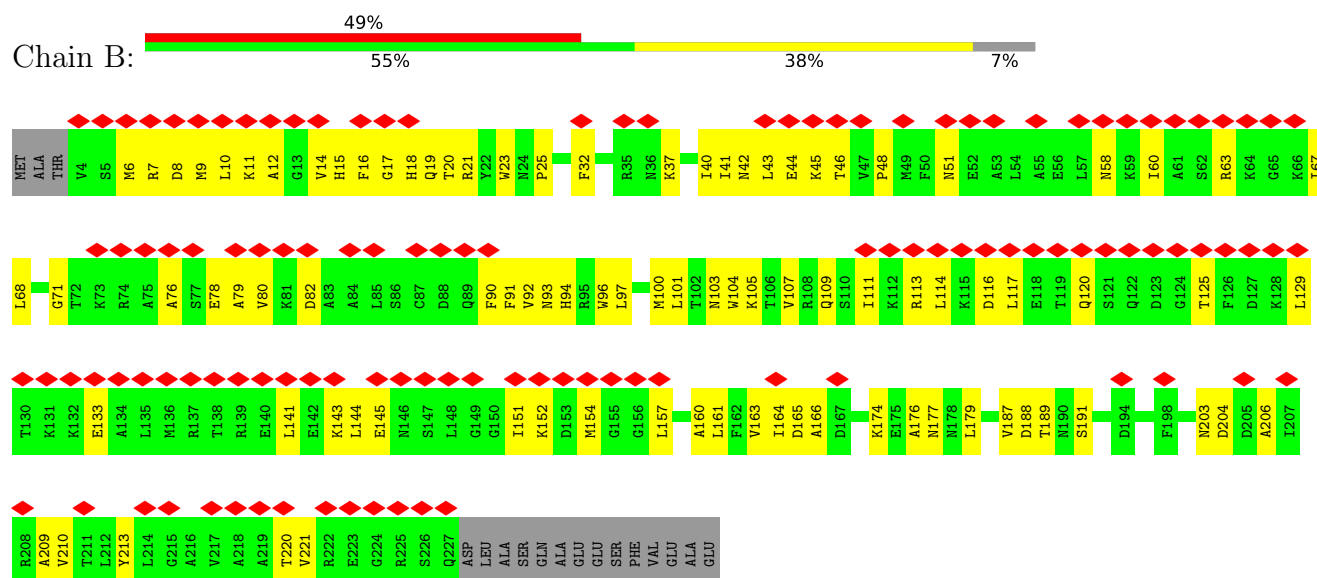
Chain A:  40% 23% 33%



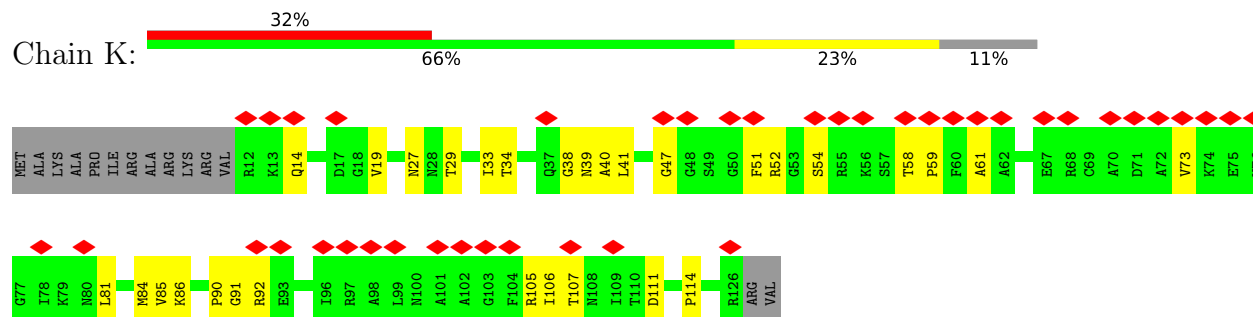




• Molecule 12: 30S ribosomal protein S2



• Molecule 13: Small ribosomal subunit protein uS11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	297347	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 ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	5.870	Depositor
Minimum map value	-2.763	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	379.72, 379.72, 379.72	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.863, 0.863, 0.863	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: D2T, PSU, G7M, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	D	0.29	0/1655	0.44	0/2216
2	E	0.28	0/1156	0.45	0/1556
3	F	0.13	0/843	0.32	0/1140
4	H	0.28	0/989	0.37	0/1326
5	L	0.44	0/945	0.60	0/1268
6	O	0.34	0/710	0.45	0/950
7	P	0.41	0/653	0.56	0/877
8	Q	0.32	0/650	0.39	0/871
9	R	0.17	0/432	0.37	0/581
10	T	0.36	0/670	0.42	0/888
11	A	0.41	0/24629	0.40	0/38420
12	B	0.35	0/1784	0.51	0/2403
13	K	0.13	0/874	0.28	0/1181
All	All	0.38	0/35990	0.41	0/53677

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1633	0	1694	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1143	0	1190	22	0
3	F	824	0	812	34	0
4	H	979	0	1031	13	0
5	L	942	0	999	29	0
6	O	702	0	721	5	0
7	P	643	0	661	2	0
8	Q	641	0	682	10	0
9	R	426	0	454	11	0
10	T	664	0	714	7	0
11	A	22039	0	11090	268	0
12	B	1753	0	1780	90	0
13	K	858	0	865	24	0
14	A	34	0	0	0	0
15	A	1996	0	0	20	0
15	D	35	0	0	1	0
15	E	5	0	0	1	0
15	H	34	0	0	0	0
15	L	48	0	0	1	0
15	O	6	0	0	0	0
15	P	56	0	0	0	0
15	Q	25	0	0	1	0
15	T	26	0	0	0	0
All	All	35512	0	22693	491	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:664:G:H22	11:A:741:G:H1	1.11	0.94
11:A:76:G:H1	11:A:93:U:H3	1.11	0.92
5:L:88:LYS:HE3	11:A:526:C:OP2	1.77	0.84
2:E:55:GLU:HG3	2:E:57:PRO:HD2	1.60	0.83
12:B:16:PHE:HA	12:B:43:LEU:HD11	1.59	0.83
1:D:9:LEU:HD12	11:A:429:U:H5'	1.61	0.80
11:A:925:G:H1'	11:A:926:G:H5''	1.64	0.80
12:B:101:LEU:O	12:B:179:LEU:HD11	1.82	0.79
12:B:163:VAL:HG12	12:B:165:ASP:H	1.48	0.79
3:F:90:MET:HE1	9:R:61:ARG:HH21	1.49	0.78
12:B:92:VAL:HG21	12:B:96:TRP:CZ3	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:LEU:HD12	11:A:429:U:H3'	1.65	0.77
11:A:86:G:H4'	11:A:87:C:H5'	1.67	0.77
5:L:44:LYS:HB2	5:L:45:PRO:HD3	1.65	0.77
12:B:92:VAL:HG21	12:B:96:TRP:HZ3	1.49	0.77
12:B:44:GLU:O	12:B:48:PRO:HD2	1.84	0.76
11:A:677:U:H3	11:A:713:G:H22	1.34	0.75
12:B:12:ALA:HB1	12:B:209:ALA:HB2	1.67	0.75
12:B:67:ILE:HD11	12:B:221:VAL:HG21	1.69	0.74
1:D:54:GLN:HA	1:D:199:LEU:HD13	1.69	0.74
11:A:673:A:H2'	11:A:674:G:C8	2.22	0.74
5:L:54:ARG:HH11	5:L:64:THR:HG23	1.51	0.73
2:E:149:SER:H	2:E:152:MET:HE3	1.54	0.73
12:B:15:HIS:NE2	12:B:46:THR:HG21	2.04	0.73
11:A:843:U:H2'	11:A:844:G:H8	1.54	0.72
3:F:37:HIS:HB2	3:F:63:ASN:HD22	1.55	0.72
11:A:1517:G:H3'	11:A:1518:A:H8	1.54	0.72
5:L:46:ASN:CG	11:A:528:C:H41	1.98	0.71
10:T:74:ARG:NH2	11:A:261:U:OP2	2.24	0.71
2:E:38:VAL:HG11	2:E:114:VAL:HG22	1.73	0.71
11:A:840:C:H2'	11:A:841:C:H5''	1.73	0.71
5:L:46:ASN:ND2	5:L:89:D2T:SB	2.64	0.70
5:L:114:ARG:HB3	5:L:119:VAL:HB	1.74	0.70
11:A:1071:C:H2'	11:A:1072:G:H8	1.56	0.70
2:E:108:GLY:HA3	11:A:9:G:H5'	1.76	0.68
11:A:77:A:H2'	11:A:78:A:C8	2.29	0.67
13:K:92:ARG:HH21	13:K:111:ASP:HB2	1.60	0.67
12:B:114:LEU:HD13	12:B:144:LEU:HB2	1.77	0.66
12:B:20:THR:HG23	12:B:37:LYS:O	1.95	0.66
11:A:728:A:H2'	11:A:729:A:C8	2.32	0.65
11:A:337:G:H2'	11:A:338:A:C8	2.31	0.65
11:A:1071:C:N4	11:A:1085:U:O4	2.20	0.65
11:A:1103:C:H5''	12:B:97:LEU:HD22	1.79	0.65
11:A:524:G:H2'	11:A:525:C:C6	2.31	0.65
12:B:93:ASN:OD1	12:B:94:HIS:ND1	2.29	0.65
5:L:79:VAL:O	5:L:103:ASP:HB3	1.97	0.65
11:A:683:G:N2	13:K:38:GLY:O	2.30	0.65
1:D:57:GLU:HB3	1:D:199:LEU:HD11	1.79	0.64
5:L:47:SER:N	11:A:529:G:O6	2.29	0.64
3:F:67:PRO:O	3:F:71:ILE:HG12	1.97	0.64
12:B:71:GLY:HA3	12:B:80:VAL:HG21	1.80	0.64
3:F:64:VAL:HG11	3:F:71:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:789:U:N3	11:A:792:A:OP2	2.28	0.63
2:E:88:VAL:HG12	2:E:93:ARG:HG2	1.79	0.63
2:E:126:LYS:NZ	11:A:9:G:OP2	2.29	0.63
11:A:841:C:O2	11:A:845:A:N6	2.32	0.63
11:A:1098:C:OP2	12:B:143:LYS:NZ	2.32	0.63
11:A:1073:U:O2	12:B:103:ASN:ND2	2.32	0.63
12:B:104:TRP:CZ3	12:B:107:VAL:HG11	2.34	0.62
13:K:105:ARG:NH1	13:K:106:ILE:O	2.32	0.62
5:L:9:ARG:NH1	11:A:880:C:OP1	2.32	0.62
6:O:2:SER:HA	6:O:35:GLN:NE2	2.14	0.62
12:B:114:LEU:HD13	12:B:144:LEU:CB	2.29	0.62
2:E:77:ASN:CG	2:E:82:GLN:HE22	2.08	0.62
11:A:925:G:C4	11:A:926:G:H2'	2.35	0.62
5:L:15:LYS:HD3	5:L:15:LYS:H	1.64	0.61
12:B:14:VAL:HA	12:B:16:PHE:CE2	2.35	0.61
12:B:23:TRP:CH2	12:B:25:PRO:HA	2.35	0.61
3:F:38:ARG:HH21	3:F:99:ALA:HA	1.66	0.61
11:A:692:U:OP2	13:K:27:ASN:ND2	2.23	0.61
6:O:3:LEU:HG	6:O:35:GLN:HG2	1.82	0.61
11:A:147:G:H2'	11:A:148:G:C8	2.36	0.61
1:D:9:LEU:CD1	11:A:429:U:H3'	2.30	0.60
5:L:110:ARG:HB2	5:L:119:VAL:HG21	1.82	0.60
11:A:1095:U:OP1	11:A:1108:G:N1	2.31	0.60
12:B:163:VAL:CG1	12:B:165:ASP:O	2.50	0.60
11:A:57:G:N7	15:A:1705:HOH:O	2.31	0.60
11:A:713:G:H2'	11:A:714:G:C8	2.37	0.60
10:T:60:ARG:NH1	11:A:195:A:OP1	2.34	0.60
13:K:19:VAL:N	13:K:34:THR:O	2.34	0.59
3:F:12:PRO:HD2	3:F:54:LEU:HD11	1.83	0.59
11:A:77:A:H2'	11:A:78:A:H8	1.66	0.59
11:A:888:G:N7	15:A:1719:HOH:O	2.32	0.59
4:H:2:SER:N	11:A:823:C:HO2'	2.01	0.58
12:B:105:LYS:O	12:B:109:GLN:HG2	2.03	0.58
11:A:676:A:H5''	13:K:114:PRO:HB3	1.85	0.58
11:A:555:U:H2'	11:A:556:C:C6	2.39	0.58
12:B:6:MET:O	12:B:10:LEU:HG	2.03	0.58
11:A:131:A:H2'	11:A:132:C:C6	2.39	0.58
1:D:95:GLU:OE1	1:D:104:ARG:NH1	2.37	0.58
11:A:459:A:H2'	11:A:460:A:C8	2.39	0.58
3:F:93:LYS:NZ	11:A:662:U:OP2	2.37	0.57
12:B:166:ALA:HB3	12:B:191:SER:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:694:A:N1	11:A:787:A:O2'	2.36	0.57
3:F:40:GLU:OE1	3:F:100:SER:OG	2.23	0.57
12:B:129:LEU:HD23	12:B:133:GLU:HG2	1.87	0.57
1:D:172:GLU:HB3	1:D:183:LYS:HE3	1.86	0.57
2:E:23:LYS:HD3	11:A:1081:A:H5'	1.85	0.57
11:A:791:G:N2	11:A:793:U:O4	2.38	0.57
11:A:679:C:H2'	11:A:680:C:C6	2.40	0.57
11:A:613:C:H2'	11:A:614:C:C6	2.40	0.57
3:F:100:SER:OG	3:F:102:MET:SD	2.58	0.57
12:B:67:ILE:HG22	12:B:160:ALA:HB3	1.87	0.57
11:A:81:A:H2'	11:A:83:C:C6	2.40	0.57
11:A:381:C:H2'	11:A:382:A:O4'	2.05	0.57
13:K:59:PRO:HD3	13:K:90:PRO:HB2	1.87	0.57
5:L:46:ASN:HA	11:A:529:G:O6	2.05	0.56
11:A:841:C:N4	11:A:844:G:OP2	2.28	0.56
1:D:9:LEU:HD13	1:D:32:CYS:HB3	1.87	0.56
12:B:187:VAL:HG13	12:B:191:SER:HB2	1.85	0.56
1:D:196:ASN:HB3	1:D:199:LEU:HG	1.87	0.56
3:F:66:ALA:HB3	3:F:71:ILE:HD11	1.87	0.56
7:P:5:ARG:HB2	11:A:376:G:H5''	1.87	0.56
11:A:472:U:H2'	11:A:473:U:C6	2.41	0.56
12:B:15:HIS:CE1	12:B:43:LEU:HD12	2.40	0.56
12:B:58:ASN:OD1	12:B:220:THR:OG1	2.20	0.56
12:B:114:LEU:HD11	12:B:145:GLU:HG2	1.87	0.56
3:F:19:PRO:HA	3:F:22:ILE:HG12	1.88	0.56
13:K:85:VAL:HG11	13:K:92:ARG:HG3	1.87	0.56
1:D:164:GLN:OE1	1:D:164:GLN:N	2.39	0.56
5:L:68:GLY:O	5:L:99:ARG:NH1	2.38	0.56
4:H:105:SER:HB2	4:H:126:ILE:HD11	1.88	0.56
10:T:39:ILE:HG23	10:T:86:LEU:HD11	1.88	0.55
11:A:1071:C:H2'	11:A:1072:G:C8	2.40	0.55
3:F:5:GLU:OE2	3:F:63:ASN:OD1	2.25	0.55
11:A:471:U:H2'	11:A:472:U:C6	2.41	0.55
12:B:96:TRP:HZ2	12:B:101:LEU:CD1	2.20	0.55
3:F:45:ARG:HH22	9:R:26:ILE:HD13	1.71	0.55
13:K:84:MET:HG2	13:K:86:LYS:HZ1	1.70	0.55
3:F:14:GLN:NE2	3:F:17:GLN:OE1	2.38	0.55
8:Q:16:LYS:HE3	11:A:275:G:H5'	1.88	0.55
11:A:679:C:H2'	11:A:680:C:H6	1.72	0.55
9:R:63:ARG:HH12	11:A:718:A:H61	1.53	0.55
11:A:17:U:H2'	11:A:18:C:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:86:G:H21	11:A:87:C:H41	1.55	0.55
3:F:90:MET:HE1	9:R:61:ARG:NH2	2.21	0.55
11:A:450:G:N7	15:A:1725:HOH:O	2.33	0.54
12:B:32:PHE:HB2	12:B:42:ASN:HA	1.89	0.54
11:A:694:A:OP1	13:K:54:SER:N	2.33	0.54
11:A:683:G:H1	11:A:707:U:H3	1.55	0.54
4:H:89:LYS:HD3	4:H:120:GLY:HA2	1.88	0.54
2:E:93:ARG:NH2	15:E:202:HOH:O	2.40	0.54
4:H:29:SER:HB3	4:H:57:PRO:HB2	1.90	0.54
11:A:548:G:N7	15:A:1723:HOH:O	2.33	0.54
12:B:48:PRO:HA	12:B:51:ASN:ND2	2.22	0.54
13:K:81:LEU:N	13:K:105:ARG:O	2.36	0.54
11:A:1103:C:C5'	12:B:97:LEU:HD22	2.38	0.54
5:L:70:GLU:OE1	11:A:521:G:H4'	2.08	0.54
11:A:746:A:H2'	11:A:747:A:C8	2.43	0.54
11:A:791:G:O6	11:A:792:A:N6	2.41	0.54
5:L:40:THR:HG22	5:L:41:THR:N	2.23	0.53
11:A:238:A:N7	15:A:1721:HOH:O	2.33	0.53
11:A:1518:A:C3'	11:A:1519:A:H5''	2.38	0.53
11:A:662:U:H2'	11:A:663:A:C8	2.43	0.53
12:B:17:GLY:HA2	12:B:41:ILE:HD12	1.88	0.53
11:A:451:A:H61	11:A:481:G:H5'	1.72	0.53
11:A:518:C:H5''	11:A:519:C:C6	2.43	0.53
12:B:209:ALA:O	12:B:213:TYR:HD1	1.91	0.53
1:D:49:SER:OG	1:D:50:ASP:N	2.41	0.53
5:L:86:ARG:HH12	5:L:88:LYS:HD2	1.73	0.53
11:A:343:U:H2'	11:A:345:C:C5	2.43	0.53
11:A:925:G:H4'	11:A:926:G:OP1	2.08	0.53
12:B:203:ASN:OD1	12:B:204:ASP:N	2.41	0.53
11:A:320:A:H2'	11:A:321:A:O4'	2.09	0.53
11:A:384:G:H2'	11:A:385:C:C6	2.43	0.53
12:B:14:VAL:CG2	12:B:206:ALA:HB2	2.39	0.52
5:L:18:LYS:NZ	11:A:910:C:OP2	2.28	0.52
12:B:163:VAL:HG12	12:B:165:ASP:O	2.10	0.52
9:R:30:LYS:HA	9:R:33:ILE:HG12	1.91	0.52
10:T:64:LYS:HE3	15:A:2549:HOH:O	2.10	0.52
11:A:590:U:H3'	15:A:1810:HOH:O	2.10	0.52
12:B:76:ALA:HB2	12:B:210:VAL:HG11	1.90	0.52
3:F:64:VAL:HG11	3:F:71:ILE:CD1	2.38	0.52
11:A:502:A:N7	15:A:1734:HOH:O	2.34	0.52
1:D:113:GLU:OE2	1:D:154:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:216:U:H2'	11:A:217:C:C6	2.45	0.52
1:D:57:GLU:CB	1:D:199:LEU:HD11	2.40	0.52
11:A:704:A:C4	11:A:705:G:C8	2.98	0.52
12:B:20:THR:HG22	12:B:21:ARG:H	1.75	0.52
12:B:7:ARG:O	12:B:11:LYS:HG3	2.10	0.52
11:A:1097:C:H5''	12:B:143:LYS:HD2	1.92	0.52
11:A:714:G:H2'	11:A:715:A:C8	2.45	0.51
11:A:860:A:H2'	11:A:861:G:O4'	2.09	0.51
11:A:458:U:H2'	11:A:459:A:C8	2.45	0.51
11:A:690:G:H2'	11:A:691:G:C8	2.45	0.51
12:B:17:GLY:HA2	12:B:41:ILE:CD1	2.40	0.51
11:A:56:U:H2'	11:A:57:G:C8	2.45	0.51
11:A:161:A:H2'	11:A:162:A:C8	2.44	0.51
11:A:344:A:H5''	11:A:345:C:H5	1.76	0.51
12:B:8:ASP:HA	12:B:11:LYS:HD2	1.92	0.51
12:B:174:LYS:HA	12:B:177:ASN:ND2	2.26	0.51
11:A:427:U:OP2	11:A:428:G:O2'	2.19	0.51
12:B:163:VAL:HG11	12:B:165:ASP:O	2.09	0.51
3:F:4:TYR:CE2	3:F:71:ILE:HG13	2.46	0.51
11:A:928:G:H2'	11:A:929:G:O4'	2.10	0.51
12:B:100:MET:HA	12:B:107:VAL:HG21	1.92	0.51
13:K:58:THR:HB	13:K:59:PRO:HD2	1.91	0.51
9:R:63:ARG:HH12	11:A:718:A:N6	2.08	0.51
11:A:31:G:O2'	11:A:48:C:N4	2.44	0.51
1:D:107:PHE:CG	1:D:145:ILE:HD11	2.45	0.51
11:A:492:C:H2'	11:A:493:A:C8	2.46	0.51
11:A:86:G:H21	11:A:87:C:N4	2.09	0.51
11:A:684:U:H1'	13:K:39:ASN:HA	1.92	0.51
11:A:1070:U:H2'	11:A:1071:C:C6	2.46	0.51
2:E:77:ASN:CG	2:E:82:GLN:NE2	2.68	0.50
5:L:18:LYS:HE2	11:A:909:A:OP1	2.11	0.50
11:A:171:A:H2'	11:A:172:A:C8	2.46	0.50
11:A:518:C:H2'	11:A:530:G:C8	2.45	0.50
11:A:1517:G:H3'	11:A:1518:A:C8	2.39	0.50
3:F:14:GLN:HB3	3:F:17:GLN:HG2	1.94	0.50
11:A:382:A:H2'	11:A:383:A:C8	2.47	0.50
12:B:68:LEU:HD13	12:B:90:PHE:HB3	1.93	0.50
12:B:157:LEU:HD13	12:B:179:LEU:HD13	1.93	0.50
11:A:91:U:H2'	11:A:92:U:C6	2.47	0.50
12:B:97:LEU:H	12:B:100:MET:CE	2.24	0.49
11:A:580:C:H2'	11:A:581:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1106:G:H2'	11:A:1107:C:C6	2.46	0.49
11:A:502:A:H2'	11:A:503:C:O4'	2.13	0.49
11:A:1532:U:H2'	11:A:1533:C:C6	2.47	0.49
11:A:1386:G:H2'	11:A:1387:G:H8	1.76	0.49
12:B:113:ARG:HH22	12:B:117:LEU:HD13	1.78	0.49
1:D:4:TYR:CE2	1:D:11:LEU:HD11	2.48	0.49
11:A:299:G:H2'	11:A:300:A:C8	2.48	0.49
11:A:841:C:C2	11:A:845:A:N6	2.81	0.49
11:A:298:A:O2'	11:A:299:G:OP1	2.29	0.48
11:A:396:C:O2'	11:A:398:U:OP1	2.29	0.48
11:A:509:A:N3	11:A:543:U:O2'	2.45	0.48
11:A:680:C:H2'	11:A:681:A:H8	1.78	0.48
12:B:117:LEU:HG	12:B:141:LEU:HG	1.94	0.48
11:A:677:U:H2'	11:A:678:U:C6	2.49	0.48
1:D:46:PRO:HB2	1:D:48:LEU:HG	1.95	0.48
11:A:204:G:H2'	11:A:205:A:H8	1.78	0.48
11:A:865:A:H5'	11:A:1078:U:O4	2.13	0.48
8:Q:18:GLU:O	11:A:254:G:O2'	2.30	0.48
2:E:156:LYS:HG2	4:H:71:VAL:HG22	1.95	0.48
9:R:50:LYS:O	9:R:54:GLN:HG2	2.13	0.48
11:A:459:A:H2'	11:A:460:A:H8	1.77	0.48
11:A:251:G:P	15:A:1991:HOH:O	2.70	0.48
11:A:747:A:H2'	11:A:748:G:O4'	2.14	0.48
12:B:20:THR:HG22	12:B:21:ARG:N	2.29	0.48
11:A:1099:G:H2'	11:A:1100:C:O4'	2.14	0.48
12:B:100:MET:HA	12:B:107:VAL:CG2	2.44	0.48
11:A:674:G:H2'	11:A:675:A:H8	1.78	0.48
12:B:16:PHE:HD1	12:B:40:ILE:HD12	1.79	0.48
12:B:120:GLN:HA	12:B:125:THR:HG23	1.95	0.48
1:D:2:ALA:HB3	11:A:404:G:N7	2.29	0.47
11:A:904:U:H2'	11:A:905:U:C6	2.49	0.47
1:D:170:TRP:CD2	1:D:186:PRO:HB3	2.49	0.47
3:F:64:VAL:CG1	3:F:71:ILE:HD11	2.44	0.47
11:A:686:U:O4	11:A:703:G:H1'	2.14	0.47
11:A:468:A:H3'	11:A:469:C:H6	1.79	0.47
12:B:111:ILE:HG12	12:B:152:LYS:HA	1.95	0.47
3:F:86:ARG:NH2	11:A:673:A:O3'	2.47	0.47
11:A:339:C:H2'	11:A:340:U:C6	2.49	0.47
2:E:110:ALA:HB1	2:E:137:VAL:HG23	1.96	0.47
11:A:180:U:H2'	11:A:181:A:H5'	1.96	0.47
11:A:751:U:H2'	11:A:752:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:924:C:H5''	11:A:925:G:H2'	1.96	0.47
11:A:1107:C:C4	11:A:1108:G:C8	3.03	0.47
3:F:10:VAL:HB	3:F:58:HIS:HB3	1.96	0.47
5:L:49:LEU:O	5:L:51:LYS:NZ	2.47	0.47
11:A:399:G:H2'	11:A:400:C:C6	2.50	0.47
12:B:67:ILE:HA	12:B:160:ALA:HB3	1.96	0.47
12:B:104:TRP:CE3	12:B:107:VAL:HG11	2.50	0.47
3:F:49:TYR:OH	3:F:86:ARG:NH1	2.41	0.47
11:A:172:A:H3'	15:A:2060:HOH:O	2.13	0.47
11:A:471:U:HO2'	11:A:472:U:P	2.38	0.47
11:A:695:A:H2'	11:A:696:A:O4'	2.15	0.47
11:A:1529:G:N7	15:A:1746:HOH:O	2.35	0.47
12:B:8:ASP:O	12:B:11:LYS:HB2	2.15	0.47
1:D:13:ARG:HG2	1:D:34:ILE:HA	1.97	0.47
9:R:63:ARG:NH1	11:A:718:A:H61	2.13	0.47
11:A:91:U:H2'	11:A:92:U:H6	1.80	0.47
11:A:110:C:H2'	11:A:111:G:O4'	2.15	0.47
2:E:26:LYS:NZ	11:A:1069:C:OP1	2.38	0.46
11:A:911:U:H2'	11:A:912:C:C6	2.49	0.46
11:A:1532:U:H2'	11:A:1533:C:H6	1.79	0.46
3:F:38:ARG:HH22	3:F:40:GLU:CD	2.23	0.46
12:B:60:ILE:O	12:B:63:ARG:HG2	2.14	0.46
13:K:29:THR:HG21	13:K:91:GLY:HA3	1.97	0.46
5:L:47:SER:O	11:A:529:G:N1	2.43	0.46
11:A:518:C:C5	11:A:529:G:H3'	2.51	0.46
12:B:12:ALA:HB3	12:B:15:HIS:HB3	1.98	0.46
3:F:35:LYS:H	3:F:65:GLU:HB3	1.80	0.46
11:A:236:A:H2'	11:A:237:G:C8	2.50	0.46
3:F:46:GLN:HG2	3:F:56:LYS:HG2	1.98	0.46
11:A:269:C:H2'	11:A:270:A:C8	2.51	0.46
11:A:371:A:H2'	11:A:372:C:O4'	2.15	0.46
3:F:90:MET:HE1	9:R:61:ARG:HE	1.81	0.46
11:A:232:G:H1'	11:A:262:A:N1	2.30	0.46
11:A:339:C:H2'	11:A:340:U:H6	1.81	0.46
11:A:691:G:H2'	11:A:692:U:C6	2.51	0.46
4:H:103:VAL:HG12	4:H:126:ILE:HD12	1.98	0.46
5:L:39:THR:HG22	5:L:51:LYS:HD3	1.98	0.46
8:Q:66:PRO:HG3	11:A:234:C:H4'	1.98	0.46
11:A:831:A:H5''	12:B:21:ARG:NH1	2.31	0.46
11:A:1086:U:C2	11:A:1087:G:C8	3.03	0.46
2:E:149:SER:N	2:E:152:MET:HE3	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:72:A:N7	15:A:1713:HOH:O	2.36	0.46
11:A:737:C:H2'	11:A:738:C:C6	2.51	0.46
11:A:925:G:C1'	11:A:926:G:H5''	2.42	0.46
4:H:11:LEU:HD22	4:H:75:ILE:HD11	1.98	0.45
11:A:1516:G:N1	11:A:1518:A:H5''	2.31	0.45
13:K:34:THR:HB	13:K:40:ALA:HA	1.98	0.45
5:L:50:ARG:NH2	11:A:522:C:H41	2.15	0.45
11:A:922:G:H2'	11:A:923:A:C8	2.51	0.45
11:A:1515:G:H2'	11:A:1516:G:O4'	2.17	0.45
11:A:1517:G:H2'	11:A:1518:A:O4'	2.16	0.45
12:B:79:ALA:HA	12:B:82:ASP:OD2	2.17	0.45
5:L:46:ASN:CG	11:A:528:C:N4	2.71	0.45
11:A:487:A:H2'	11:A:488:C:O4'	2.15	0.45
11:A:821:G:H2'	11:A:822:U:C6	2.51	0.45
11:A:1507:A:C2	11:A:1530:G:C4	3.05	0.45
1:D:152:GLN:O	1:D:155:VAL:HG22	2.16	0.45
11:A:202:G:O2'	11:A:468:A:H8	1.99	0.45
1:D:95:GLU:CD	1:D:104:ARG:HH12	2.25	0.45
3:F:90:MET:HE3	11:A:736:C:H5''	1.97	0.45
5:L:110:ARG:HD2	5:L:110:ARG:HA	1.81	0.45
10:T:36:TYR:OH	11:A:259:G:OP1	2.28	0.45
11:A:613:C:H2'	11:A:614:C:H6	1.81	0.45
11:A:777:A:H2'	11:A:778:G:C8	2.52	0.45
1:D:11:LEU:HB3	1:D:63:ARG:HD3	1.99	0.45
2:E:56:VAL:HB	2:E:57:PRO:HD3	1.98	0.45
11:A:180:U:C2'	11:A:181:A:H5'	2.47	0.45
11:A:268:U:H2'	11:A:269:C:C6	2.52	0.45
11:A:864:A:H2'	11:A:865:A:C8	2.52	0.45
11:A:1069:C:H2'	11:A:1070:U:O4'	2.16	0.45
6:O:74:ASP:OD2	6:O:77:ARG:HG3	2.17	0.45
9:R:21:ILE:HD13	9:R:54:GLN:HG3	1.98	0.45
11:A:688:G:O2'	11:A:704:A:N1	2.42	0.45
11:A:1070:U:H2'	11:A:1071:C:H6	1.82	0.45
12:B:113:ARG:NH1	12:B:116:ASP:OD1	2.50	0.45
11:A:460:A:H2'	11:A:461:A:C8	2.53	0.44
12:B:18:HIS:O	12:B:19:GLN:HB2	2.16	0.44
12:B:23:TRP:CZ3	12:B:25:PRO:HA	2.52	0.44
13:K:41:LEU:H	13:K:41:LEU:HD23	1.82	0.44
1:D:171:LEU:C	1:D:171:LEU:HD12	2.42	0.44
6:O:23:GLY:HA3	11:A:750:C:O2	2.17	0.44
1:D:37:ALA:O	1:D:42:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:665:A:N3	11:A:732:C:H2'	2.32	0.44
11:A:737:C:H2'	11:A:738:C:H6	1.82	0.44
12:B:60:ILE:HA	12:B:63:ARG:HE	1.82	0.44
4:H:102:ALA:HB3	4:H:113:ASP:HB3	2.00	0.44
11:A:62:U:OP1	11:A:385:C:O2'	2.31	0.44
12:B:32:PHE:HA	12:B:42:ASN:HD22	1.82	0.44
11:A:43:C:H5'	15:A:3040:HOH:O	2.16	0.44
11:A:264:C:H2'	11:A:265:G:O4'	2.17	0.44
13:K:47:GLY:O	13:K:52:ARG:NH1	2.50	0.44
11:A:744:C:H2'	11:A:745:G:C8	2.53	0.44
10:T:82:GLN:O	10:T:86:LEU:HG	2.17	0.44
1:D:99:ASP:OD1	1:D:100:ASN:N	2.51	0.44
11:A:2:A:N3	11:A:613:C:O2'	2.50	0.44
12:B:161:LEU:HD22	12:B:176:ALA:HB2	2.00	0.44
11:A:514:C:H2'	11:A:515:G:C8	2.53	0.43
5:L:66:TYR:OH	11:A:522:C:OP2	2.27	0.43
11:A:458:U:H2'	11:A:459:A:H8	1.84	0.43
11:A:867:G:O2'	11:A:873:A:N1	2.50	0.43
12:B:78:GLU:H	12:B:78:GLU:CD	2.25	0.43
13:K:59:PRO:HB3	13:K:91:GLY:HA2	2.00	0.43
11:A:471:U:O2'	11:A:472:U:OP1	2.31	0.43
11:A:579:A:H2'	11:A:580:C:C6	2.53	0.43
11:A:845:A:C5	11:A:846:G:H1'	2.53	0.43
11:A:1518:A:H2'	11:A:1519:A:H5''	1.98	0.43
1:D:54:GLN:HB3	1:D:203:LEU:HB2	2.00	0.43
9:R:32:TYR:CG	9:R:55:LEU:HD21	2.53	0.43
11:A:705:G:C5	11:A:706:A:C8	3.06	0.43
11:A:815:A:N7	11:A:1509:C:O2'	2.45	0.43
11:A:235:C:H2'	11:A:236:A:C8	2.53	0.43
11:A:1519:A:H3'	11:A:1520:C:O4'	2.19	0.43
8:Q:57:ASP:OD1	8:Q:81:LYS:HD3	2.18	0.43
11:A:41:G:H2'	11:A:42:G:C8	2.54	0.43
11:A:900:A:H2'	11:A:901:A:C8	2.54	0.43
11:A:924:C:H3'	11:A:925:G:H2'	2.01	0.43
1:D:2:ALA:N	11:A:405:U:O4	2.52	0.43
1:D:58:LYS:HD3	1:D:203:LEU:HD23	2.01	0.43
8:Q:28:PHE:HZ	15:A:2836:HOH:O	2.01	0.43
13:K:51:PHE:HD2	13:K:61:ALA:HB2	1.84	0.43
11:A:689:C:C2	11:A:690:G:C8	3.07	0.43
13:K:84:MET:SD	13:K:84:MET:N	2.91	0.43
1:D:150:LYS:HG2	1:D:178:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:LEU:HD11	2:E:96:MET:HB3	2.00	0.43
2:E:108:GLY:O	2:E:112:ARG:HB2	2.19	0.43
11:A:12:U:H4'	11:A:526:C:H4'	2.01	0.42
11:A:672:U:H2'	11:A:673:A:C8	2.54	0.42
11:A:1109:C:H2'	11:A:1110:A:O4'	2.19	0.42
12:B:80:VAL:HG12	12:B:91:PHE:HB2	2.00	0.42
8:Q:41:THR:HG22	11:A:280:C:C2	2.54	0.42
11:A:113:G:H2'	11:A:114:U:C6	2.54	0.42
11:A:241:G:N7	15:A:1761:HOH:O	2.37	0.42
11:A:362:G:N7	15:A:1755:HOH:O	2.36	0.42
11:A:1105:A:H2'	11:A:1106:G:H8	1.84	0.42
1:D:3:ARG:HD2	15:D:333:HOH:O	2.19	0.42
11:A:1090:U:H2'	11:A:1091:U:C6	2.54	0.42
12:B:18:HIS:HD2	12:B:19:GLN:HG2	1.84	0.42
13:K:33:ILE:HG21	13:K:73:VAL:HG11	2.02	0.42
11:A:57:G:H2'	11:A:58:C:C6	2.54	0.42
1:D:19:LEU:HD22	1:D:64:ILE:HG13	2.01	0.42
11:A:302:G:O2'	11:A:556:C:H5''	2.20	0.42
11:A:736:C:H2'	11:A:737:C:C6	2.55	0.42
5:L:70:GLU:HG2	15:L:231:HOH:O	2.17	0.42
11:A:685:G:O2'	11:A:686:U:H5''	2.20	0.42
1:D:144:SER:HB2	1:D:179:GLU:HG2	2.01	0.42
3:F:82:ASP:OD1	3:F:82:ASP:N	2.52	0.42
4:H:7:ILE:O	4:H:11:LEU:HG	2.20	0.42
8:Q:69:LYS:HB2	11:A:266:G:H3'	2.02	0.42
11:A:471:U:H2'	11:A:472:U:H6	1.82	0.42
11:A:501:C:H2'	11:A:502:A:C8	2.54	0.42
12:B:19:GLN:HG2	12:B:188:ASP:OD2	2.20	0.42
12:B:103:ASN:O	12:B:107:VAL:HG23	2.19	0.42
3:F:37:HIS:HB2	3:F:63:ASN:ND2	2.29	0.42
4:H:108:LYS:HA	4:H:108:LYS:HD3	1.81	0.42
11:A:313:A:H2'	11:A:314:C:C6	2.54	0.42
11:A:680:C:H2'	11:A:681:A:C8	2.54	0.42
11:A:925:G:N3	11:A:926:G:H2'	2.34	0.42
1:D:14:ARG:NE	11:A:543:U:OP1	2.53	0.42
1:D:39:GLY:HA3	11:A:542:G:H5'	2.01	0.42
2:E:108:GLY:O	2:E:112:ARG:CB	2.67	0.42
5:L:40:THR:CG2	5:L:41:THR:N	2.83	0.42
5:L:88:LYS:CE	11:A:526:C:OP2	2.58	0.42
8:Q:18:GLU:HG3	15:Q:102:HOH:O	2.19	0.42
11:A:518:C:C6	11:A:529:G:H2'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:117:LEU:HD12	12:B:120:GLN:HG3	2.01	0.42
11:A:79:G:H2'	11:A:80:A:C8	2.55	0.42
11:A:604:G:H2'	11:A:605:U:O4'	2.20	0.42
11:A:1074:G:O2'	11:A:1101:A:N1	2.42	0.42
1:D:9:LEU:CD1	11:A:429:U:H5'	2.42	0.41
11:A:852:G:N7	15:A:1764:HOH:O	2.37	0.41
12:B:90:PHE:CE2	12:B:154:MET:HG2	2.54	0.41
4:H:50:LYS:HE2	4:H:52:GLU:HG3	2.03	0.41
11:A:108:G:H5'	11:A:109:A:H5'	2.02	0.41
11:A:865:A:H2'	11:A:866:C:C6	2.55	0.41
11:A:1072:G:H2'	11:A:1073:U:C6	2.54	0.41
12:B:19:GLN:HB2	12:B:189:THR:OG1	2.20	0.41
2:E:64:MET:O	2:E:68:ARG:HG3	2.20	0.41
8:Q:6:ARG:HE	8:Q:6:ARG:HB3	1.70	0.41
11:A:321:A:H2'	11:A:322:C:C6	2.55	0.41
3:F:38:ARG:NH2	3:F:99:ALA:HA	2.34	0.41
3:F:88:MET:HE2	3:F:90:MET:SD	2.60	0.41
4:H:3:MET:HE2	15:A:3234:HOH:O	2.19	0.41
4:H:39:VAL:O	4:H:43:GLU:HG2	2.20	0.41
5:L:44:LYS:CB	5:L:45:PRO:HD3	2.44	0.41
11:A:1106:G:H2'	11:A:1107:C:H6	1.83	0.41
12:B:117:LEU:HD12	12:B:117:LEU:HA	1.80	0.41
6:O:2:SER:CA	6:O:35:GLN:NE2	2.82	0.41
10:T:33:LYS:HB2	10:T:33:LYS:HE3	1.80	0.41
11:A:58:C:O2'	11:A:388:G:N7	2.43	0.41
11:A:204:G:H2'	11:A:205:A:C8	2.56	0.41
12:B:67:ILE:CD1	12:B:221:VAL:HG21	2.43	0.41
12:B:143:LYS:HE3	12:B:143:LYS:HB3	1.81	0.41
2:E:76:LEU:HD12	2:E:76:LEU:C	2.46	0.41
11:A:769:G:H4'	11:A:1513:A:H4'	2.02	0.41
11:A:1508:A:H2'	11:A:1509:C:O4'	2.21	0.41
1:D:128:ARG:HB3	1:D:128:ARG:NH1	2.36	0.41
3:F:38:ARG:NH2	3:F:40:GLU:OE2	2.51	0.41
11:A:37:U:O2'	11:A:500:G:H4'	2.20	0.41
11:A:636:U:H2'	11:A:637:C:C6	2.56	0.41
11:A:676:A:O2'	11:A:677:U:H5'	2.21	0.41
11:A:831:A:OP1	12:B:21:ARG:HD2	2.20	0.41
12:B:15:HIS:CE1	12:B:46:THR:HG21	2.56	0.41
12:B:42:ASN:HB3	12:B:45:LYS:HB2	2.02	0.41
11:A:6:G:O2'	11:A:7:A:H8	2.03	0.41
11:A:120:A:C4'	15:A:2297:HOH:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:149:SER:O	2:E:153:VAL:HG12	2.20	0.41
3:F:25:TYR:O	3:F:29:ILE:HG12	2.21	0.41
11:A:176:C:H2'	11:A:177:G:N3	2.36	0.41
11:A:663:A:H5'	11:A:836:G:OP1	2.21	0.41
11:A:824:G:H5'	15:A:1970:HOH:O	2.20	0.41
11:A:1097:C:C5'	12:B:143:LYS:HD2	2.51	0.41
12:B:9:MET:HB3	12:B:15:HIS:ND1	2.35	0.41
13:K:14:GLN:HE21	13:K:14:GLN:HB3	1.68	0.41
3:F:42:TRP:HB2	3:F:59:TYR:HB2	2.03	0.41
11:A:33:A:H2'	11:A:34:C:C6	2.55	0.41
11:A:130:A:H1'	11:A:263:A:O2'	2.20	0.41
11:A:539:A:H2'	11:A:540:G:C8	2.55	0.41
12:B:90:PHE:HE2	12:B:151:ILE:HA	1.86	0.41
7:P:53:ASP:OD2	7:P:56:ARG:HG2	2.22	0.40
11:A:35:G:H2'	11:A:36:C:C6	2.56	0.40
13:K:81:LEU:O	13:K:107:THR:N	2.54	0.40
13:K:81:LEU:HD13	13:K:81:LEU:HA	1.93	0.40
1:D:26:ARG:HH12	11:A:411:A:P	2.45	0.40
11:A:881:G:H2'	11:A:882:C:O4'	2.20	0.40
11:A:918:A:H2'	11:A:919:A:O4'	2.21	0.40
8:Q:58:VAL:HB	8:Q:80:GLU:HB3	2.04	0.40
12:B:164:ILE:HD12	12:B:164:ILE:HA	1.93	0.40
11:A:20:U:H2'	11:A:21:G:O4'	2.22	0.40
12:B:43:LEU:HD22	12:B:43:LEU:H	1.86	0.40
2:E:149:SER:OG	2:E:152:MET:HG2	2.22	0.40
11:A:262:A:H2'	11:A:263:A:C8	2.56	0.40
11:A:788:U:H2'	11:A:789:U:O4'	2.22	0.40
11:A:926:G:N2	11:A:927:G:N3	2.69	0.40
11:A:1513:A:H2'	11:A:1514:G:C8	2.56	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	D	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
2	E	153/167 (92%)	149 (97%)	4 (3%)	0	100	100
3	F	99/135 (73%)	95 (96%)	4 (4%)	0	100	100
4	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
5	L	118/124 (95%)	112 (95%)	6 (5%)	0	100	100
6	O	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
7	P	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
8	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
9	R	50/75 (67%)	50 (100%)	0	0	100	100
10	T	83/87 (95%)	83 (100%)	0	0	100	100
12	B	222/241 (92%)	209 (94%)	13 (6%)	0	100	100
13	K	113/129 (88%)	104 (92%)	9 (8%)	0	100	100
All	All	1408/1548 (91%)	1359 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	D	171/173 (99%)	171 (100%)	0	100	100
2	E	118/126 (94%)	118 (100%)	0	100	100
3	F	88/116 (76%)	88 (100%)	0	100	100
4	H	104/105 (99%)	104 (100%)	0	100	100
5	L	101/103 (98%)	101 (100%)	0	100	100
6	O	75/77 (97%)	75 (100%)	0	100	100
7	P	65/65 (100%)	65 (100%)	0	100	100
8	Q	73/78 (94%)	73 (100%)	0	100	100
9	R	45/65 (69%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	T	65/66 (98%)	65 (100%)	0	100	100
12	B	186/199 (94%)	186 (100%)	0	100	100
13	K	88/99 (89%)	88 (100%)	0	100	100
All	All	1179/1272 (93%)	1179 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	70	ASN
2	E	82	GLN
3	F	37	HIS
3	F	63	ASN
3	F	94	HIS
4	H	4	GLN
4	H	21	ASN
6	O	35	GLN
8	Q	9	GLN
10	T	61	GLN
10	T	82	GLN
12	B	19	GLN
12	B	24	ASN
12	B	39	HIS
13	K	21	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1022/1542 (66%)	161 (15%)	8 (0%)

All (161) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	6	G
11	A	9	G
11	A	32	A
11	A	39	G
11	A	47	C

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Mol	Chain	Res	Type
11	A	48	C
11	A	50	A
11	A	51	A
11	A	54	C
11	A	55	A
11	A	70	U
11	A	71	A
11	A	75	G
11	A	80	A
11	A	81	A
11	A	82	G
11	A	83	C
11	A	85	U
11	A	86	G
11	A	88	U
11	A	89	U
11	A	90	C
11	A	91	U
11	A	109	A
11	A	116	A
11	A	119	A
11	A	120	A
11	A	122	G
11	A	130	A
11	A	131	A
11	A	149	A
11	A	164	G
11	A	181	A
11	A	183	C
11	A	189	A
11	A	196	A
11	A	197	A
11	A	200	G
11	A	204	G
11	A	209	U
11	A	210	C
11	A	211	G
11	A	212	G
11	A	243	A
11	A	245	U
11	A	247	G
11	A	251	G

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Mol	Chain	Res	Type
11	A	254	G
11	A	262	A
11	A	266	G
11	A	267	C
11	A	280	C
11	A	289	G
11	A	299	G
11	A	316	C
11	A	321	A
11	A	328	C
11	A	332	G
11	A	344	A
11	A	352	C
11	A	354	G
11	A	356	A
11	A	367	U
11	A	372	C
11	A	384	G
11	A	392	C
11	A	398	U
11	A	406	G
11	A	412	A
11	A	413	G
11	A	421	U
11	A	422	C
11	A	423	G
11	A	424	G
11	A	429	U
11	A	446	G
11	A	467	U
11	A	468	A
11	A	472	U
11	A	481	G
11	A	484	G
11	A	486	U
11	A	511	C
11	A	512	U
11	A	518	C
11	A	521	G
11	A	524	G
11	A	527	G7M
11	A	531	U

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Mol	Chain	Res	Type
11	A	532	A
11	A	533	A
11	A	547	A
11	A	559	A
11	A	562	U
11	A	572	A
11	A	573	A
11	A	576	C
11	A	596	A
11	A	619	U
11	A	633	G
11	A	650	G
11	A	653	U
11	A	665	A
11	A	684	U
11	A	686	U
11	A	687	A
11	A	695	A
11	A	702	A
11	A	703	G
11	A	718	A
11	A	719	C
11	A	721	G
11	A	724	G
11	A	734	G
11	A	748	G
11	A	755	G
11	A	786	G
11	A	794	A
11	A	815	A
11	A	817	C
11	A	821	G
11	A	828	U
11	A	841	C
11	A	842	U
11	A	845	A
11	A	846	G
11	A	849	G
11	A	872	A
11	A	885	G
11	A	901	A
11	A	902	G

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Mol	Chain	Res	Type
11	A	914	A
11	A	925	G
11	A	926	G
11	A	927	G
11	A	928	G
11	A	930	C
11	A	934	C
11	A	935	A
11	A	1065	U
11	A	1070	U
11	A	1085	U
11	A	1089	G
11	A	1094	G
11	A	1095	U
11	A	1097	C
11	A	1101	A
11	A	1104	G
11	A	1108	G
11	A	1389	C
11	A	1391	U
11	A	1508	A
11	A	1518	A
11	A	1519	A
11	A	1520	C
11	A	1522	U
11	A	1529	G
11	A	1530	G
11	A	1531	A
11	A	1532	U
11	A	1535	C

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	85	U
11	A	109	A
11	A	298	A
11	A	428	G
11	A	471	U
11	A	925	G
11	A	1530	G
11	A	1531	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
11	PSU	A	516	11,14	18,21,22	1.05	1 (5%)	21,30,33	2.01	6 (28%)
5	D2T	L	89	5	8,9,10	1.42	1 (12%)	6,11,13	1.49	1 (16%)
11	G7M	A	527	11	23,26,27	0.73	1 (4%)	34,39,42	0.61	1 (2%)

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
11	PSU	A	516	11,14	-	0/7/25/26	0/2/2/2
5	D2T	L	89	5	-	3/7/12/14	-
11	G7M	A	527	11	-	1/7/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	516	PSU	C6-C5	3.28	1.38	1.35
11	A	527	G7M	C8-N7	2.48	1.37	1.33
5	L	89	D2T	CB1-SB	-2.01	1.75	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	516	PSU	N1-C2-N3	5.10	120.55	115.17
11	A	516	PSU	C4-N3-C2	-4.95	119.55	126.37
11	A	516	PSU	O2-C2-N1	-2.66	120.05	122.79
11	A	516	PSU	C6-N1-C2	-2.30	120.55	122.69
11	A	516	PSU	C6-C5-C4	2.29	119.72	118.17
11	A	516	PSU	O4'-C1'-C2'	2.21	108.21	105.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	527	G7M	N9-C8-N7	-2.12	107.34	112.48
5	L	89	D2T	O-C-CA	-2.11	119.36	124.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	89	D2T	CG-CB-SB-CB1
5	L	89	D2T	SB-CB-CG-OD1
11	A	527	G7M	C4'-C5'-O5'-P
5	L	89	D2T	SB-CB-CG-OD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	89	D2T	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 34 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

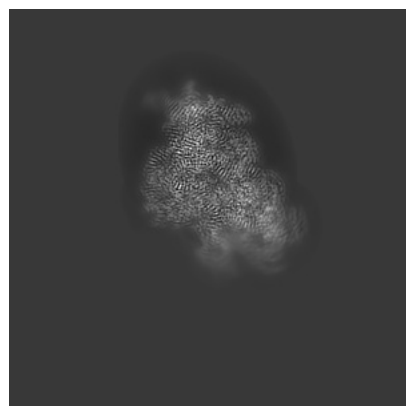
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67203. These allow visual inspection of the internal detail of the map and identification of artifacts.

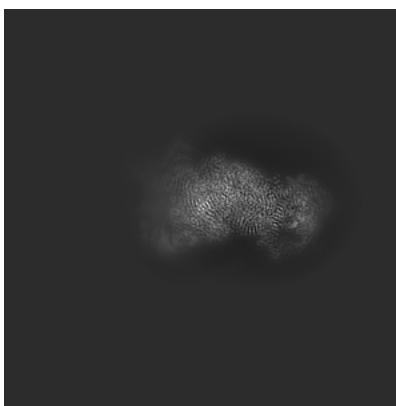
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

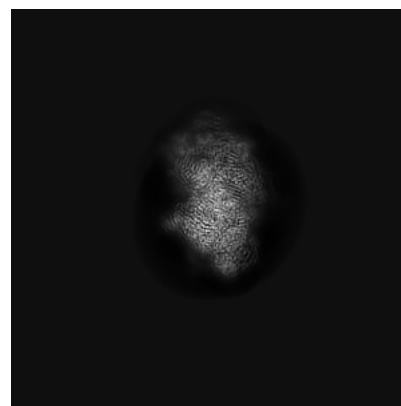
6.1.1 Primary map



X

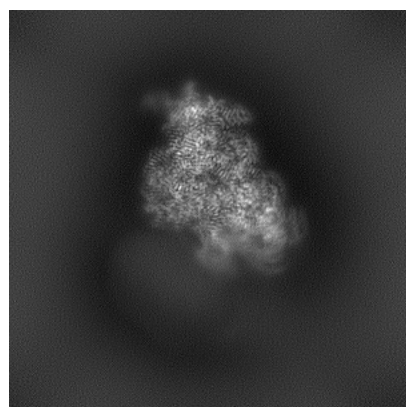


Y

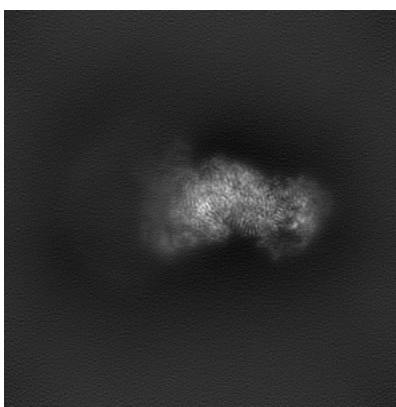


Z

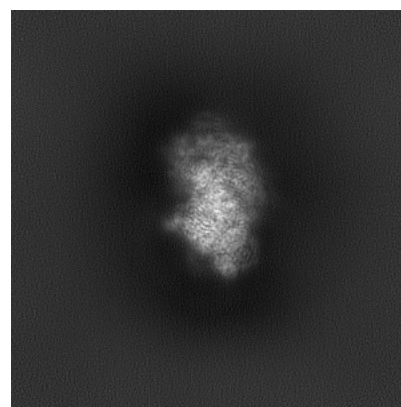
6.1.2 Raw map



X



Y

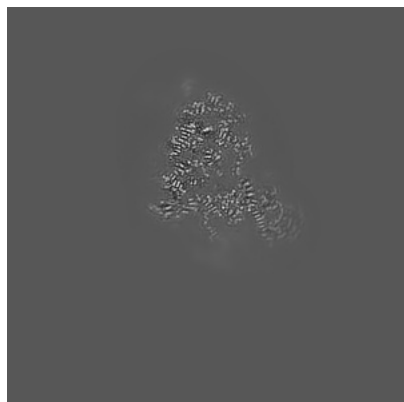


Z

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

6.2 Central slices [i](#)

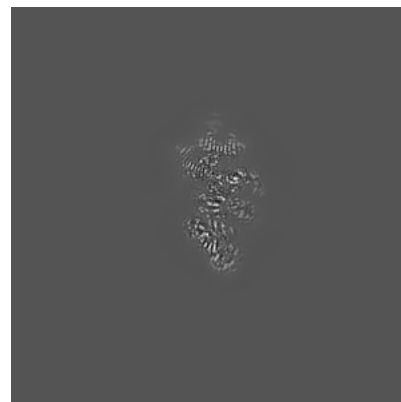
6.2.1 Primary map



X Index: 220

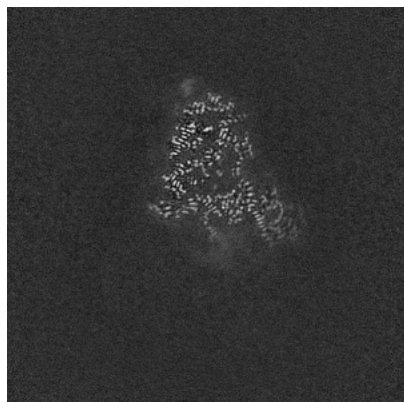


Y Index: 220

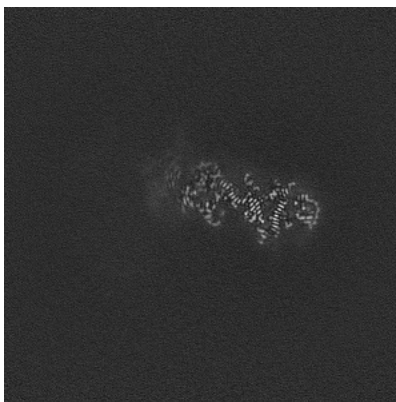


Z Index: 220

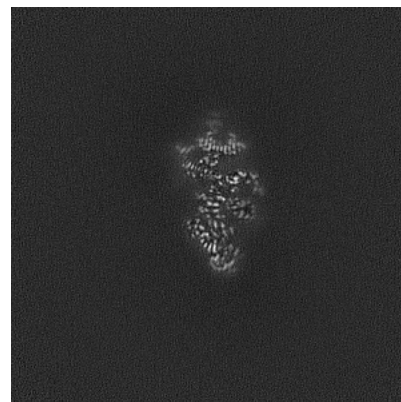
6.2.2 Raw map



X Index: 220



Y Index: 220

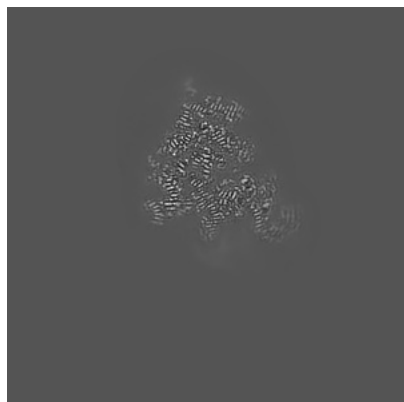


Z Index: 220

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

6.3 Largest variance slices [i](#)

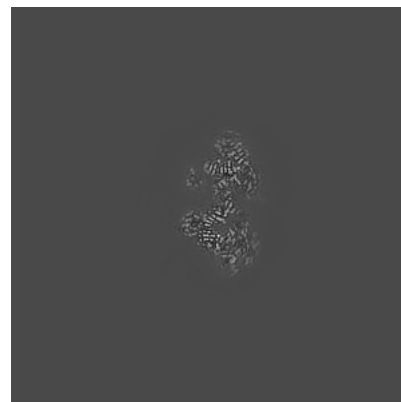
6.3.1 Primary map



X Index: 226

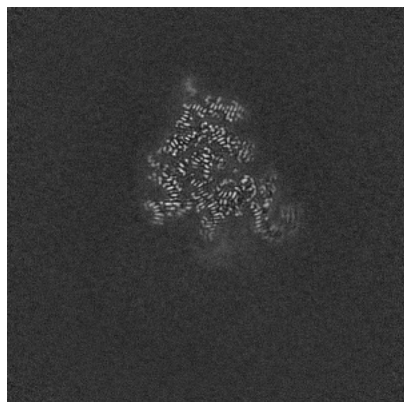


Y Index: 199

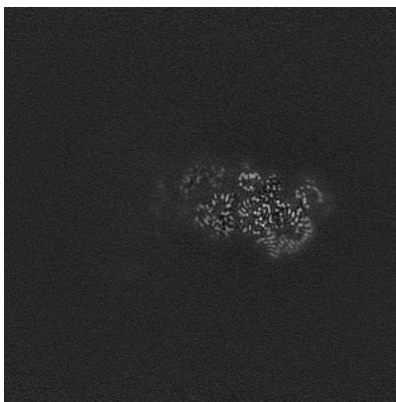


Z Index: 245

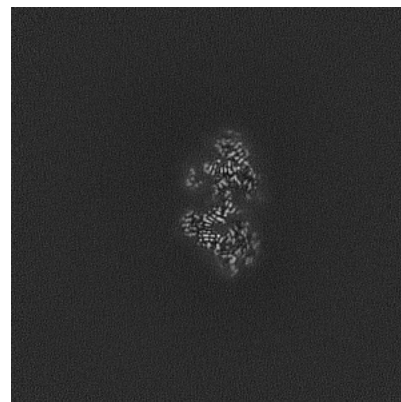
6.3.2 Raw map



X Index: 226



Y Index: 206

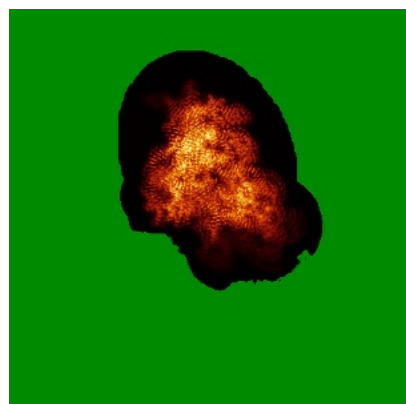


Z Index: 245

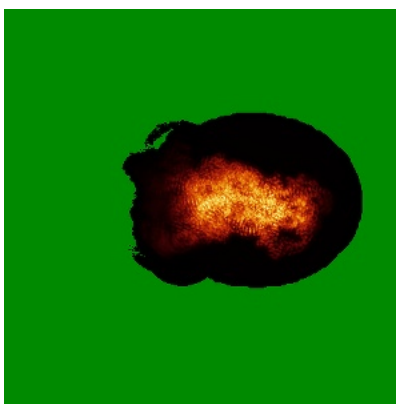
The images above show the largest variance slices of the map in three orthogonal directions.

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

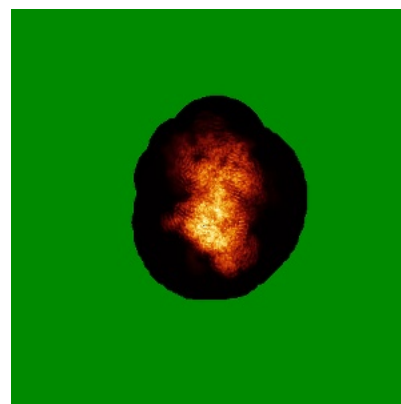
6.4.1 Primary map



X

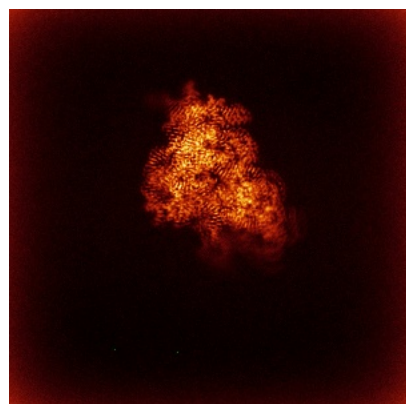


Y

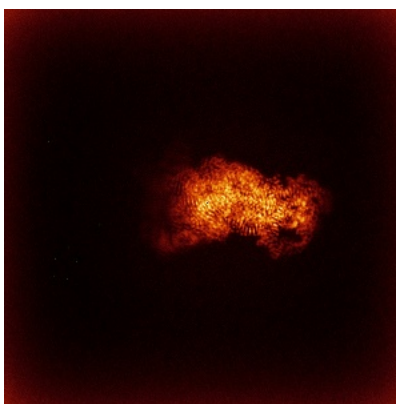


Z

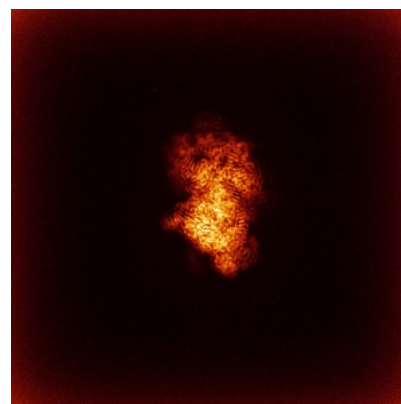
6.4.2 Raw map



X



Y

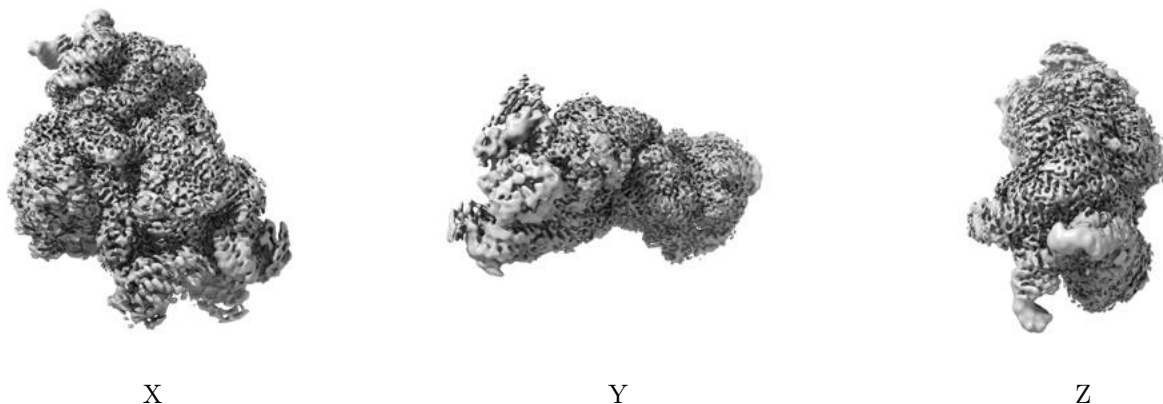


Z

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.

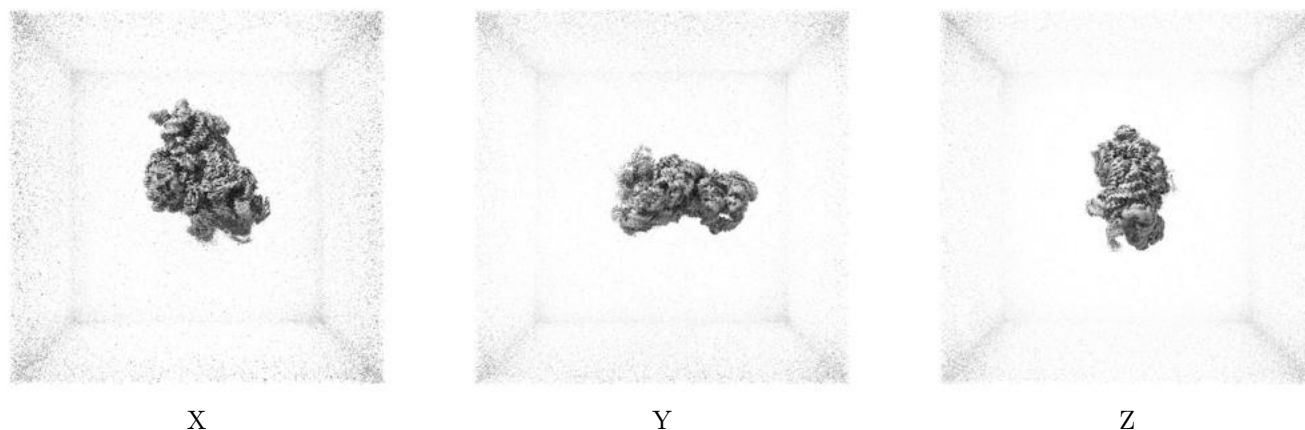
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

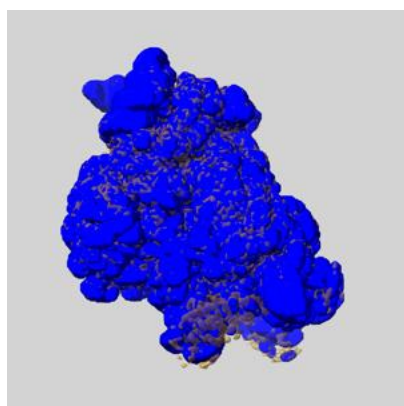
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

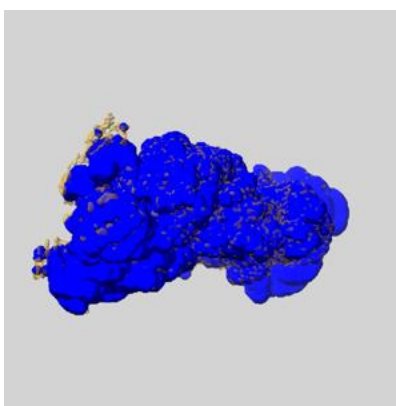
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

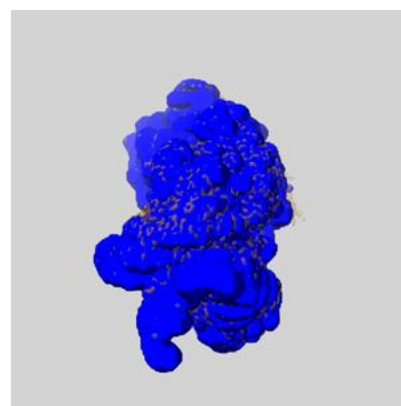
6.6.1 emd_67203_msk_1.map [i](#)



X



Y

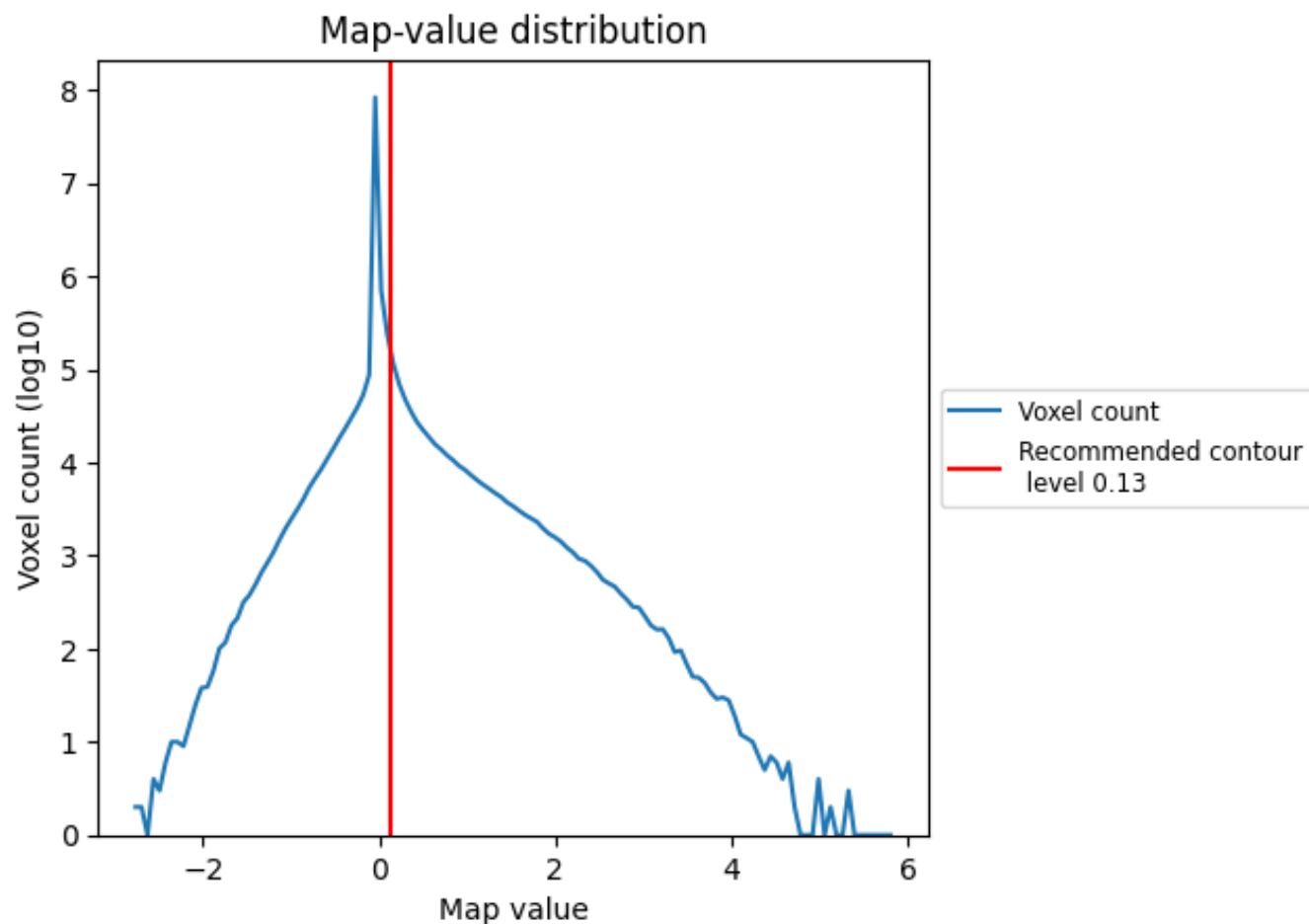


Z

7 Map analysis [i](#)

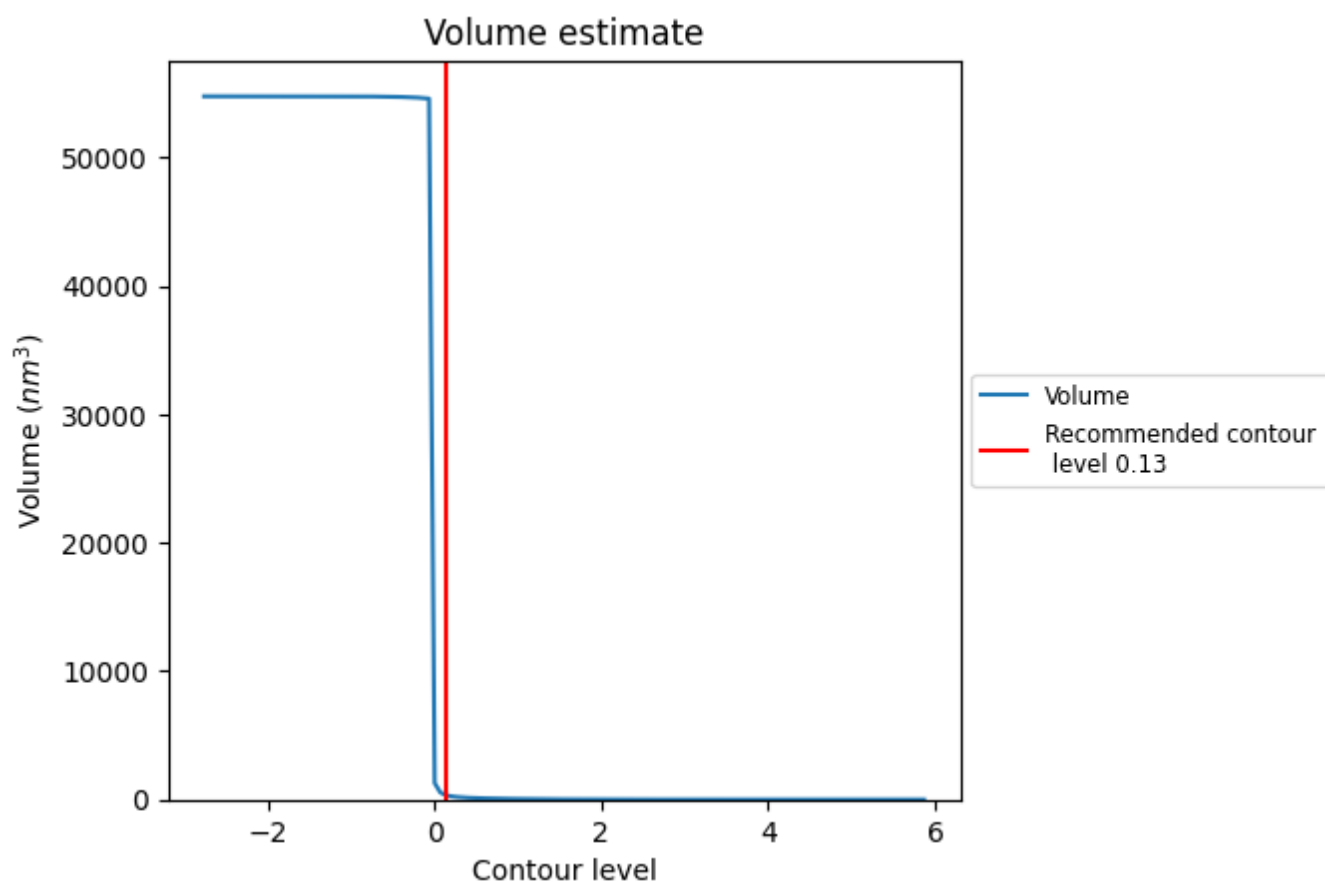
This section contains the results of statistical analysis of the map.

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.

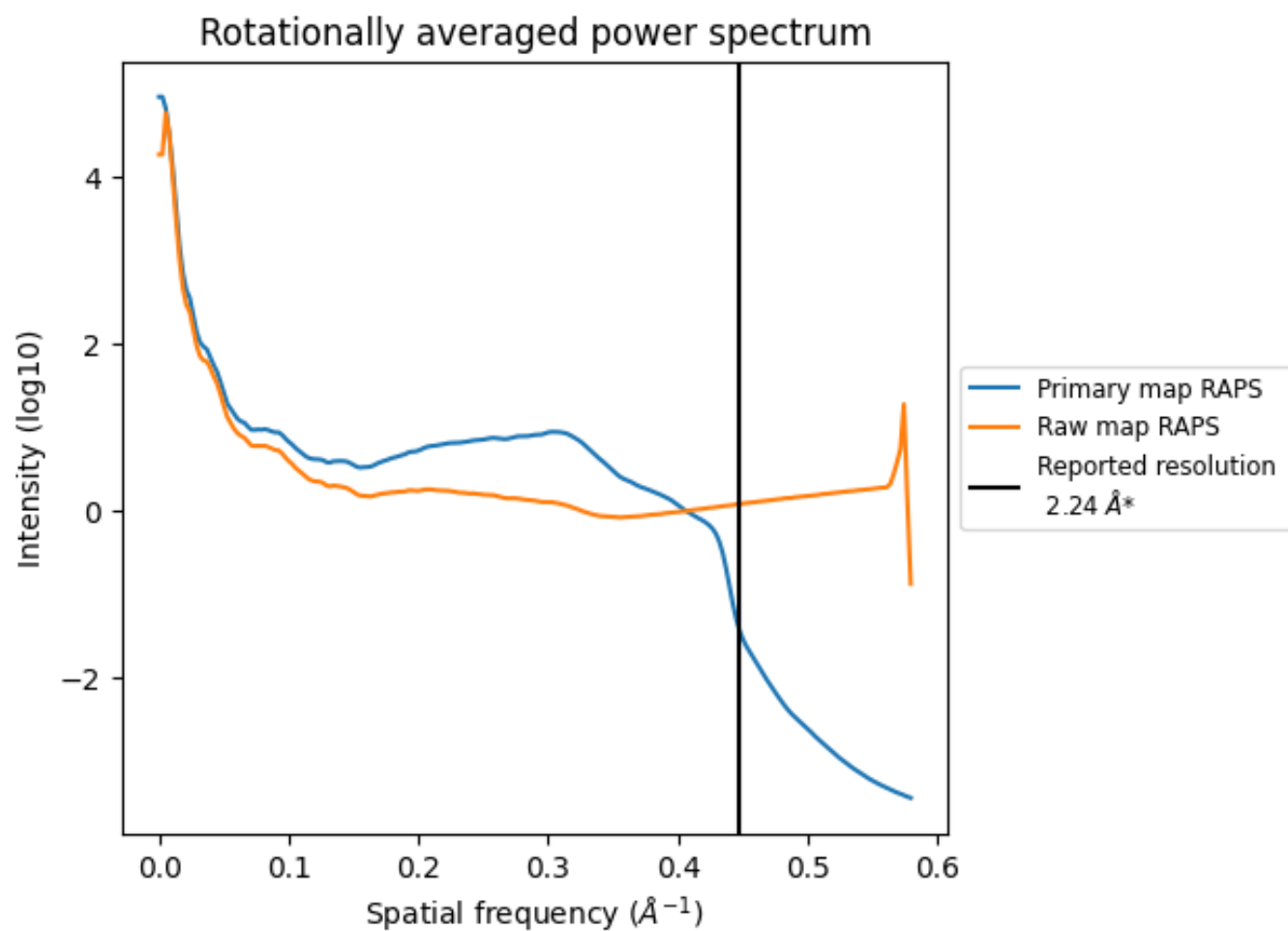
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365 nm^3 ; this corresponds to an approximate mass of 330 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 ⓘ

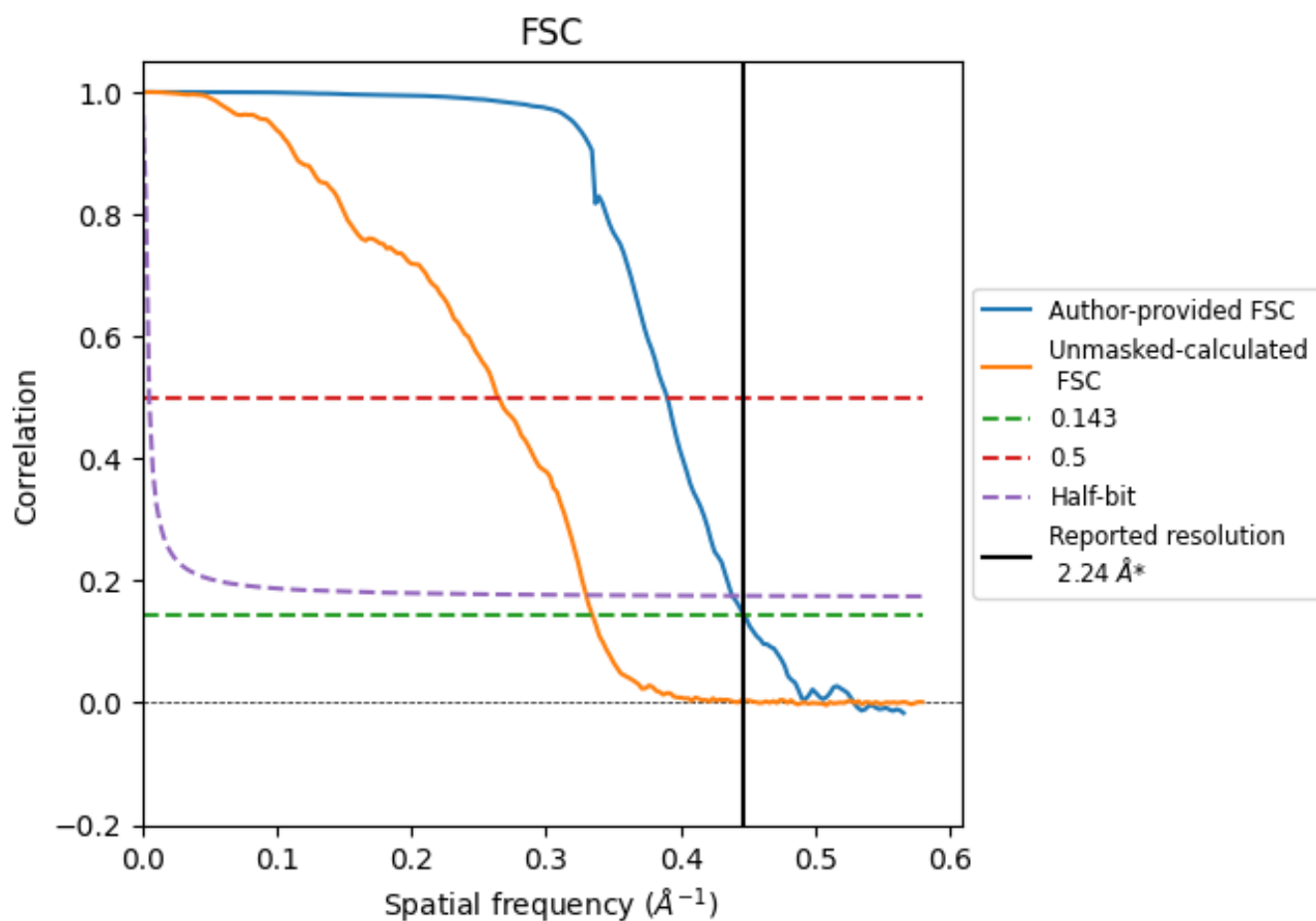


*Reported resolution corresponds to spatial frequency of 0.446 \AA^{-1}

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 0.446 \AA^{-1}

8.2 Resolution estimates [i](#)

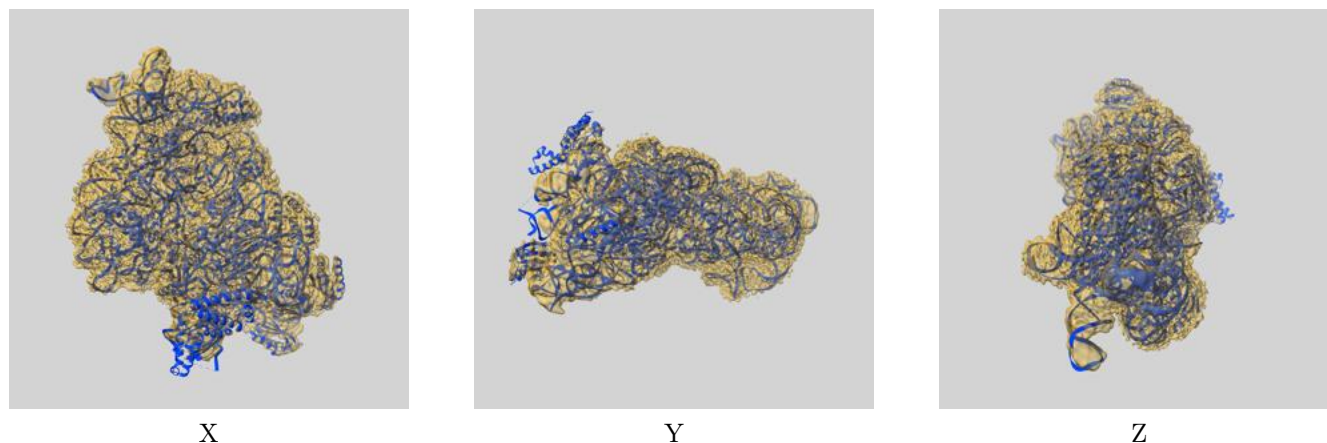
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.24	2.57	2.28
Unmasked-calculated*	2.99	3.78	3.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.24 by more than 10 %

9 Map-model fit [i](#)

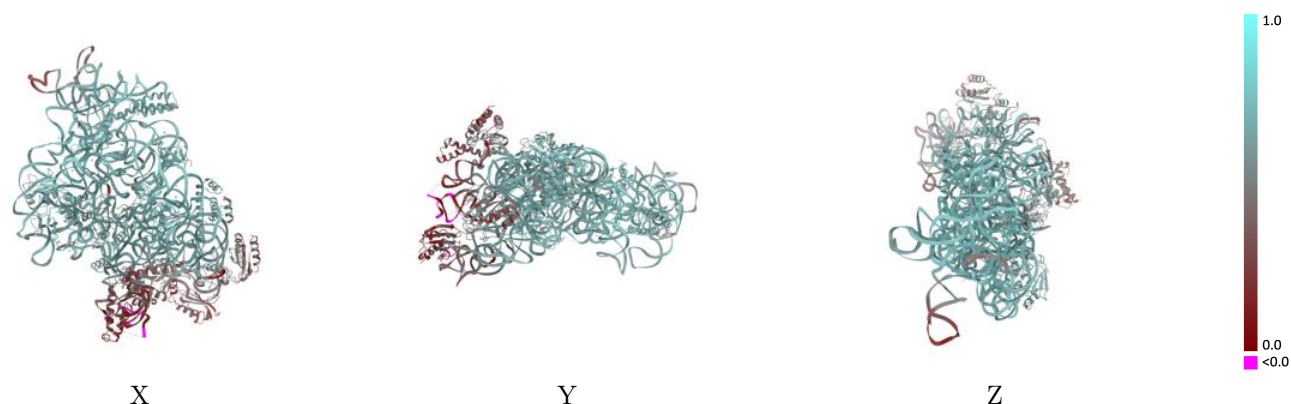
This section contains information regarding the fit between EMDB map EMD-67203 and PDB model 9XTE. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



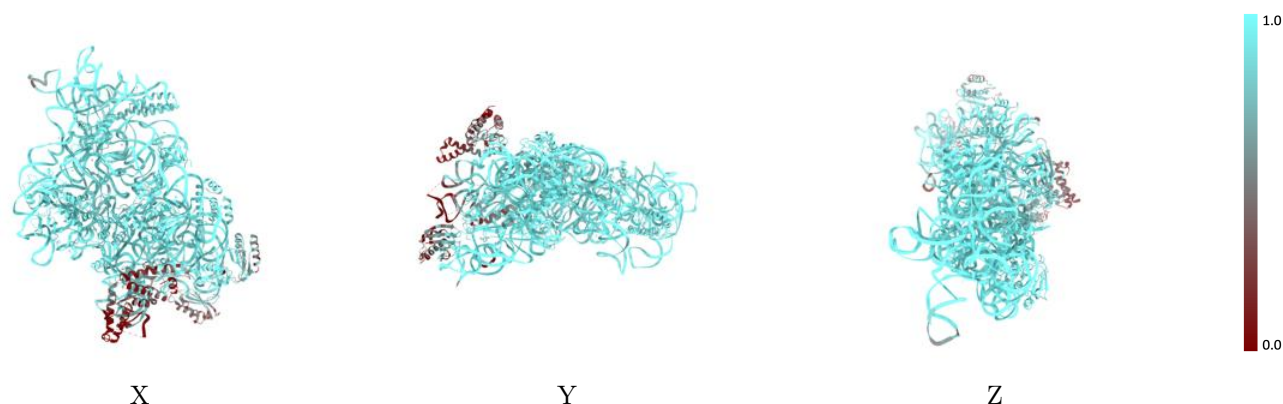
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



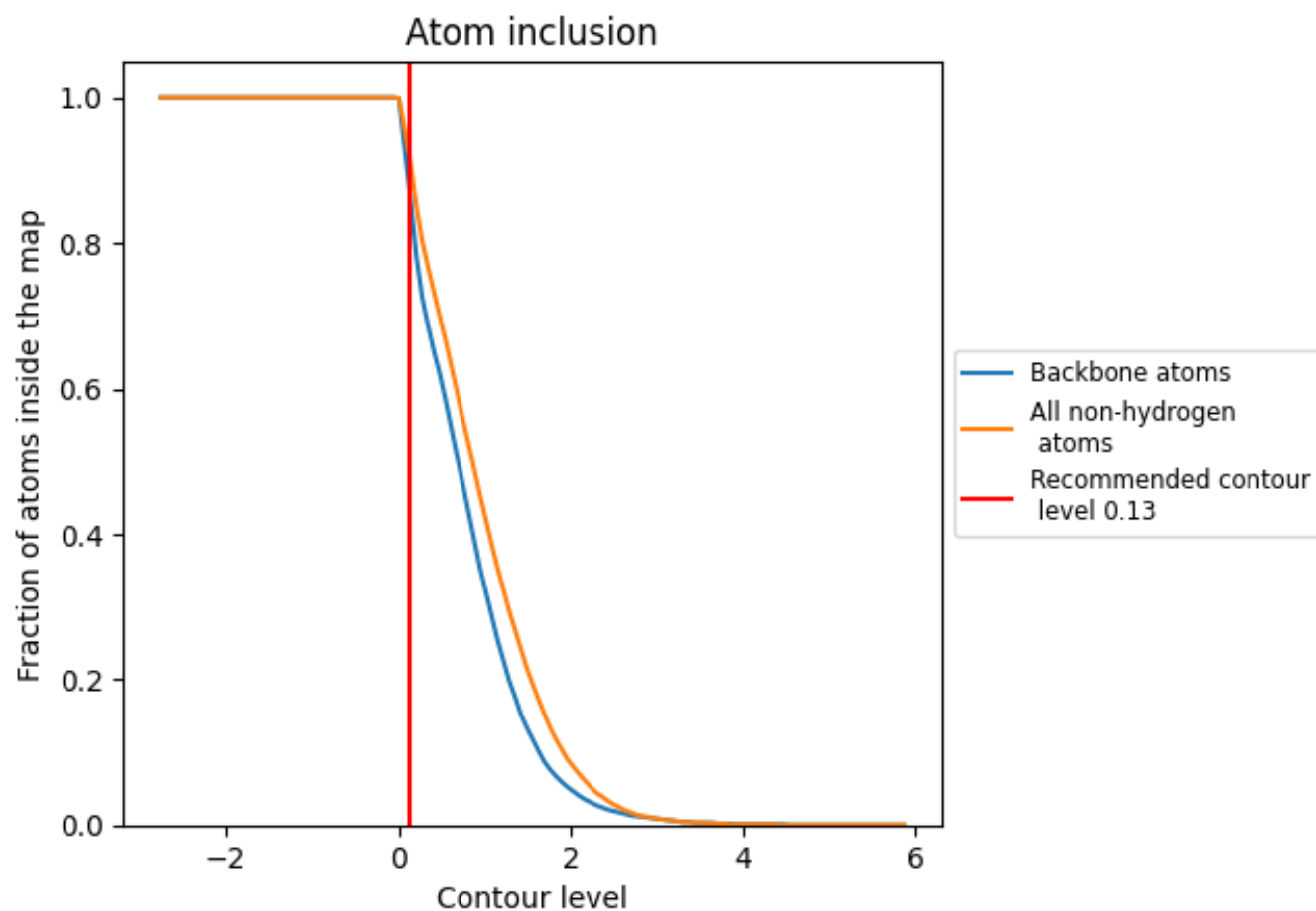
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 92% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9170	<div></div> 0.6050
A	<div></div> 0.9600	<div></div> 0.6280
B	<div></div> 0.4130	<div></div> 0.3580
D	<div></div> 0.9720	<div></div> 0.6350
E	<div></div> 0.9610	<div></div> 0.6260
F	<div></div> 0.7440	<div></div> 0.4000
H	<div></div> 0.9790	<div></div> 0.6780
K	<div></div> 0.5380	<div></div> 0.2920
L	<div></div> 0.9840	<div></div> 0.6840
O	<div></div> 0.9660	<div></div> 0.6090
P	<div></div> 0.9790	<div></div> 0.7210
Q	<div></div> 0.9920	<div></div> 0.6710
R	<div></div> 0.9310	<div></div> 0.5590
T	<div></div> 0.9830	<div></div> 0.6750

1.0

0.0

<0.0