



Full wwPDB EM Validation Report ⓘ

Oct 1, 2025 – 02:13 PM JST

PDB ID : 9V1K / pdb_00009v1k
EMDB ID : EMD-64696
Title : Cryo- EM structure of small subunit (head) of 75S ribosome with P- tRNA from *Entamoeba histolytica*
Authors : Sharma, S.; Mishra, S.; Gourinath, S.; Kaushal, P.S.
Deposited on : 2025-05-19
Resolution : 3.40 Å (reported)
Based on initial models : 5XXB, 4UG0

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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

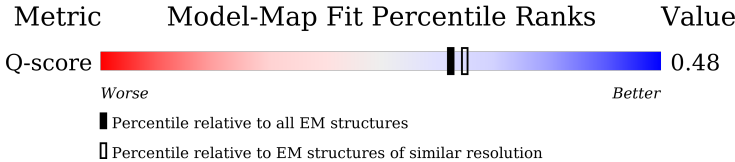
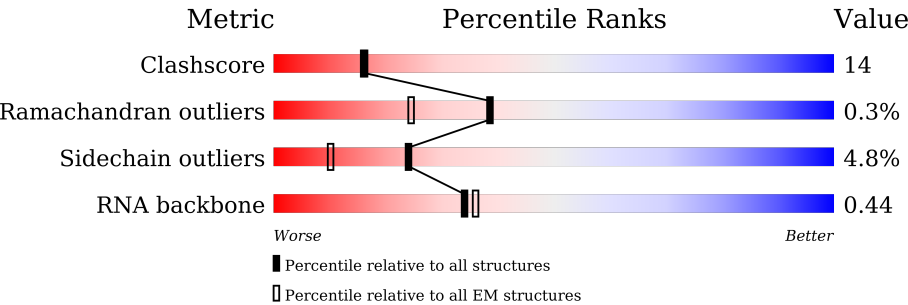
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	sA	137	<div> <div>40%</div> <div>9%</div> <div>49%</div> </div>
2	sD	69	<div> <div>59%</div> <div>26%</div> <div>13%</div> </div>
3	sE	56	<div> <div>62%</div> <div>32%</div> </div>

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Mol	Chain	Length	Quality of chain
4	sG	321	
5	sa	1947	
6	sd	244	
7	sg	206	
8	sl	127	
9	sq	144	
10	ss	158	
11	st	117	
12	su	155	
13	sv	155	
14	sw	118	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 22456 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 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	sA	70	Total	C	N	O	S	0	0
			554	359	93	98	4		

- Molecule 2 is a protein called 40S ribosomal protein S28, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	sD	60	Total	C	N	O	S	0	0
			468	289	93	84	2		

- Molecule 3 is a protein called Ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	sE	55	Total	C	N	O	S	0	0
			442	273	90	75	4		

- Molecule 4 is a protein called Guanine nucleotide-binding protein subunit beta 2-like 1, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	sG	181	Total	C	N	O	S	0	0
			1395	880	248	258	9		

- Molecule 5 is a RNA chain called 17S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	sa	475	Total	C	N	O	P	0	0
			10153	4544	1840	3294	475		

- Molecule 6 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	sd	214	Total	C	N	O	S	0	0
			1656	1048	303	294	11		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	sg	184	Total	C	N	O	S	0	0
			1463	924	264	264	11		

- Molecule 8 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	sl	71	Total	C	N	O	S	0	0
			579	380	99	91	9		

- Molecule 9 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	sq	105	Total	C	N	O	S	0	0
			842	543	150	144	5		

- Molecule 10 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	ss	141	Total	C	N	O	S	0	0
			1104	713	198	189	4		

- Molecule 11 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	st	76	Total	C	N	O	S	0	0
			629	399	123	106	1		

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	su	144	Total	C	N	O	S	0	0
			1163	722	233	202	6		

- Molecule 13 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	sv	155	Total	C	N	O	S	0	0
			1245	796	223	217	9		

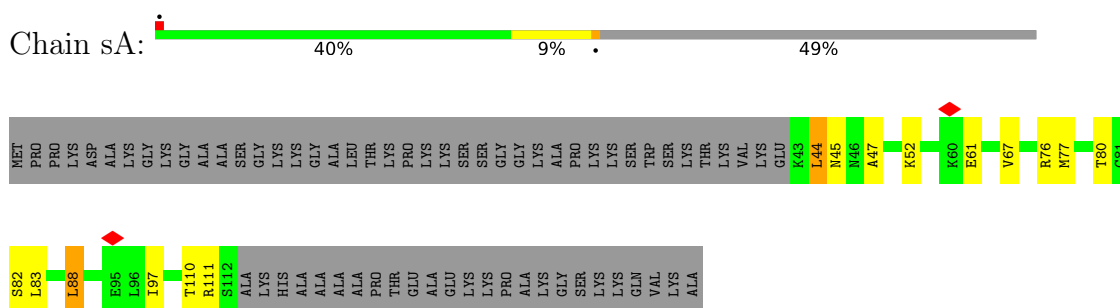
- Molecule 14 is a protein called 40S ribosomal protein S20, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	sw	98	Total	C	N	O	S	0	0
			763	481	134	143	5		

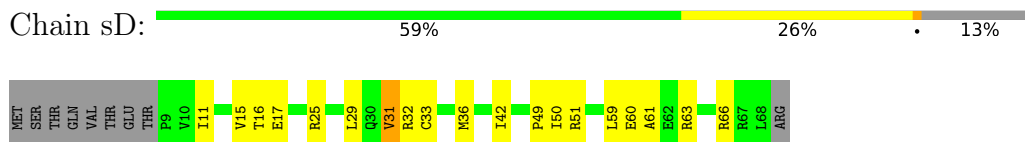
3 Residue-property plots [i](#)

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

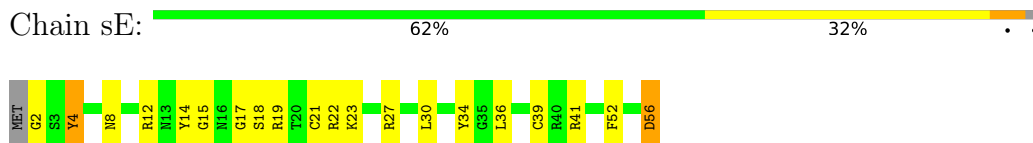
- Molecule 1: 40S ribosomal protein S25



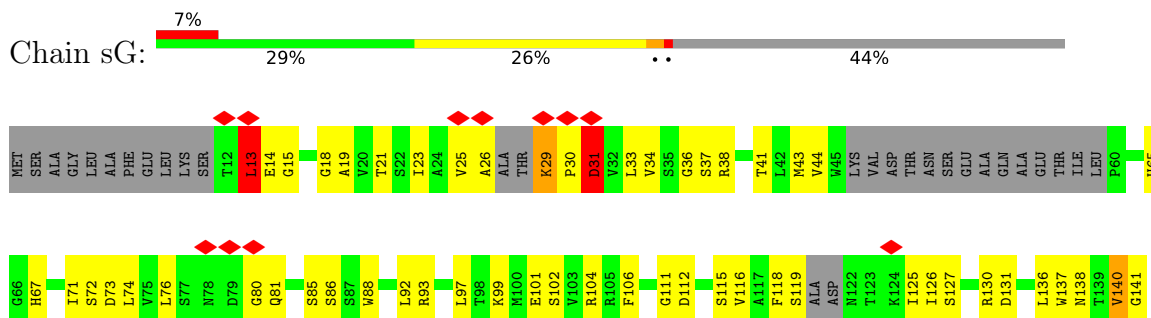
- Molecule 2: 40S ribosomal protein S28, putative

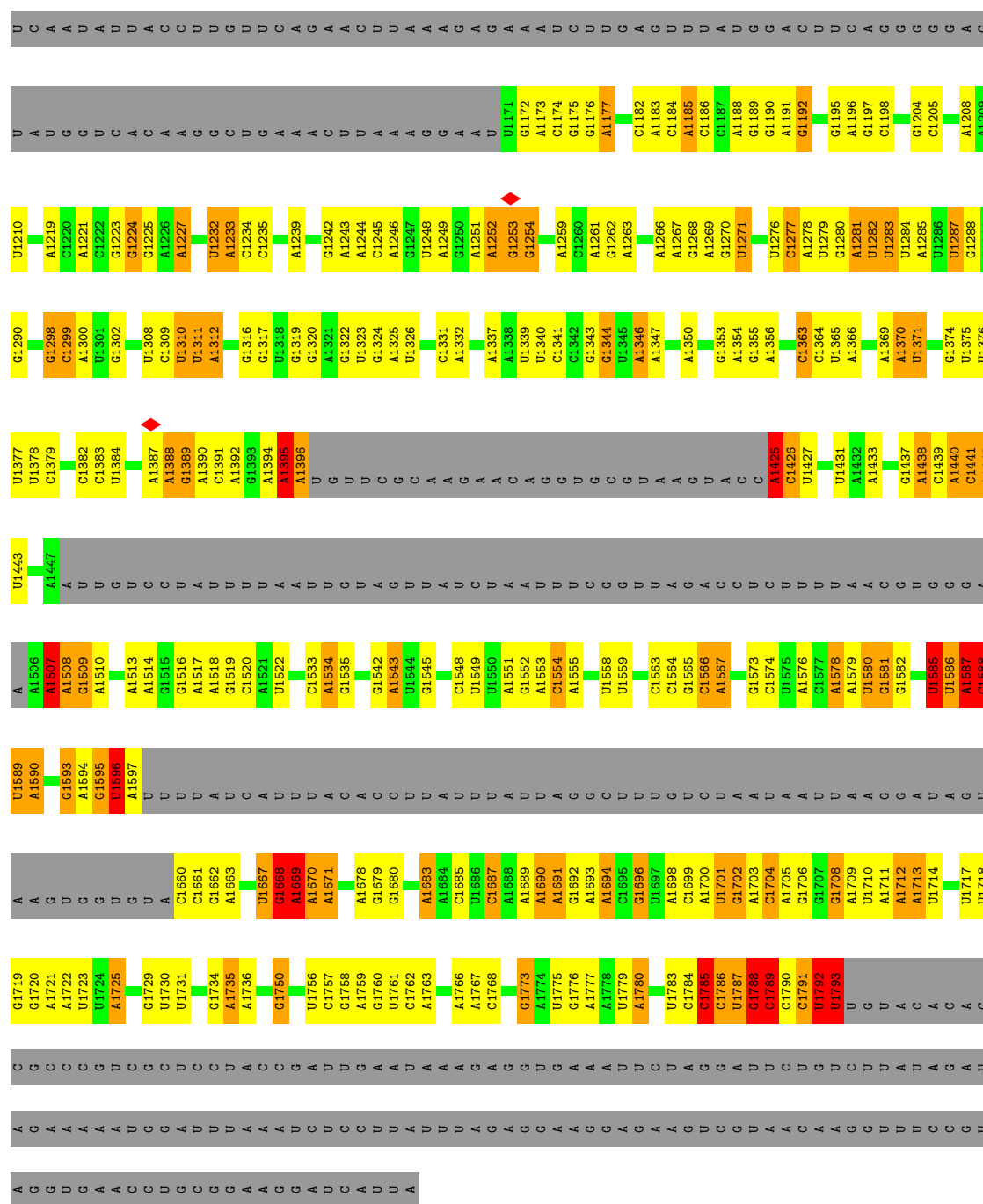


- Molecule 3: Ribosomal protein S29, putative

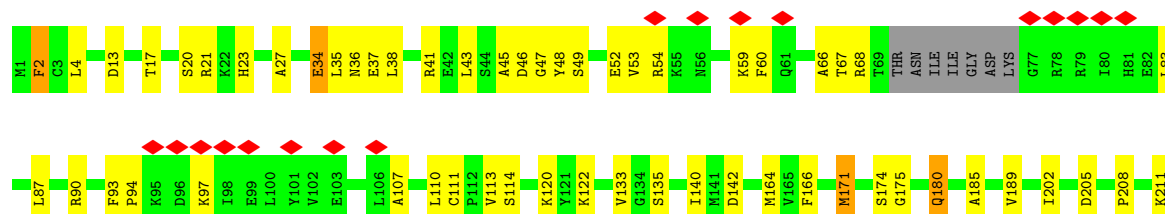


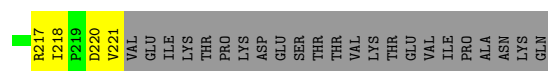
- Molecule 4: Guanine nucleotide-binding protein subunit beta 2-like 1, putative





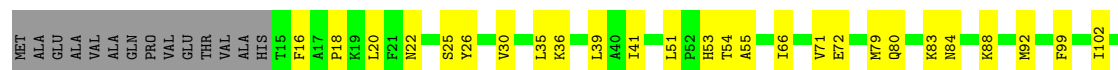
• Molecule 6: 40S ribosomal protein S3





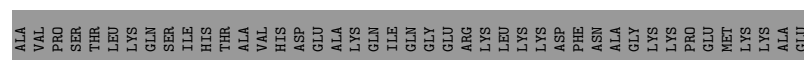
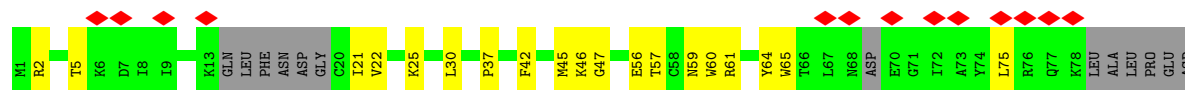
- Molecule 7: Small ribosomal subunit protein uS7

Chain sg: 70% 19% 11%



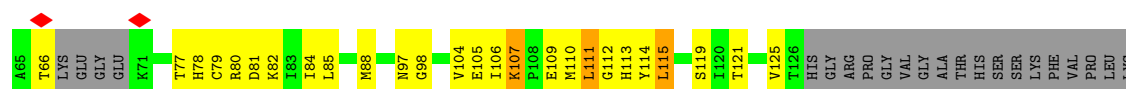
- Molecule 8: 40S ribosomal protein S10, putative

Chain sl: 10% 41% 15% 44%



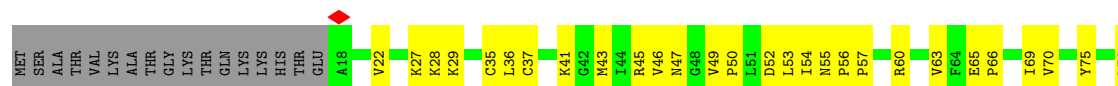
- Molecule 9: 40S ribosomal protein S15, putative

Chain sq: 6% 38% 32% 27%



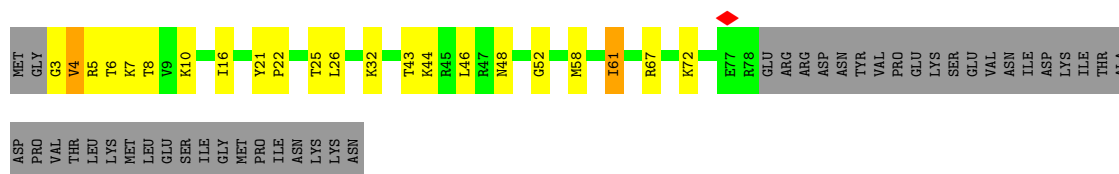
- Molecule 10: 40S ribosomal protein S16, putative

Chain ss: 64% 25% 11%

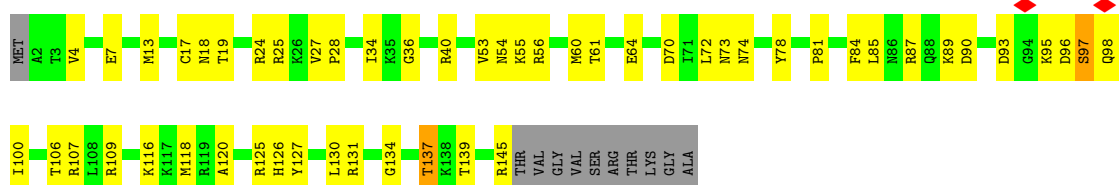


- Molecule 11: 40S ribosomal protein S17, putative

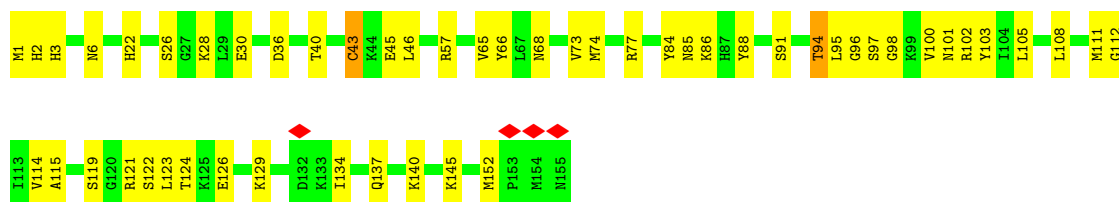
Chain st: 46% 17% 35%



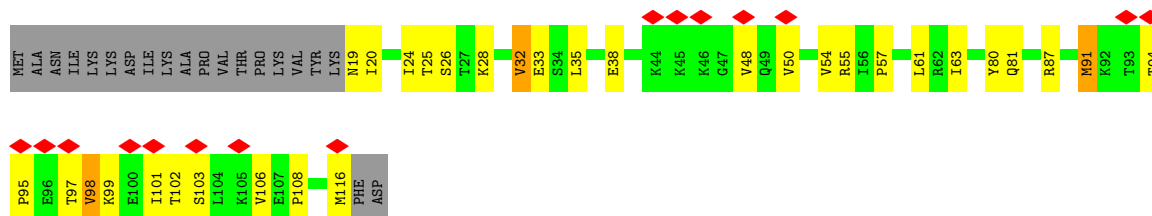
- Molecule 12: Small ribosomal subunit protein uS13



- Molecule 13: Small ribosomal subunit protein eS19



- Molecule 14: 40S ribosomal protein S20, putative



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53764	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.106	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	16.402	Depositor
Minimum map value	-5.883	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.8	Depositor
Map size (\AA)	224.70001, 224.70001, 224.70001	wwPDB
Map dimensions	210, 210, 210	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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	sA	0.19	0/561	0.36	0/757
2	sD	0.19	0/470	0.33	0/630
3	sE	0.25	0/449	0.37	0/595
4	sG	0.24	0/1415	0.51	0/1896
5	sa	0.45	12/11368 (0.1%)	0.63	36/17709 (0.2%)
6	sd	0.19	0/1676	0.34	0/2243
7	sg	0.21	0/1484	0.29	0/1994
8	sl	0.18	0/590	0.27	0/791
9	sq	0.18	0/856	0.32	0/1143
10	ss	0.24	0/1121	0.33	0/1503
11	st	0.20	0/637	0.26	0/852
12	su	0.20	0/1181	0.33	0/1584
13	sv	0.22	0/1271	0.29	0/1708
14	sw	0.22	0/772	0.40	0/1039
All	All	0.35	12/23851 (0.1%)	0.52	36/34444 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	sG	0	1
9	sq	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	sa	1585	U	O3'-P	-11.42	1.44	1.61
5	sa	1508	A	O3'-P	-7.01	1.50	1.61
5	sa	1789	C	O3'-P	-6.94	1.50	1.61
5	sa	1787	U	O3'-P	-6.86	1.50	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	sa	1588	C	O3'-P	-6.45	1.51	1.61
5	sa	1586	U	O3'-P	-6.32	1.51	1.61
5	sa	1791	C	O3'-P	-6.26	1.51	1.61
5	sa	1790	C	O3'-P	-6.09	1.52	1.61
5	sa	1595	G	O3'-P	-5.92	1.52	1.61
5	sa	1668	G	O3'-P	-5.82	1.52	1.61
5	sa	1425	A	O3'-P	-5.16	1.53	1.61
5	sa	1509	G	O3'-P	-5.11	1.53	1.61

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	sa	1586	U	C1'-C2'-O2'	-24.88	71.08	108.40
5	sa	1509	G	C1'-C2'-O2'	-20.38	77.83	108.40
5	sa	1788	G	C1'-C2'-O2'	-16.00	84.39	108.40
5	sa	1596	U	C1'-C2'-O2'	-14.86	86.11	108.40
5	sa	1588	C	C1'-C2'-O2'	-14.82	86.18	108.40
5	sa	1786	C	C1'-C2'-O2'	-14.64	86.43	108.40
5	sa	1785	C	C1'-C2'-O2'	-12.42	89.77	108.40
5	sa	1589	U	C1'-C2'-O2'	-12.04	90.34	108.40
5	sa	1596	U	C3'-C2'-O2'	-10.38	95.13	110.70
5	sa	1587	A	C1'-C2'-O2'	-10.10	93.25	108.40
5	sa	1667	U	C2'-C3'-O3'	-9.56	99.36	113.70
5	sa	1790	C	C1'-C2'-O2'	-9.21	94.58	108.40
5	sa	1508	A	C4'-C3'-O3'	-9.17	99.25	113.00
5	sa	1790	C	C3'-C2'-O2'	8.99	124.19	110.70
5	sa	1507	A	C1'-C2'-O2'	-8.87	95.10	108.40
5	sa	1792	U	C3'-C2'-O2'	-8.50	97.95	110.70
5	sa	1789	C	C1'-C2'-O2'	-8.42	95.77	108.40
5	sa	1786	C	C2'-C3'-O3'	-7.20	102.89	113.70
5	sa	1509	G	C2'-C3'-O3'	-7.15	102.98	113.70
5	sa	1791	C	C4'-C3'-O3'	-6.96	102.56	113.00
5	sa	1667	U	C1'-C2'-O2'	-6.53	98.61	108.40
5	sa	1668	G	C2'-C3'-O3'	-6.41	104.08	113.70
5	sa	1789	C	C4'-C3'-O3'	-6.29	103.56	113.00
5	sa	1507	A	C2'-C3'-O3'	-6.19	104.42	113.70
5	sa	1791	C	C2'-C3'-O3'	6.05	122.78	113.70
5	sa	1395	A	C4'-C3'-O3'	-6.03	103.95	113.00
5	sa	1589	U	C3'-C2'-O2'	-5.60	102.30	110.70
5	sa	1588	C	C2'-C3'-O3'	-5.52	105.42	113.70
5	sa	1785	C	O4'-C4'-C3'	-5.50	98.50	104.00
5	sa	1793	U	C1'-C2'-O2'	5.43	116.55	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	sa	1586	U	C2'-C3'-O3'	-5.41	105.59	113.70
5	sa	1788	G	O4'-C4'-C3'	-5.39	98.61	104.00
5	sa	1669	A	C4'-C3'-O3'	5.24	117.25	109.40
5	sa	1586	U	C3'-C2'-O2'	5.15	118.42	110.70
5	sa	1596	U	C2'-C3'-O3'	-5.08	106.08	113.70
5	sa	1587	A	O5'-P-OP1	-5.04	92.89	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	sG	31	ASP	Peptide
9	sq	111	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	sA	554	0	609	11	0
2	sD	468	0	500	11	0
3	sE	442	0	444	17	0
4	sG	1395	0	1380	66	0
5	sa	10153	0	5105	261	0
6	sd	1656	0	1753	45	0
7	sg	1463	0	1526	27	0
8	sl	579	0	612	16	0
9	sq	842	0	913	36	0
10	ss	1104	0	1185	28	0
11	st	629	0	676	19	0
12	su	1163	0	1202	39	0
13	sv	1245	0	1285	40	0
14	sw	763	0	826	20	0
All	All	22456	0	18016	562	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 (562) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:1668:G:C8	5:sa:1668:G:H5'	1.97	1.00
5:sa:1750:G:N2	5:sa:1776:G:O2'	2.05	0.89
5:sa:1668:G:H2'	5:sa:1669:A:H5'	1.59	0.84
4:sG:203:THR:HG21	4:sG:248:GLN:HA	1.59	0.82
5:sa:1667:U:H2'	5:sa:1668:G:C8	2.17	0.79
5:sa:1172:G:H2'	5:sa:1173:A:H8	1.49	0.78
3:sE:14:TYR:HB3	5:sa:1763:A:C8	2.19	0.77
12:su:70:ASP:OD1	12:su:74:ASN:ND2	2.18	0.76
9:sq:111:LEU:O	9:sq:113:HIS:N	2.19	0.74
5:sa:1383:C:H5	5:sa:1389:G:H1	1.32	0.74
5:sa:1784:C:H4'	5:sa:1785:C:OP1	1.85	0.73
7:sg:99:PHE:HA	7:sg:102:ILE:HD12	1.71	0.73
2:sD:36:MET:SD	2:sD:36:MET:N	2.55	0.73
14:sw:35:LEU:HD21	14:sw:106:VAL:HG12	1.71	0.73
5:sa:1441:C:O2'	5:sa:1442:A:O5'	2.07	0.73
5:sa:1364:C:O2'	5:sa:1366:A:N7	2.21	0.72
9:sq:77:THR:HG22	9:sq:79:CYS:H	1.53	0.72
10:ss:35:CYS:SG	10:ss:36:LEU:N	2.63	0.72
10:ss:141:ALA:O	10:ss:143:LYS:NZ	2.22	0.72
5:sa:1792:U:O5'	5:sa:1792:U:H6	1.73	0.72
5:sa:1760:G:OP2	5:sa:1762:C:N4	2.22	0.71
5:sa:1507:A:H5''	5:sa:1507:A:H8	1.54	0.71
5:sa:1198:C:OP1	12:su:131:ARG:NH2	2.24	0.71
14:sw:116:MET:HE2	14:sw:116:MET:HA	1.73	0.71
5:sa:1717:U:O4	9:sq:39:ARG:NH2	2.23	0.71
7:sg:195:LYS:NZ	7:sg:199:GLU:OE2	2.24	0.70
13:sv:43:CYS:SG	13:sv:94:THR:OG1	2.49	0.70
5:sa:1669:A:O2'	5:sa:1670:A:O5'	2.10	0.70
5:sa:1776:G:OP1	7:sg:53:HIS:NE2	2.23	0.70
12:su:36:GLY:HA3	12:su:100:ILE:HA	1.75	0.69
8:sl:56:GLU:HG3	8:sl:65:TRP:HE1	1.57	0.69
3:sE:17:GLY:O	3:sE:27:ARG:NH2	2.21	0.69
7:sg:22:ASN:ND2	13:sv:152:MET:SD	2.66	0.68
4:sG:14:GLU:OE2	4:sG:305:LYS:NZ	2.26	0.68
5:sa:1391:C:H2'	5:sa:1392:A:H8	1.59	0.68
11:st:43:THR:HG22	11:st:46:LEU:H	1.59	0.68
5:sa:1668:G:N2	5:sa:1669:A:C4	2.62	0.68
6:sd:107:ALA:HB1	6:sd:110:LEU:HB2	1.76	0.67
5:sa:1441:C:HO2'	5:sa:1442:A:H8	1.40	0.67
5:sa:1593:G:O6	5:sa:1594:A:N6	2.27	0.67
10:ss:57:PRO:HA	10:ss:60:ARG:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:sE:41:ARG:NH2	5:sa:1224:G:OP2	2.27	0.67
5:sa:1581:G:H2'	5:sa:1582:G:H8	1.59	0.67
5:sa:1596:U:C4	5:sa:1680:G:C6	2.81	0.67
5:sa:1312:A:N1	5:sa:1353:G:O2'	2.27	0.67
4:sG:92:LEU:HB2	4:sG:106:PHE:HB2	1.77	0.67
9:sq:36:LEU:O	9:sq:41:ARG:NH2	2.28	0.67
13:sv:28:LYS:HE3	13:sv:111:MET:HB3	1.75	0.67
6:sd:52:GLU:OE1	6:sd:54:ARG:NH2	2.28	0.66
5:sa:1722:A:OP1	9:sq:43:SER:OG	2.13	0.66
1:sA:44:LEU:HD12	5:sa:1701:U:H5'	1.76	0.66
5:sa:1441:C:O2'	5:sa:1442:A:H8	1.78	0.66
5:sa:1267:A:OP1	9:sq:58:LYS:NZ	2.28	0.66
4:sG:99:LYS:HD2	4:sG:99:LYS:O	1.96	0.65
5:sa:1251:A:O2'	5:sa:1281:A:N1	2.29	0.65
2:sD:60:GLU:HG3	2:sD:63:ARG:HD3	1.77	0.65
5:sa:1437:G:N7	11:st:44:LYS:NZ	2.43	0.65
10:ss:98:GLN:HE22	10:ss:134:ALA:HA	1.62	0.65
5:sa:1394:A:C4	5:sa:1395:A:C8	2.85	0.65
13:sv:115:ALA:N	13:sv:122:SER:O	2.30	0.65
5:sa:1586:U:OP1	13:sv:57:ARG:NE	2.29	0.65
6:sd:54:ARG:HG3	14:sw:108:PRO:HG3	1.77	0.65
13:sv:97:SER:O	13:sv:101:ASN:ND2	2.29	0.65
6:sd:21:ARG:HA	6:sd:21:ARG:HH11	1.62	0.65
4:sG:125:ILE:O	4:sG:137:TRP:N	2.31	0.64
13:sv:105:LEU:HD13	13:sv:121:ARG:HD2	1.79	0.64
1:sA:76:ARG:HB2	1:sA:77:MET:HE2	1.78	0.64
2:sD:49:PRO:HD3	5:sa:1780:A:H5'	1.78	0.64
4:sG:138:ASN:HD21	4:sG:140:VAL:HG12	1.63	0.64
5:sa:1387:A:O2'	5:sa:1388:A:O4'	2.15	0.64
6:sd:4:LEU:HD12	8:sl:37:PRO:HB3	1.80	0.63
5:sa:1284:U:N3	5:sa:1285:A:N7	2.47	0.63
2:sD:60:GLU:N	2:sD:60:GLU:OE1	2.32	0.63
4:sG:104:ARG:NH1	4:sG:140:VAL:O	2.32	0.63
5:sa:1789:C:H5''	5:sa:1789:C:H6	1.62	0.63
5:sa:1587:A:C2	5:sa:1693:A:C2	2.87	0.63
4:sG:73:ASP:OD2	4:sG:116:VAL:N	2.30	0.62
4:sG:37:SER:OG	4:sG:38:ARG:N	2.32	0.62
4:sG:303:ASP:OD1	4:sG:303:ASP:N	2.33	0.62
6:sd:140:ILE:HD13	6:sd:202:ILE:HD11	1.80	0.62
7:sg:127:SER:OG	7:sg:138:ARG:NH1	2.33	0.62
10:ss:41:LYS:NZ	13:sv:1:MET:SD	2.61	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:su:96:ASP:OD1	12:su:97:SER:N	2.33	0.62
7:sg:54:THR:OG1	7:sg:72:GLU:OE1	2.17	0.62
5:sa:1667:U:P	13:sv:121:ARG:HH22	2.23	0.62
5:sa:1699:C:H4'	5:sa:1705:A:N6	2.14	0.62
12:su:87:ARG:HB3	12:su:97:SER:HA	1.81	0.62
5:sa:1761:U:H3	5:sa:1766:A:H2	1.47	0.61
5:sa:1308:U:OP2	5:sa:1309:C:O2'	2.13	0.61
5:sa:1712:A:O2'	5:sa:1713:A:OP1	2.16	0.61
4:sG:25:VAL:HG22	4:sG:33:LEU:HD13	1.82	0.61
5:sa:1581:G:H2'	5:sa:1582:G:C8	2.34	0.61
13:sv:108:LEU:HA	13:sv:111:MET:HE3	1.82	0.61
5:sa:1668:G:C8	5:sa:1668:G:C5'	2.79	0.61
5:sa:1671:A:N3	5:sa:1729:G:O2'	2.24	0.61
5:sa:1196:A:H2'	5:sa:1197:G:H8	1.66	0.60
5:sa:1516:G:N2	5:sa:1519:G:OP2	2.32	0.60
5:sa:1719:G:N7	9:sq:46:ARG:NH1	2.49	0.60
5:sa:1722:A:OP1	9:sq:114:TYR:OH	2.19	0.60
13:sv:85:ASN:HB3	13:sv:91:SER:HB3	1.83	0.60
14:sw:33:GLU:OE2	14:sw:87:ARG:NE	2.24	0.60
10:ss:37:CYS:SG	10:ss:78:LEU:HD22	2.42	0.60
4:sG:177:ASN:ND2	4:sG:198:THR:O	2.35	0.59
5:sa:1596:U:C5	5:sa:1680:G:C6	2.91	0.59
5:sa:1578:A:OP1	7:sg:166:ARG:NH1	2.35	0.59
4:sG:159:VAL:HG12	4:sG:172:SER:HB2	1.85	0.59
1:sA:80:THR:HG22	1:sA:82:SER:H	1.68	0.59
4:sG:73:ASP:OD1	4:sG:74:LEU:N	2.35	0.59
12:su:90:ASP:OD2	12:su:107:ARG:NH2	2.36	0.59
12:su:97:SER:OG	12:su:98:GLN:N	2.35	0.59
4:sG:26:ALA:HB2	4:sG:76:LEU:HD13	1.84	0.59
6:sd:35:LEU:HD13	6:sd:87:LEU:HD11	1.83	0.59
13:sv:30:GLU:OE2	13:sv:103:TYR:OH	2.16	0.59
5:sa:1589:U:H3'	5:sa:1589:U:H6	1.67	0.59
5:sa:1756:U:OP1	13:sv:91:SER:OG	2.20	0.59
5:sa:1172:G:H2'	5:sa:1173:A:C8	2.34	0.59
5:sa:1341:C:O2'	11:st:10:LYS:NZ	2.36	0.58
5:sa:1439:C:H2'	5:sa:1440:A:H4'	1.85	0.58
5:sa:1322:G:N2	5:sa:1325:A:OP2	2.34	0.58
6:sd:49:SER:O	6:sd:49:SER:OG	2.20	0.58
5:sa:1668:G:C2	5:sa:1669:A:C8	2.91	0.58
12:su:118:MET:HE3	12:su:120:ALA:HB2	1.85	0.58
5:sa:1586:U:P	13:sv:57:ARG:HH21	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:ss:109:GLN:HB2	10:ss:117:LYS:HD2	1.86	0.58
4:sG:26:ALA:HB1	4:sG:80:GLY:HA2	1.84	0.58
5:sa:1661:C:H2'	5:sa:1662:G:H8	1.68	0.57
5:sa:1298:G:H4'	5:sa:1299:C:H5'	1.85	0.57
5:sa:1174:C:H2'	5:sa:1175:G:C8	2.40	0.57
5:sa:1579:A:H4'	5:sa:1580:U:H5'	1.87	0.57
12:su:73:ASN:O	12:su:98:GLN:NE2	2.34	0.57
4:sG:112:ASP:OD2	4:sG:130:ARG:NE	2.35	0.57
4:sG:152:HIS:HE2	4:sG:172:SER:HG	1.49	0.57
5:sa:1441:C:C2	5:sa:1442:A:C8	2.92	0.57
5:sa:1510:A:OP1	11:st:3:GLY:N	2.38	0.57
5:sa:1668:G:C2'	5:sa:1669:A:H5'	2.33	0.57
5:sa:1690:A:O2'	5:sa:1691:A:H8	1.87	0.56
6:sd:34:GLU:OE1	8:sl:59:ASN:ND2	2.38	0.56
10:ss:50:PRO:HD2	10:ss:53:LEU:HD12	1.87	0.56
14:sw:50:VAL:HA	14:sw:91:MET:HE1	1.87	0.56
5:sa:1589:U:H3'	5:sa:1589:U:C6	2.40	0.56
14:sw:101:ILE:HG22	14:sw:103:SER:H	1.69	0.56
4:sG:67:HIS:NE2	4:sG:93:ARG:HB2	2.21	0.56
5:sa:1586:U:H2'	5:sa:1587:A:O5'	2.05	0.56
5:sa:1587:A:H5''	5:sa:1588:C:OP2	2.04	0.56
6:sd:122:LYS:NZ	6:sd:135:SER:OG	2.39	0.56
4:sG:34:VAL:HG21	4:sG:97:LEU:HD21	1.88	0.56
12:su:81:PRO:HG2	12:su:84:PHE:HB2	1.86	0.56
2:sD:29:LEU:HD22	2:sD:50:ILE:HG22	1.88	0.56
5:sa:1188:A:N3	5:sa:1779:U:O2'	2.32	0.56
5:sa:1719:G:N1	5:sa:1722:A:OP2	2.39	0.56
5:sa:1712:A:H2'	5:sa:1713:A:C8	2.41	0.55
5:sa:1669:A:O2'	5:sa:1670:A:P	2.65	0.55
4:sG:23:ILE:HG23	4:sG:33:LEU:HD11	1.88	0.55
5:sa:1196:A:H2'	5:sa:1197:G:C8	2.41	0.55
6:sd:45:ALA:O	6:sd:68:ARG:NH1	2.39	0.55
14:sw:94:THR:OG1	14:sw:97:THR:OG1	2.22	0.55
4:sG:19:ALA:HB3	4:sG:38:ARG:HD2	1.87	0.55
5:sa:1287:U:H2'	5:sa:1288:G:C8	2.40	0.55
5:sa:1509:G:O5'	11:st:4:VAL:HG23	2.06	0.55
5:sa:1566:C:H5'	12:su:130:LEU:HD22	1.88	0.55
5:sa:1324:G:H2'	5:sa:1325:A:C8	2.42	0.55
5:sa:1596:U:C5	5:sa:1680:G:O6	2.60	0.55
5:sa:1232:U:H3	5:sa:1563:C:H5	1.55	0.55
5:sa:1277:C:H2'	5:sa:1278:A:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:1543:A:OP2	6:sd:41:ARG:NH2	2.35	0.55
5:sa:1595:G:O2'	5:sa:1661:C:O2	2.25	0.55
6:sd:43:LEU:HD11	6:sd:83:LEU:HD11	1.88	0.54
4:sG:34:VAL:HG12	4:sG:74:LEU:HD11	1.89	0.54
5:sa:1223:G:OP1	5:sa:1224:G:O2'	2.20	0.54
2:sD:33:CYS:N	2:sD:42:ILE:O	2.41	0.54
4:sG:99:LYS:HE3	4:sG:101:GLU:HB3	1.88	0.54
5:sa:1195:G:C2	5:sa:1196:A:C8	2.95	0.54
5:sa:1244:A:O2'	8:sl:47:GLY:HA2	2.06	0.54
4:sG:248:GLN:HG2	4:sG:288:ILE:HG22	1.88	0.54
5:sa:1590:A:N3	5:sa:1773:G:O2'	2.32	0.54
5:sa:1667:U:H2'	5:sa:1668:G:N7	2.22	0.54
5:sa:1669:A:H2'	5:sa:1669:A:OP2	2.07	0.54
6:sd:120:LYS:HG3	6:sd:189:VAL:HB	1.90	0.54
5:sa:1589:U:C6	5:sa:1589:U:C3'	2.91	0.54
12:su:85:LEU:HG	12:su:97:SER:HB3	1.90	0.54
5:sa:1395:A:H5'	5:sa:1396:A:OP2	2.08	0.53
5:sa:1396:A:C2	5:sa:1425:A:C5	2.95	0.53
5:sa:1396:A:N1	5:sa:1425:A:C6	2.75	0.53
12:su:72:LEU:HB3	12:su:100:ILE:HD13	1.90	0.53
10:ss:52:ASP:OD2	13:sv:2:HIS:NE2	2.35	0.53
13:sv:65:VAL:HG11	13:sv:114:VAL:HG12	1.90	0.53
5:sa:1389:G:H2'	5:sa:1390:A:H8	1.74	0.53
5:sa:1396:A:C6	5:sa:1425:A:N6	2.77	0.53
5:sa:1507:A:H8	5:sa:1507:A:C5'	2.22	0.53
5:sa:1585:U:OP1	13:sv:40:THR:OG1	2.20	0.53
6:sd:94:PRO:HD2	6:sd:97:LYS:HD3	1.90	0.53
6:sd:49:SER:OG	6:sd:111:CYS:SG	2.45	0.53
13:sv:119:SER:O	13:sv:119:SER:OG	2.20	0.53
4:sG:284:ALA:O	4:sG:302:VAL:HG13	2.09	0.53
5:sa:1507:A:H5''	5:sa:1507:A:C8	2.40	0.53
5:sa:1709:A:H2'	5:sa:1710:U:O4'	2.09	0.53
7:sg:53:HIS:HB2	7:sg:92:MET:SD	2.49	0.53
3:sE:4:TYR:HB3	6:sd:2:PHE:CD1	2.44	0.53
4:sG:300:GLY:HA2	4:sG:306:ILE:HA	1.90	0.53
5:sa:1442:A:H2'	5:sa:1443:U:H6	1.73	0.53
4:sG:73:ASP:O	4:sG:86:SER:N	2.40	0.53
6:sd:37:GLU:OE1	8:sl:60:TRP:NE1	2.35	0.53
11:st:25:THR:OG1	11:st:26:LEU:N	2.42	0.53
4:sG:29:LYS:HB3	4:sG:30:PRO:HD3	1.91	0.52
5:sa:1513:A:H2'	5:sa:1514:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:1588:C:C3'	5:sa:1588:C:C6	2.92	0.52
8:sl:56:GLU:HG3	8:sl:65:TRP:NE1	2.24	0.52
10:ss:22:VAL:HG22	10:ss:37:CYS:HB3	1.91	0.52
3:sE:52:PHE:HB3	14:sw:80:TYR:HB3	1.91	0.52
5:sa:1363:C:H1'	5:sa:1517:A:C4	2.44	0.52
5:sa:1391:C:H2'	5:sa:1392:A:C8	2.41	0.52
5:sa:1595:G:OP1	6:sd:23:HIS:NE2	2.32	0.52
6:sd:13:ASP:HB2	6:sd:27:ALA:HB1	1.90	0.52
5:sa:1343:G:H2'	5:sa:1344:G:C8	2.45	0.52
3:sE:56:ASP:OD1	3:sE:56:ASP:N	2.42	0.52
9:sq:56:VAL:HA	9:sq:59:LEU:HB2	1.90	0.52
4:sG:156:VAL:HA	4:sG:174:GLY:HA2	1.92	0.52
5:sa:1431:U:H4'	14:sw:57:PRO:HG3	1.92	0.52
5:sa:1776:G:H5''	7:sg:88:LYS:HB2	1.91	0.52
13:sv:6:ASN:OD1	13:sv:6:ASN:N	2.42	0.52
5:sa:1183:A:C4	5:sa:1788:G:N2	2.78	0.52
5:sa:1731:U:OP1	12:su:40:ARG:NE	2.43	0.52
6:sd:60:PHE:HD2	6:sd:93:PHE:HE1	1.57	0.52
11:st:6:THR:HG22	11:st:7:LYS:H	1.74	0.52
12:su:87:ARG:HB2	12:su:99:LEU:HD12	1.92	0.52
1:sA:88:LEU:HD13	1:sA:97:ILE:HD12	1.91	0.51
4:sG:30:PRO:O	4:sG:31:ASP:HB2	2.09	0.51
5:sa:1310:U:C2	5:sa:1311:U:H5	2.28	0.51
5:sa:1395:A:H2'	5:sa:1396:A:C8	2.45	0.51
6:sd:59:LYS:HA	6:sd:97:LYS:HB2	1.91	0.51
5:sa:1438:A:N6	5:sa:1518:A:N7	2.59	0.51
5:sa:1758:G:H2'	5:sa:1759:A:H8	1.76	0.51
4:sG:18:GLY:O	4:sG:304:LYS:HG3	2.11	0.51
5:sa:1567:A:OP2	12:su:145:ARG:NH2	2.26	0.51
6:sd:36:ASN:OD1	6:sd:48:TYR:OH	2.12	0.51
5:sa:1680:G:H1'	5:sa:1685:C:O2	2.11	0.51
5:sa:1701:U:O2'	5:sa:1702:G:O5'	2.29	0.51
5:sa:1704:C:O2'	12:su:25:ARG:NH2	2.44	0.51
5:sa:1730:U:H2'	5:sa:1731:U:C6	2.46	0.51
6:sd:53:VAL:HG12	6:sd:53:VAL:O	2.12	0.50
2:sD:16:THR:OG1	2:sD:32:ARG:O	2.19	0.50
5:sa:1720:G:O2'	9:sq:49:LYS:HE2	2.11	0.50
5:sa:1725:A:H5''	12:su:134:GLY:HA3	1.94	0.50
5:sa:1573:G:O2'	5:sa:1768:C:OP1	2.28	0.50
12:su:87:ARG:NE	12:su:90:ASP:OD1	2.41	0.50
5:sa:1668:G:N2	5:sa:1669:A:N9	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:sG:15:GLY:O	4:sG:43:MET:HE2	2.11	0.50
9:sq:32:PHE:HZ	9:sq:111:LEU:HD13	1.77	0.50
5:sa:1185:A:H2'	5:sa:1186:C:C6	2.46	0.50
9:sq:61:LYS:HA	9:sq:64:LYS:HD2	1.92	0.50
5:sa:1227:A:N6	5:sa:1564:C:O5'	2.43	0.49
5:sa:1437:G:OP1	11:st:32:LYS:NZ	2.31	0.49
7:sg:25:SER:OG	7:sg:26:TYR:N	2.43	0.49
9:sq:52:HIS:NE2	9:sq:81:ASP:OD1	2.37	0.49
12:su:24:ARG:O	12:su:56:ARG:NH1	2.33	0.49
13:sv:74:MET:HA	13:sv:77:ARG:HB2	1.94	0.49
14:sw:26:SER:HB3	14:sw:32:VAL:HG13	1.94	0.49
5:sa:1279:U:H2'	5:sa:1280:G:C8	2.48	0.49
5:sa:1698:A:H4'	12:su:54:ASN:HD21	1.77	0.49
7:sg:120:ASN:ND2	7:sg:183:SER:O	2.46	0.49
10:ss:54:ILE:HG22	10:ss:56:PRO:HD2	1.95	0.49
4:sG:21:THR:O	4:sG:287:SER:HB2	2.12	0.49
11:st:5:ARG:HB2	11:st:10:LYS:HE3	1.95	0.49
2:sD:15:VAL:HG22	2:sD:31:VAL:HG21	1.95	0.49
4:sG:93:ARG:NH1	4:sG:102:SER:OG	2.45	0.49
6:sd:220:ASP:OD1	6:sd:221:VAL:N	2.45	0.49
12:su:34:ILE:HG22	12:su:36:GLY:H	1.77	0.49
5:sa:1284:U:C2	5:sa:1285:A:N7	2.80	0.49
5:sa:1734:G:H4'	5:sa:1735:A:O5'	2.11	0.49
9:sq:109:GLU:N	9:sq:109:GLU:OE1	2.45	0.49
4:sG:72:SER:HB3	4:sG:88:TRP:HE1	1.78	0.49
4:sG:219:ASP:OD1	4:sG:219:ASP:N	2.44	0.49
5:sa:1262:G:H2'	5:sa:1263:A:H8	1.76	0.49
4:sG:119:SER:HB3	4:sG:161:PHE:CE2	2.48	0.49
1:sA:76:ARG:HB2	1:sA:77:MET:CE	2.43	0.49
3:sE:2:GLY:N	5:sa:1259:A:OP1	2.46	0.49
1:sA:82:SER:OG	5:sa:1700:A:OP2	2.27	0.48
13:sv:45:GLU:N	13:sv:45:GLU:OE1	2.46	0.48
5:sa:1596:U:O4	5:sa:1680:G:C5	2.65	0.48
5:sa:1376:U:H2'	5:sa:1377:U:C6	2.48	0.48
10:ss:69:ILE:HG22	10:ss:70:VAL:HG13	1.95	0.48
5:sa:1580:U:O2'	7:sg:84:ASN:OD1	2.25	0.48
5:sa:1661:C:H2'	5:sa:1662:G:C8	2.47	0.48
5:sa:1789:C:H5''	5:sa:1789:C:C6	2.46	0.48
4:sG:74:LEU:HA	4:sG:85:SER:HA	1.94	0.48
5:sa:1376:U:H2'	5:sa:1377:U:H6	1.79	0.48
5:sa:1669:A:OP2	5:sa:1669:A:H8	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:sg:30:VAL:HB	7:sg:36:LYS:HD2	1.96	0.48
9:sq:105:GLU:HG2	9:sq:107:LYS:HD3	1.95	0.48
14:sw:24:ILE:HG13	14:sw:32:VAL:HG12	1.96	0.48
2:sD:11:ILE:HD11	2:sD:61:ALA:HB2	1.96	0.48
5:sa:1669:A:N3	5:sa:1671:A:OP2	2.46	0.48
10:ss:45:ARG:HH11	10:ss:45:ARG:HG2	1.78	0.48
5:sa:1196:A:O2'	5:sa:1736:A:N3	2.41	0.48
5:sa:1793:U:H6	5:sa:1793:U:C5'	2.27	0.48
7:sg:79:MET:O	7:sg:79:MET:HG2	2.14	0.48
9:sq:80:ARG:HH12	9:sq:119:SER:HB3	1.79	0.48
5:sa:1254:G:N2	5:sa:1280:G:O2'	2.46	0.48
5:sa:1712:A:HO2'	5:sa:1713:A:P	2.33	0.48
7:sg:80:GLN:O	7:sg:84:ASN:ND2	2.44	0.48
14:sw:50:VAL:HG12	14:sw:91:MET:HE1	1.95	0.48
5:sa:1282:U:H2'	5:sa:1283:U:H5'	1.96	0.47
5:sa:1425:A:H2'	5:sa:1425:A:N3	2.29	0.47
1:sa:52:LYS:HG2	12:su:4:VAL:HG11	1.96	0.47
5:sa:1721:A:O2'	9:sq:81:ASP:OD2	2.25	0.47
2:sD:66:ARG:HD2	2:sD:66:ARG:HA	1.70	0.47
3:sE:21:CYS:HB2	3:sE:39:CYS:HB3	1.96	0.47
4:sG:106:PHE:CE2	4:sG:141:GLY:HA2	2.50	0.47
5:sa:1183:A:C6	5:sa:1788:G:N1	2.83	0.47
5:sa:1668:G:N1	5:sa:1669:A:C5	2.82	0.47
5:sa:1756:U:H2'	5:sa:1757:C:C6	2.49	0.47
4:sG:36:GLY:HA3	4:sG:71:ILE:HG21	1.96	0.47
5:sa:1340:U:OP1	5:sa:1353:G:N2	2.47	0.47
5:sa:1396:A:O3'	5:sa:1425:A:P	2.72	0.47
5:sa:1566:C:OP1	12:su:125:ARG:NH2	2.30	0.47
9:sq:52:HIS:HB3	9:sq:82:LYS:HD3	1.96	0.47
13:sv:73:VAL:HG21	13:sv:102:ARG:HG3	1.96	0.47
3:sE:4:TYR:HB3	6:sd:2:PHE:HD1	1.77	0.47
5:sa:1587:A:C8	5:sa:1587:A:H3'	2.50	0.47
5:sa:1708:G:N2	5:sa:1735:A:OP2	2.46	0.47
7:sg:35:LEU:HD21	7:sg:148:ARG:HH11	1.80	0.47
12:su:116:LYS:HB2	12:su:116:LYS:HE3	1.72	0.47
13:sv:26:SER:HB3	13:sv:28:LYS:HD3	1.95	0.47
5:sa:1208:A:N3	5:sa:1235:C:O2'	2.46	0.47
5:sa:1353:G:OP1	6:sd:174:SER:N	2.48	0.47
5:sa:1588:C:C6	5:sa:1588:C:H3'	2.49	0.47
6:sd:111:CYS:HB3	6:sd:114:SER:OG	2.15	0.47
5:sa:1775:U:H5'	10:ss:90:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:sg:20:LEU:HD21	7:sg:71:VAL:HG11	1.97	0.47
3:sE:14:TYR:OH	5:sa:1719:G:O3'	2.22	0.46
11:st:32:LYS:HB2	11:st:32:LYS:HE3	1.79	0.46
5:sa:1204:G:H21	5:sa:1567:A:H62	1.62	0.46
6:sd:2:PHE:HB2	6:sd:4:LEU:HG	1.97	0.46
4:sG:136:LEU:HD13	4:sG:145:ALA:HB3	1.98	0.46
5:sa:1309:C:H1'	5:sa:1310:U:OP2	2.15	0.46
9:sq:59:LEU:HD23	9:sq:59:LEU:HA	1.79	0.46
5:sa:1183:A:C6	5:sa:1788:G:C2	3.03	0.46
7:sg:39:LEU:HB3	7:sg:41:ILE:HD11	1.97	0.46
7:sg:30:VAL:HG13	7:sg:119:ILE:HD11	1.97	0.46
7:sg:108:LYS:HB3	7:sg:108:LYS:HE2	1.71	0.46
13:sv:68:ASN:N	13:sv:68:ASN:OD1	2.49	0.46
4:sG:161:PHE:CE1	4:sG:170:PHE:HB3	2.51	0.46
5:sa:1388:A:H2'	5:sa:1389:G:O4'	2.15	0.46
5:sa:1596:U:O2'	5:sa:1660:C:O2	2.28	0.46
6:sd:218:ILE:HG21	11:st:16:ILE:HG12	1.98	0.46
5:sa:1343:G:H5''	11:st:67:ARG:NH1	2.29	0.46
5:sa:1425:A:C8	5:sa:1425:A:H5''	2.51	0.46
5:sa:1565:G:H2'	5:sa:1565:G:N3	2.31	0.46
5:sa:1581:G:C2	5:sa:1582:G:C5	3.04	0.46
13:sv:112:GLY:O	13:sv:124:THR:OG1	2.33	0.46
10:ss:28:LYS:HG3	10:ss:29:LYS:H	1.81	0.45
13:sv:126:GLU:CD	13:sv:126:GLU:H	2.23	0.45
10:ss:75:TYR:HA	10:ss:78:LEU:HD12	1.97	0.45
5:sa:1233:A:H5''	5:sa:1234:C:OP2	2.16	0.45
5:sa:1669:A:HO2'	5:sa:1670:A:P	2.36	0.45
5:sa:1759:A:H2'	5:sa:1760:G:H8	1.81	0.45
6:sd:60:PHE:CD2	6:sd:93:PHE:HE1	2.32	0.45
3:sE:34:TYR:OH	5:sa:1594:A:OP1	2.25	0.45
5:sa:1426:C:O2'	5:sa:1427:U:H5'	2.17	0.45
13:sv:77:ARG:HD2	13:sv:98:GLY:HA2	1.98	0.45
4:sG:34:VAL:HG22	4:sG:44:VAL:HG22	1.98	0.45
4:sG:81:GLN:O	4:sG:97:LEU:N	2.33	0.45
5:sa:1182:C:H2'	5:sa:1183:A:H8	1.82	0.45
8:sl:45:MET:HE2	8:sl:45:MET:HB2	1.87	0.45
12:su:107:ARG:HD2	12:su:107:ARG:HA	1.51	0.45
14:sw:20:ILE:HG22	14:sw:91:MET:HB2	1.98	0.45
4:sG:153:SER:N	4:sG:176:ASP:OD2	2.50	0.45
5:sa:1396:A:N6	5:sa:1425:A:N6	2.65	0.45
5:sa:1709:A:C2	5:sa:1735:A:C8	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:sG:102:SER:OG	4:sG:102:SER:O	2.29	0.45
9:sq:56:VAL:O	9:sq:60:LEU:HG	2.17	0.45
14:sw:55:ARG:HG2	14:sw:87:ARG:NH1	2.31	0.45
4:sG:137:TRP:HA	4:sG:143:CYS:HA	1.98	0.44
9:sq:82:LYS:O	9:sq:115:LEU:HB2	2.16	0.44
5:sa:1245:C:H2'	5:sa:1246:A:C8	2.52	0.44
5:sa:1261:A:H2'	5:sa:1262:G:H8	1.82	0.44
5:sa:1390:A:O2'	13:sv:6:ASN:ND2	2.51	0.44
5:sa:1394:A:H2'	5:sa:1395:A:O4'	2.17	0.44
5:sa:1691:A:H3'	5:sa:1692:G:H8	1.83	0.44
6:sd:133:VAL:HG11	6:sd:166:PHE:CD2	2.52	0.44
7:sg:51:LEU:HD23	7:sg:51:LEU:HA	1.80	0.44
3:sE:14:TYR:HB3	5:sa:1763:A:H8	1.74	0.44
7:sg:83:LYS:HB2	7:sg:83:LYS:HE3	1.56	0.44
5:sa:1662:G:O2'	5:sa:1687:C:N4	2.50	0.44
5:sa:1756:U:H2'	5:sa:1757:C:H6	1.82	0.44
9:sq:97:ASN:OD1	9:sq:98:GLY:N	2.46	0.44
12:su:85:LEU:HD23	12:su:96:ASP:HA	1.99	0.44
3:sE:22:ARG:NH1	3:sE:36:LEU:O	2.50	0.44
4:sG:157:SER:N	4:sG:173:ALA:O	2.51	0.44
12:su:116:LYS:HE2	12:su:127:TYR:HB2	1.99	0.44
5:sa:1439:C:O2'	5:sa:1440:A:OP1	2.33	0.44
10:ss:65:GLU:O	10:ss:69:ILE:HG13	2.17	0.44
5:sa:1245:C:H2'	5:sa:1246:A:H8	1.82	0.44
9:sq:19:LYS:HD2	9:sq:35:MET:HE1	1.99	0.44
5:sa:1757:C:H2'	5:sa:1758:G:H8	1.83	0.44
7:sg:16:PHE:CE2	7:sg:18:PRO:HG3	2.53	0.44
13:sv:46:LEU:HA	13:sv:46:LEU:HD23	1.86	0.44
1:sA:45:ASN:O	1:sA:45:ASN:ND2	2.51	0.44
5:sa:1252:A:N6	5:sa:1281:A:O2'	2.51	0.44
5:sa:1346:A:H4'	5:sa:1347:A:O5'	2.18	0.44
13:sv:66:TYR:HA	13:sv:123:LEU:HD11	1.98	0.44
3:sE:15:GLY:O	3:sE:19:ARG:NH2	2.51	0.43
4:sG:152:HIS:NE2	4:sG:172:SER:OG	2.34	0.43
5:sa:1185:A:H2'	5:sa:1186:C:H6	1.81	0.43
5:sa:1284:U:C2	5:sa:1285:A:C8	3.06	0.43
5:sa:1319:G:C6	5:sa:1320:G:N7	2.86	0.43
5:sa:1354:A:H2'	5:sa:1355:G:O4'	2.18	0.43
5:sa:1371:U:H5	5:sa:1683:A:N7	2.15	0.43
5:sa:1553:A:O2'	5:sa:1554:C:H5''	2.17	0.43
5:sa:1585:U:O2'	5:sa:1586:U:H5'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:ss:27:LYS:HB2	10:ss:27:LYS:HE3	1.78	0.43
12:su:7:GLU:N	12:su:7:GLU:OE1	2.51	0.43
14:sw:99:LYS:HB3	14:sw:102:THR:HB	2.00	0.43
5:sa:1248:U:H2'	5:sa:1249:A:H8	1.82	0.43
5:sa:1356:A:H61	6:sd:175:GLY:CA	2.31	0.43
5:sa:1439:C:O2	5:sa:1441:C:H5'	2.19	0.43
5:sa:1370:A:N6	5:sa:1427:U:O2'	2.51	0.43
12:su:27:VAL:HG23	12:su:55:LYS:O	2.19	0.43
4:sG:137:TRP:CE3	4:sG:143:CYS:HB2	2.54	0.43
5:sa:1574:C:O2'	13:sv:88:TYR:O	2.26	0.43
5:sa:1691:A:C8	5:sa:1692:G:C8	3.06	0.43
5:sa:1793:U:H6	5:sa:1793:U:H5''	1.82	0.43
11:st:58:MET:HE3	11:st:58:MET:HB3	1.89	0.43
4:sG:41:THR:HG22	4:sG:65:HIS:CE1	2.54	0.43
5:sa:1712:A:H2'	5:sa:1713:A:H8	1.82	0.43
6:sd:164:MET:HE2	6:sd:164:MET:HB3	1.91	0.43
9:sq:28:PRO:HG2	9:sq:31:ASP:HB2	2.00	0.43
12:su:60:MET:HE3	12:su:60:MET:HB2	1.74	0.43
13:sv:84:TYR:CE1	13:sv:86:LYS:HG3	2.54	0.43
3:sE:12:ARG:NH2	5:sa:1558:U:OP1	2.47	0.43
4:sG:142:LYS:HD2	4:sG:142:LYS:HA	1.73	0.43
4:sG:180:LYS:HB2	4:sG:181:THR:HG23	1.99	0.43
5:sa:1284:U:C4	5:sa:1285:A:N7	2.86	0.43
5:sa:1374:G:H2'	5:sa:1375:U:C6	2.54	0.43
9:sq:29:GLU:O	9:sq:33:VAL:HG23	2.18	0.43
9:sq:54:ARG:HE	9:sq:54:ARG:HB3	1.56	0.43
9:sq:106:ILE:HA	9:sq:110:MET:SD	2.59	0.43
11:st:6:THR:HB	11:st:8:THR:HG22	2.00	0.43
5:sa:1382:C:H2'	5:sa:1383:C:O2	2.19	0.43
5:sa:1565:G:OP1	12:su:137:THR:N	2.50	0.43
6:sd:113:VAL:HG22	6:sd:185:ALA:HB2	2.01	0.43
10:ss:28:LYS:O	10:ss:29:LYS:C	2.61	0.43
12:su:64:GLU:N	12:su:64:GLU:OE1	2.52	0.43
1:sA:110:THR:OG1	1:sA:111:ARG:N	2.52	0.43
4:sG:26:ALA:CB	4:sG:80:GLY:HA2	2.47	0.43
4:sG:176:ASP:OD1	4:sG:176:ASP:N	2.51	0.43
10:ss:85:THR:O	10:ss:85:THR:OG1	2.33	0.43
5:sa:1302:G:C4	5:sa:1543:A:C2	3.07	0.43
6:sd:171:MET:HB2	6:sd:171:MET:HE2	1.65	0.43
6:sd:180:GLN:H	6:sd:180:GLN:HG3	1.71	0.43
7:sg:143:VAL:HG13	7:sg:147:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:sv:22:HIS:CG	13:sv:134:ILE:HD11	2.54	0.43
5:sa:1384:U:OP1	13:sv:129:LYS:HE2	2.19	0.43
11:st:48:ASN:O	11:st:52:GLY:N	2.47	0.42
2:sD:51:ARG:HH22	7:sg:66:ILE:HD13	1.83	0.42
4:sG:127:SER:OG	4:sG:137:TRP:NE1	2.49	0.42
5:sa:1268:G:N7	9:sq:54:ARG:HD3	2.35	0.42
8:sl:57:THR:HG23	8:sl:64:TYR:HB2	2.01	0.42
9:sq:85:LEU:O	9:sq:88:MET:HG2	2.19	0.42
4:sG:286:MET:HG3	4:sG:302:VAL:HG12	2.02	0.42
5:sa:1667:U:H2'	5:sa:1668:G:H5'	2.00	0.42
11:st:72:LYS:HB2	11:st:72:LYS:HE2	1.72	0.42
5:sa:1548:C:H2'	5:sa:1549:U:C6	2.54	0.42
6:sd:90:ARG:HB2	8:sl:64:TYR:HE2	1.85	0.42
12:su:18:ASN:ND2	12:su:18:ASN:O	2.53	0.42
5:sa:1433:A:OP1	14:sw:87:ARG:NH2	2.38	0.42
10:ss:37:CYS:HG	10:ss:78:LEU:HD22	1.83	0.42
10:ss:43:MET:HE3	13:sv:3:HIS:HB2	2.00	0.42
12:su:17:CYS:O	12:su:19:THR:HG23	2.20	0.42
13:sv:77:ARG:HB3	13:sv:95:LEU:HD12	2.02	0.42
8:sl:30:LEU:HA	8:sl:37:PRO:HA	2.01	0.42
3:sE:23:LYS:HE3	3:sE:23:LYS:HB2	1.89	0.42
4:sG:138:ASN:ND2	4:sG:140:VAL:HG12	2.33	0.42
4:sG:153:SER:OG	4:sG:176:ASP:OD2	2.33	0.42
5:sa:1253:G:O2'	5:sa:1254:G:OP1	2.31	0.42
5:sa:1425:A:C8	5:sa:1425:A:C5'	3.03	0.42
5:sa:1589:U:H6	5:sa:1589:U:C3'	2.31	0.42
6:sd:142:ASP:OD1	6:sd:142:ASP:N	2.51	0.42
4:sG:111:GLY:H	4:sG:131:ASP:HB2	1.84	0.42
5:sa:1394:A:C2	5:sa:1395:A:C8	3.08	0.42
8:sl:25:LYS:HB3	8:sl:61:ARG:HD2	2.01	0.42
11:st:61:ILE:HD13	11:st:61:ILE:HA	1.94	0.42
5:sa:1283:U:HO2'	5:sa:1284:U:H5	1.68	0.42
5:sa:1668:G:H2'	5:sa:1668:G:N3	2.35	0.42
9:sq:51:LYS:HG3	9:sq:79:CYS:SG	2.60	0.42
13:sv:137:GLN:HA	13:sv:140:LYS:HE3	2.02	0.42
5:sa:1175:G:O2'	5:sa:1177:A:OP1	2.34	0.42
5:sa:1548:C:H2'	5:sa:1549:U:H6	1.85	0.42
5:sa:1596:U:H1'	5:sa:1660:C:O2	2.19	0.42
6:sd:38:LEU:HD13	8:sl:64:TYR:CE1	2.55	0.42
6:sd:205:ASP:O	6:sd:208:PRO:HD2	2.19	0.41
5:sa:1204:G:C6	5:sa:1205:C:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:sq:111:LEU:HD23	9:sq:111:LEU:HA	1.93	0.41
14:sw:28:LYS:HE3	14:sw:28:LYS:HB2	1.90	0.41
4:sG:72:SER:HB3	4:sG:88:TRP:NE1	2.36	0.41
5:sa:1533:C:H3'	5:sa:1534:A:H4'	2.00	0.41
5:sa:1679:G:H21	5:sa:1685:C:H1'	1.85	0.41
11:st:21:TYR:N	11:st:22:PRO:HD2	2.35	0.41
5:sa:1669:A:C2	5:sa:1671:A:OP2	2.74	0.41
12:su:27:VAL:HB	12:su:28:PRO:HD3	2.02	0.41
12:su:70:ASP:OD2	12:su:78:TYR:OH	2.28	0.41
12:su:89:LYS:HA	12:su:95:LYS:HG3	2.01	0.41
4:sG:283:SER:O	4:sG:284:ALA:C	2.63	0.41
5:sa:1391:C:C2	5:sa:1392:A:C8	3.09	0.41
5:sa:1394:A:N3	5:sa:1395:A:C8	2.89	0.41
9:sq:57:LYS:HE2	9:sq:57:LYS:HB3	1.65	0.41
5:sa:1189:G:H2'	5:sa:1190:G:C8	2.56	0.41
5:sa:1300:A:C6	5:sa:1545:G:C5	3.08	0.41
9:sq:59:LEU:HA	9:sq:62:ILE:HD12	2.01	0.41
9:sq:107:LYS:H	9:sq:110:MET:CG	2.34	0.41
4:sG:13:LEU:HD12	4:sG:306:ILE:HD13	2.03	0.41
5:sa:1172:G:C4	5:sa:1173:A:C8	3.09	0.41
5:sa:1182:C:H2'	5:sa:1183:A:C8	2.55	0.41
10:ss:28:LYS:HD2	10:ss:28:LYS:HA	1.73	0.41
14:sw:61:LEU:O	14:sw:81:GLN:HA	2.20	0.41
5:sa:1355:G:H21	11:st:8:THR:HG21	1.86	0.41
5:sa:1387:A:O2'	5:sa:1388:A:C8	2.73	0.41
5:sa:1394:A:O2'	5:sa:1395:A:P	2.78	0.41
5:sa:1440:A:H2	5:sa:1441:C:H41	1.67	0.41
5:sa:1442:A:H2'	5:sa:1443:U:C6	2.54	0.41
5:sa:1789:C:C6	5:sa:1789:C:C5'	3.04	0.41
6:sd:211:LYS:HD2	6:sd:217:ARG:NH1	2.34	0.41
10:ss:63:VAL:O	10:ss:66:PRO:HD2	2.21	0.41
13:sv:77:ARG:O	13:sv:96:GLY:N	2.48	0.41
5:sa:1559:U:O2'	9:sq:78:HIS:ND1	2.45	0.41
5:sa:1596:U:C4	5:sa:1680:G:C5	3.09	0.41
5:sa:1696:G:H2'	5:sa:1696:G:N3	2.36	0.41
5:sa:1699:C:H4'	5:sa:1705:A:H61	1.81	0.41
6:sd:43:LEU:O	6:sd:47:GLY:N	2.40	0.41
8:sl:42:PHE:HE1	8:sl:46:LYS:HD2	1.86	0.41
9:sq:84:ILE:HG21	9:sq:110:MET:O	2.21	0.41
13:sv:145:LYS:HB3	13:sv:145:LYS:HE2	1.91	0.41
4:sG:73:ASP:HB3	4:sG:115:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:1377:U:H2'	5:sa:1378:U:H6	1.86	0.41
5:sa:1693:A:O2'	5:sa:1694:A:OP1	2.32	0.41
8:sl:45:MET:HB3	8:sl:65:TRP:CE2	2.56	0.41
13:sv:43:CYS:HG	13:sv:94:THR:HG1	1.60	0.41
14:sw:95:PRO:HA	14:sw:98:VAL:HG13	2.03	0.41
4:sG:177:ASN:HA	4:sG:201:ILE:HD11	2.03	0.40
5:sa:1191:A:H2'	5:sa:1192:G:O4'	2.21	0.40
5:sa:1377:U:H2'	5:sa:1378:U:C6	2.56	0.40
5:sa:1394:A:O2'	5:sa:1395:A:OP1	2.34	0.40
1:sA:80:THR:HG23	5:sa:1700:A:H2'	2.04	0.40
1:sA:83:LEU:HD23	1:sA:83:LEU:HA	1.91	0.40
3:sE:8:ASN:HD22	3:sE:8:ASN:HA	1.61	0.40
7:sg:55:ALA:O	10:ss:137:ARG:NH2	2.54	0.40
8:sl:75:LEU:HD23	8:sl:75:LEU:HA	1.75	0.40
10:ss:52:ASP:O	10:ss:53:LEU:HD23	2.22	0.40
5:sa:1662:G:C2	5:sa:1663:A:H1'	2.56	0.40
7:sg:16:PHE:CZ	7:sg:18:PRO:HG3	2.56	0.40
8:sl:21:ILE:HD12	8:sl:22:VAL:H	1.86	0.40
10:ss:46:VAL:O	10:ss:49:VAL:HG22	2.21	0.40
5:sa:1271:U:O2	5:sa:1271:U:O4'	2.39	0.40
5:sa:1375:U:H5'	10:ss:83:ARG:HH21	1.87	0.40
5:sa:1395:A:C2	5:sa:1396:A:C5	3.09	0.40
5:sa:1396:A:HO3'	5:sa:1425:A:P	2.44	0.40
6:sd:46:ASP:OD1	6:sd:66:ALA:HB1	2.21	0.40
12:su:106:THR:HA	12:su:109:ARG:HG2	2.03	0.40
5:sa:1189:G:H2'	5:sa:1190:G:H8	1.86	0.40
5:sa:1585:U:C2'	5:sa:1586:U:H5'	2.52	0.40
6:sd:60:PHE:HD2	6:sd:93:PHE:CE1	2.37	0.40
14:sw:98:VAL:HB	14:sw:99:LYS:H	1.70	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	sA	68/137 (50%)	62 (91%)	5 (7%)	1 (2%)	8	30
2	sD	58/69 (84%)	53 (91%)	5 (9%)	0	100	100
3	sE	53/56 (95%)	46 (87%)	7 (13%)	0	100	100
4	sG	159/321 (50%)	140 (88%)	17 (11%)	2 (1%)	10	33
6	sd	210/244 (86%)	193 (92%)	17 (8%)	0	100	100
7	sg	180/206 (87%)	171 (95%)	9 (5%)	0	100	100
8	sl	65/127 (51%)	61 (94%)	4 (6%)	0	100	100
9	sq	101/144 (70%)	91 (90%)	9 (9%)	1 (1%)	13	39
10	ss	139/158 (88%)	129 (93%)	10 (7%)	0	100	100
11	st	74/117 (63%)	73 (99%)	1 (1%)	0	100	100
12	su	142/155 (92%)	131 (92%)	11 (8%)	0	100	100
13	sv	153/155 (99%)	143 (94%)	10 (6%)	0	100	100
14	sw	96/118 (81%)	89 (93%)	6 (6%)	1 (1%)	13	39
All	All	1498/2007 (75%)	1382 (92%)	111 (7%)	5 (0%)	38	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	sq	112	GLY
14	sw	98	VAL
4	sG	13	LEU
1	sA	47	ALA
4	sG	31	ASP

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	sA	65/112 (58%)	61 (94%)	4 (6%)	15	40
2	sD	50/59 (85%)	46 (92%)	4 (8%)	10	31
3	sE	45/46 (98%)	41 (91%)	4 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	sG	157/272 (58%)	149 (95%)	8 (5%)	20	46
6	sd	178/206 (86%)	171 (96%)	7 (4%)	27	53
7	sg	164/178 (92%)	162 (99%)	2 (1%)	67	80
8	sl	64/111 (58%)	62 (97%)	2 (3%)	35	60
9	sq	94/127 (74%)	87 (93%)	7 (7%)	11	35
10	ss	114/128 (89%)	110 (96%)	4 (4%)	31	56
11	st	68/106 (64%)	66 (97%)	2 (3%)	37	61
12	su	122/130 (94%)	114 (93%)	8 (7%)	14	39
13	sv	132/132 (100%)	128 (97%)	4 (3%)	36	61
14	sw	89/107 (83%)	81 (91%)	8 (9%)	8	27
All	All	1342/1714 (78%)	1278 (95%)	64 (5%)	24	48

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	sA	44	LEU
1	sA	61	GLU
1	sA	67	VAL
1	sA	88	LEU
2	sD	17	GLU
2	sD	25	ARG
2	sD	31	VAL
2	sD	59	LEU
3	sE	4	TYR
3	sE	18	SER
3	sE	30	LEU
3	sE	56	ASP
4	sG	13	LEU
4	sG	29	LYS
4	sG	118	PHE
4	sG	126	ILE
4	sG	140	VAL
4	sG	172	SER
4	sG	203	THR
4	sG	306	ILE
6	sd	2	PHE
6	sd	17	THR
6	sd	20	SER

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Mol	Chain	Res	Type
6	sd	34	GLU
6	sd	67	THR
6	sd	171	MET
6	sd	180	GLN
7	sg	171	LEU
7	sg	184	LYS
8	sl	2	ARG
8	sl	5	THR
9	sq	35	MET
9	sq	66	THR
9	sq	104	VAL
9	sq	107	LYS
9	sq	115	LEU
9	sq	121	THR
9	sq	125	VAL
10	ss	47	ASN
10	ss	55	ASN
10	ss	84	VAL
10	ss	89	GLN
11	st	4	VAL
11	st	61	ILE
12	su	13	MET
12	su	53	VAL
12	su	61	THR
12	su	93	ASP
12	su	97	SER
12	su	126	HIS
12	su	137	THR
12	su	139	THR
13	sv	36	ASP
13	sv	43	CYS
13	sv	94	THR
13	sv	100	VAL
14	sw	19	ASN
14	sw	25	THR
14	sw	32	VAL
14	sw	38	GLU
14	sw	48	VAL
14	sw	54	VAL
14	sw	63	ILE
14	sw	91	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	sA	45	ASN
3	sE	8	ASN
6	sd	61	GLN
6	sd	176	ASN
7	sg	81	HIS
7	sg	103	HIS
8	sl	31	HIS
8	sl	40	GLN
10	ss	74	ASN
10	ss	89	GLN
10	ss	118	ASN
12	su	73	ASN
13	sv	6	ASN
13	sv	101	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	sa	472/1947 (24%)	127 (26%)	0

All (127) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	sa	1176	G
5	sa	1177	A
5	sa	1184	C
5	sa	1185	A
5	sa	1192	G
5	sa	1210	U
5	sa	1219	A
5	sa	1221	A
5	sa	1224	G
5	sa	1225	G
5	sa	1227	A
5	sa	1232	U
5	sa	1233	A
5	sa	1239	A
5	sa	1242	G
5	sa	1243	A
5	sa	1252	A
5	sa	1253	G

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Mol	Chain	Res	Type
5	sa	1254	G
5	sa	1266	A
5	sa	1269	A
5	sa	1270	G
5	sa	1271	U
5	sa	1276	U
5	sa	1277	C
5	sa	1281	A
5	sa	1282	U
5	sa	1283	U
5	sa	1287	U
5	sa	1290	G
5	sa	1298	G
5	sa	1299	C
5	sa	1310	U
5	sa	1311	U
5	sa	1312	A
5	sa	1316	G
5	sa	1317	G
5	sa	1323	U
5	sa	1326	U
5	sa	1331	C
5	sa	1332	A
5	sa	1337	A
5	sa	1339	U
5	sa	1344	G
5	sa	1346	A
5	sa	1350	A
5	sa	1363	C
5	sa	1365	U
5	sa	1369	A
5	sa	1370	A
5	sa	1371	U
5	sa	1379	C
5	sa	1388	A
5	sa	1389	G
5	sa	1395	A
5	sa	1396	A
5	sa	1425	A
5	sa	1426	C
5	sa	1438	A
5	sa	1440	A

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Mol	Chain	Res	Type
5	sa	1441	C
5	sa	1442	A
5	sa	1507	A
5	sa	1508	A
5	sa	1520	C
5	sa	1522	U
5	sa	1534	A
5	sa	1535	G
5	sa	1542	G
5	sa	1543	A
5	sa	1551	A
5	sa	1552	G
5	sa	1554	C
5	sa	1555	A
5	sa	1566	C
5	sa	1567	A
5	sa	1576	A
5	sa	1578	A
5	sa	1580	U
5	sa	1581	G
5	sa	1585	U
5	sa	1587	A
5	sa	1588	C
5	sa	1590	A
5	sa	1593	G
5	sa	1596	U
5	sa	1597	A
5	sa	1668	G
5	sa	1669	A
5	sa	1670	A
5	sa	1671	A
5	sa	1678	A
5	sa	1683	A
5	sa	1687	C
5	sa	1689	A
5	sa	1690	A
5	sa	1691	A
5	sa	1694	A
5	sa	1696	G
5	sa	1701	U
5	sa	1702	G
5	sa	1703	A

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Mol	Chain	Res	Type
5	sa	1704	C
5	sa	1706	G
5	sa	1708	G
5	sa	1711	A
5	sa	1712	A
5	sa	1713	A
5	sa	1714	U
5	sa	1718	U
5	sa	1723	U
5	sa	1725	A
5	sa	1735	A
5	sa	1750	G
5	sa	1767	A
5	sa	1773	G
5	sa	1777	A
5	sa	1780	A
5	sa	1783	U
5	sa	1785	C
5	sa	1786	C
5	sa	1787	U
5	sa	1788	G
5	sa	1789	C
5	sa	1791	C
5	sa	1792	U
5	sa	1793	U

There are no RNA pucker outliers to report.

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](#)

There are no ligands in this entry.

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.

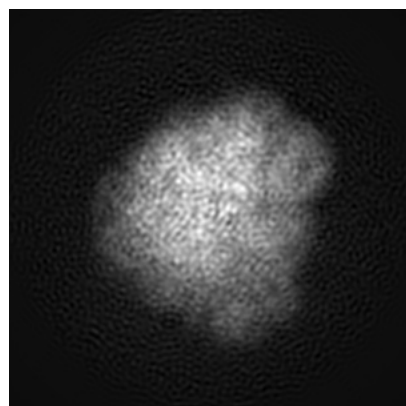
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64696. These allow visual inspection of the internal detail of the map and identification of artifacts.

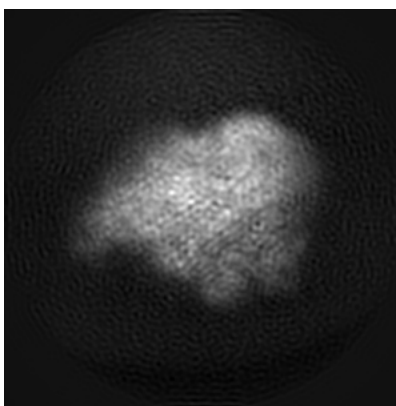
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

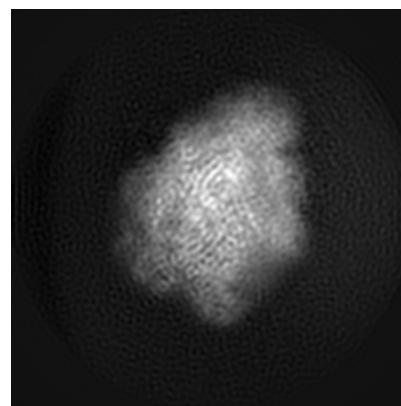
6.1.1 Primary map



X

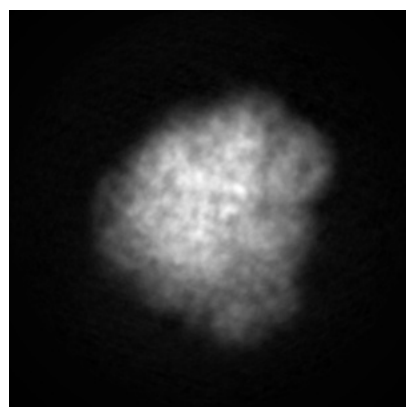


Y

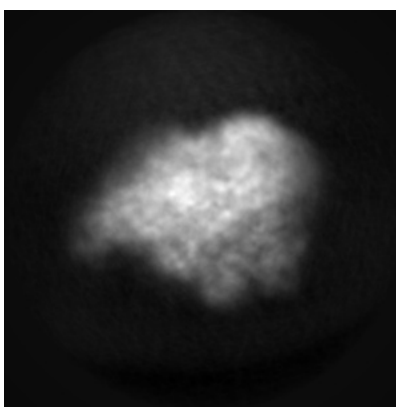


Z

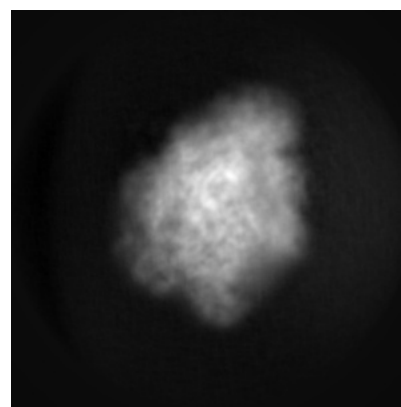
6.1.2 Raw map



X



Y

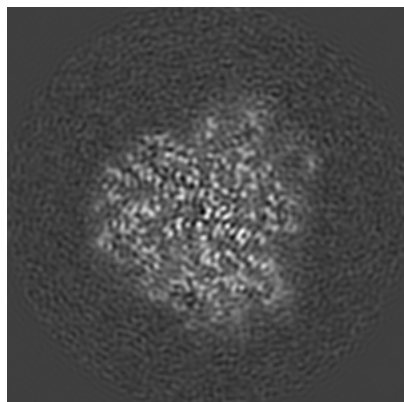


Z

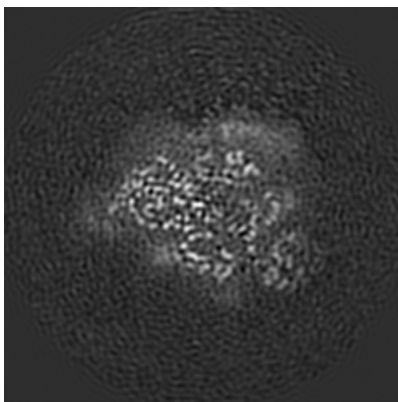
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

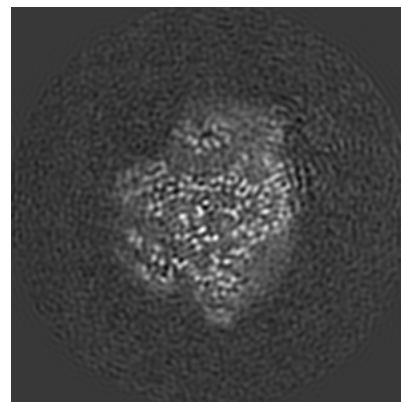
6.2.1 Primary map



X Index: 105

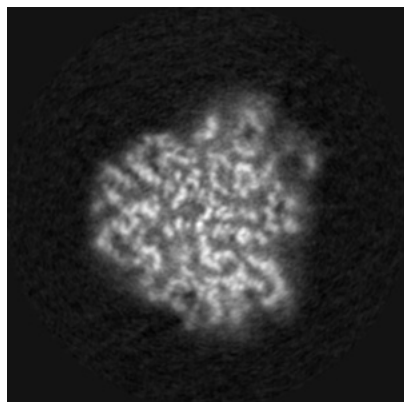


Y Index: 105

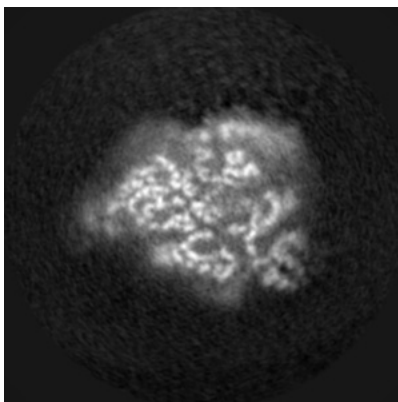


Z Index: 105

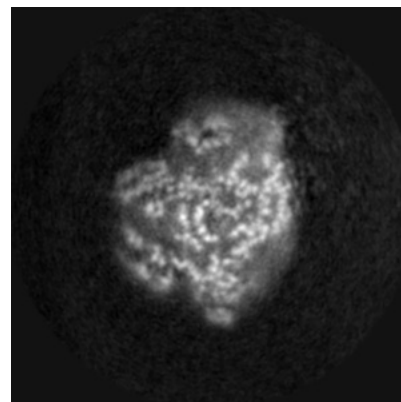
6.2.2 Raw map



X Index: 105



Y Index: 105

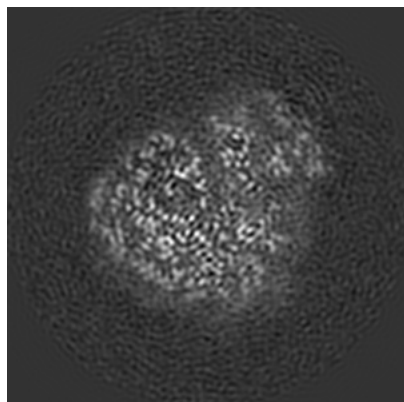


Z Index: 105

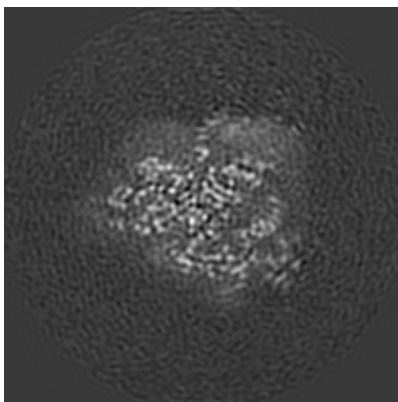
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

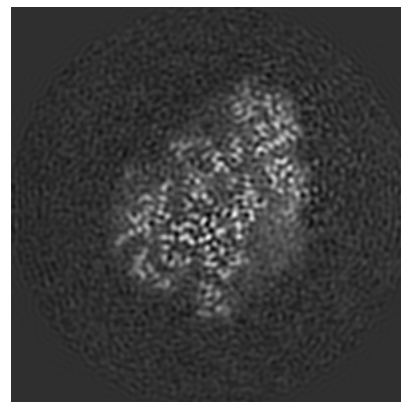
6.3.1 Primary map



X Index: 113

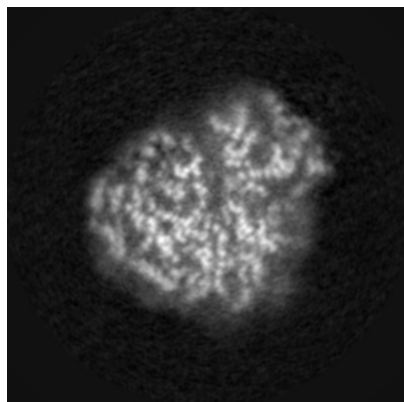


Y Index: 102

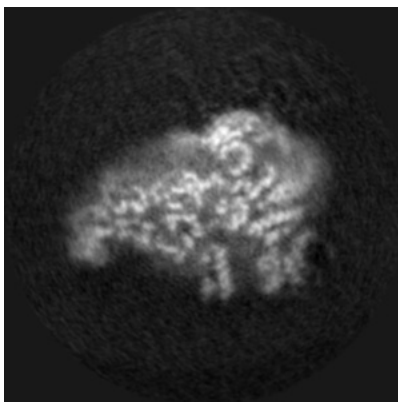


Z Index: 119

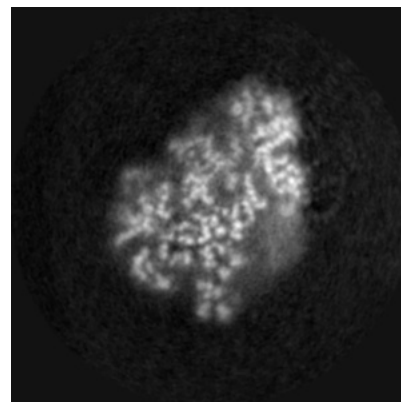
6.3.2 Raw map



X Index: 114



Y Index: 122

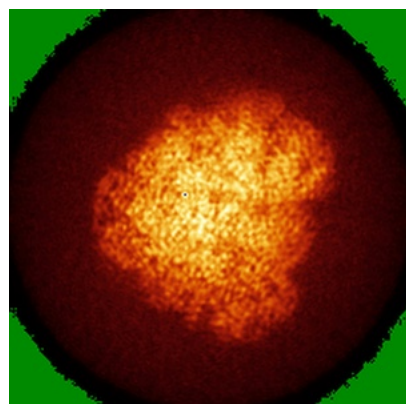


Z Index: 118

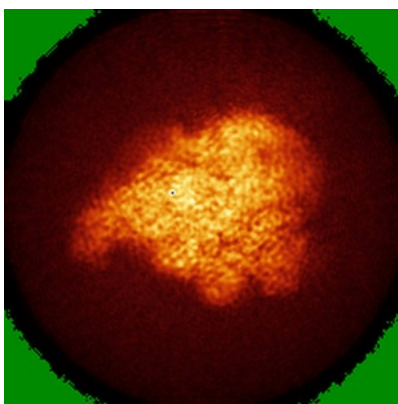
The images above show the largest variance slices of the map in three orthogonal directions.

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

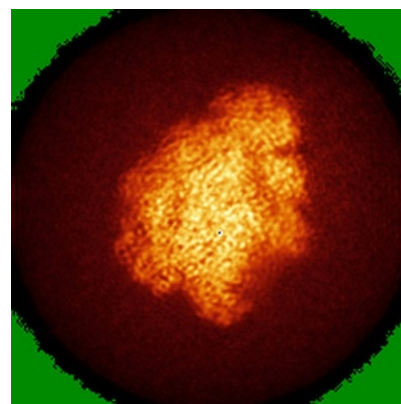
6.4.1 Primary map



X

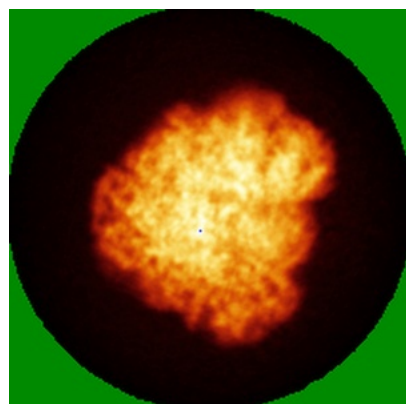


Y

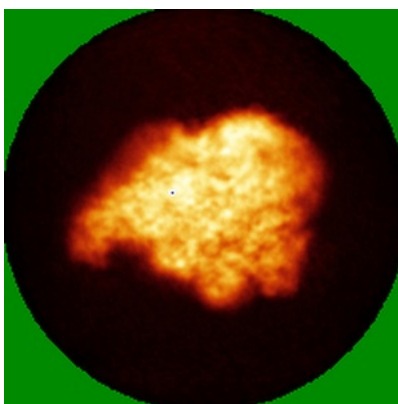


Z

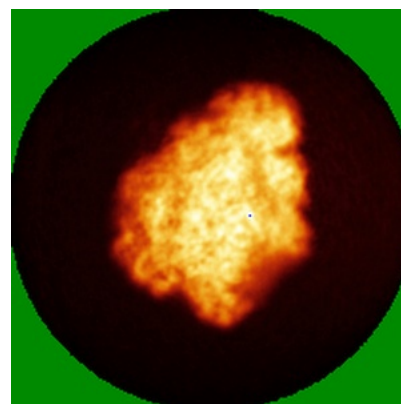
6.4.2 Raw map



X



Y

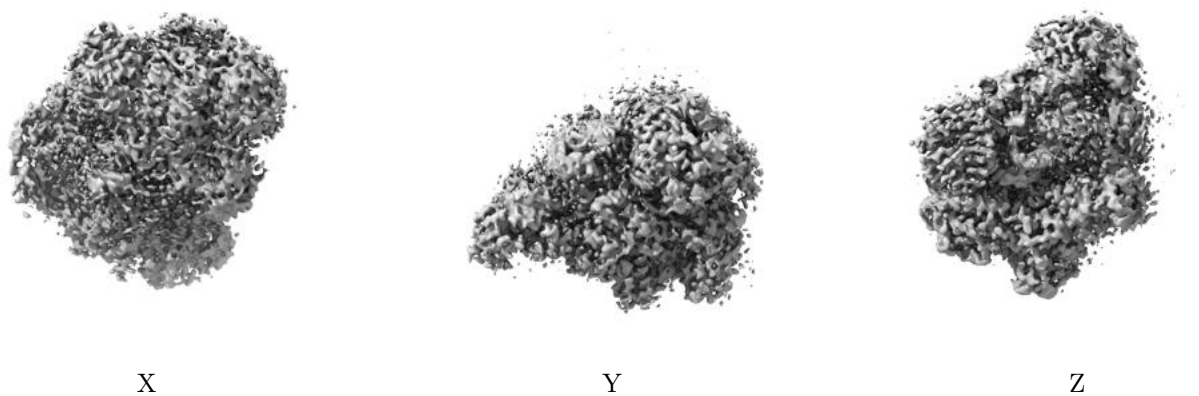


Z

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 2.8. 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.

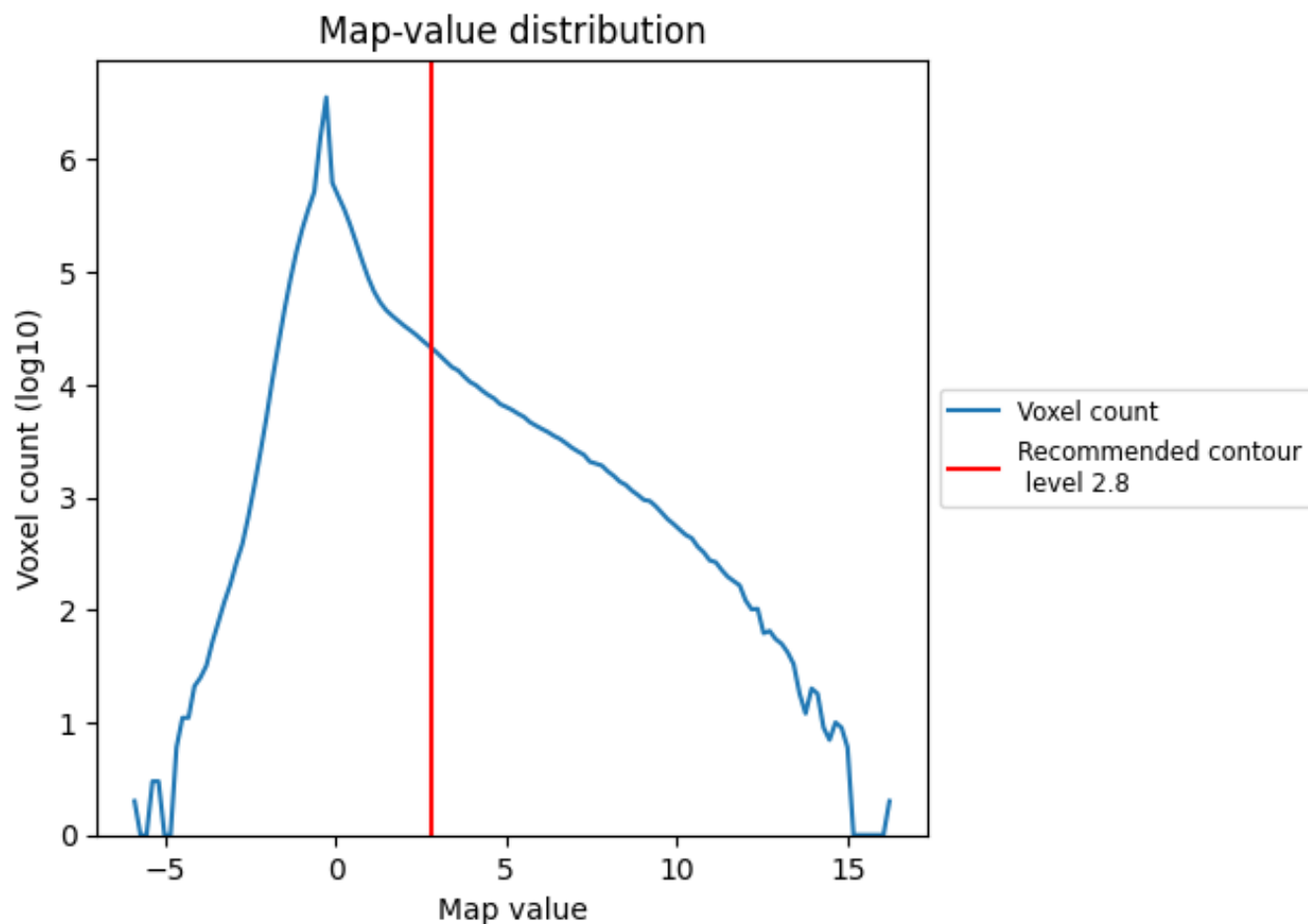
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

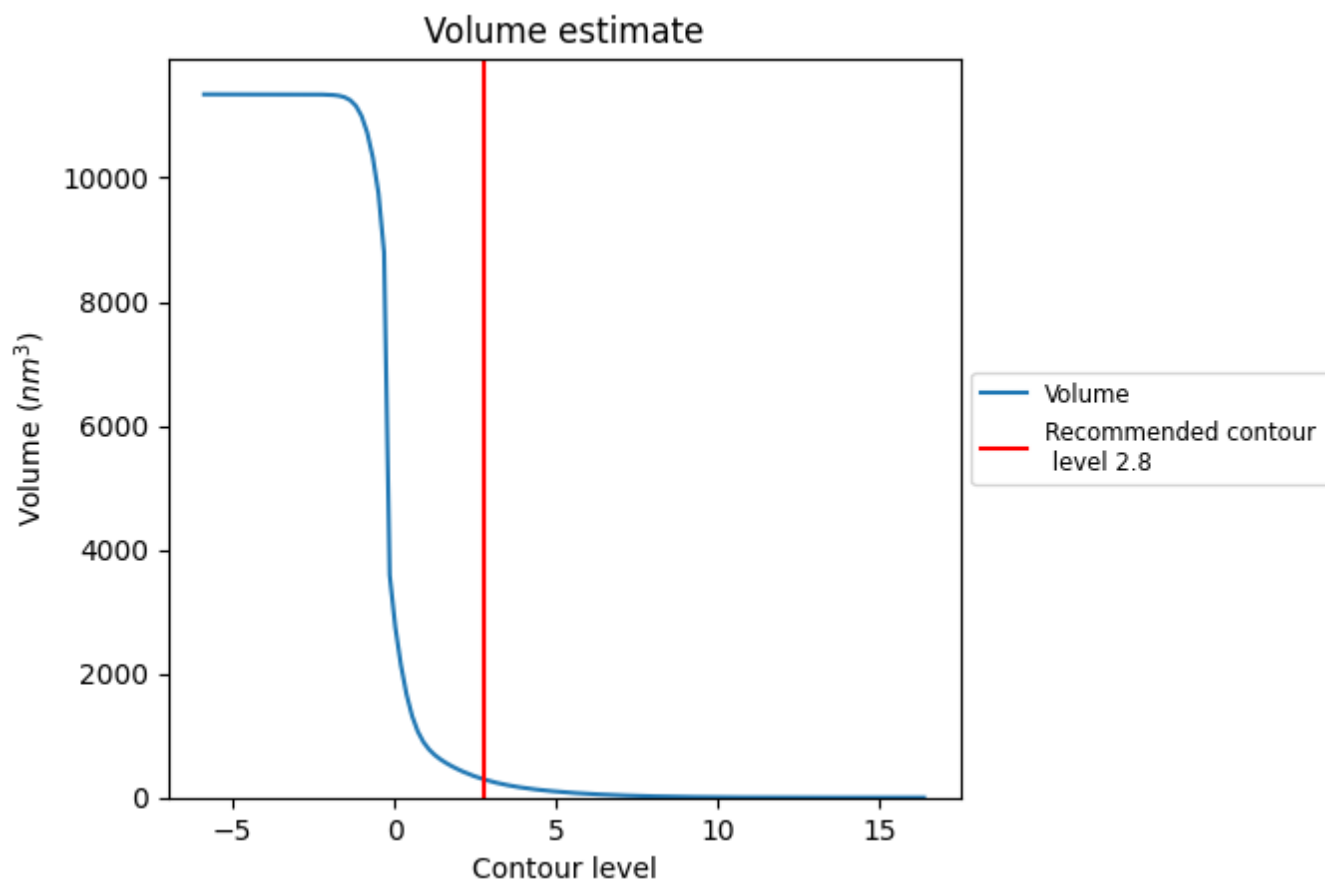
This section contains the results of statistical analysis of the map.

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.

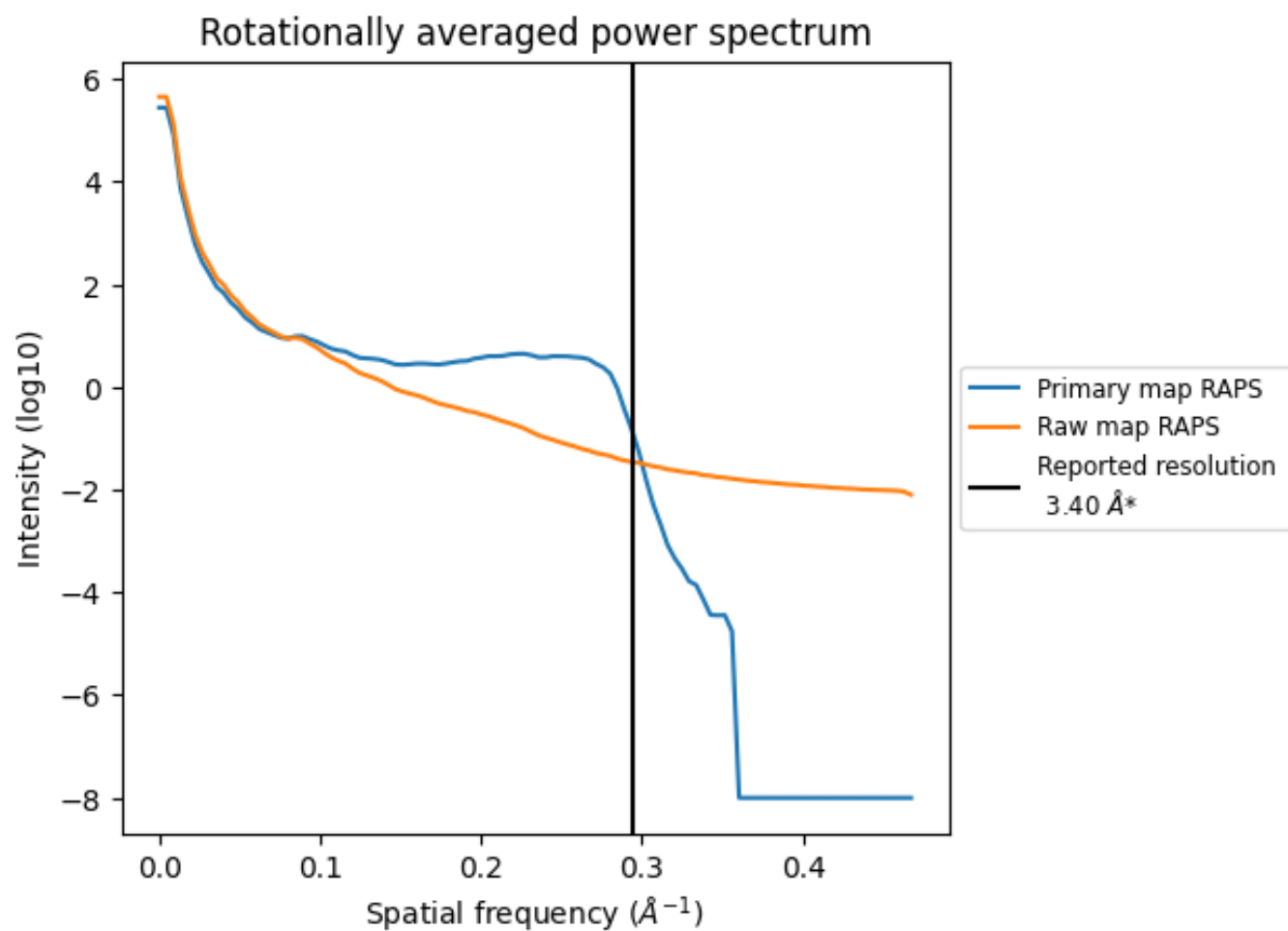
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290 nm^3 ; this corresponds to an approximate mass of 262 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 ⓘ

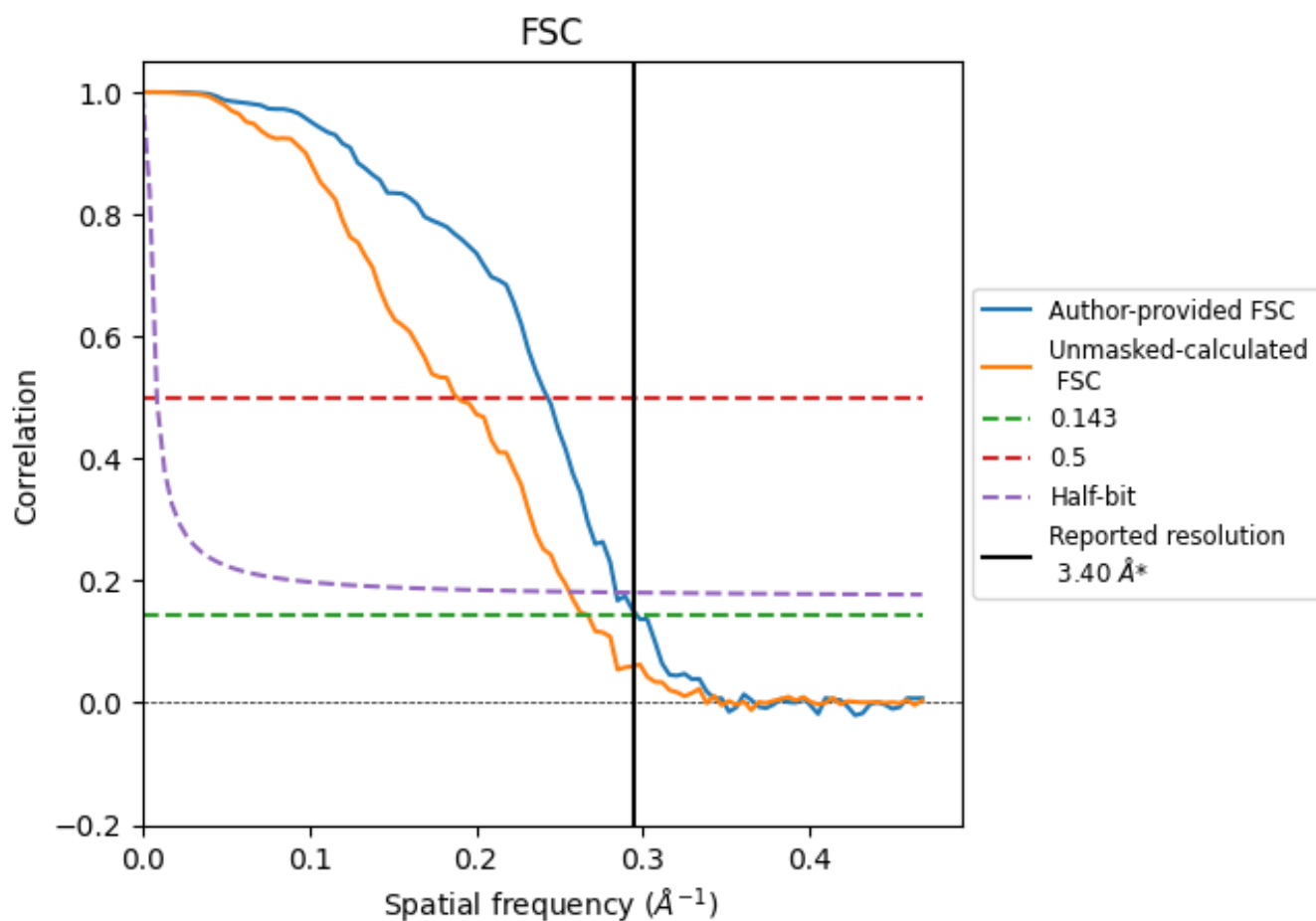


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

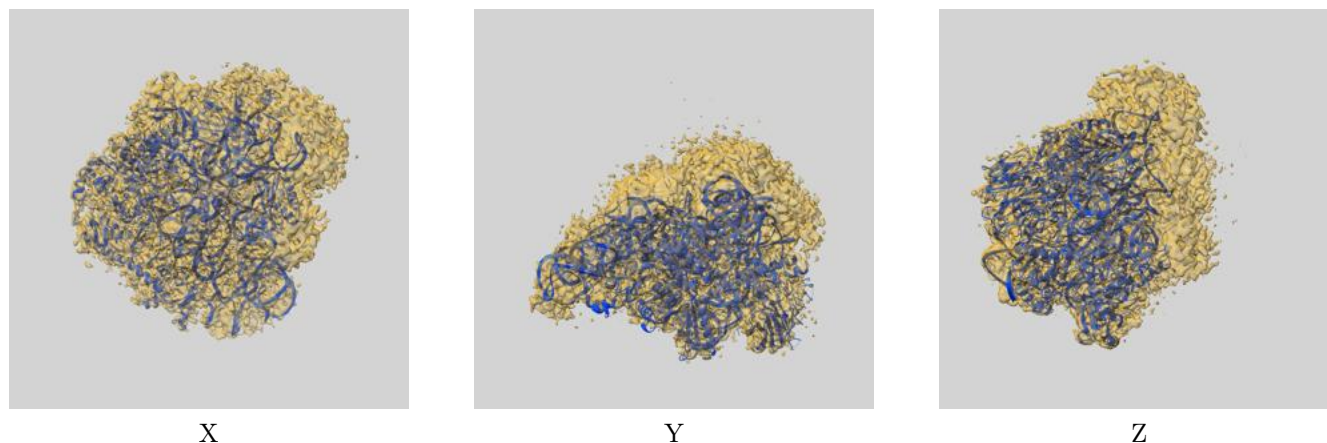
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	4.12	3.52
Unmasked-calculated*	3.74	5.30	3.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

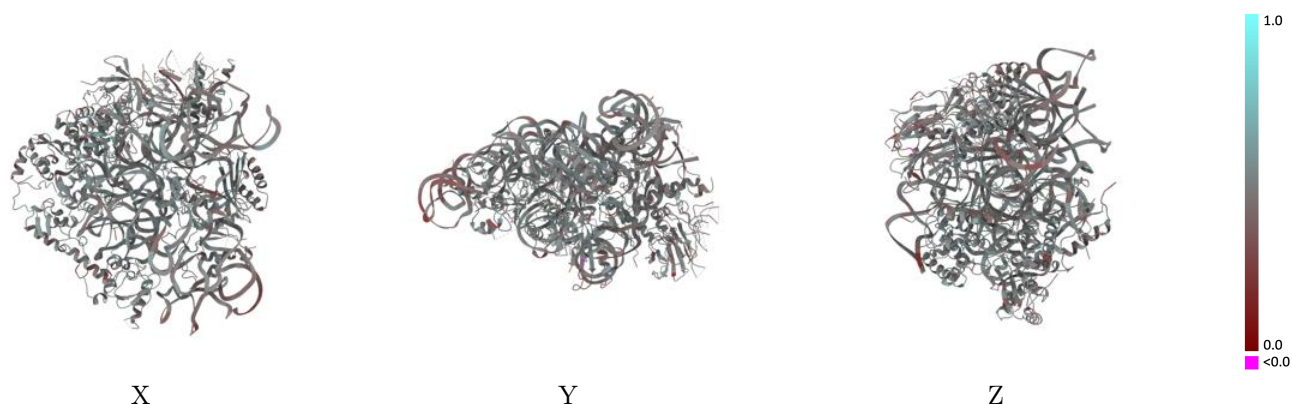
This section contains information regarding the fit between EMDB map EMD-64696 and PDB model 9V1K. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



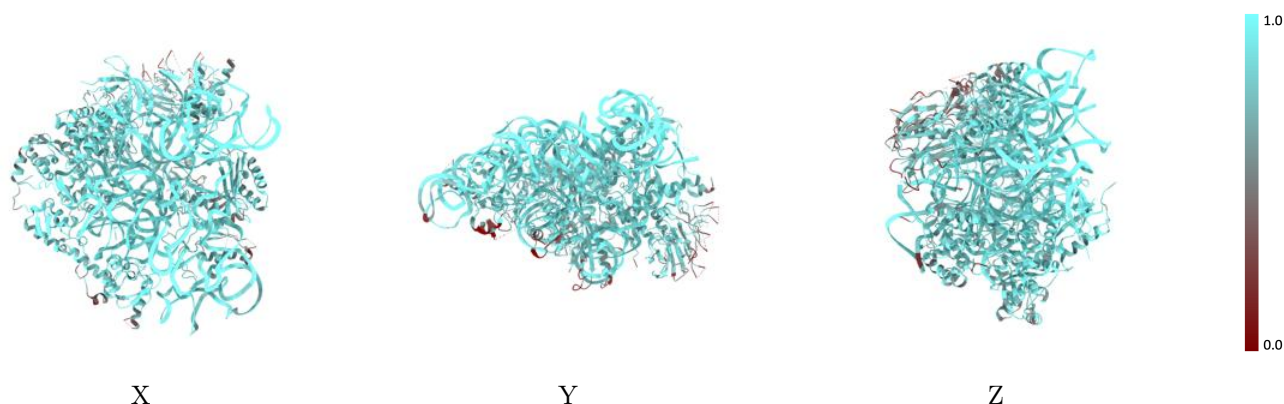
The images above show the 3D surface view of the map at the recommended contour level 2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



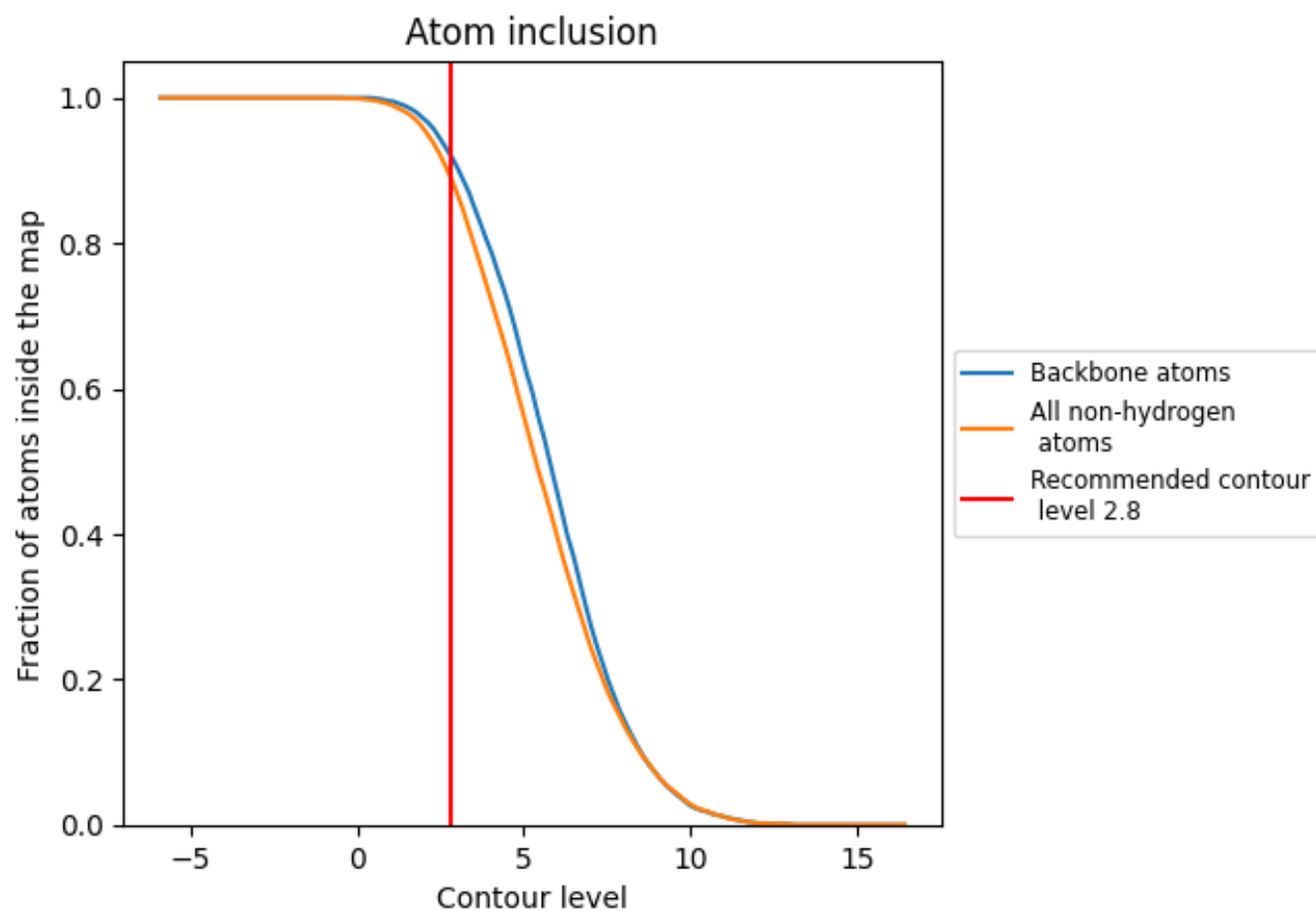
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.8).































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.4800
sA	 0.8120	 0.4730
sD	 0.8910	 0.4660
sE	 0.9620	 0.5160
sG	 0.6830	 0.4630
sa	 0.9610	 0.4720
sd	 0.8020	 0.4750
sg	 0.9080	 0.4990
sl	 0.7100	 0.4940
sq	 0.8500	 0.4920
ss	 0.8940	 0.5100
st	 0.8620	 0.4810
su	 0.9010	 0.4860
sv	 0.8610	 0.5070
sw	 0.7370	 0.4630

