



Full wwPDB EM Validation Report ⓘ

May 27, 2026 – 07:38 pm BST

PDB ID : 28YE / pdb_000028ye
EMDB ID : EMD-56961
Title : 50S ribosomal subunit with E-tRNA and RsfS from the alphaproteobacteria
Asaia platycodi
Authors : Chan, L.I.; Omae, K.; Amikura, K.; Suzuki, S.; Melnikov, S.M.
Deposited on : 2026-02-27
Resolution : 2.98 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:

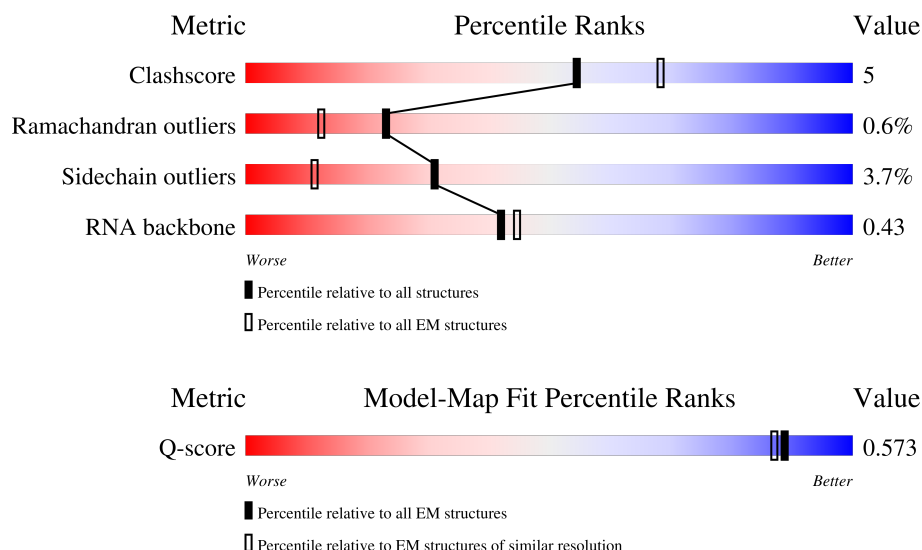
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.98 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.





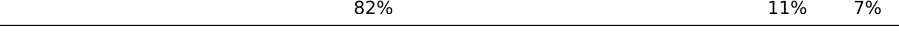
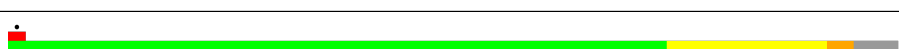



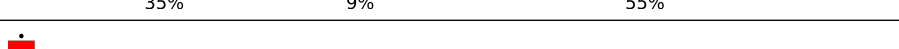



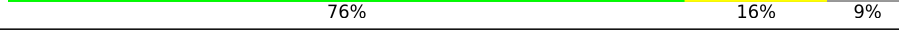

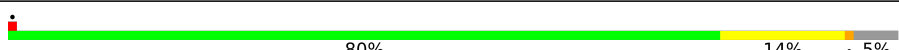


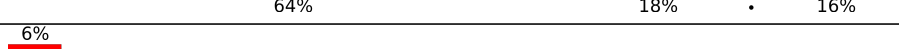



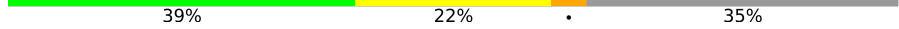



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13236 (2.48 - 3.48)

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	Z	41	
2	A	276	
3	B	2726	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	67	
5	D	44	
6	E	55	
7	F	67	
8	H	61	
9	I	77	
10	J	100	
11	K	88	
12	L	212	
13	M	106	
14	N	113	
15	O	143	
16	P	104	
17	Q	128	
18	S	141	
19	T	138	
20	U	161	
21	V	122	
22	W	158	
23	X	192	
24	Y	178	
25	a	204	
26	b	227	
27	c	18	
28	d	113	

Continued on next page...

Mol	Chain	Length	Quality of chain
29	R	127	
30	G	152	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 79050 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 Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	41	Total	C	N	O	S	0	0
			343	208	79	53	3		

- Molecule 2 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	274	Total	C	N	O	S	0	0
			2116	1311	420	378	7		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	2455	Total	C	N	O	P	0	0
			52721	23513	9732	17021	2455		

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	66	Total	C	N	O	S	0	0
			517	322	102	87	6		

- Molecule 5 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	44	Total	C	N	O	S	0	0
			368	223	88	55	2		

- Molecule 6 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	51	Total	C	N	O	S	0	0
			412	262	77	72	1		

- Molecule 7 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	63	Total	C	N	O	S	0	0
			481	289	102	84	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	58	Total	C	N	O	S	0	0
			435	267	86	81	1		

- Molecule 9 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	64	Total	C	N	O	S	0	0
			502	309	101	92			

- Molecule 10 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			771	472	157	141	1		

- Molecule 11 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	72	Total	C	N	O	S	0	0
			529	325	110	92	2		

- Molecule 12 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	95	Total	C	N	O	S	0	0
			733	462	143	126	2		

- Molecule 13 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	105	Total	C	N	O	S	0	0
			795	495	157	141	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	111	Total	C	N	O	S	0	0
			858	541	160	153	4		

- Molecule 15 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	122	Total	C	N	O	S	0	0
			959	594	196	167	2		

- Molecule 16 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	104	Total	C	N	O	S	0	0
			794	496	153	144	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	117	Total	C	N	O	S	0	0
			946	596	188	161	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	129	Total	C	N	O	S	0	0
			1003	622	196	180	5		

- Molecule 19 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	135	Total	C	N	O	S	0	0
			1048	672	203	170	3		

- Molecule 20 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	153	Total	C	N	O	S	0	0
			1124	696	221	205	2		

- Molecule 21 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	122	Total	C	N	O	S	0	0
			933	587	177	165	4		

- Molecule 22 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	154	Total	C	N	O	S	0	0
			1201	756	227	214	4		

- Molecule 23 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	161	Total	C	N	O	S	0	0
			1250	768	242	237	3		

- Molecule 24 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	175	Total	C	N	O	S	0	0
			1342	846	244	249	3		

- Molecule 25 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	204	Total	C	N	O	S	0	0
			1529	959	291	276	3		

- Molecule 26 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	222	Total	C	N	O	S	0	0
			1686	1053	317	307	9		

- Molecule 27 is a RNA chain called E-site tRNA (heterogeneous fragment modelled as poly-U with the CCA-end).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	18	Total	C	N	O	P	0	0
			362	163	41	140	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	73	Total	C	N	O	P	0	0
			1559	696	283	508	72		

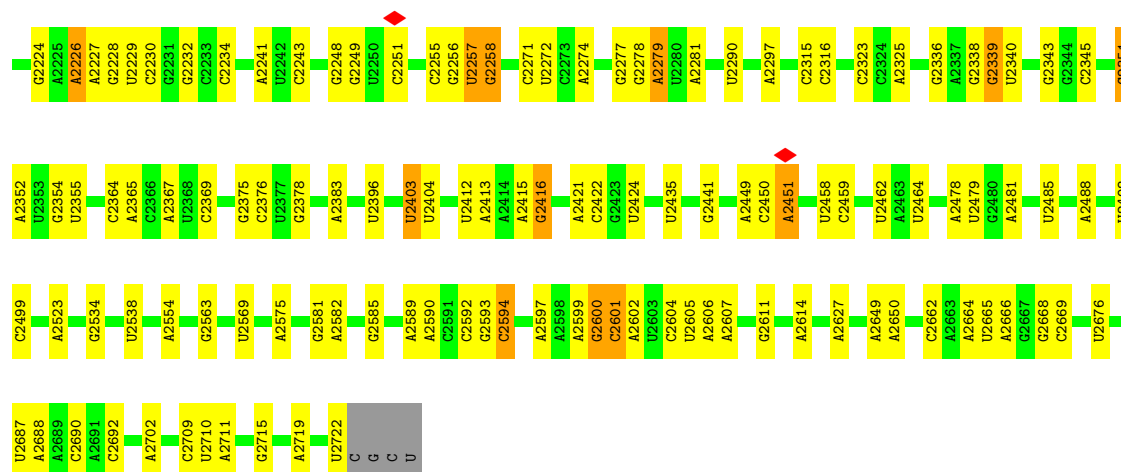
- Molecule 29 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	R	118	Total	C	N	O	S	0	0
			941	585	186	169	1		

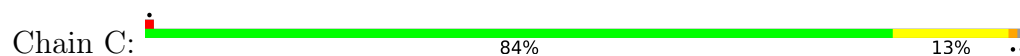
- Molecule 30 is a protein called Ribosome silencing factor S.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	103	Total	C	N	O	S	0	0
			792	498	137	154	3		





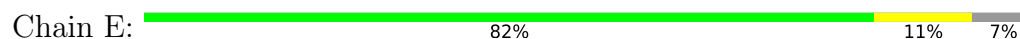
- Molecule 4: Large ribosomal subunit protein bL35



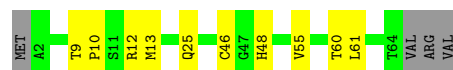
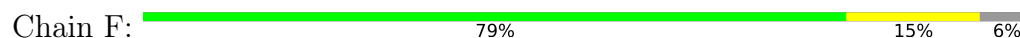
- Molecule 5: Large ribosomal subunit protein bL34



- Molecule 6: Large ribosomal subunit protein bL33



- Molecule 7: Large ribosomal subunit protein bL32



- Molecule 8: Large ribosomal subunit protein uL30



- Molecule 9: Large ribosomal subunit protein uL29

Chain I:  64% 18% 17%



- Molecule 10: Large ribosomal subunit protein bL28

Chain J:  71% 26%




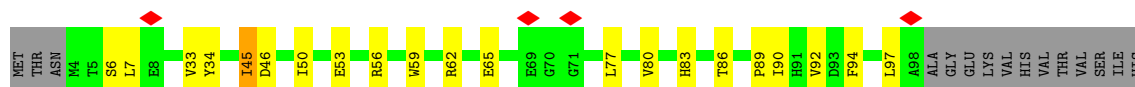
- Molecule 11: Large ribosomal subunit protein bL27

Chain K:  60% 22% 18%




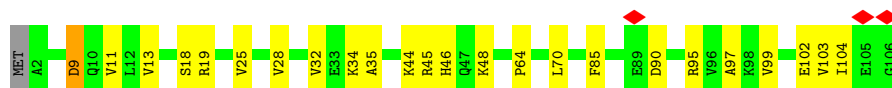
- Molecule 12: Large ribosomal subunit protein bL25

Chain L:  35% 9% 55%



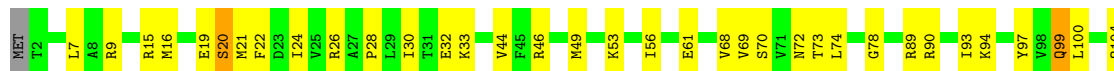
- Molecule 13: Large ribosomal subunit protein uL24

Chain M:  76% 22%



- Molecule 14: Large ribosomal subunit protein uL23

Chain N:  63% 34%





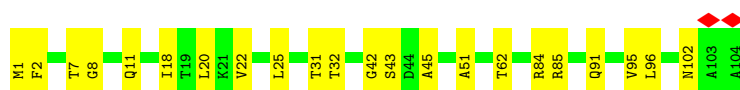
- Molecule 15: Large ribosomal subunit protein uL22

Chain O: 76% 9% 15%



- Molecule 16: Large ribosomal subunit protein bL21

Chain P: 79% 21%



- Molecule 17: Large ribosomal subunit protein bL20

Chain Q: 76% 16% 9%



- Molecule 18: Large ribosomal subunit protein bL17

Chain S: 77% 14% 9%



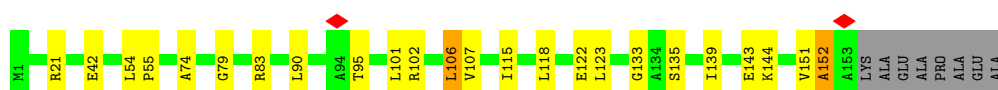
- Molecule 19: Large ribosomal subunit protein uL16

Chain T: 80% 16% 2%



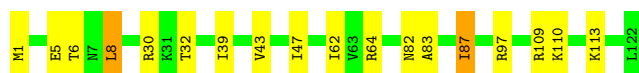
- Molecule 20: Large ribosomal subunit protein uL15

Chain U: 80% 14% 5%

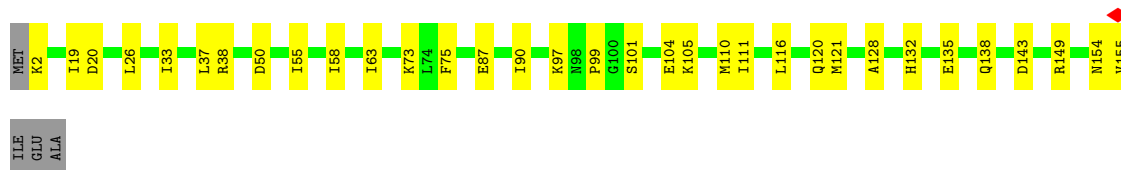
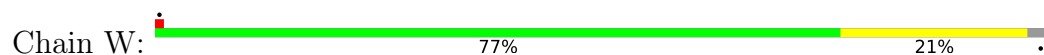


- Molecule 21: Large ribosomal subunit protein uL14

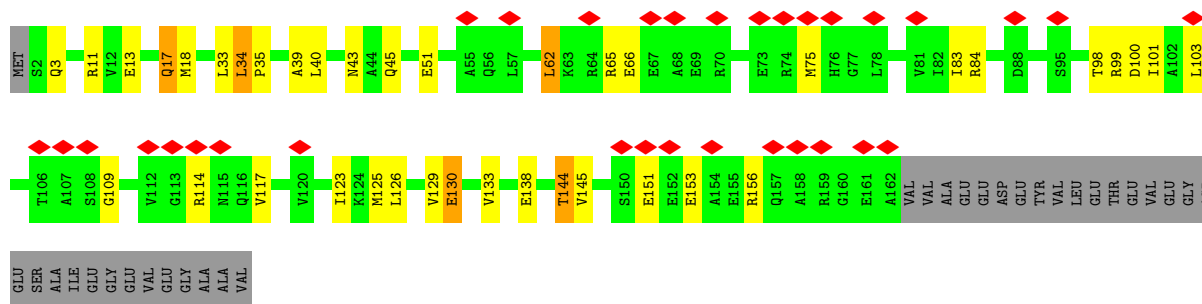
Chain V: 85% 13% 2%



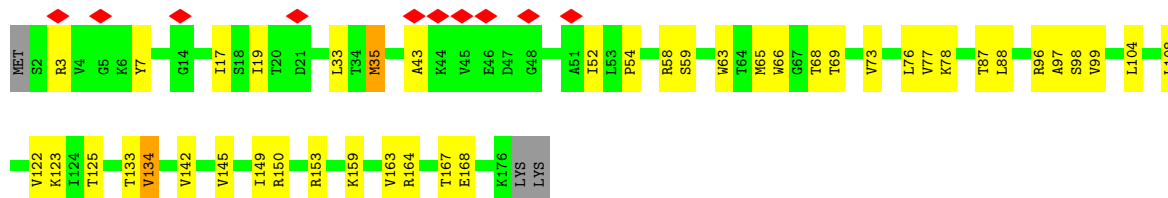
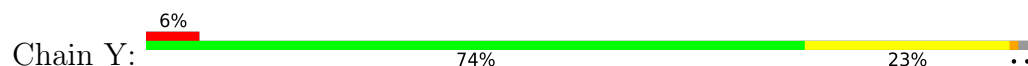
- Molecule 22: Large ribosomal subunit protein uL13



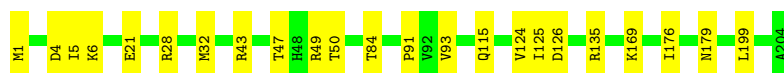
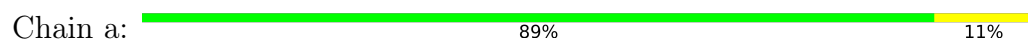
- Molecule 23: Large ribosomal subunit protein bL9



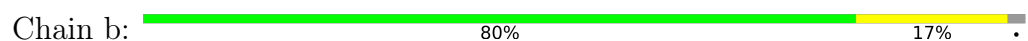
- Molecule 24: Large ribosomal subunit protein uL6



- Molecule 25: Large ribosomal subunit protein uL4

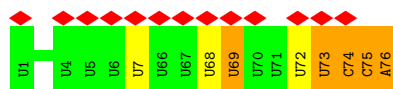


- Molecule 26: Large ribosomal subunit protein uL3

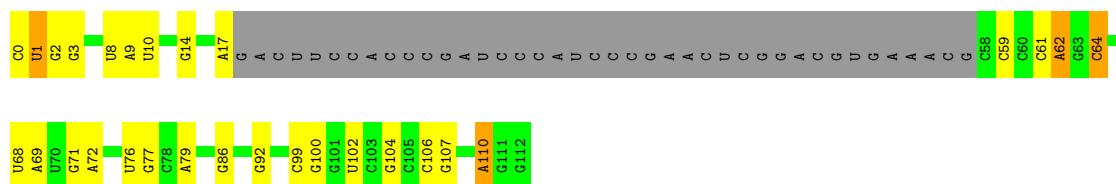




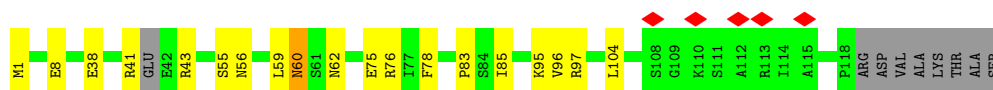
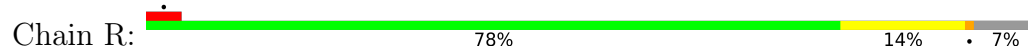
- Molecule 27: E-site tRNA (heterogeneous fragment modelled as poly-U with the CCA-end)



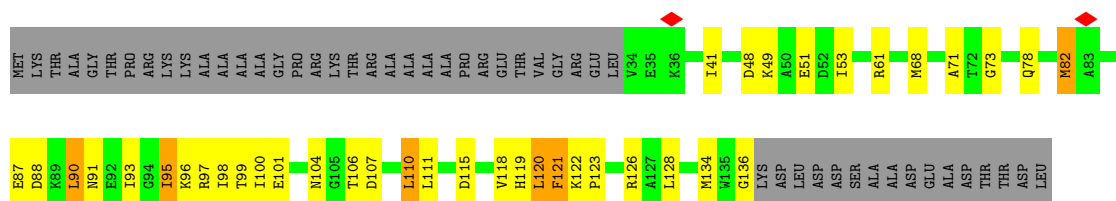
- Molecule 28: 5S rRNA (fragment)



- Molecule 29: Large ribosomal subunit protein bL19



- Molecule 30: Ribosome silencing factor S



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48969	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	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.716	Depositor
Minimum map value	-1.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.166	Depositor
Map size (\AA)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.95, 0.95, 0.95	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	Z	0.36	0/344	0.64	0/449
2	A	0.42	0/2158	0.64	0/2902
3	B	0.47	0/59040	0.42	6/92094 (0.0%)
4	C	0.45	0/526	0.51	0/697
5	D	0.50	0/371	0.56	0/484
6	E	0.39	0/418	0.47	0/560
7	F	0.44	0/491	0.53	0/659
8	H	0.37	0/437	0.56	0/583
9	I	0.36	0/504	0.67	0/674
10	J	0.40	0/777	0.48	0/1044
11	K	0.45	0/533	0.57	0/710
12	L	0.32	0/746	0.61	2/1007 (0.2%)
13	M	0.36	0/802	0.55	0/1071
14	N	0.39	0/864	0.70	0/1159
15	O	0.45	0/969	0.56	0/1299
16	P	0.40	0/801	0.53	0/1079
17	Q	0.48	0/958	0.56	0/1281
18	S	0.43	0/1015	0.56	0/1361
19	T	0.39	0/1070	0.57	0/1437
20	U	0.44	0/1133	0.58	0/1511
21	V	0.41	0/944	0.58	0/1268
22	W	0.42	0/1223	0.53	0/1651
23	X	0.30	0/1261	0.63	0/1700
24	Y	0.31	0/1365	0.56	0/1846
25	a	0.44	0/1552	0.53	0/2094
26	b	0.42	0/1712	0.52	0/2298
27	c	0.23	0/397	0.54	0/609
28	d	0.35	0/1742	0.44	0/2713
29	R	0.40	0/953	0.46	0/1281
30	G	0.34	0/802	0.66	0/1085
All	All	0.45	0/85908	0.46	8/128606 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2711	A	OP1-P-OP2	-13.84	78.07	119.60
3	B	2710	U	OP1-P-O3'	-11.02	74.93	108.00
3	B	2711	A	O5'-P-OP2	-10.84	75.48	108.00
3	B	2711	A	O5'-P-OP1	8.38	133.13	108.00
3	B	2710	U	OP2-P-O3'	8.24	132.71	108.00
12	L	45	ILE	CA-C-N	-5.61	105.71	122.71
12	L	45	ILE	C-N-CA	-5.61	105.71	122.71
3	B	2710	U	O3'-P-O5'	-5.30	96.04	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	343	0	389	13	0
2	A	2116	0	2157	49	0
3	B	52721	0	26545	236	0
4	C	517	0	559	8	0
5	D	368	0	410	4	0
6	E	412	0	433	6	0
7	F	481	0	480	6	0
8	H	435	0	465	9	0
9	I	502	0	529	15	0
10	J	771	0	817	17	0
11	K	529	0	553	10	0
12	L	733	0	768	15	0
13	M	795	0	866	16	0
14	N	858	0	942	35	0
15	O	959	0	1017	7	0
16	P	794	0	848	14	0
17	Q	946	0	994	12	0
18	S	1003	0	1049	15	0
19	T	1048	0	1126	18	0
20	U	1124	0	1189	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	933	0	1006	15	0
22	W	1201	0	1253	26	0
23	X	1250	0	1284	28	0
24	Y	1342	0	1394	36	0
25	a	1529	0	1600	19	0
26	b	1686	0	1746	25	0
27	c	362	0	185	3	0
28	d	1559	0	792	7	0
29	R	941	0	978	14	0
30	G	792	0	797	34	0
All	All	79050	0	53171	674	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 5.

All (674) 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)
3:B:680:A:H62	3:B:699:G:H21	0.96	0.94
9:I:10:LEU:HD21	9:I:57:ILE:HD12	1.54	0.89
3:B:1588:U:O2	3:B:1601:G:O6	1.92	0.88
3:B:2600:G:C8	24:Y:3:ARG:HB2	2.09	0.88
23:X:101:ILE:HD11	23:X:145:VAL:HG21	1.56	0.86
3:B:827:C:H2'	3:B:828:G:H8	1.43	0.84
2:A:21:ARG:HH11	3:B:1449:C:H5''	1.43	0.82
26:b:6:ILE:HG13	26:b:53:MET:HE3	1.60	0.81
14:N:99:GLN:O	14:N:99:GLN:NE2	2.14	0.79
3:B:836:A:H2'	3:B:837:G:H8	1.46	0.79
10:J:16:ASN:HD22	10:J:24:LYS:HB3	1.47	0.79
3:B:1284:A:N1	3:B:1480:C:N3	2.31	0.79
22:W:73:LYS:HB3	22:W:90:ILE:HD11	1.64	0.79
19:T:64:VAL:HG13	19:T:106:ILE:HG22	1.67	0.77
3:B:680:A:N6	3:B:699:G:H21	1.79	0.77
3:B:2424:U:H5'	26:b:150:ARG:HB2	1.68	0.75
1:Z:7:LEU:HD21	1:Z:40:GLN:HB2	1.68	0.75
3:B:1367:U:H3	3:B:1372:A:H62	1.36	0.74
2:A:183:LEU:HD12	2:A:269:ILE:HD11	1.70	0.73
3:B:458:A:H5''	13:M:48:LYS:HD2	1.69	0.73
12:L:45:ILE:HD12	12:L:50:ILE:HD11	1.71	0.72
10:J:12:VAL:H	10:J:31:PRO:HD3	1.52	0.72
16:P:11:GLN:OE1	17:Q:91:ASP:HB2	1.88	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:51:LEU:HD21	18:S:70:LEU:HD22	1.72	0.70
3:B:1659:A:H2'	3:B:1660:A:C8	2.26	0.70
30:G:107:ASP:HB2	30:G:122:LYS:HG3	1.72	0.70
3:B:1139:G:H21	16:P:91:GLN:HE22	1.39	0.69
3:B:2607:A:H1'	24:Y:65:MET:HE1	1.75	0.69
30:G:96:LYS:H	30:G:97:ARG:NH1	1.90	0.69
10:J:69:LEU:O	10:J:85:LYS:HE3	1.94	0.68
8:H:11:GLN:HG2	8:H:34:ILE:HA	1.77	0.67
22:W:19:ILE:HD12	22:W:33:ILE:HD11	1.77	0.67
3:B:1916:U:H3	3:B:2279:A:H2	1.43	0.67
29:R:97:ARG:HG2	29:R:97:ARG:HH11	1.59	0.67
8:H:15:ALA:O	8:H:18:ARG:HG2	1.94	0.67
24:Y:96:ARG:HH22	24:Y:98:SER:HB3	1.60	0.67
3:B:1411:U:H2'	3:B:1412:C:C6	2.29	0.67
3:B:895:C:H2'	3:B:896:G:H8	1.60	0.66
3:B:836:A:H2'	3:B:837:G:C8	2.29	0.66
26:b:14:ARG:HE	29:R:60:ASN:HB3	1.60	0.66
15:O:85:THR:HG22	15:O:118:VAL:HB	1.76	0.66
3:B:827:C:H2'	3:B:828:G:C8	2.29	0.65
10:J:18:VAL:HG22	10:J:24:LYS:HD3	1.77	0.65
2:A:23:GLU:O	2:A:24:LEU:HD23	1.95	0.65
24:Y:134:VAL:HG22	24:Y:142:VAL:HG13	1.79	0.64
27:c:75:C:H1'	27:c:76:A:H5'	1.79	0.64
2:A:94:ILE:HG22	2:A:102:ALA:H	1.61	0.64
30:G:99:THR:HG22	30:G:101:GLU:H	1.62	0.64
3:B:2226:A:H2'	3:B:2227:A:C8	2.33	0.63
10:J:11:GLY:HA2	10:J:31:PRO:HG3	1.80	0.63
3:B:2600:G:H8	24:Y:3:ARG:HB2	1.63	0.63
3:B:257:G:C8	3:B:258:U:H1'	2.34	0.63
18:S:49:GLU:HG2	18:S:94:TYR:HD1	1.64	0.63
18:S:44:ILE:HD12	18:S:47:VAL:HB	1.79	0.63
30:G:107:ASP:O	30:G:121:PHE:HB3	1.99	0.63
3:B:379:A:H4'	3:B:380:U:H5''	1.81	0.63
25:a:1:MET:N	25:a:1:MET:HE2	2.14	0.63
19:T:41:ARG:HD2	19:T:94:VAL:HG21	1.80	0.62
1:Z:4:ARG:HH11	1:Z:4:ARG:HG2	1.64	0.62
3:B:1710:A:H2'	3:B:1711:A:C8	2.34	0.62
30:G:96:LYS:HG2	30:G:97:ARG:HH11	1.64	0.62
3:B:680:A:H62	3:B:699:G:N2	1.81	0.62
24:Y:54:PRO:HD3	24:Y:66:TRP:CE2	2.35	0.62
21:V:109:ARG:HG3	21:V:109:ARG:HH11	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:195:VAL:HG12	2:A:196:SER:H	1.65	0.61
3:B:1540:G:H4'	21:V:6:THR:HG22	1.82	0.61
2:A:182:ARG:HG2	2:A:183:LEU:H	1.66	0.61
19:T:37:LEU:HB2	19:T:128:LYS:O	2.01	0.61
16:P:31:THR:HG22	16:P:32:THR:H	1.64	0.61
3:B:933:A:H61	19:T:83:MET:HE2	1.65	0.61
3:B:837:G:H2'	3:B:838:C:C6	2.35	0.61
3:B:1411:U:H2'	3:B:1412:C:H6	1.64	0.61
22:W:33:ILE:HD12	22:W:55:ILE:HG21	1.82	0.60
10:J:16:ASN:ND2	10:J:24:LYS:HB3	2.15	0.60
12:L:83:HIS:HB2	12:L:90:ILE:HD11	1.81	0.60
14:N:19:GLU:HA	14:N:22:PHE:HB2	1.84	0.60
19:T:46:GLN:OE1	19:T:126:PRO:HD3	2.01	0.60
4:C:23:MET:HE2	4:C:47:PRO:HB2	1.83	0.60
2:A:160:THR:HB	2:A:177:GLN:HG3	1.82	0.60
14:N:49:MET:HE3	14:N:49:MET:O	2.01	0.59
17:Q:88:ILE:HG23	17:Q:90:ILE:HG13	1.83	0.59
21:V:1:MET:HB3	21:V:32:THR:HB	1.82	0.59
3:B:1463:G:H2'	3:B:1464:G:C8	2.37	0.59
14:N:93:ILE:HG22	14:N:94:LYS:H	1.67	0.59
21:V:39:ILE:HD13	21:V:62:ILE:HD11	1.85	0.59
23:X:11:ARG:HG3	23:X:17:GLN:NE2	2.17	0.59
13:M:45:ARG:HG3	13:M:46:HIS:N	2.16	0.59
3:B:1665:A:H3'	3:B:1666:G:C8	2.39	0.58
9:I:26:LYS:HB3	14:N:22:PHE:CD2	2.38	0.58
1:Z:14:ASP:HB2	1:Z:36:MET:SD	2.43	0.58
1:Z:22:ARG:HH12	3:B:2604:C:H3'	1.68	0.58
20:U:107:VAL:HG11	20:U:115:ILE:HD12	1.85	0.58
3:B:1284:A:N6	3:B:1480:C:O2	2.34	0.58
11:K:26:PHE:O	11:K:29:GLU:HG3	2.03	0.58
29:R:97:ARG:HG2	29:R:97:ARG:NH1	2.18	0.58
3:B:973:A:H2'	3:B:974:A:C8	2.39	0.58
30:G:95:ILE:HG22	30:G:98:ILE:HD11	1.86	0.57
3:B:1413:U:H2'	3:B:1414:G:H8	1.70	0.57
3:B:268:G:H1	3:B:332:C:H41	1.51	0.57
10:J:38:LEU:HD23	10:J:65:LEU:HD13	1.86	0.57
3:B:1318:G:N2	14:N:97:TYR:HB3	2.20	0.57
3:B:1318:G:OP2	3:B:1318:G:H8	1.87	0.57
2:A:146:LEU:HD21	2:A:154:ILE:HD11	1.87	0.57
18:S:43:GLU:HA	18:S:43:GLU:OE1	2.03	0.57
24:Y:69:THR:O	24:Y:73:VAL:HG23	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:14:ARG:HG3	2:A:14:ARG:HH11	1.70	0.56
3:B:43:A:H2'	3:B:44:A:C8	2.40	0.56
6:E:33:LYS:HB3	6:E:51:GLU:HG2	1.87	0.56
8:H:16:ILE:H	8:H:16:ILE:HD12	1.70	0.56
14:N:16:MET:HG2	14:N:20:SER:HB3	1.87	0.56
19:T:29:PHE:HB3	19:T:65:TRP:CE3	2.41	0.56
3:B:837:G:H2'	3:B:838:C:H6	1.70	0.56
19:T:36:ALA:HB2	19:T:103:LEU:HD21	1.88	0.56
18:S:104:TYR:CD1	18:S:104:TYR:O	2.59	0.56
3:B:1705:A:HO2'	3:B:1706:G:H8	1.54	0.56
3:B:1873:C:H2'	3:B:1874:C:C6	2.40	0.55
3:B:2068:U:H2'	3:B:2069:C:C6	2.40	0.55
24:Y:153:ARG:O	24:Y:163:VAL:HG12	2.06	0.55
3:B:2315:C:N4	3:B:2316:C:H41	2.04	0.55
2:A:29:PRO:HB3	2:A:63:ARG:NH1	2.22	0.55
17:Q:58:ARG:HA	17:Q:61:TRP:CE3	2.41	0.55
22:W:99:PRO:HG2	22:W:128:ALA:HB2	1.88	0.55
2:A:94:ILE:HG22	2:A:102:ALA:N	2.20	0.55
3:B:394:U:H2'	3:B:395:C:C6	2.41	0.55
24:Y:73:VAL:O	24:Y:77:VAL:HG22	2.07	0.55
30:G:87:GLU:OE2	30:G:100:ILE:HD11	2.07	0.55
3:B:828:G:C6	3:B:896:G:C6	2.95	0.55
2:A:273:LYS:HG3	2:A:275:GLY:H	1.71	0.55
3:B:128:G:H2'	3:B:129:A:C8	2.42	0.55
24:Y:58:ARG:HG3	24:Y:63:TRP:CH2	2.42	0.54
3:B:271:A:H2'	3:B:272:G:O4'	2.07	0.54
3:B:2593:G:HO2'	3:B:2594:C:H6	1.53	0.54
14:N:53:LYS:O	14:N:56:ILE:C	2.51	0.54
23:X:34:LEU:H	23:X:35:PRO:CD	2.20	0.54
3:B:1919:A:H2'	3:B:1920:C:C6	2.42	0.54
3:B:901:G:N2	8:H:49:MET:HE1	2.23	0.54
3:B:728:G:H2'	3:B:729:U:C6	2.43	0.54
3:B:1001:A:N6	3:B:1101:G:H2'	2.23	0.54
22:W:90:ILE:HD12	22:W:90:ILE:H	1.72	0.54
3:B:785:U:O2	3:B:1227:G:H5'	2.07	0.54
24:Y:96:ARG:HG3	24:Y:96:ARG:HH11	1.72	0.54
22:W:90:ILE:HD12	22:W:90:ILE:N	2.23	0.54
19:T:29:PHE:HB3	19:T:65:TRP:CZ3	2.43	0.53
25:a:84:THR:HG22	25:a:84:THR:O	2.08	0.53
26:b:54:SER:HB2	26:b:78:LYS:HB2	1.89	0.53
2:A:222:GLY:HA2	2:A:225:MET:HE3	1.88	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1284:A:H2'	3:B:1285:A:O4'	2.08	0.53
3:B:1360:A:H2'	3:B:1361:A:C8	2.43	0.53
24:Y:164:ARG:HB2	24:Y:168:GLU:OE1	2.09	0.53
25:a:6:LYS:HB2	25:a:125:ILE:HG22	1.91	0.53
25:a:50:THR:HG23	25:a:91:PRO:HD2	1.90	0.53
20:U:106:LEU:H	20:U:106:LEU:HD23	1.73	0.53
2:A:159:GLY:H	2:A:195:VAL:HB	1.74	0.53
1:Z:13:ARG:HB3	1:Z:36:MET:SD	2.49	0.53
24:Y:78:LYS:HD2	24:Y:78:LYS:O	2.08	0.53
2:A:143:ASN:OD1	2:A:152:GLY:HA3	2.09	0.53
18:S:45:ARG:HB3	18:S:46:PRO:HD3	1.91	0.53
2:A:131:PRO:HD3	2:A:189:MET:HE2	1.90	0.53
3:B:208:C:H5	3:B:218:G:H21	1.57	0.52
3:B:257:G:H3'	3:B:258:U:H4'	1.90	0.52
3:B:63:A:C2	9:I:59:THR:HG22	2.44	0.52
20:U:101:LEU:HD22	20:U:106:LEU:HD12	1.91	0.52
27:c:73:U:H5''	27:c:74:C:H5''	1.90	0.52
3:B:2169:C:H5''	3:B:2170:G:OP1	2.09	0.52
11:K:40:GLN:HG3	11:K:42:GLY:O	2.09	0.52
30:G:53:ILE:HD12	30:G:53:ILE:O	2.10	0.52
3:B:1420:A:H4'	3:B:1421:U:OP2	2.09	0.52
12:L:80:VAL:HG22	12:L:92:VAL:HG13	1.91	0.52
3:B:883:A:H2'	3:B:884:A:C8	2.45	0.52
30:G:96:LYS:HG2	30:G:97:ARG:NH1	2.24	0.52
3:B:1413:U:H2'	3:B:1414:G:C8	2.45	0.52
1:Z:2:LYS:HD3	1:Z:4:ARG:HD2	1.92	0.52
3:B:36:G:H5''	3:B:37:G:OP1	2.10	0.52
16:P:95:VAL:O	16:P:96:LEU:HD23	2.09	0.52
8:H:25:THR:HG23	8:H:49:MET:HG2	1.92	0.52
9:I:52:ARG:HH11	9:I:52:ARG:HG3	1.75	0.52
24:Y:3:ARG:HG2	24:Y:7:TYR:HE2	1.75	0.52
3:B:613:C:H2'	3:B:614:U:C6	2.45	0.52
22:W:26:LEU:HB2	22:W:63:ILE:HD12	1.92	0.52
13:M:95:ARG:HH21	13:M:104:ILE:HG21	1.75	0.51
18:S:46:PRO:O	18:S:50:LYS:HG3	2.10	0.51
30:G:49:LYS:HE2	30:G:51:GLU:OE1	2.09	0.51
26:b:35:VAL:HG12	26:b:93:ALA:HA	1.92	0.51
3:B:2375:G:C6	3:B:2376:C:C4	2.97	0.51
3:B:1699:G:H2'	3:B:1700:C:H6	1.75	0.51
13:M:85:PHE:HE1	13:M:95:ARG:HG2	1.75	0.51
14:N:21:MET:HA	14:N:24:ILE:HD12	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:G:104:ASN:O	30:G:106:THR:HG22	2.10	0.51
23:X:11:ARG:HD2	23:X:138:GLU:OE1	2.10	0.51
15:O:70:ALA:O	15:O:76:LEU:HB2	2.10	0.51
24:Y:145:VAL:O	24:Y:149:ILE:HG22	2.11	0.51
20:U:123:LEU:HD23	20:U:123:LEU:H	1.75	0.51
25:a:49:ARG:HG3	25:a:93:VAL:HG23	1.92	0.51
3:B:1912:C:H2'	3:B:1913:C:C6	2.46	0.51
4:C:13:ARG:HG3	4:C:13:ARG:HH11	1.76	0.51
10:J:37:THR:OG1	10:J:48:ARG:HD2	2.10	0.51
11:K:37:ILE:HG22	11:K:38:VAL:HG23	1.93	0.51
21:V:109:ARG:HG3	21:V:109:ARG:NH1	2.26	0.51
2:A:17:VAL:HG12	2:A:204:HIS:H	1.75	0.50
2:A:122:THR:H	2:A:130:MET:HE3	1.75	0.50
3:B:1699:G:H2'	3:B:1700:C:C6	2.46	0.50
7:F:10:PRO:HA	7:F:13:MET:HE3	1.92	0.50
9:I:28:GLU:OE1	9:I:28:GLU:HA	2.11	0.50
20:U:144:LYS:HE3	20:U:144:LYS:HA	1.93	0.50
24:Y:58:ARG:HG3	24:Y:63:TRP:CZ3	2.46	0.50
23:X:65:ARG:O	23:X:65:ARG:HG2	2.11	0.50
3:B:1174:U:H2'	3:B:1175:U:C6	2.47	0.50
9:I:27:ARG:HA	14:N:22:PHE:HZ	1.76	0.50
16:P:84:ARG:O	16:P:85:ARG:HG2	2.10	0.50
30:G:86:VAL:O	30:G:90:LEU:HD22	2.12	0.50
2:A:62:TYR:HE2	3:B:1673:C:H5''	1.77	0.50
22:W:132:HIS:CE1	22:W:135:GLU:HG2	2.46	0.50
24:Y:19:ILE:HG13	24:Y:19:ILE:O	2.10	0.50
3:B:1388:G:H2'	3:B:1389:A:C8	2.47	0.50
30:G:100:ILE:HG22	30:G:100:ILE:O	2.12	0.50
3:B:1913:C:H2'	3:B:1914:U:H6	1.77	0.49
2:A:145:GLU:HG2	2:A:151:GLY:O	2.12	0.49
21:V:64:ARG:HB2	21:V:83:ALA:HB3	1.94	0.49
3:B:1588:U:O2	3:B:1601:G:C6	2.64	0.49
22:W:50:ASP:OD1	22:W:120:GLN:HG3	2.12	0.49
3:B:835:G:H2'	3:B:836:A:O4'	2.12	0.49
14:N:44:VAL:HG22	14:N:97:TYR:CD1	2.47	0.49
24:Y:88:LEU:HD23	24:Y:163:VAL:HG22	1.95	0.49
3:B:2056:A:C2	3:B:2066:G:N1	2.76	0.49
3:B:2257:U:O2'	3:B:2258:G:H8	1.96	0.49
22:W:73:LYS:HB3	22:W:90:ILE:CD1	2.38	0.49
3:B:1705:A:O2'	3:B:1706:G:H8	1.95	0.49
26:b:149:GLN:OE1	26:b:153:PRO:HG2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:21:ARG:HB2	2:A:24:LEU:HD11	1.95	0.49
9:I:11:ARG:HG2	9:I:60:VAL:HG13	1.94	0.49
12:L:34:TYR:CD1	12:L:34:TYR:C	2.91	0.49
14:N:16:MET:HB3	14:N:21:MET:HE2	1.93	0.49
14:N:28:PRO:O	14:N:30:ILE:HG13	2.13	0.49
14:N:61:GLU:HG2	14:N:68:VAL:HG23	1.94	0.49
3:B:834:A:H2'	3:B:835:G:O4'	2.13	0.49
30:G:41:ILE:HD12	30:G:90:LEU:HD11	1.95	0.49
9:I:25:LEU:HD23	9:I:54:ILE:HD13	1.94	0.48
16:P:2:PHE:CE1	16:P:42:GLY:HA3	2.47	0.48
2:A:154:ILE:HG21	2:A:176:LEU:HD22	1.95	0.48
3:B:417:G:H21	25:a:47:THR:HG22	1.77	0.48
1:Z:21:ARG:HG3	1:Z:21:ARG:O	2.13	0.48
9:I:27:ARG:HA	14:N:22:PHE:CZ	2.48	0.48
14:N:104:GLN:N	14:N:104:GLN:OE1	2.46	0.48
26:b:125:ARG:HA	26:b:166:MET:HE3	1.95	0.48
3:B:2120:G:H2'	3:B:2121:U:C6	2.48	0.48
1:Z:22:ARG:HB2	1:Z:27:TYR:CE1	2.48	0.48
13:M:97:ALA:HB2	13:M:104:ILE:HD11	1.95	0.48
28:d:0:C:H2'	28:d:1:U:C6	2.48	0.48
29:R:95:LYS:HD2	29:R:96:VAL:N	2.29	0.48
29:R:104:LEU:HD22	29:R:104:LEU:H	1.78	0.48
3:B:2:A:H2'	3:B:3:G:C8	2.49	0.48
14:N:110:ALA:C	14:N:111:LYS:HE2	2.38	0.48
16:P:1:MET:HB2	16:P:43:SER:HA	1.95	0.48
3:B:1404:U:H4'	3:B:1404:U:OP1	2.14	0.48
3:B:1609:G:H2'	3:B:1610:G:C8	2.49	0.48
3:B:1776:A:H2'	3:B:1777:G:O4'	2.13	0.48
23:X:75:MET:HE1	23:X:109:GLY:HA2	1.94	0.48
3:B:840:C:H42	3:B:882:A:H61	1.60	0.48
3:B:896:G:C2	3:B:897:A:C5	3.02	0.48
3:B:1397:A:H2'	3:B:1398:A:C8	2.49	0.48
3:B:2190:G:H2'	3:B:2191:C:C6	2.49	0.48
24:Y:3:ARG:HG2	24:Y:7:TYR:CE2	2.48	0.48
3:B:1114:G:H21	22:W:110:MET:HE2	1.78	0.48
3:B:1705:A:C2'	3:B:1706:G:H8	2.26	0.48
13:M:11:VAL:HG21	13:M:70:LEU:HD22	1.96	0.48
13:M:85:PHE:CE1	13:M:95:ARG:HG2	2.49	0.48
14:N:99:GLN:HE21	14:N:99:GLN:C	2.17	0.48
3:B:2421:A:C8	26:b:150:ARG:HD2	2.49	0.48
18:S:73:GLU:O	18:S:77:THR:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:209:GLY:HA2	3:B:738:A:H5'	1.96	0.47
3:B:394:U:H2'	3:B:395:C:H6	1.79	0.47
3:B:1659:A:H2'	3:B:1660:A:H8	1.77	0.47
14:N:69:VAL:HB	14:N:99:GLN:HG3	1.96	0.47
16:P:51:ALA:HB2	17:Q:88:ILE:HG13	1.95	0.47
17:Q:62:ILE:HG13	17:Q:92:ARG:HD3	1.96	0.47
25:a:21:GLU:H	25:a:21:GLU:CD	2.21	0.47
3:B:787:U:H2'	3:B:788:C:H6	1.79	0.47
3:B:1435:C:H2'	3:B:1436:U:O4'	2.14	0.47
3:B:2421:A:N7	26:b:151:GLN:HG2	2.30	0.47
9:I:25:LEU:HB3	9:I:54:ILE:HD11	1.95	0.47
9:I:26:LYS:HB3	14:N:22:PHE:CE2	2.49	0.47
17:Q:72:GLN:OE1	17:Q:72:GLN:HA	2.14	0.47
3:B:1629:G:C2	3:B:1631:C:OP1	2.67	0.47
12:L:80:VAL:CG2	12:L:92:VAL:HG13	2.44	0.47
23:X:99:ARG:CZ	23:X:114:ARG:HD2	2.44	0.47
25:a:1:MET:HE2	25:a:1:MET:H2	1.79	0.47
4:C:22:VAL:O	4:C:50:MET:HG3	2.13	0.47
8:H:10:LYS:HB2	8:H:37:GLU:OE1	2.14	0.47
23:X:62:LEU:O	23:X:66:GLU:HG2	2.14	0.47
24:Y:59:SER:O	24:Y:63:TRP:HB2	2.15	0.47
29:R:78:PHE:HB3	29:R:85:ILE:HD11	1.95	0.47
1:Z:36:MET:O	1:Z:36:MET:HG3	2.15	0.47
9:I:13:LYS:HB3	9:I:13:LYS:HE2	1.65	0.47
30:G:111:LEU:HB2	30:G:118:VAL:HG22	1.97	0.47
3:B:728:G:H2'	3:B:729:U:H6	1.80	0.47
19:T:27:LEU:HD23	19:T:105:GLU:OE2	2.14	0.47
20:U:102:ARG:HA	20:U:107:VAL:HG22	1.96	0.47
3:B:270:A:H2'	3:B:271:A:C8	2.50	0.47
3:B:2226:A:H2'	3:B:2227:A:H8	1.77	0.47
8:H:54:ALA:HA	8:H:57:ILE:HD11	1.97	0.47
20:U:42:GLU:O	20:U:42:GLU:HG2	2.15	0.47
23:X:13:GLU:OE1	23:X:13:GLU:HA	2.15	0.47
24:Y:33:LEU:HD12	24:Y:76:LEU:HG	1.97	0.47
24:Y:104:LEU:HD21	24:Y:149:ILE:HD12	1.97	0.47
11:K:71:ARG:HD2	11:K:75:GLY:HA2	1.97	0.47
28:d:76:U:H2'	28:d:77:G:C8	2.50	0.47
3:B:883:A:C8	19:T:13:HIS:ND1	2.83	0.47
3:B:1114:G:N2	22:W:110:MET:HE2	2.30	0.47
3:B:2097:C:H2'	3:B:2098:U:O4'	2.15	0.47
3:B:2592:C:H2'	3:B:2593:G:H5''	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:163:VAL:HG22	24:Y:163:VAL:O	2.15	0.47
28:d:62:A:H61	28:d:102:U:H2'	1.80	0.47
3:B:542:G:H2'	3:B:1878:A:N7	2.29	0.47
3:B:1588:U:H2'	3:B:1589:G:C8	2.51	0.46
24:Y:52:ILE:HD12	24:Y:52:ILE:O	2.15	0.46
1:Z:4:ARG:HE	1:Z:10:ALA:HB2	1.79	0.46
2:A:34:THR:HG23	2:A:63:ARG:HG2	1.97	0.46
2:A:76:GLY:HA3	2:A:96:TYR:HA	1.97	0.46
3:B:256:A:H1'	3:B:258:U:N3	2.30	0.46
4:C:57:THR:O	4:C:60:GLN:HG2	2.15	0.46
15:O:104:ARG:H	15:O:104:ARG:HG2	1.56	0.46
3:B:2177:A:H2'	3:B:2178:U:C6	2.49	0.46
28:d:71:G:H2'	28:d:72:A:O4'	2.15	0.46
3:B:29:A:H1'	25:a:47:THR:HG23	1.97	0.46
3:B:417:G:N2	25:a:47:THR:HG22	2.29	0.46
3:B:2257:U:HO2'	3:B:2258:G:H8	1.59	0.46
4:C:31:HIS:ND1	4:C:31:HIS:C	2.74	0.46
3:B:343:U:H5'	3:B:345:G:H21	1.79	0.46
3:B:2498:U:H2'	3:B:2499:C:H6	1.80	0.46
3:B:2601:C:H3'	3:B:2602:A:H8	1.81	0.46
15:O:45:ILE:HG23	15:O:60:ARG:HD2	1.96	0.46
26:b:53:MET:HG2	26:b:54:SER:N	2.30	0.46
7:F:46:CYS:SG	7:F:48:HIS:HB2	2.56	0.46
29:R:8:GLU:HG2	29:R:59:LEU:HB3	1.96	0.46
3:B:2488:A:H5''	22:W:97:LYS:HG3	1.97	0.46
12:L:65:GLU:OE2	12:L:65:GLU:HA	2.14	0.46
16:P:20:LEU:HD13	16:P:22:VAL:HG13	1.98	0.46
29:R:41:ARG:HH12	29:R:43:ARG:HE	1.64	0.46
2:A:19:ILE:HG23	2:A:203:GLN:OE1	2.15	0.46
2:A:72:PHE:HD1	2:A:72:PHE:O	1.99	0.46
3:B:1913:C:H2'	3:B:1914:U:C6	2.50	0.46
22:W:149:ARG:HG2	22:W:149:ARG:NH1	2.31	0.46
24:Y:150:ARG:HG2	24:Y:150:ARG:O	2.15	0.46
28:d:69:A:C6	28:d:99:C:C2	3.04	0.46
3:B:1504:A:C6	3:B:1511:A:N6	2.84	0.46
3:B:1588:U:C2	3:B:1601:G:O6	2.68	0.46
3:B:1666:G:H2'	3:B:1667:A:C8	2.51	0.46
3:B:177:A:H2'	3:B:178:C:C6	2.51	0.46
3:B:942:G:H2'	3:B:943:U:C6	2.51	0.46
6:E:15:ALA:O	6:E:16:GLU:HG2	2.15	0.46
10:J:67:SER:O	10:J:71:THR:HG22	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:149:ARG:HG2	22:W:149:ARG:HH11	1.81	0.46
3:B:303:A:H2'	3:B:303:A:N3	2.32	0.45
3:B:2194:G:N3	3:B:2230:C:H2'	2.31	0.45
14:N:78:GLY:HA3	14:N:90:ARG:O	2.17	0.45
18:S:24:MET:HG2	18:S:44:ILE:HG21	1.97	0.45
30:G:61:ARG:NH2	30:G:136:GLY:HA2	2.31	0.45
3:B:931:U:H5	19:T:41:ARG:HH12	1.63	0.45
3:B:2176:A:H2'	3:B:2177:A:C8	2.51	0.45
3:B:2523:A:H4'	21:V:30:ARG:HG3	1.97	0.45
10:J:69:LEU:HB3	10:J:85:LYS:HG3	1.99	0.45
12:L:46:ASP:OD2	12:L:46:ASP:C	2.58	0.45
17:Q:83:LEU:HD23	17:Q:83:LEU:HA	1.74	0.45
23:X:130:GLU:OE2	23:X:144:THR:HG22	2.17	0.45
3:B:2351:G:H5''	3:B:2352:A:H5''	1.97	0.45
11:K:33:ALA:O	11:K:61:ALA:HB3	2.16	0.45
12:L:6:SER:O	12:L:7:LEU:HD23	2.16	0.45
18:S:25:ALA:HB2	18:S:44:ILE:HD11	1.98	0.45
2:A:14:ARG:HG3	2:A:14:ARG:NH1	2.32	0.45
21:V:47:ILE:HD12	21:V:47:ILE:O	2.16	0.45
25:a:5:ILE:HD13	25:a:124:VAL:HG12	1.98	0.45
3:B:607:G:H2'	3:B:608:C:C6	2.51	0.45
3:B:1174:U:H2'	3:B:1175:U:H6	1.82	0.45
18:S:2:ARG:O	18:S:2:ARG:HG2	2.16	0.45
26:b:110:VAL:HG11	26:b:194:ILE:HG23	1.98	0.45
2:A:196:SER:O	2:A:198:PRO:HD3	2.17	0.45
3:B:268:G:H22	3:B:332:C:H5	1.65	0.45
3:B:1651:G:H2'	3:B:1652:C:H6	1.81	0.45
3:B:1676:A:H4'	3:B:1677:U:H5''	1.98	0.45
3:B:2135:G:H4'	3:B:2136:A:O4'	2.16	0.45
16:P:18:ILE:HD13	16:P:18:ILE:HA	1.75	0.45
20:U:21:ARG:HE	20:U:21:ARG:HB3	1.63	0.45
25:a:1:MET:HE2	25:a:1:MET:H1	1.81	0.45
26:b:28:LEU:HD13	26:b:204:ILE:HD11	1.99	0.45
3:B:787:U:H2'	3:B:788:C:C6	2.51	0.45
3:B:2451:A:N3	3:B:2451:A:H2'	2.32	0.45
25:a:169:LYS:HE2	25:a:169:LYS:HB3	1.78	0.45
2:A:63:ARG:CD	2:A:84:ASP:HB2	2.47	0.45
3:B:2044:C:H2'	3:B:2045:U:C6	2.52	0.45
13:M:95:ARG:NH2	13:M:104:ILE:HG21	2.32	0.45
15:O:54:ARG:O	15:O:57:GLN:HG3	2.17	0.45
3:B:71:G:C6	3:B:72:G:N7	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:258:U:H2'	3:B:259:G:O4'	2.16	0.45
3:B:1868:A:H5'	7:F:9:THR:HG21	1.98	0.45
3:B:2485:U:H4'	26:b:82:GLU:OE2	2.17	0.45
18:S:95:THR:HG22	18:S:115:MET:HG2	1.99	0.45
24:Y:167:THR:HG23	24:Y:167:THR:O	2.16	0.45
2:A:187:GLU:N	2:A:187:GLU:OE1	2.50	0.44
3:B:1153:G:O5'	3:B:1153:G:H8	1.99	0.44
13:M:102:GLU:HG2	13:M:103:VAL:H	1.81	0.44
20:U:90:LEU:O	20:U:90:LEU:HG	2.17	0.44
21:V:97:ARG:NH2	30:G:134:MET:HB3	2.32	0.44
24:Y:123:LYS:HB2	24:Y:123:LYS:HE2	1.65	0.44
30:G:98:ILE:N	30:G:98:ILE:HD12	2.32	0.44
3:B:931:U:H5	19:T:41:ARG:NH1	2.16	0.44
8:H:15:ALA:O	8:H:16:ILE:C	2.60	0.44
25:a:126:ASP:OD1	25:a:126:ASP:C	2.60	0.44
3:B:256:A:H1'	3:B:258:U:C2	2.52	0.44
3:B:258:U:H5'	3:B:259:G:OP2	2.17	0.44
3:B:829:G:H2'	3:B:830:G:C8	2.52	0.44
3:B:1155:U:H2'	3:B:1156:A:C8	2.52	0.44
22:W:33:ILE:O	22:W:37:LEU:HB2	2.17	0.44
26:b:42:GLU:CD	26:b:42:GLU:H	2.25	0.44
3:B:717:C:OP1	26:b:136:GLY:HA2	2.18	0.44
3:B:896:G:N1	3:B:897:A:C5	2.86	0.44
3:B:2449:A:O2'	3:B:2450:C:H5'	2.18	0.44
22:W:138:GLN:H	22:W:138:GLN:HG3	1.63	0.44
3:B:2369:C:C6	3:B:2416:G:H1'	2.52	0.44
11:K:46:MET:HE1	11:K:76:ARG:HE	1.83	0.44
26:b:39:ARG:O	26:b:47:THR:HA	2.18	0.44
29:R:76:ARG:HG2	29:R:78:PHE:CZ	2.53	0.44
30:G:61:ARG:HH22	30:G:136:GLY:HA2	1.82	0.44
1:Z:10:ALA:HA	1:Z:13:ARG:HG3	2.00	0.44
3:B:457:C:H4'	13:M:46:HIS:ND1	2.32	0.44
23:X:51:GLU:HA	23:X:51:GLU:OE2	2.17	0.44
2:A:26:LYS:H	2:A:26:LYS:HG2	1.60	0.44
3:B:933:A:H61	19:T:83:MET:CE	2.30	0.44
7:F:61:LEU:HD12	7:F:61:LEU:HA	1.78	0.44
16:P:95:VAL:C	16:P:96:LEU:HD23	2.42	0.44
19:T:59:LYS:O	19:T:60:ARG:HG2	2.17	0.44
2:A:28:LYS:HD2	2:A:28:LYS:HA	1.65	0.44
3:B:1493:G:O2'	5:D:1:MET:HG3	2.17	0.44
9:I:26:LYS:O	14:N:22:PHE:HE2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:74:ALA:HB3	20:U:115:ILE:HD13	1.99	0.44
21:V:113:LYS:HD3	30:G:110:LEU:HD23	1.99	0.44
26:b:20:GLY:HA2	29:R:83:PRO:HG2	2.00	0.44
29:R:55:SER:HB3	29:R:62:ASN:OD1	2.18	0.44
3:B:1303:U:H2'	3:B:1304:A:C8	2.53	0.44
3:B:2364:C:H2'	3:B:2365:A:H8	1.83	0.44
13:M:44:LYS:NZ	13:M:44:LYS:HB3	2.33	0.44
14:N:94:LYS:HE2	14:N:94:LYS:HB3	1.54	0.44
17:Q:48:ARG:O	17:Q:48:ARG:HG2	2.18	0.44
23:X:101:ILE:HG13	23:X:145:VAL:HG11	2.00	0.44
2:A:20:ASP:OD2	2:A:20:ASP:C	2.60	0.43
3:B:154:G:C2	3:B:155:G:C8	3.05	0.43
22:W:116:LEU:O	22:W:116:LEU:HD12	2.18	0.43
30:G:82:MET:O	30:G:86:VAL:HG23	2.17	0.43
30:G:87:GLU:OE1	30:G:98:ILE:HB	2.18	0.43
30:G:88:ASP:HA	30:G:91:ASN:ND2	2.33	0.43
2:A:71:LYS:HE3	2:A:74:VAL:HG11	2.00	0.43
2:A:158:ALA:HB3	3:B:1677:U:O2'	2.18	0.43
3:B:162:A:O2'	3:B:163:G:H5'	2.18	0.43
3:B:1651:G:H2'	3:B:1652:C:C6	2.53	0.43
12:L:53:GLU:C	12:L:53:GLU:OE2	2.61	0.43
14:N:70:SER:H	14:N:99:GLN:HB3	1.83	0.43
3:B:679:A:C2	3:B:701:A:H1'	2.54	0.43
3:B:2375:G:C5	3:B:2376:C:C5	3.07	0.43
3:B:2589:A:H2'	3:B:2590:A:C8	2.52	0.43
5:D:34:ARG:NH2	5:D:39:ARG:HD2	2.33	0.43
14:N:72:ASN:OD1	14:N:72:ASN:N	2.50	0.43
26:b:12:MET:HE2	26:b:12:MET:HB3	1.83	0.43
30:G:115:ASP:OD1	30:G:115:ASP:N	2.51	0.43
3:B:138:A:H2'	3:B:139:U:C6	2.53	0.43
3:B:1665:A:H3'	3:B:1666:G:H8	1.83	0.43
3:B:2498:U:H2'	3:B:2499:C:C6	2.53	0.43
22:W:143:ASP:OD2	22:W:143:ASP:C	2.61	0.43
3:B:807:A:H2'	3:B:808:G:C8	2.54	0.43
14:N:53:LYS:O	14:N:56:ILE:O	2.37	0.43
29:R:76:ARG:HG2	29:R:78:PHE:CE1	2.53	0.43
3:B:20:U:H2'	3:B:21:G:C8	2.54	0.43
3:B:146:A:C8	3:B:153:A:C2	3.07	0.43
3:B:1126:G:H2'	3:B:1127:U:C6	2.54	0.43
6:E:40:ASP:C	6:E:40:ASP:OD1	2.61	0.43
23:X:33:LEU:O	23:X:34:LEU:HD23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:68:U:O2'	27:c:69:U:H5'	2.19	0.43
30:G:121:PHE:CE1	30:G:126:ARG:HD3	2.54	0.43
3:B:926:G:C2	3:B:927:G:C8	3.07	0.43
3:B:1102:A:H8	3:B:1102:A:OP1	2.02	0.43
3:B:1867:A:H4'	17:Q:34:ILE:HD12	1.99	0.43
23:X:18:MET:HB2	23:X:18:MET:HE2	1.72	0.43
23:X:43:ASN:C	23:X:43:ASN:OD1	2.61	0.43
30:G:71:ALA:HB3	30:G:120:LEU:HB3	2.00	0.43
3:B:1543:A:C8	21:V:5:GLU:HG3	2.54	0.43
20:U:54:LEU:HD12	20:U:55:PRO:HD2	2.00	0.43
2:A:88:THR:OG1	2:A:158:ALA:HB2	2.19	0.43
3:B:1334:C:H2'	3:B:1335:G:O4'	2.19	0.43
3:B:1487:G:O2'	5:D:3:ARG:HD2	2.19	0.43
7:F:12:ARG:O	7:F:12:ARG:HG3	2.18	0.43
15:O:14:GLU:HB3	15:O:120:ALA:HA	2.01	0.43
23:X:84:ARG:HB3	23:X:84:ARG:NH1	2.34	0.43
25:a:28:ARG:O	25:a:32:MET:HG3	2.19	0.43
11:K:19:ARG:HA	11:K:19:ARG:HD3	1.86	0.42
14:N:89:ARG:HD2	14:N:90:ARG:N	2.33	0.42
23:X:45:GLN:OE1	23:X:45:GLN:C	2.62	0.42
30:G:97:ARG:HD3	30:G:97:ARG:N	2.33	0.42
3:B:2228:G:H2'	3:B:2229:U:C6	2.54	0.42
10:J:12:VAL:HA	10:J:29:PHE:O	2.19	0.42
10:J:33:LEU:HA	10:J:33:LEU:HD23	1.77	0.42
11:K:33:ALA:O	11:K:35:ASN:N	2.52	0.42
22:W:75:PHE:O	22:W:87:GLU:HA	2.19	0.42
24:Y:43:ALA:HB2	24:Y:52:ILE:HG22	2.01	0.42
2:A:108:GLN:OE1	2:A:198:PRO:HG3	2.20	0.42
3:B:1196:C:H4'	3:B:1197:G:OP2	2.19	0.42
22:W:20:ASP:OD2	22:W:20:ASP:C	2.61	0.42
23:X:138:GLU:OE1	23:X:138:GLU:HA	2.20	0.42
3:B:85:A:H2'	3:B:86:A:O4'	2.19	0.42
20:U:133:GLY:HA2	20:U:151:VAL:HG23	2.00	0.42
22:W:97:LYS:HA	22:W:97:LYS:HD3	1.70	0.42
30:G:128:LEU:HD23	30:G:128:LEU:HA	1.70	0.42
3:B:916:A:O5'	3:B:916:A:H8	2.03	0.42
3:B:1595:A:H2'	3:B:1596:A:C8	2.54	0.42
5:D:34:ARG:CZ	5:D:39:ARG:HD2	2.49	0.42
9:I:23:LEU:HD23	9:I:23:LEU:HA	1.84	0.42
12:L:89:PRO:C	12:L:90:ILE:HD13	2.45	0.42
17:Q:35:ALA:O	17:Q:39:VAL:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:139:ILE:O	20:U:143:GLU:HG3	2.20	0.42
24:Y:159:LYS:HA	24:Y:159:LYS:HD3	1.80	0.42
28:d:110:A:H8	28:d:110:A:OP2	2.00	0.42
2:A:44:ASN:HD22	2:A:50:THR:CG2	2.32	0.42
3:B:988:U:H2'	3:B:989:G:C8	2.54	0.42
3:B:1271:U:C4	3:B:1272:C:C5	3.08	0.42
10:J:66:ASP:O	10:J:70:ILE:HG13	2.19	0.42
18:S:44:ILE:O	18:S:44:ILE:HG23	2.20	0.42
19:T:91:GLU:HA	19:T:91:GLU:OE1	2.19	0.42
3:B:235:C:H5'	3:B:2243:C:O2'	2.19	0.42
3:B:837:G:N3	3:B:838:C:C5	2.88	0.42
12:L:59:TRP:CE3	12:L:77:LEU:HD23	2.54	0.42
15:O:79:ASP:OD2	15:O:79:ASP:C	2.62	0.42
22:W:154:ASN:OD1	22:W:154:ASN:C	2.62	0.42
24:Y:96:ARG:HH12	24:Y:97:ALA:C	2.28	0.42
3:B:257:G:H8	3:B:258:U:H1'	1.81	0.42
3:B:626:A:H8	3:B:626:A:OP2	2.03	0.42
3:B:1396:G:H2'	3:B:1397:A:C8	2.54	0.42
3:B:2226:A:H8	3:B:2226:A:H5''	1.85	0.42
9:I:53:ALA:O	9:I:57:ILE:HD13	2.20	0.42
14:N:26:ARG:HB2	14:N:46:ARG:HD2	2.01	0.42
14:N:44:VAL:HG22	14:N:97:TYR:HD1	1.84	0.42
21:V:87:ILE:O	21:V:87:ILE:HG13	2.19	0.42
23:X:98:THR:HA	23:X:101:ILE:HG22	2.01	0.42
2:A:184:VAL:HG22	2:A:185:ARG:H	1.84	0.42
3:B:2068:U:H2'	3:B:2069:C:H6	1.83	0.42
3:B:2085:U:H2'	3:B:2086:G:O4'	2.19	0.42
17:Q:48:ARG:HH21	17:Q:49:ASP:CG	2.27	0.42
23:X:39:ALA:O	23:X:40:LEU:HD23	2.20	0.42
23:X:153:GLU:HG2	23:X:156:ARG:HE	1.83	0.42
24:Y:108:LEU:HD23	24:Y:108:LEU:HA	1.91	0.42
26:b:7:ALA:O	26:b:53:MET:HE1	2.20	0.42
3:B:580:A:H2'	3:B:581:A:C8	2.55	0.42
3:B:612:U:C2	3:B:613:C:C5	3.08	0.42
3:B:1506:A:H2'	3:B:1507:G:C8	2.55	0.42
3:B:2120:G:OP1	11:K:18:GLY:HA3	2.19	0.42
3:B:2315:C:C2	3:B:2316:C:C5	3.08	0.42
13:M:32:VAL:HG23	13:M:34:LYS:HD2	2.02	0.42
26:b:182:ASP:OD2	26:b:185:ARG:HG3	2.20	0.42
3:B:883:A:H2'	3:B:884:A:H8	1.83	0.41
3:B:1152:U:H5''	3:B:1153:G:OP2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1318:G:H21	14:N:97:TYR:HB3	1.83	0.41
23:X:153:GLU:HA	23:X:156:ARG:HG3	2.02	0.41
28:d:64:C:OP1	28:d:64:C:O4'	2.38	0.41
30:G:48:ASP:OD1	30:G:48:ASP:O	2.38	0.41
3:B:1155:U:H2'	3:B:1156:A:H8	1.85	0.41
3:B:1550:A:O5'	3:B:1550:A:H8	2.02	0.41
6:E:40:ASP:HB2	6:E:49:PHE:CZ	2.56	0.41
10:J:85:LYS:O	10:J:89:LEU:HD23	2.20	0.41
21:V:110:LYS:HG3	30:G:101:GLU:HB2	2.02	0.41
23:X:123:ILE:HD12	23:X:129:VAL:HG21	2.02	0.41
24:Y:35:MET:HB3	24:Y:35:MET:HE3	1.76	0.41
3:B:75:A:C2	3:B:93:A:C5	3.08	0.41
3:B:1147:A:O2'	3:B:1148:U:H5'	2.20	0.41
3:B:1416:U:H2'	3:B:1417:C:C6	2.55	0.41
12:L:56:ARG:HB3	12:L:62:ARG:HH22	1.85	0.41
20:U:123:LEU:H	20:U:123:LEU:CD2	2.32	0.41
30:G:73:GLY:O	30:G:122:LYS:HA	2.20	0.41
3:B:837:G:H2'	3:B:838:C:C5	2.56	0.41
3:B:2043:U:H2'	3:B:2044:C:H6	1.85	0.41
4:C:29:LYS:HB3	4:C:29:LYS:HE3	1.74	0.41
23:X:83:ILE:HD12	23:X:83:ILE:HA	1.90	0.41
2:A:23:GLU:C	2:A:24:LEU:HD23	2.45	0.41
2:A:93:LEU:HD12	2:A:94:ILE:H	1.85	0.41
3:B:128:G:H5''	14:N:15:ARG:NH1	2.34	0.41
3:B:1118:C:H5	22:W:155:VAL:HG12	1.85	0.41
6:E:40:ASP:HB2	6:E:49:PHE:HZ	1.84	0.41
17:Q:108:GLU:O	17:Q:112:LEU:HG	2.20	0.41
24:Y:17:ILE:HD12	24:Y:17:ILE:N	2.36	0.41
2:A:128:ASN:O	2:A:192:VAL:HG23	2.20	0.41
2:A:157:SER:O	2:A:160:THR:HG23	2.20	0.41
3:B:1445:A:H2'	3:B:1446:U:O4'	2.20	0.41
3:B:1934:U:H2'	3:B:1935:U:C6	2.55	0.41
12:L:97:LEU:HD23	12:L:97:LEU:HA	1.81	0.41
14:N:106:ILE:HD12	14:N:107:ASP:H	1.85	0.41
23:X:99:ARG:NH1	23:X:114:ARG:HD2	2.36	0.41
26:b:152:ASP:HB3	26:b:153:PRO:HD3	2.01	0.41
3:B:237:A:OP1	4:C:7:LYS:HE3	2.21	0.41
3:B:1153:G:O5'	3:B:1153:G:C8	2.74	0.41
3:B:1503:U:C4	3:B:1504:A:N7	2.89	0.41
3:B:2364:C:H2'	3:B:2365:A:C8	2.56	0.41
12:L:83:HIS:HB3	12:L:86:THR:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:106:ILE:HD12	14:N:107:ASP:N	2.36	0.41
18:S:33:GLN:O	18:S:33:GLN:HG3	2.19	0.41
24:Y:87:THR:HG23	24:Y:133:THR:HG22	2.02	0.41
1:Z:4:ARG:O	1:Z:40:GLN:HA	2.20	0.41
2:A:228:VAL:HG13	2:A:229:ASP:OD1	2.20	0.41
3:B:75:A:C8	3:B:90:U:C4	3.08	0.41
3:B:2064:C:H2'	3:B:2065:U:C6	2.55	0.41
6:E:16:GLU:HG3	6:E:16:GLU:O	2.20	0.41
10:J:96:ALA:O	10:J:100:ALA:HB3	2.21	0.41
11:K:45:MET:O	11:K:59:LEU:HD11	2.21	0.41
14:N:32:GLU:CG	14:N:33:LYS:N	2.84	0.41
14:N:74:LEU:HD23	14:N:97:TYR:HE2	1.85	0.41
23:X:151:GLU:H	23:X:151:GLU:CD	2.29	0.41
25:a:43:ARG:H	25:a:43:ARG:HG2	1.68	0.41
29:R:8:GLU:HG2	29:R:59:LEU:CB	2.51	0.41
1:Z:37:LYS:HB2	1:Z:37:LYS:HE3	1.81	0.41
2:A:146:LEU:HA	2:A:146:LEU:HD22	1.89	0.41
2:A:221:ARG:O	2:A:224:VAL:HG22	2.21	0.41
3:B:1227:G:H3'	3:B:1228:C:H5'	2.03	0.41
3:B:2403:U:H2'	3:B:2404:U:C6	2.56	0.41
8:H:29:LEU:O	8:H:38:ARG:HG2	2.21	0.41
10:J:35:GLU:O	10:J:36:ILE:HD12	2.20	0.41
12:L:33:VAL:HA	12:L:94:PHE:O	2.21	0.41
13:M:13:VAL:HG11	13:M:18:SER:HB2	2.01	0.41
13:M:35:ALA:O	13:M:64:PRO:HA	2.21	0.41
16:P:7:THR:HG23	16:P:8:GLY:N	2.36	0.41
16:P:25:LEU:HD13	16:P:25:LEU:HA	1.83	0.41
20:U:79:GLY:O	20:U:83:ARG:HB2	2.20	0.41
21:V:109:ARG:HA	21:V:109:ARG:HD2	1.91	0.41
25:a:47:THR:HG22	25:a:47:THR:O	2.21	0.41
25:a:199:LEU:HD12	25:a:199:LEU:HA	1.93	0.41
26:b:50:GLN:HA	26:b:82:GLU:HB3	2.02	0.41
26:b:109:ASP:OD1	26:b:174:LEU:HA	2.21	0.41
29:R:41:ARG:NH1	29:R:43:ARG:HH21	2.17	0.41
30:G:78:GLN:HG2	30:G:82:MET:HE2	2.02	0.41
3:B:923:G:C5	3:B:924:U:C4	3.08	0.41
3:B:926:G:C2	3:B:927:G:N7	2.89	0.41
13:M:9:ASP:O	13:M:25:VAL:HG23	2.21	0.41
20:U:151:VAL:HG13	20:U:152:ALA:N	2.36	0.41
23:X:100:ASP:HA	23:X:103:LEU:HD23	2.03	0.41
24:Y:78:LYS:HD2	24:Y:78:LYS:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:55:LYS:HD2	26:b:75:GLU:OE2	2.21	0.41
3:B:1442:A:H5'	3:B:1442:A:N3	2.36	0.40
3:B:1669:A:H2'	3:B:1670:C:C6	2.56	0.40
24:Y:52:ILE:HD13	24:Y:66:TRP:CD1	2.56	0.40
26:b:47:THR:HG23	26:b:47:THR:O	2.21	0.40
3:B:506:A:H4'	3:B:507:G:C8	2.56	0.40
3:B:1279:A:OP2	3:B:1481:G:H2'	2.21	0.40
3:B:1601:G:O2'	3:B:1602:U:C6	2.73	0.40
7:F:25:GLN:H	7:F:25:GLN:HG2	1.68	0.40
10:J:12:VAL:HG11	10:J:28:ARG:NH1	2.36	0.40
16:P:31:THR:HG22	16:P:32:THR:N	2.34	0.40
21:V:8:LEU:HB3	21:V:82:ASN:HB2	2.03	0.40
3:B:52:G:O2'	3:B:53:C:H5''	2.22	0.40
3:B:824:C:H2'	3:B:825:C:H6	1.87	0.40
3:B:843:G:N1	3:B:881:C:C4	2.89	0.40
3:B:932:A:O2'	3:B:933:A:H5'	2.20	0.40
4:C:50:MET:HB3	4:C:50:MET:HE2	1.70	0.40
22:W:38:ARG:HD3	22:W:111:ILE:HD13	2.03	0.40
30:G:73:GLY:O	30:G:123:PRO:HD3	2.21	0.40
3:B:106:U:O2'	3:B:116:A:N3	2.53	0.40
3:B:895:C:C2	3:B:896:G:C8	3.09	0.40
3:B:1270:G:H8	3:B:1270:G:H5''	1.86	0.40
3:B:1396:G:H2'	3:B:1397:A:H8	1.87	0.40
13:M:90:ASP:OD1	13:M:90:ASP:C	2.65	0.40
22:W:101:SER:O	22:W:105:LYS:HB2	2.21	0.40
25:a:6:LYS:HB3	25:a:6:LYS:HE3	1.58	0.40
30:G:121:PHE:HE1	30:G:126:ARG:HD3	1.85	0.40
2:A:108:GLN:O	2:A:110:VAL:HG23	2.22	0.40
2:A:208:ALA:O	2:A:212:ARG:HG2	2.21	0.40
3:B:525:G:H2'	3:B:526:U:H6	1.86	0.40
3:B:2338:G:O2'	3:B:2339:G:H5'	2.21	0.40
18:S:106:ASP:OD2	18:S:106:ASP:N	2.54	0.40
19:T:7:THR:HG22	19:T:8:LYS:H	1.87	0.40
19:T:43:THR:OG1	19:T:46:GLN:HG3	2.21	0.40
19:T:76:THR:OG1	19:T:91:GLU:HG3	2.22	0.40
23:X:126:LEU:HD23	23:X:126:LEU:HA	1.87	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	Z	39/41 (95%)	33 (85%)	6 (15%)	0	100	100
2	A	272/276 (99%)	245 (90%)	24 (9%)	3 (1%)	11	40
4	C	64/67 (96%)	58 (91%)	6 (9%)	0	100	100
5	D	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
6	E	49/55 (89%)	47 (96%)	2 (4%)	0	100	100
7	F	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
8	H	56/61 (92%)	51 (91%)	4 (7%)	1 (2%)	6	28
9	I	62/77 (80%)	53 (86%)	8 (13%)	1 (2%)	7	31
10	J	97/100 (97%)	93 (96%)	3 (3%)	1 (1%)	12	42
11	K	70/88 (80%)	60 (86%)	9 (13%)	1 (1%)	9	34
12	L	93/212 (44%)	89 (96%)	4 (4%)	0	100	100
13	M	103/106 (97%)	93 (90%)	10 (10%)	0	100	100
14	N	109/113 (96%)	97 (89%)	12 (11%)	0	100	100
15	O	120/143 (84%)	109 (91%)	11 (9%)	0	100	100
16	P	102/104 (98%)	92 (90%)	9 (9%)	1 (1%)	12	42
17	Q	115/128 (90%)	113 (98%)	2 (2%)	0	100	100
18	S	127/141 (90%)	112 (88%)	15 (12%)	0	100	100
19	T	133/138 (96%)	121 (91%)	11 (8%)	1 (1%)	16	47
20	U	151/161 (94%)	130 (86%)	17 (11%)	4 (3%)	4	20
21	V	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	16	47
22	W	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
23	X	159/192 (83%)	142 (89%)	14 (9%)	3 (2%)	6	27
24	Y	173/178 (97%)	160 (92%)	13 (8%)	0	100	100
25	a	202/204 (99%)	186 (92%)	16 (8%)	0	100	100
26	b	220/227 (97%)	205 (93%)	15 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	R	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
30	G	101/152 (66%)	84 (83%)	16 (16%)	1 (1%)	12	42
All	All	3108/3482 (89%)	2831 (91%)	259 (8%)	18 (1%)	23	53

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	73	ASP
8	H	16	ILE
9	I	23	LEU
20	U	106	LEU
23	X	133	VAL
11	K	34	GLY
16	P	45	ALA
20	U	135	SER
20	U	152	ALA
21	V	87	ILE
23	X	34	LEU
2	A	30	VAL
2	A	52	ARG
10	J	12	VAL
20	U	122	GLU
19	T	89	SER
23	X	117	VAL
30	G	95	ILE

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	Z	37/37 (100%)	34 (92%)	3 (8%)	11	36
2	A	220/222 (99%)	208 (94%)	12 (6%)	19	51
4	C	56/57 (98%)	55 (98%)	1 (2%)	51	76
5	D	37/37 (100%)	36 (97%)	1 (3%)	39	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	E	44/47 (94%)	44 (100%)	0	100	100
7	F	52/56 (93%)	50 (96%)	2 (4%)	29	61
8	H	46/48 (96%)	45 (98%)	1 (2%)	45	73
9	I	51/60 (85%)	50 (98%)	1 (2%)	48	75
10	J	85/86 (99%)	80 (94%)	5 (6%)	18	48
11	K	51/61 (84%)	50 (98%)	1 (2%)	48	75
12	L	75/167 (45%)	75 (100%)	0	100	100
13	M	85/86 (99%)	81 (95%)	4 (5%)	23	56
14	N	94/95 (99%)	87 (93%)	7 (7%)	13	40
15	O	100/112 (89%)	99 (99%)	1 (1%)	68	83
16	P	83/83 (100%)	81 (98%)	2 (2%)	43	72
17	Q	92/100 (92%)	88 (96%)	4 (4%)	26	58
18	S	104/113 (92%)	104 (100%)	0	100	100
19	T	105/107 (98%)	103 (98%)	2 (2%)	50	75
20	U	107/111 (96%)	105 (98%)	2 (2%)	50	75
21	V	102/102 (100%)	100 (98%)	2 (2%)	48	75
22	W	130/133 (98%)	126 (97%)	4 (3%)	35	66
23	X	132/156 (85%)	126 (96%)	6 (4%)	24	57
24	Y	146/149 (98%)	140 (96%)	6 (4%)	27	60
25	a	155/155 (100%)	150 (97%)	5 (3%)	34	65
26	b	175/175 (100%)	167 (95%)	8 (5%)	24	57
29	R	98/105 (93%)	93 (95%)	5 (5%)	21	53
30	G	83/117 (71%)	75 (90%)	8 (10%)	8	29
All	All	2545/2777 (92%)	2452 (96%)	93 (4%)	31	62

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	3	ILE
1	Z	25	ARG
1	Z	35	ARG
2	A	34	THR
2	A	35	GLU
2	A	83	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	124	VAL
2	A	125	LYS
2	A	128	ASN
2	A	130	MET
2	A	146	LEU
2	A	156	ARG
2	A	180	GLU
2	A	188	CYS
2	A	189	MET
4	C	31	HIS
5	D	16	HIS
7	F	55	VAL
7	F	60	THR
8	H	57	ILE
9	I	40	GLN
10	J	2	SER
10	J	36	ILE
10	J	47	VAL
10	J	51	LEU
10	J	60	GLU
11	K	83	LEU
13	M	9	ASP
13	M	19	ARG
13	M	28	VAL
13	M	99	VAL
14	N	7	LEU
14	N	9	ARG
14	N	20	SER
14	N	73	THR
14	N	99	GLN
14	N	100	LEU
14	N	108	LEU
15	O	58	GLU
16	P	62	THR
16	P	102	ASN
17	Q	4	VAL
17	Q	27	ARG
17	Q	57	PHE
17	Q	85	LYS
19	T	7	THR
19	T	103	LEU
20	U	95	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	U	118	LEU
21	V	8	LEU
21	V	43	VAL
22	W	2	LYS
22	W	58	ILE
22	W	104	GLU
22	W	121	MET
23	X	3	GLN
23	X	17	GLN
23	X	62	LEU
23	X	125	MET
23	X	130	GLU
23	X	144	THR
24	Y	35	MET
24	Y	68	THR
24	Y	99	VAL
24	Y	122	VAL
24	Y	125	THR
24	Y	134	VAL
25	a	4	ASP
25	a	115	GLN
25	a	135	ARG
25	a	176	ILE
25	a	179	ASN
26	b	27	VAL
26	b	44	ASP
26	b	63	LYS
26	b	72	THR
26	b	81	VAL
26	b	132	GLU
26	b	151	GLN
26	b	203	MET
29	R	1	MET
29	R	38	GLU
29	R	56	ASN
29	R	60	ASN
29	R	75	GLU
30	G	68	MET
30	G	82	MET
30	G	90	LEU
30	G	93	ILE
30	G	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	G	119	HIS
30	G	120	LEU
30	G	121	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	5	ASN
2	A	163	GLN
2	A	220	ASN
7	F	20	HIS
7	F	32	ASN
8	H	58	GLN
10	J	82	GLN
13	M	47	GLN
16	P	87	ASN
16	P	89	HIS
16	P	91	GLN
18	S	88	GLN
20	U	38	GLN
22	W	81	HIS
23	X	31	ASN
24	Y	107	ASN
25	a	89	HIS
25	a	179	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	c	16/18 (88%)	7 (43%)	0
28	d	71/113 (62%)	21 (29%)	0
3	B	2446/2726 (89%)	467 (19%)	10 (0%)
All	All	2533/2857 (88%)	495 (19%)	10 (0%)

All (495) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	B	3	G
3	B	25	U
3	B	30	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	33	G
3	B	36	G
3	B	37	G
3	B	42	G
3	B	46	G
3	B	50	U
3	B	52	G
3	B	53	C
3	B	54	A
3	B	62	A
3	B	65	A
3	B	66	G
3	B	69	A
3	B	91	U
3	B	92	G
3	B	93	A
3	B	99	G
3	B	102	U
3	B	104	U
3	B	108	A
3	B	109	A
3	B	110	U
3	B	115	A
3	B	125	A
3	B	145	G
3	B	149	A
3	B	151	A
3	B	167	A
3	B	182	A
3	B	185	A
3	B	201	G
3	B	202	A
3	B	208	C
3	B	210	U
3	B	215	A
3	B	234	G
3	B	235	C
3	B	244	G
3	B	252	G
3	B	253	G
3	B	257	G
3	B	258	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	259	G
3	B	261	C
3	B	262	C
3	B	269	A
3	B	270	A
3	B	271	A
3	B	272	G
3	B	303	A
3	B	304	U
3	B	305	G
3	B	307	G
3	B	309	G
3	B	310	A
3	B	326	A
3	B	327	G
3	B	328	U
3	B	329	G
3	B	330	U
3	B	331	U
3	B	333	A
3	B	339	G
3	B	340	U
3	B	343	U
3	B	344	U
3	B	347	G
3	B	361	G
3	B	371	G
3	B	380	U
3	B	381	G
3	B	386	G
3	B	387	A
3	B	402	U
3	B	432	A
3	B	442	G
3	B	448	G
3	B	450	U
3	B	451	G
3	B	452	A
3	B	455	A
3	B	456	G
3	B	466	G
3	B	469	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	478	A
3	B	480	A
3	B	499	U
3	B	505	C
3	B	506	A
3	B	507	G
3	B	509	C
3	B	535	A
3	B	545	U
3	B	547	A
3	B	559	G
3	B	565	G
3	B	571	A
3	B	574	G
3	B	575	A
3	B	579	U
3	B	587	U
3	B	588	A
3	B	594	A
3	B	607	G
3	B	609	G
3	B	610	A
3	B	612	U
3	B	618	U
3	B	619	A
3	B	627	U
3	B	628	G
3	B	629	A
3	B	660	U
3	B	662	U
3	B	668	U
3	B	673	A
3	B	680	A
3	B	697	C
3	B	698	U
3	B	699	G
3	B	701	A
3	B	704	G
3	B	712	C
3	B	714	C
3	B	721	U
3	B	739	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	748	A
3	B	749	G
3	B	750	G
3	B	756	A
3	B	758	G
3	B	759	G
3	B	762	A
3	B	765	C
3	B	766	A
3	B	776	A
3	B	779	G
3	B	780	C
3	B	786	C
3	B	801	U
3	B	802	G
3	B	820	U
3	B	822	G
3	B	823	C
3	B	826	U
3	B	829	G
3	B	832	G
3	B	839	A
3	B	845	U
3	B	847	G
3	B	880	C
3	B	883	A
3	B	887	C
3	B	888	C
3	B	889	G
3	B	892	U
3	B	900	A
3	B	904	U
3	B	914	A
3	B	919	G
3	B	931	U
3	B	932	A
3	B	934	G
3	B	946	A
3	B	947	G
3	B	956	A
3	B	960	C
3	B	969	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	975	G
3	B	984	A
3	B	986	C
3	B	999	G
3	B	1004	G
3	B	1005	A
3	B	1006	U
3	B	1008	U
3	B	1009	G
3	B	1010	G
3	B	1101	G
3	B	1108	U
3	B	1110	A
3	B	1111	C
3	B	1112	G
3	B	1113	G
3	B	1119	A
3	B	1132	A
3	B	1143	G
3	B	1147	A
3	B	1148	U
3	B	1150	U
3	B	1151	U
3	B	1152	U
3	B	1153	G
3	B	1162	G
3	B	1196	C
3	B	1197	G
3	B	1215	G
3	B	1226	U
3	B	1227	G
3	B	1228	C
3	B	1230	A
3	B	1233	G
3	B	1248	G
3	B	1249	A
3	B	1251	A
3	B	1266	C
3	B	1277	A
3	B	1278	A
3	B	1291	C
3	B	1298	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	1315	G
3	B	1318	G
3	B	1324	G
3	B	1329	U
3	B	1332	G
3	B	1342	A
3	B	1345	G
3	B	1347	C
3	B	1356	U
3	B	1358	G
3	B	1360	A
3	B	1365	G
3	B	1372	A
3	B	1378	G
3	B	1389	A
3	B	1395	C
3	B	1401	C
3	B	1402	A
3	B	1403	A
3	B	1404	U
3	B	1405	A
3	B	1406	U
3	B	1407	G
3	B	1408	U
3	B	1409	U
3	B	1412	C
3	B	1419	U
3	B	1420	A
3	B	1421	U
3	B	1422	U
3	B	1423	G
3	B	1426	U
3	B	1428	G
3	B	1432	A
3	B	1433	G
3	B	1434	G
3	B	1435	C
3	B	1437	U
3	B	1438	U
3	B	1440	G
3	B	1441	G
3	B	1442	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	1443	G
3	B	1446	U
3	B	1447	U
3	B	1449	C
3	B	1451	G
3	B	1453	A
3	B	1456	U
3	B	1457	A
3	B	1462	U
3	B	1466	G
3	B	1468	A
3	B	1469	U
3	B	1470	A
3	B	1481	G
3	B	1482	A
3	B	1484	A
3	B	1491	C
3	B	1492	A
3	B	1505	G
3	B	1508	A
3	B	1521	U
3	B	1522	U
3	B	1523	G
3	B	1548	G
3	B	1549	C
3	B	1578	A
3	B	1587	A
3	B	1588	U
3	B	1590	U
3	B	1591	G
3	B	1593	G
3	B	1594	C
3	B	1597	C
3	B	1602	U
3	B	1613	C
3	B	1615	G
3	B	1620	G
3	B	1621	G
3	B	1628	C
3	B	1630	A
3	B	1631	C
3	B	1633	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	1635	U
3	B	1638	G
3	B	1641	A
3	B	1657	C
3	B	1658	G
3	B	1659	A
3	B	1664	G
3	B	1665	A
3	B	1668	G
3	B	1671	G
3	B	1673	C
3	B	1676	A
3	B	1677	U
3	B	1678	A
3	B	1684	U
3	B	1686	A
3	B	1702	G
3	B	1704	A
3	B	1705	A
3	B	1726	G
3	B	1777	G
3	B	1778	G
3	B	1784	A
3	B	1785	A
3	B	1786	A
3	B	1794	U
3	B	1802	G
3	B	1803	U
3	B	1811	U
3	B	1812	G
3	B	1815	C
3	B	1818	A
3	B	1819	U
3	B	1820	G
3	B	1839	U
3	B	1840	G
3	B	1841	U
3	B	1845	C
3	B	1850	U
3	B	1854	C
3	B	1871	C
3	B	1878	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	1879	A
3	B	1881	A
3	B	1887	G
3	B	1888	G
3	B	1891	C
3	B	1900	A
3	B	1903	C
3	B	1904	G
3	B	1908	A
3	B	1909	G
3	B	1910	A
3	B	1917	G
3	B	1924	U
3	B	1939	G
3	B	1940	U
3	B	2046	A
3	B	2047	A
3	B	2051	A
3	B	2055	C
3	B	2074	A
3	B	2087	G
3	B	2092	U
3	B	2099	G
3	B	2117	A
3	B	2118	G
3	B	2128	G
3	B	2132	C
3	B	2136	A
3	B	2137	U
3	B	2169	C
3	B	2170	G
3	B	2171	A
3	B	2183	U
3	B	2184	A
3	B	2194	G
3	B	2196	C
3	B	2199	U
3	B	2203	A
3	B	2206	G
3	B	2210	G
3	B	2221	G
3	B	2224	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	2226	A
3	B	2232	G
3	B	2234	C
3	B	2241	A
3	B	2248	G
3	B	2249	G
3	B	2251	C
3	B	2255	C
3	B	2256	G
3	B	2257	U
3	B	2258	G
3	B	2271	C
3	B	2272	U
3	B	2274	A
3	B	2277	G
3	B	2278	G
3	B	2279	A
3	B	2281	A
3	B	2290	U
3	B	2297	A
3	B	2323	C
3	B	2325	A
3	B	2336	G
3	B	2339	G
3	B	2340	U
3	B	2343	G
3	B	2345	C
3	B	2351	G
3	B	2354	G
3	B	2355	U
3	B	2367	A
3	B	2378	G
3	B	2383	A
3	B	2396	U
3	B	2403	U
3	B	2412	U
3	B	2413	A
3	B	2415	A
3	B	2416	G
3	B	2422	C
3	B	2435	U
3	B	2441	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	2451	A
3	B	2458	U
3	B	2459	C
3	B	2462	U
3	B	2464	U
3	B	2478	A
3	B	2479	U
3	B	2481	A
3	B	2534	G
3	B	2538	U
3	B	2554	A
3	B	2563	G
3	B	2569	U
3	B	2575	A
3	B	2581	G
3	B	2582	A
3	B	2585	G
3	B	2594	C
3	B	2597	A
3	B	2599	A
3	B	2600	G
3	B	2601	C
3	B	2606	A
3	B	2611	G
3	B	2614	A
3	B	2627	A
3	B	2649	A
3	B	2650	A
3	B	2662	C
3	B	2664	A
3	B	2665	U
3	B	2666	A
3	B	2668	G
3	B	2669	C
3	B	2676	U
3	B	2687	U
3	B	2688	A
3	B	2690	C
3	B	2692	C
3	B	2702	A
3	B	2709	C
3	B	2715	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	2719	A
3	B	2722	U
27	c	7	U
27	c	69	U
27	c	72	U
27	c	73	U
27	c	74	C
27	c	75	C
27	c	76	A
28	d	1	U
28	d	2	G
28	d	3	G
28	d	8	U
28	d	9	A
28	d	10	U
28	d	14	G
28	d	17	A
28	d	59	C
28	d	61	C
28	d	62	A
28	d	64	C
28	d	68	U
28	d	79	A
28	d	86	G
28	d	92	G
28	d	100	G
28	d	104	G
28	d	106	C
28	d	107	G
28	d	110	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	B	2	A
3	B	270	A
3	B	303	A
3	B	327	G
3	B	608	C
3	B	1196	C
3	B	1406	U
3	B	1420	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	2256	G
3	B	2605	U

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	c	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	7:U	O3'	66:U	P	16.63

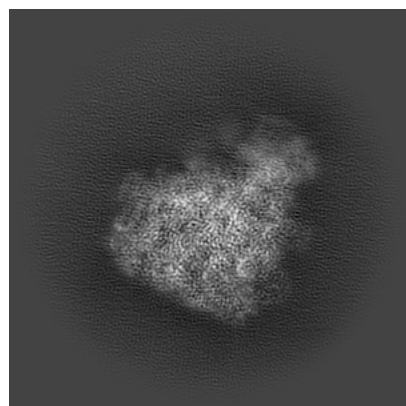
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56961. These allow visual inspection of the internal detail of the map and identification of artifacts.

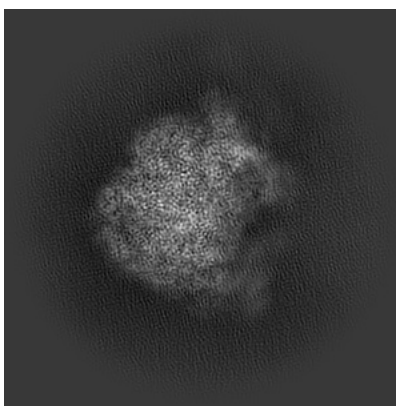
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

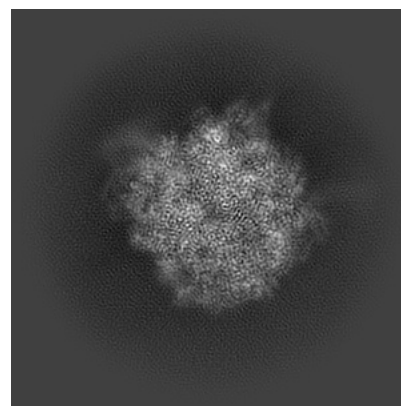
6.1.1 Primary map



X

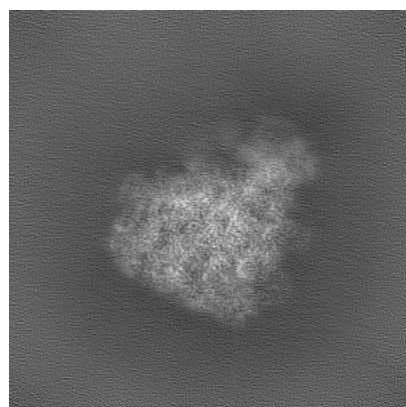


Y

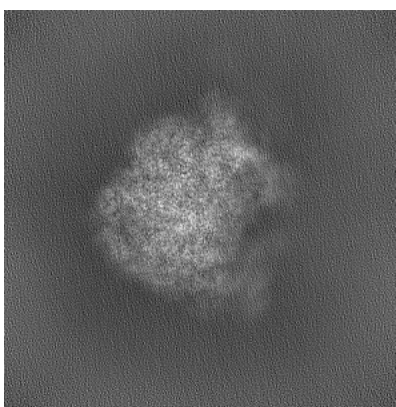


Z

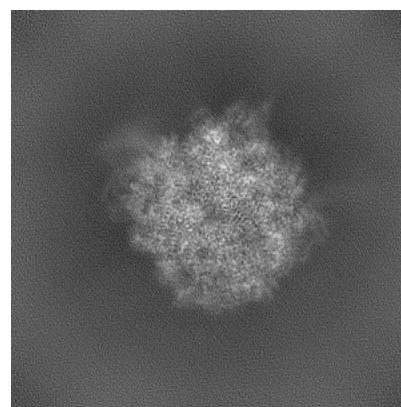
6.1.2 Raw map



X



Y

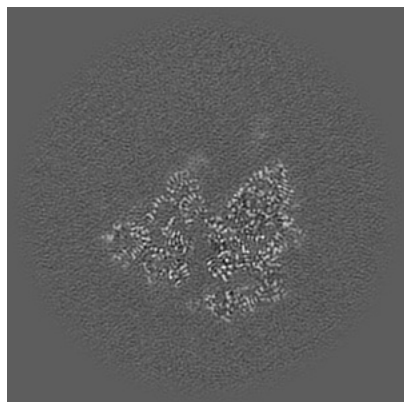


Z

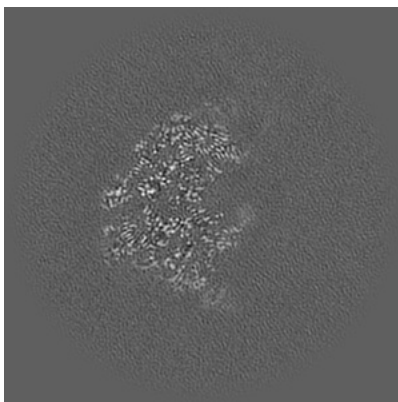
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

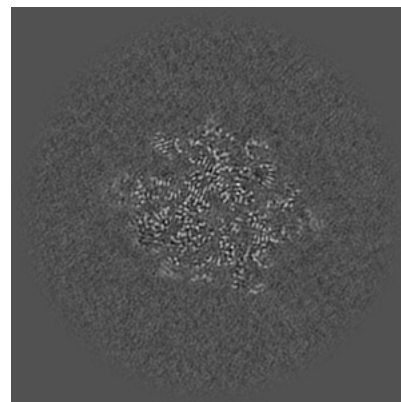
6.2.1 Primary map



X Index: 200

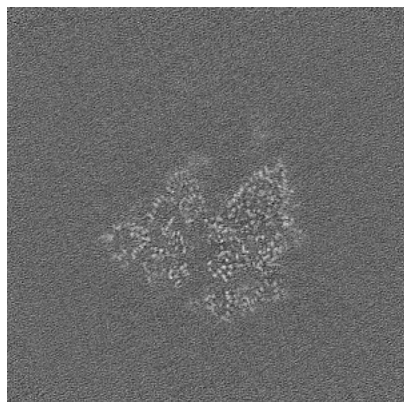


Y Index: 200

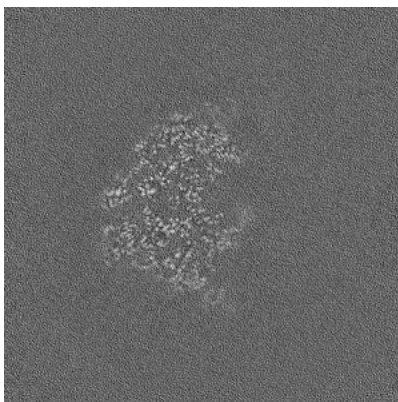


Z Index: 200

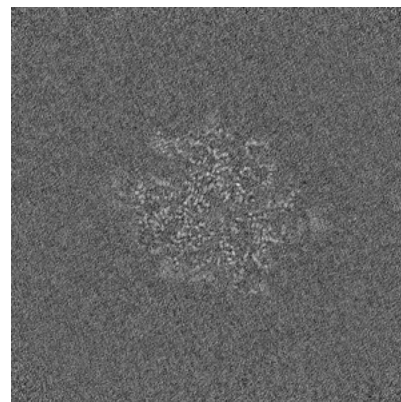
6.2.2 Raw map



X Index: 200



Y Index: 200

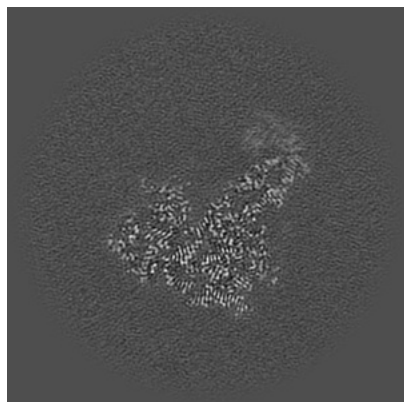


Z Index: 200

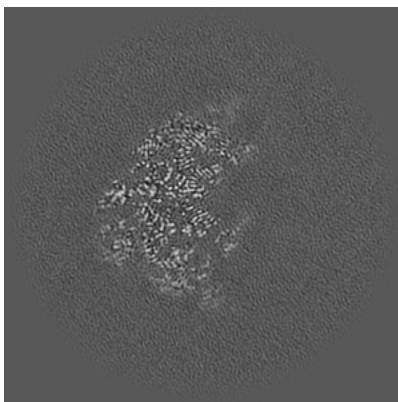
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

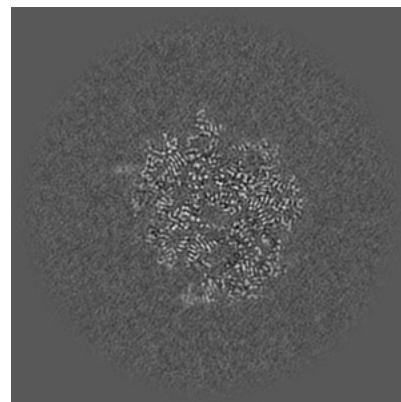
6.3.1 Primary map



X Index: 215

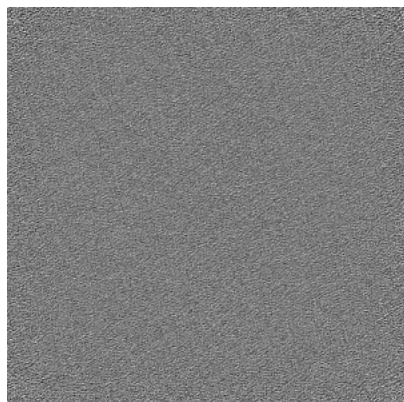


Y Index: 204

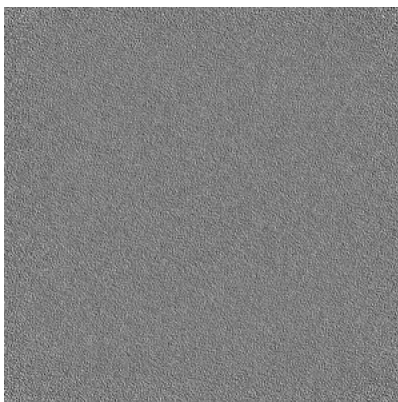


Z Index: 182

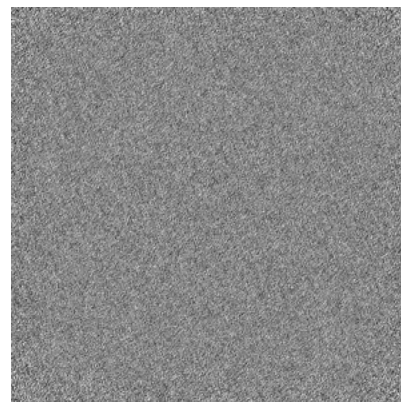
6.3.2 Raw map



X Index: 0



Y Index: 0

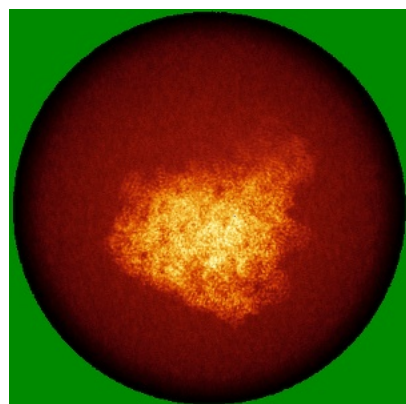


Z Index: 0

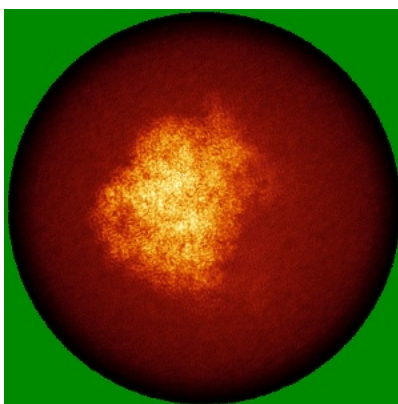
The images above show the largest variance slices of the map in three orthogonal directions.

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

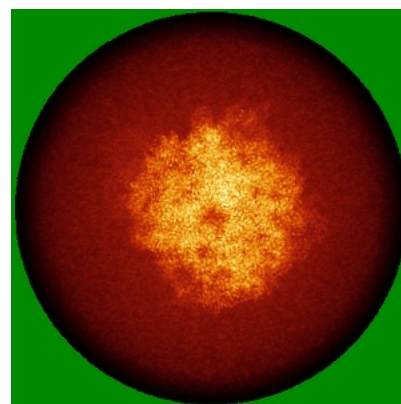
6.4.1 Primary map



X

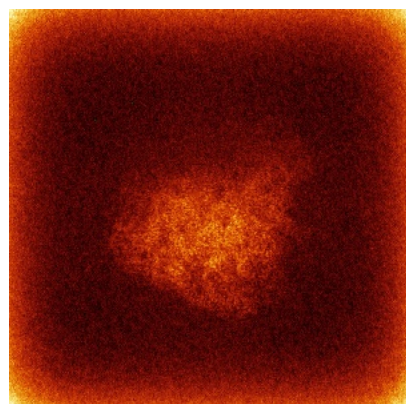


Y

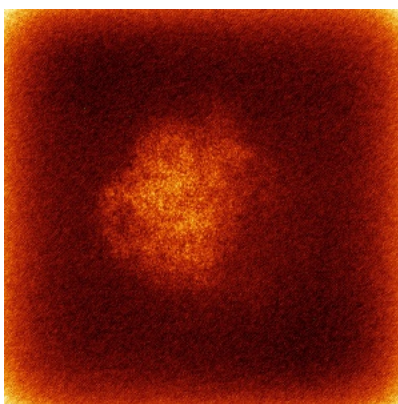


Z

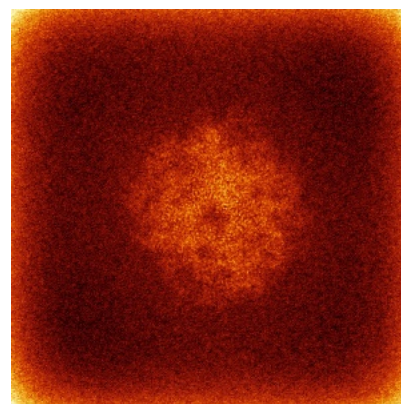
6.4.2 Raw map



X



Y

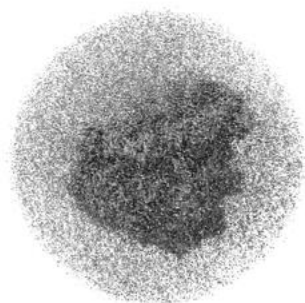


Z

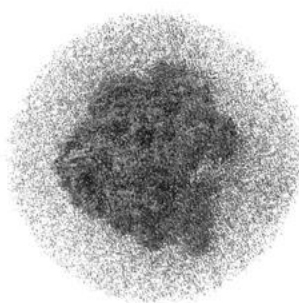
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

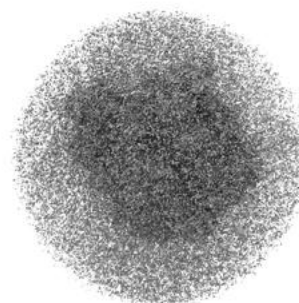
6.5.1 Primary map



X



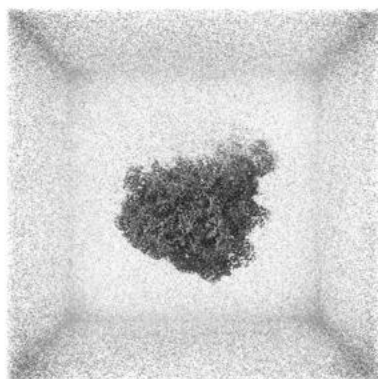
Y



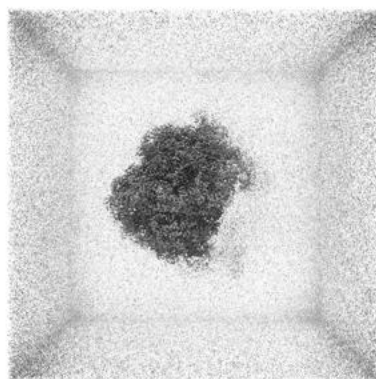
Z

The images above show the 3D surface view of the map at the recommended contour level 0.166. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

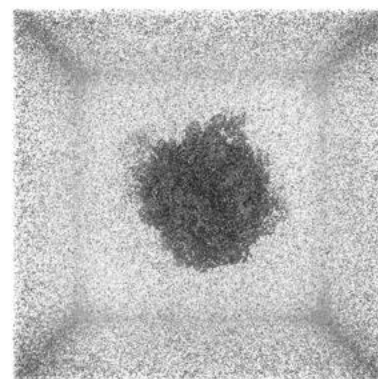
6.5.2 Raw map



X



Y



Z

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

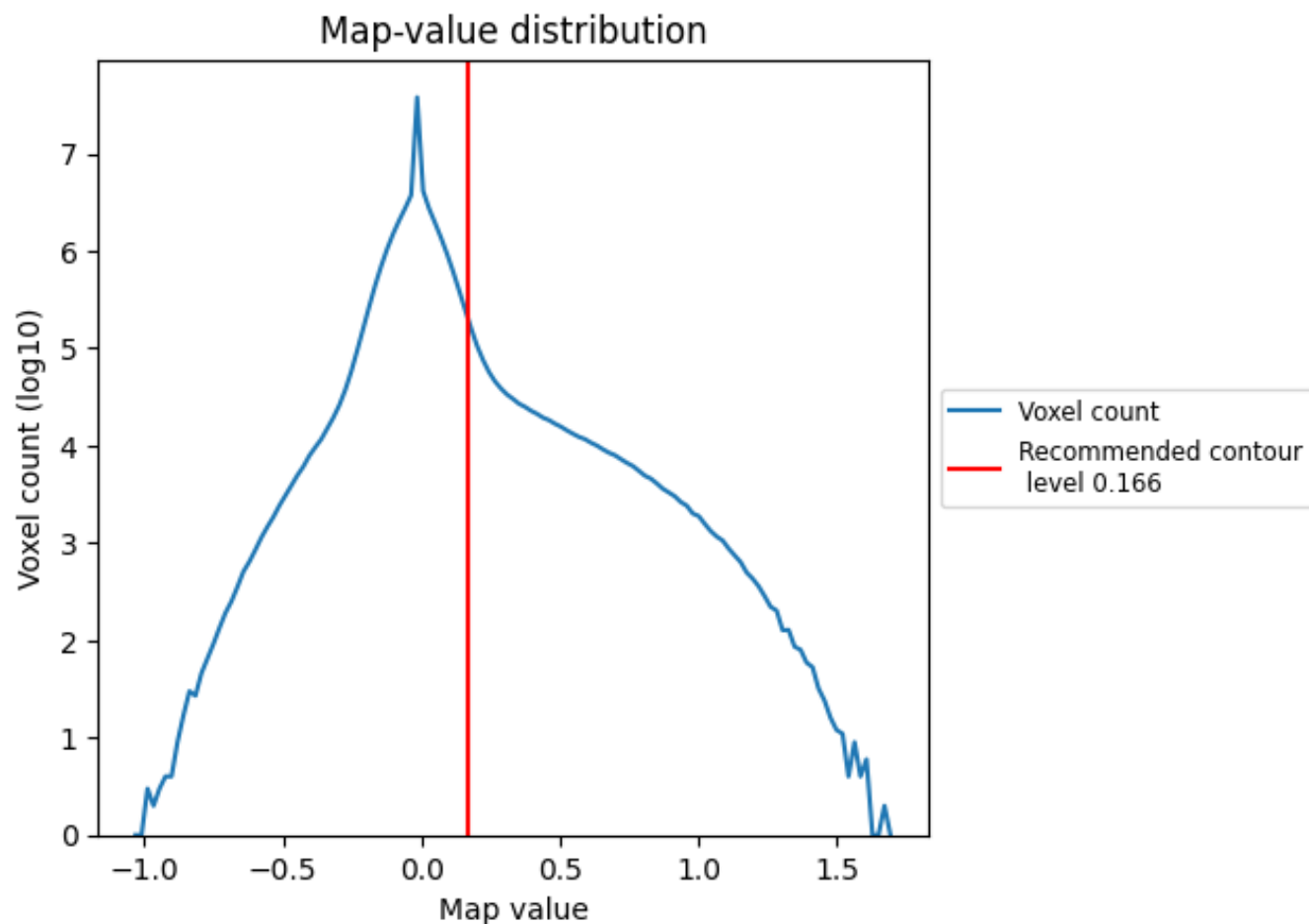
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

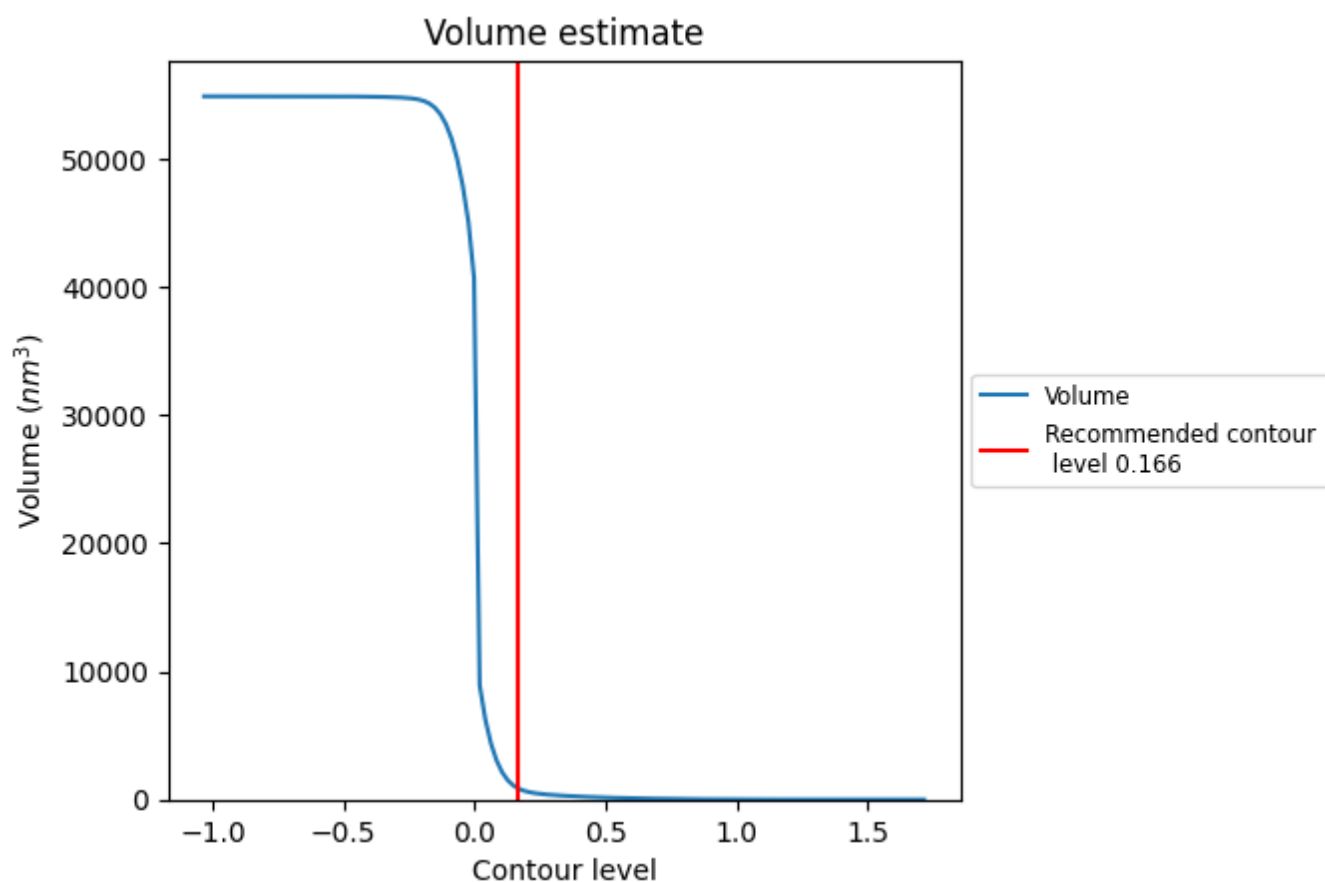
This section contains the results of statistical analysis of the map.

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.

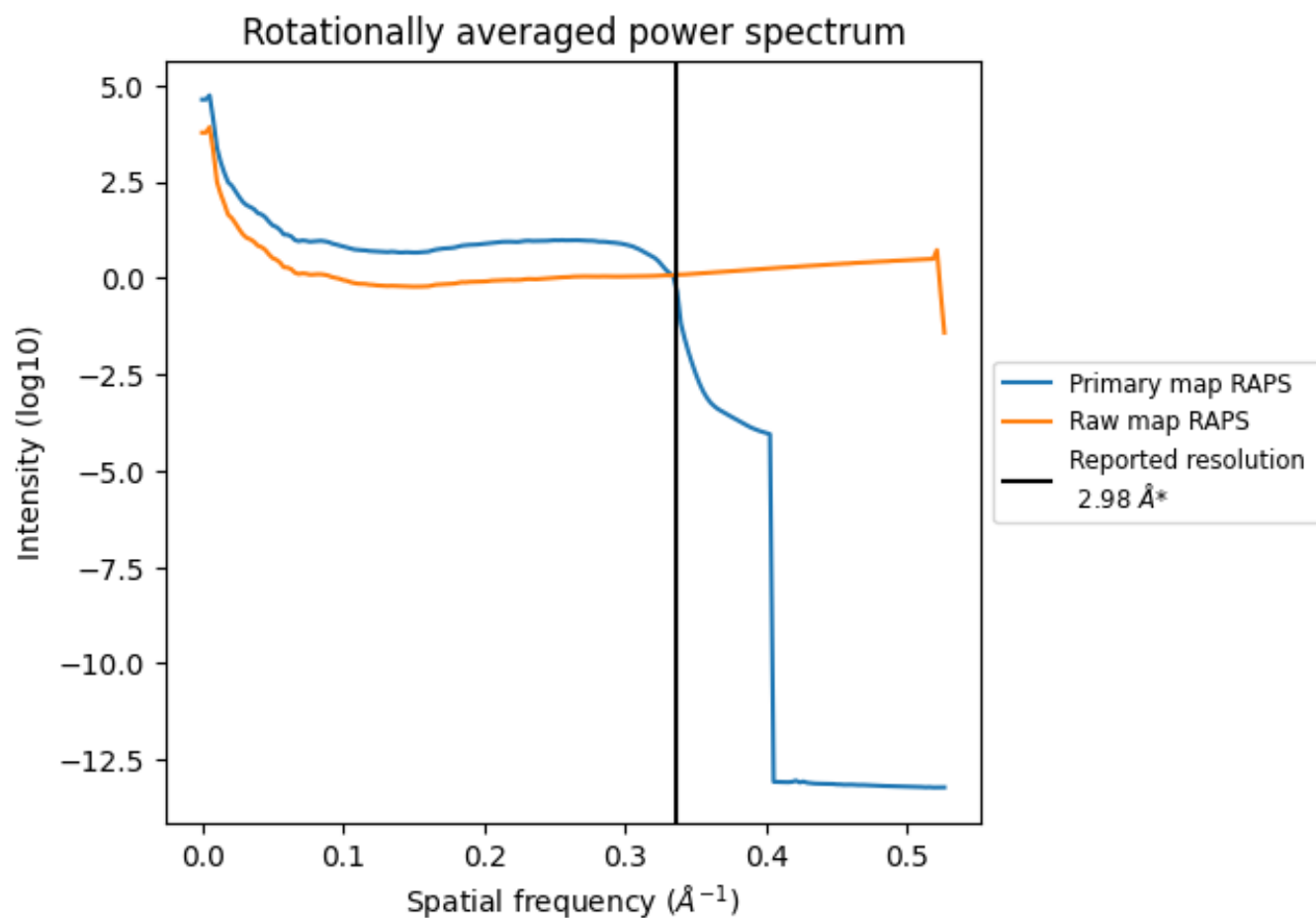
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 888 nm³; this corresponds to an approximate mass of 802 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 ⓘ

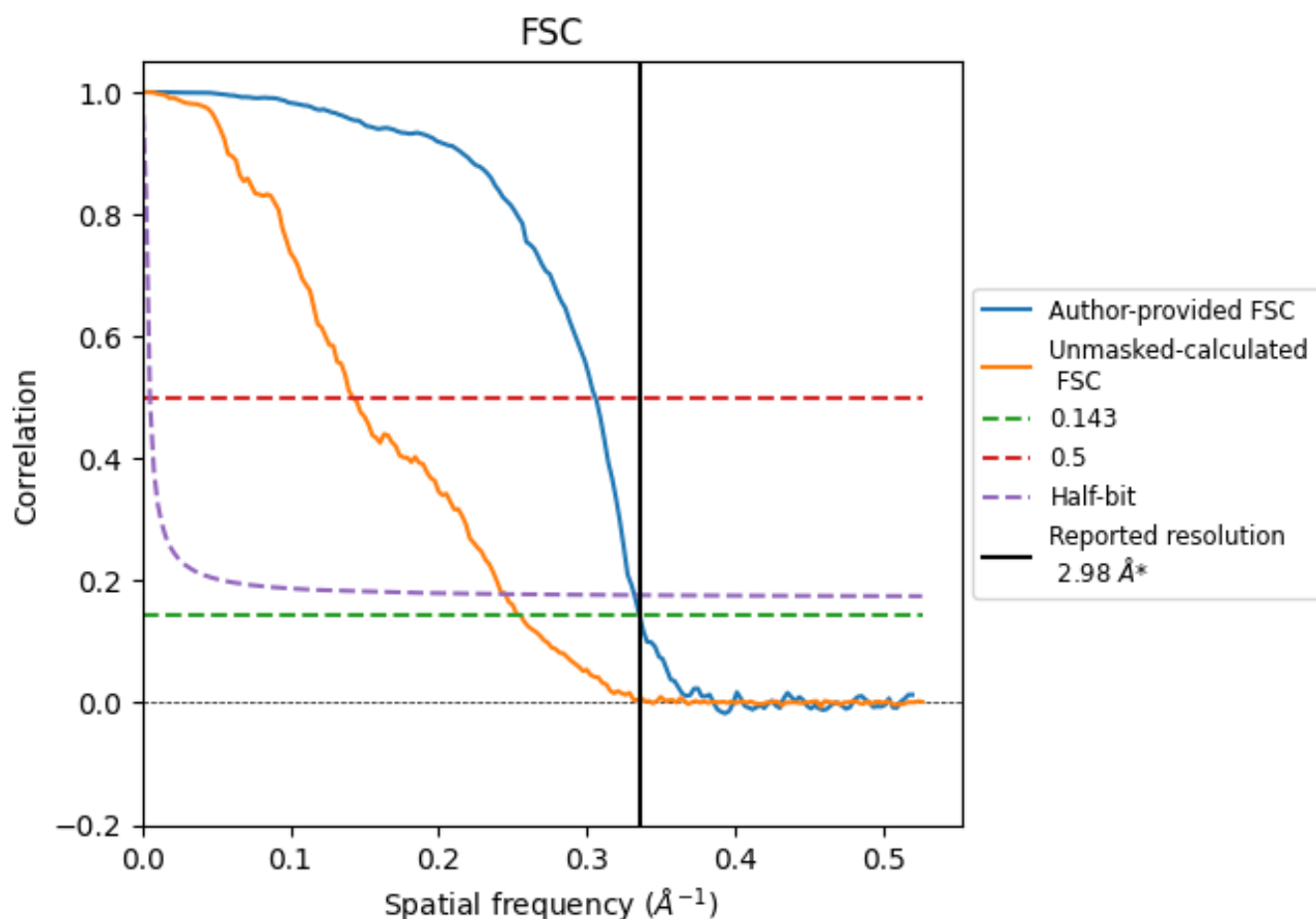


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.336 \AA^{-1}

8.2 Resolution estimates [i](#)

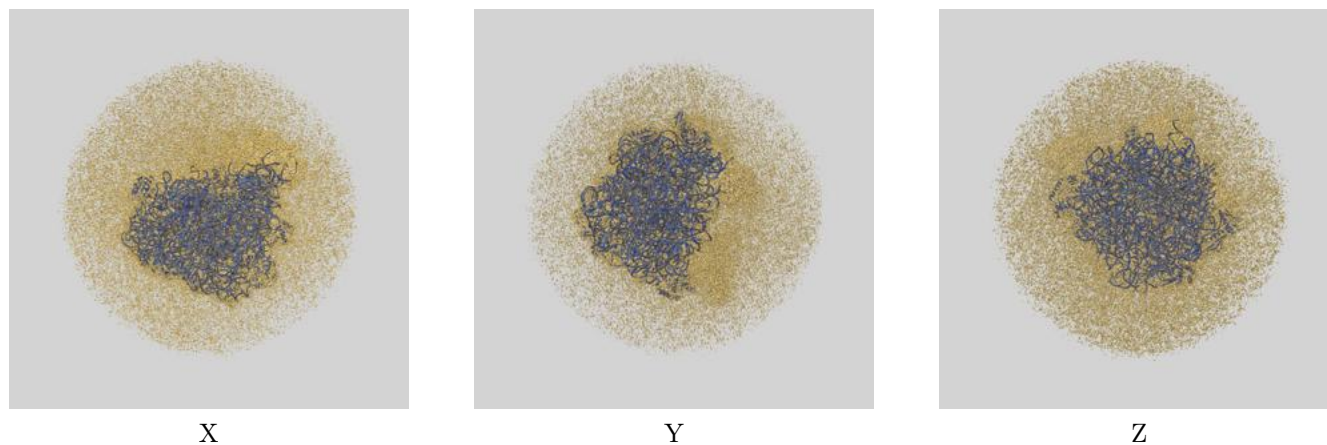
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.27	3.01
Unmasked-calculated*	3.92	7.04	4.08

*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 3.92 differs from the reported value 2.98 by more than 10 %

9 Map-model fit [i](#)

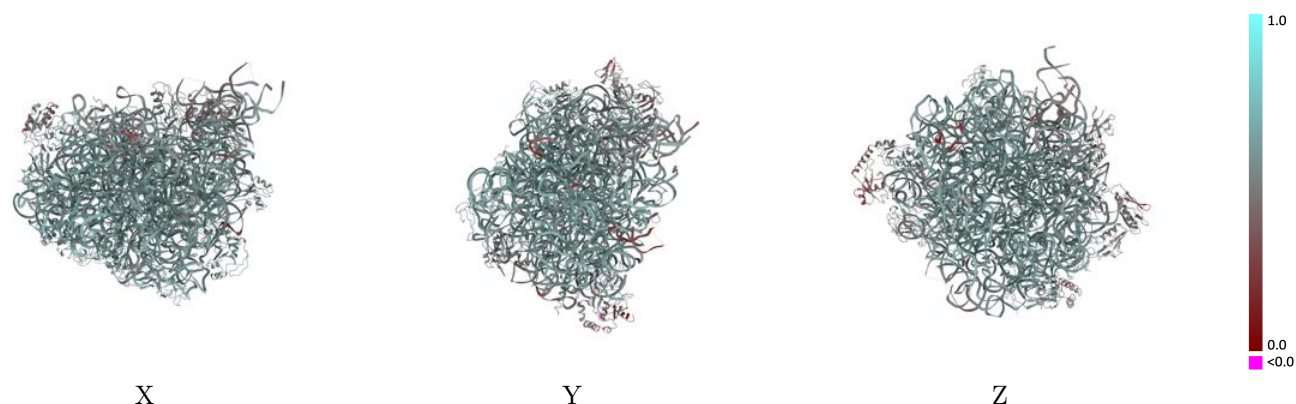
This section contains information regarding the fit between EMDB map EMD-56961 and PDB model 28YE. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



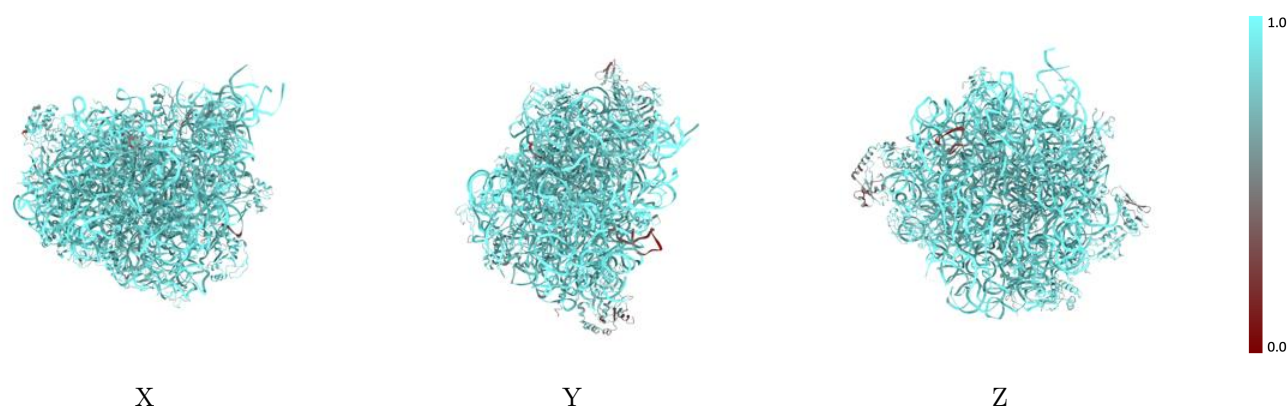
The images above show the 3D surface view of the map at the recommended contour level 0.166 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



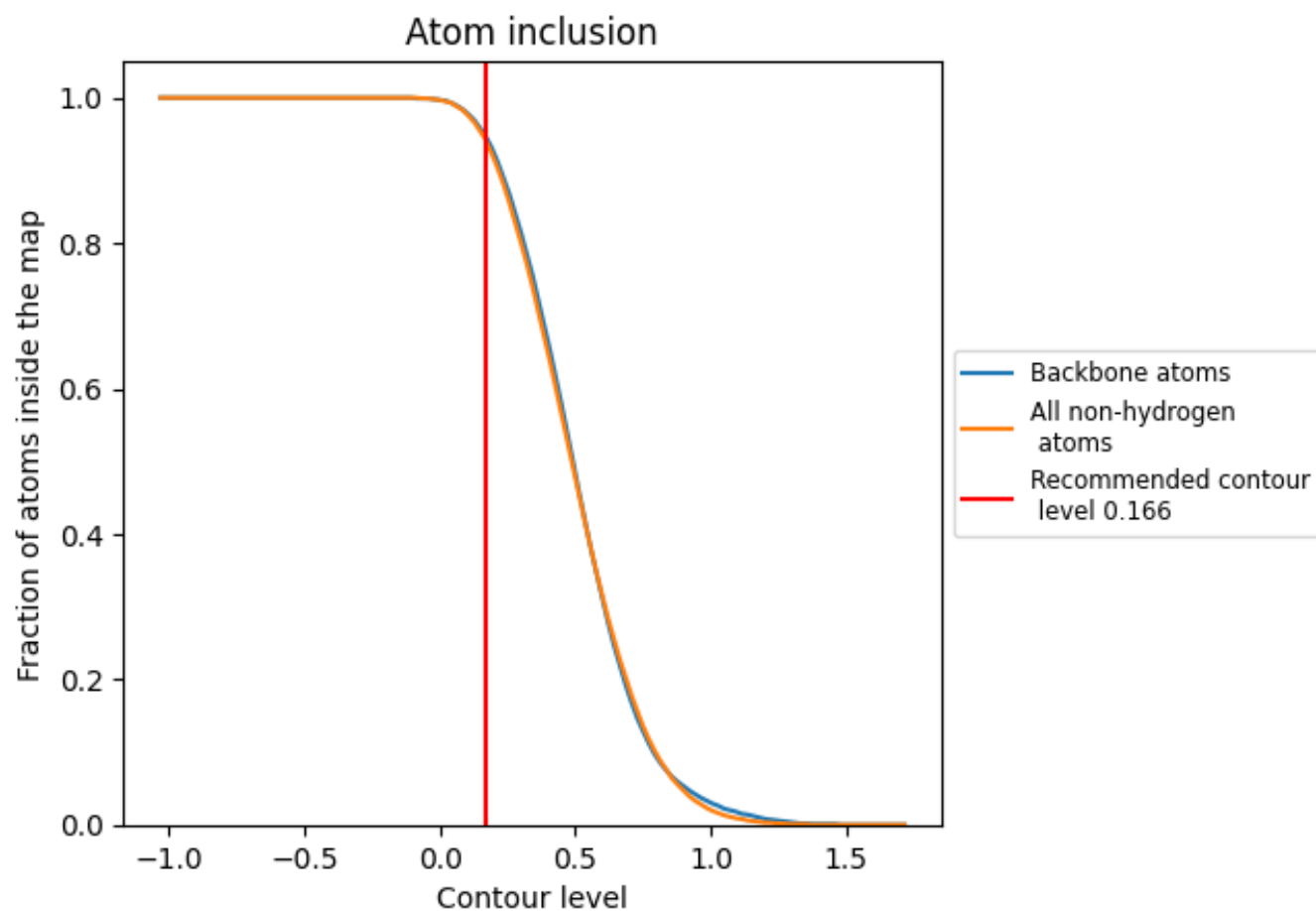
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.166).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.166) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9440	 0.5730
A	 0.9080	 0.5610
B	 0.9700	 0.5860
C	 0.9560	 0.6050
D	 0.9570	 0.6060
E	 0.9500	 0.5850
F	 0.9490	 0.6070
G	 0.8380	 0.4670
H	 0.9220	 0.5620
I	 0.8560	 0.5080
J	 0.8970	 0.5590
K	 0.9140	 0.5540
L	 0.8050	 0.4570
M	 0.8920	 0.5550
N	 0.8760	 0.5180
O	 0.9450	 0.6040
P	 0.9070	 0.5580
Q	 0.9350	 0.5780
R	 0.9010	 0.5790
S	 0.9560	 0.5990
T	 0.8900	 0.5380
U	 0.9300	 0.5780
V	 0.9230	 0.5820
W	 0.9360	 0.5780
X	 0.6570	 0.4120
Y	 0.7850	 0.4640
Z	 0.8760	 0.5400
a	 0.9480	 0.5970
b	 0.9530	 0.6000
c	 0.3290	 0.2500
d	 0.9200	 0.5140

