



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:20 AM JST

PDB ID : 7WTM
EMDB ID : EMD-32791
Title : Cryo-EM structure of a yeast pre-40S ribosomal subunit - State Dis-E
Authors : Cheng, J.; La Venuta, G.; Lau, B.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on : 2022-02-05
Resolution : 3.50 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

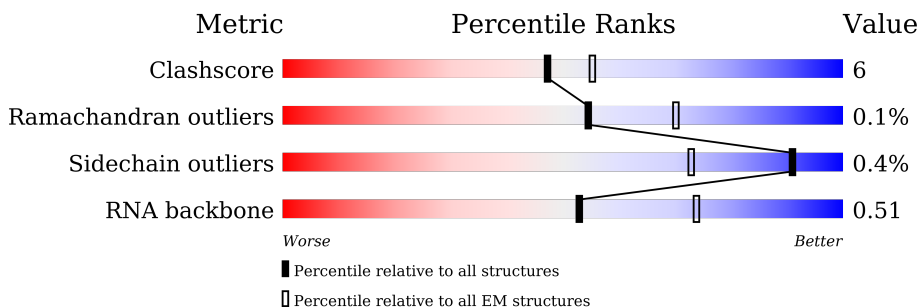
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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





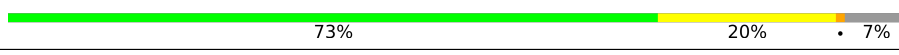



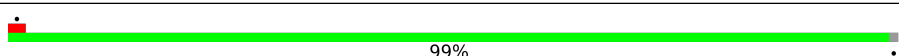
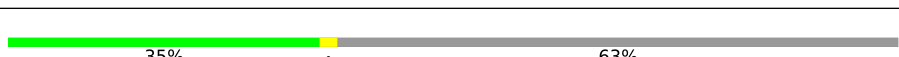
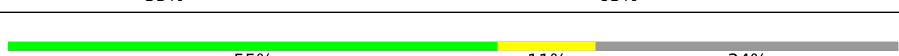

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	C2	1800	
2	SB	255	
3	SE	261	
4	SG	236	
5	SH	190	
6	SI	200	
7	SJ	197	

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Mol	Chain	Length	Quality of chain
8	SL	156	 79% 14% 6%
9	SN	151	 85% 14%
10	SO	137	 73% 20% 7%
11	SW	130	 86% 13%
12	SX	145	 6% 77% 23%
13	SY	135	 80% 19%
14	Sb	82	 99%
15	Se	63	 35% 63%
16	CA	274	 55% 11% 34%
17	JL	318	 23% 76% 13% 11%

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 44623 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C2	1106	23575	10547	4185	7737	1106	0	0

- Molecule 2 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	216	1722	1091	312	315	4	0	0

- Molecule 3 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SE	260	2068	1316	389	360	3	0	0

- Molecule 4 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SG	218	1755	1102	337	313	3	0	0

- Molecule 5 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	SH	185	1486	954	266	266	0	0

- Molecule 6 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SI	188	1489	925	298	264	2	0	0

- Molecule 7 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SJ	185	1494	943	289	261	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SL	146	1168	747	221	197	3	0	0

- Molecule 9 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SN	150	1192	759	224	207	2	0	0

- Molecule 10 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SO	128	949	582	188	176	3	0	0

- Molecule 11 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SW	129	1021	650	188	180	3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SX	144	1121	708	220	191	2	0	0

- Molecule 13 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	SY	134	1073	676	208	189	0	0

- Molecule 14 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Sb	81	610	382	110	113	5	0	0

- Molecule 15 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	Se	23	201	130	41	30	0	0

- Molecule 16 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	CA	181	1436	917	261	254	4	0	0

- Molecule 17 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	JL	283	2262	1439	401	408	14	0	0

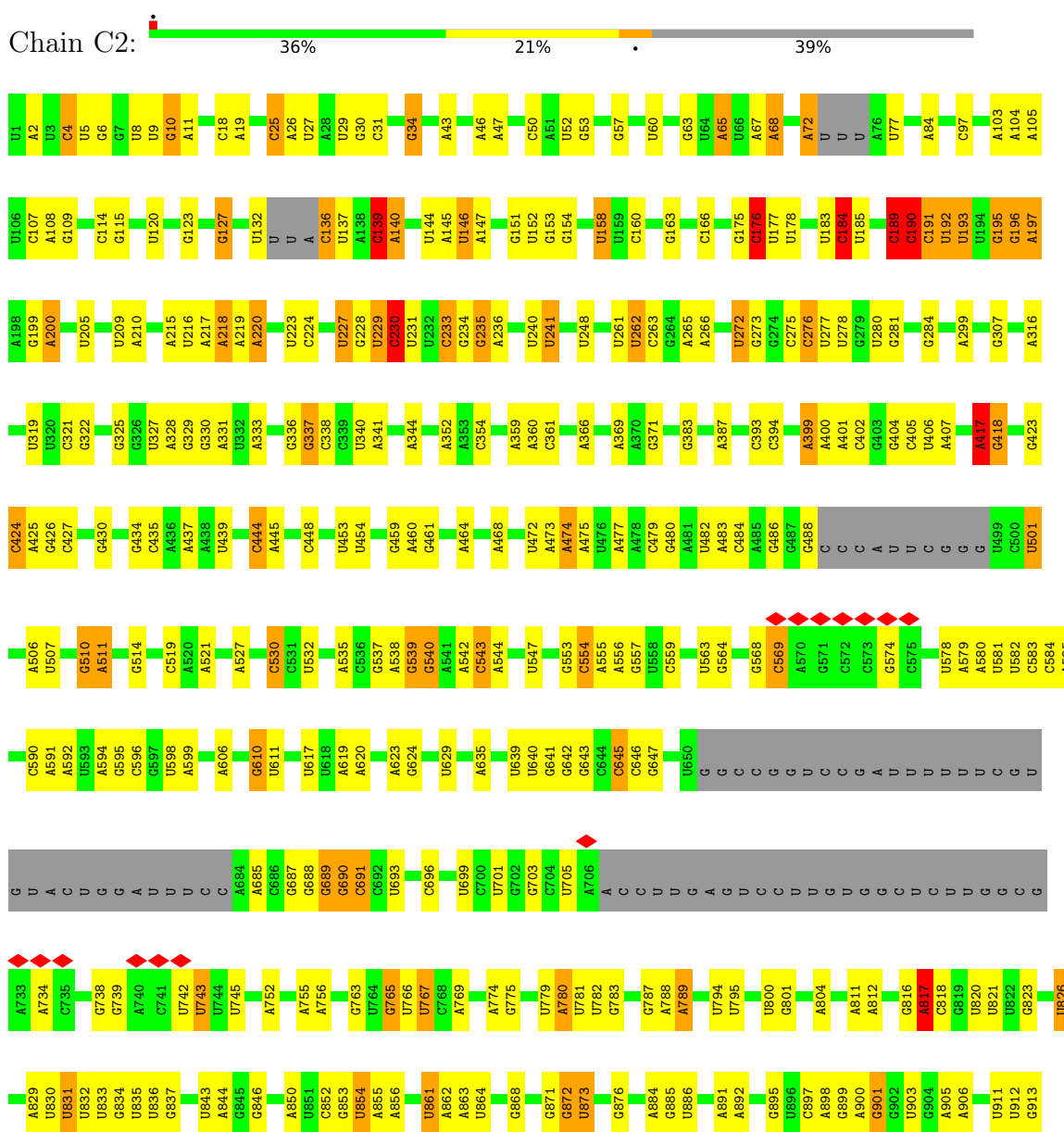
- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

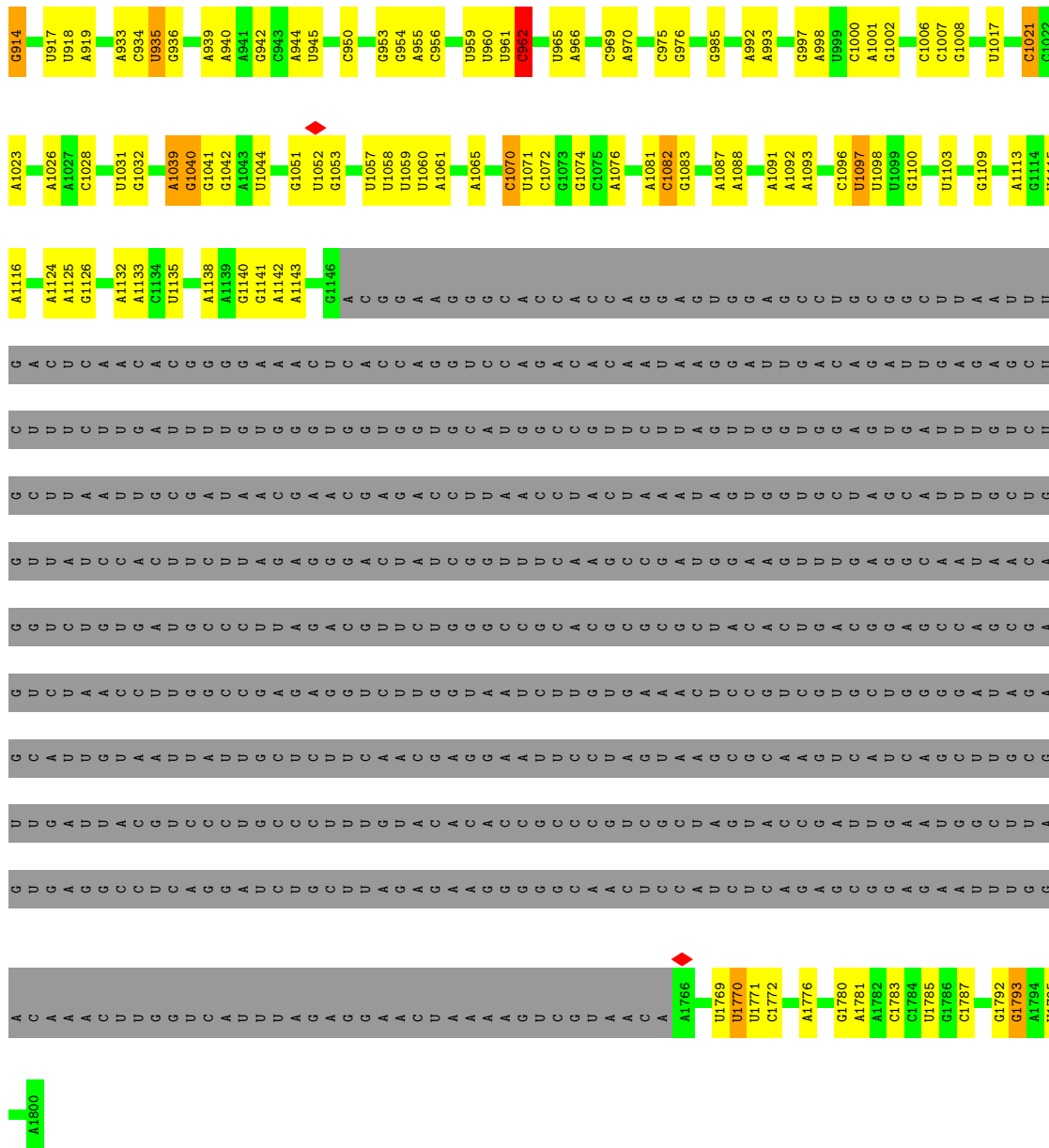
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
18	Sb	1	1	1	0

3 Residue-property plots

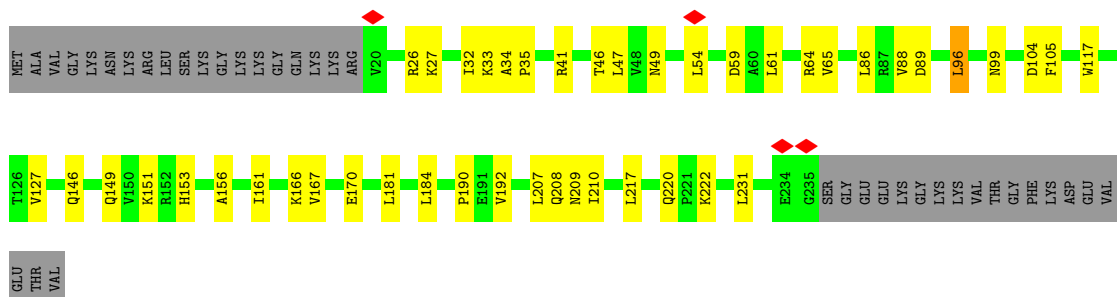
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 18S rRNA

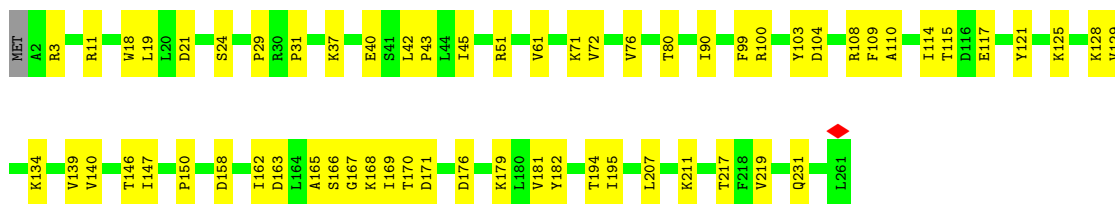
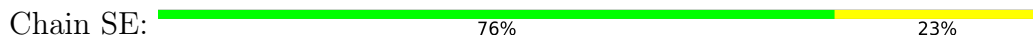




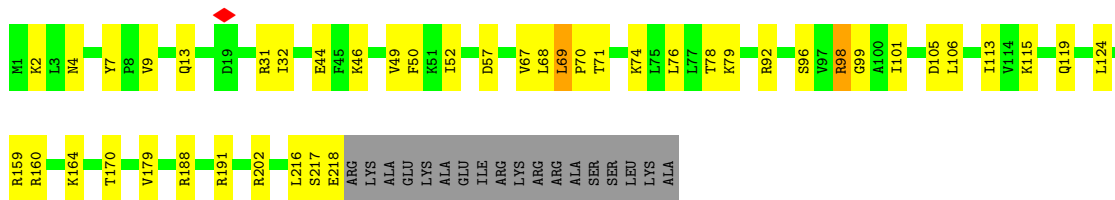
● Molecule 2: 40S ribosomal protein S1-A



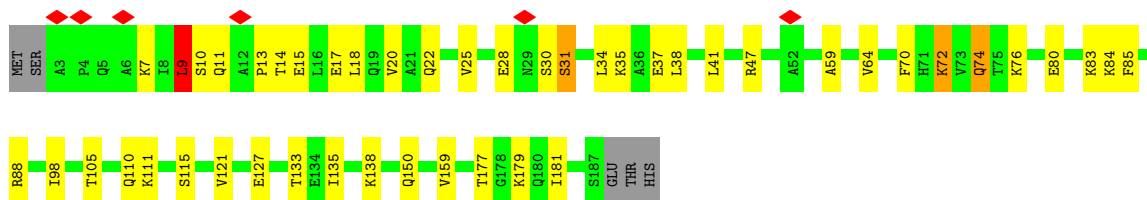
● Molecule 3: 40S ribosomal protein S4-A



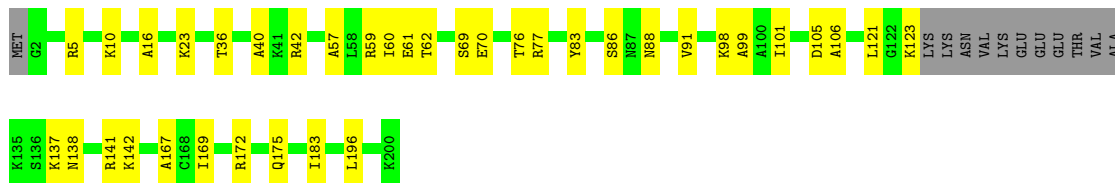
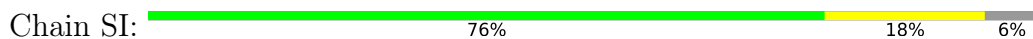
• Molecule 4: 40S ribosomal protein S6-A



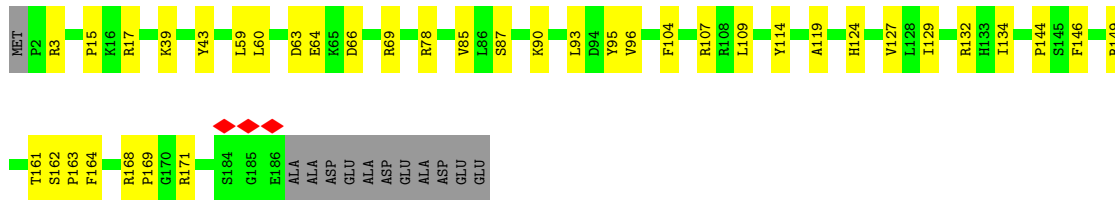
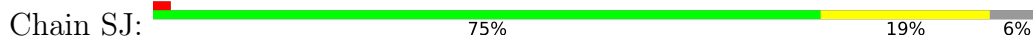
• Molecule 5: 40S ribosomal protein S7-A



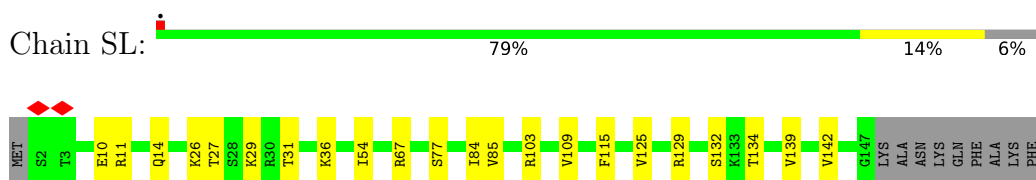
• Molecule 6: 40S ribosomal protein S8-A



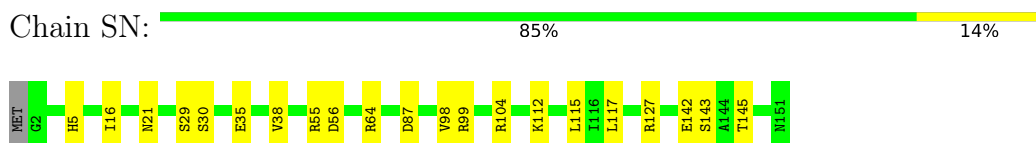
• Molecule 7: 40S ribosomal protein S9-A



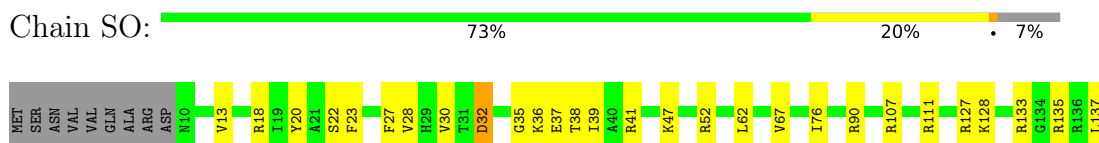
- Molecule 8: 40S ribosomal protein S11-A



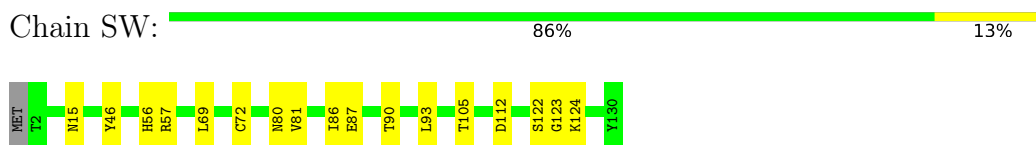
- Molecule 9: 40S ribosomal protein S13



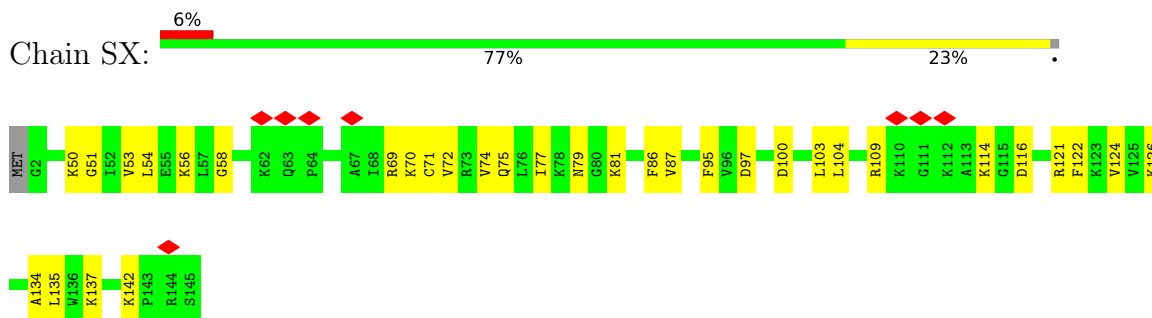
- Molecule 10: 40S ribosomal protein S14-A



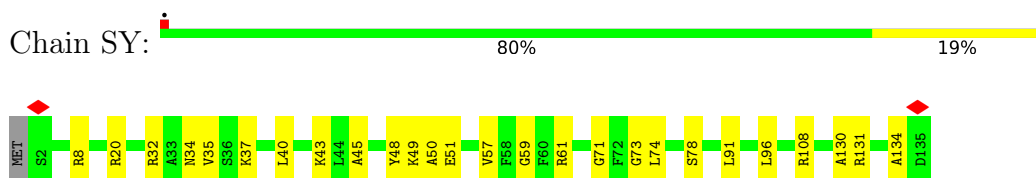
- Molecule 11: 40S ribosomal protein S22-A



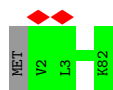
- Molecule 12: 40S ribosomal protein S23-A



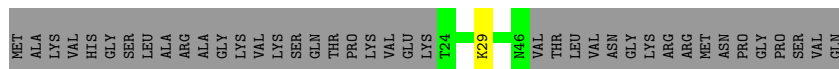
- Molecule 13: 40S ribosomal protein S24-A



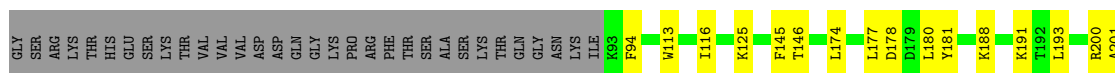
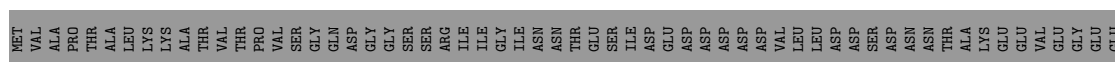
- Molecule 14: 40S ribosomal protein S27-A



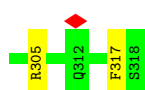
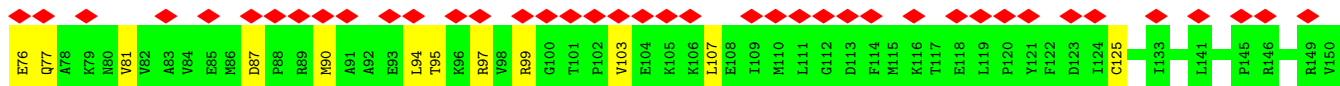
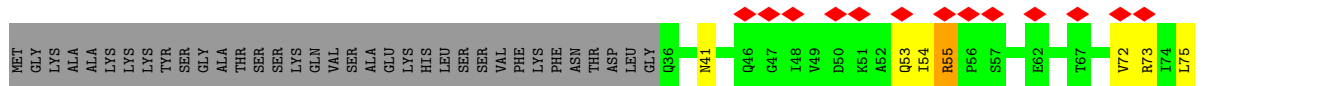
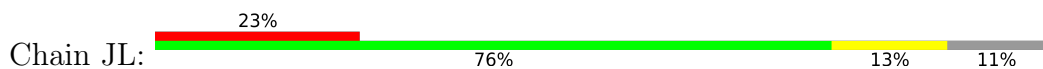
- Molecule 15: 40S ribosomal protein S30-A



- Molecule 16: Pre-rRNA-processing protein PNO1



- Molecule 17: Dimethyladenosine transferase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6122	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.388	Depositor
Minimum map value	-0.197	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	376.92, 376.92, 376.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.047, 1.047, 1.047	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	C2	0.64	1/26373 (0.0%)	1.03	89/41079 (0.2%)
2	SB	0.31	0/1748	0.62	2/2352 (0.1%)
3	SE	0.46	0/2109	0.68	0/2839
4	SG	0.31	0/1779	0.64	1/2379 (0.0%)
5	SH	0.31	0/1511	0.69	1/2036 (0.0%)
6	SI	0.38	0/1514	0.68	0/2021
7	SJ	0.33	0/1519	0.62	0/2035
8	SL	0.44	0/1194	0.61	0/1610
9	SN	0.37	0/1215	0.63	0/1638
10	SO	0.31	0/960	0.67	1/1290 (0.1%)
11	SW	0.41	0/1038	0.69	2/1395 (0.1%)
12	SX	0.34	0/1139	0.65	0/1518
13	SY	0.40	0/1087	0.71	0/1449
14	Sb	0.32	0/620	0.64	0/838
15	Se	0.28	0/205	0.65	0/271
16	CA	0.31	0/1462	0.61	0/1969
17	JL	0.27	0/2305	0.59	1/3116 (0.0%)
All	All	0.53	1/47778 (0.0%)	0.89	97/69835 (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
5	SH	0	4
9	SN	0	1
13	SY	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C2	474	A	N9-C4	-5.25	1.34	1.37

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	190	C	N3-C2-O2	-12.00	113.50	121.90
1	C2	645	C	N3-C2-O2	-11.02	114.19	121.90
1	C2	646	C	N3-C2-O2	-9.81	115.03	121.90
1	C2	190	C	N1-C2-O2	9.64	124.68	118.90
1	C2	453	U	C2-N1-C1'	9.26	128.81	117.70
1	C2	50	C	N3-C2-O2	-9.02	115.58	121.90
4	SG	69	LEU	CA-CB-CG	8.84	135.64	115.30
1	C2	453	U	N1-C2-O2	8.67	128.87	122.80
1	C2	645	C	N1-C2-O2	7.93	123.66	118.90
1	C2	646	C	C6-N1-C2	-7.88	117.15	120.30
1	C2	453	U	N3-C2-O2	-7.64	116.85	122.20
1	C2	956	C	N3-C2-O2	-7.58	116.59	121.90
1	C2	479	C	N3-C2-O2	-7.49	116.66	121.90
1	C2	861	U	C2-N1-C1'	7.28	126.44	117.70
1	C2	430	G	C5-C6-O6	7.14	132.89	128.60
1	C2	10	G	N3-C4-C5	-7.12	125.04	128.60
1	C2	795	U	N3-C2-O2	-6.98	117.31	122.20
17	JL	164	LEU	CA-CB-CG	6.95	131.29	115.30
1	C2	965	U	C2-N1-C1'	6.91	126.00	117.70
1	C2	10	G	C4-N9-C1'	6.75	135.28	126.50
1	C2	189	C	N1-C2-O2	6.74	122.94	118.90
1	C2	864	U	N1-C2-O2	6.74	127.52	122.80
1	C2	864	U	N3-C2-O2	-6.72	117.50	122.20
11	SW	93	LEU	CA-CB-CG	6.72	130.75	115.30
1	C2	120	U	N3-C2-O2	-6.70	117.51	122.20
1	C2	120	U	N1-C2-O2	6.54	127.38	122.80
1	C2	10	G	N3-C4-N9	6.50	129.90	126.00
1	C2	430	G	N9-C4-C5	6.49	108.00	105.40
1	C2	430	G	N3-C4-N9	-6.48	122.11	126.00
1	C2	224	C	N3-C2-O2	-6.39	117.43	121.90
1	C2	795	U	C2-N1-C1'	6.39	125.37	117.70
1	C2	272	U	P-O3'-C3'	6.37	127.34	119.70
1	C2	430	G	N1-C6-O6	-6.29	116.12	119.90
1	C2	872	G	C5-C6-O6	6.27	132.36	128.60
1	C2	872	G	N1-C6-O6	-6.25	116.15	119.90
1	C2	144	U	C2-N1-C1'	6.24	125.19	117.70
1	C2	935	U	N1-C2-O2	6.23	127.16	122.80
1	C2	453	U	C6-N1-C1'	-6.20	112.52	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	962	C	N3-C2-O2	-6.20	117.56	121.90
1	C2	956	C	N1-C2-O2	6.17	122.60	118.90
1	C2	191	C	O4'-C1'-N1	6.16	113.13	108.20
1	C2	934	C	C2-N1-C1'	6.12	125.53	118.80
1	C2	195	G	N1-C2-N2	-6.08	110.73	116.20
1	C2	934	C	N1-C2-O2	6.05	122.53	118.90
1	C2	795	U	N1-C2-O2	6.03	127.02	122.80
1	C2	935	U	N3-C2-O2	-5.98	118.02	122.20
1	C2	645	C	C6-N1-C2	-5.96	117.92	120.30
10	SO	32	ASP	CB-CG-OD2	5.96	123.66	118.30
5	SH	9	LEU	CA-CB-CG	5.95	128.97	115.30
1	C2	479	C	N1-C2-O2	5.92	122.45	118.90
1	C2	195	G	N3-C2-N2	5.90	124.03	119.90
1	C2	690	G	C8-N9-C4	-5.90	104.04	106.40
1	C2	1021	C	C6-N1-C2	-5.90	117.94	120.30
1	C2	767	U	N3-C2-O2	-5.85	118.10	122.20
1	C2	184	C	N1-C2-O2	5.81	122.39	118.90
1	C2	569	C	N1-C2-O2	5.77	122.36	118.90
1	C2	176	C	C6-N1-C1'	5.76	127.72	120.80
1	C2	691	C	C2-N1-C1'	5.76	125.14	118.80
1	C2	224	C	C6-N1-C2	-5.69	118.03	120.30
1	C2	864	U	C2-N1-C1'	5.68	124.52	117.70
1	C2	276	C	N3-C2-O2	-5.66	117.94	121.90
1	C2	1021	C	C5-C6-N1	5.64	123.82	121.00
1	C2	934	C	N3-C2-O2	-5.62	117.97	121.90
2	SB	54	LEU	CA-CB-CG	5.59	128.16	115.30
1	C2	1070	C	C2-N1-C1'	5.55	124.90	118.80
1	C2	1097	U	P-O3'-C3'	5.51	126.31	119.70
11	SW	112	ASP	CB-CG-OD1	5.47	123.23	118.30
1	C2	1021	C	C2-N1-C1'	5.43	124.78	118.80
1	C2	743	U	C2-N1-C1'	5.42	124.20	117.70
1	C2	417	A	P-O3'-C3'	5.41	126.19	119.70
1	C2	934	C	C6-N1-C2	-5.39	118.14	120.30
1	C2	136	C	P-O3'-C3'	5.39	126.16	119.70
1	C2	691	C	N1-C2-O2	5.37	122.12	118.90
1	C2	689	G	N1-C6-O6	-5.37	116.68	119.90
1	C2	767	U	C2-N1-C1'	5.37	124.15	117.70
1	C2	139	C	P-O3'-C3'	5.36	126.13	119.70
1	C2	10	G	C8-N9-C1'	-5.35	120.05	127.00
1	C2	690	G	N7-C8-N9	5.34	115.77	113.10
1	C2	935	U	C5-C4-O4	5.32	129.09	125.90
1	C2	767	U	N1-C2-O2	5.30	126.51	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	610	G	C4-N9-C1'	5.28	133.37	126.50
1	C2	901	G	O4'-C1'-N9	5.26	112.41	108.20
1	C2	962	C	C6-N1-C2	-5.25	118.20	120.30
1	C2	184	C	N3-C2-O2	-5.24	118.23	121.90
1	C2	530	C	N1-C2-O2	5.24	122.04	118.90
1	C2	861	U	C6-N1-C1'	-5.19	113.94	121.20
1	C2	817	A	P-O3'-C3'	5.18	125.92	119.70
1	C2	144	U	C6-N1-C1'	-5.16	113.97	121.20
1	C2	230	C	N1-C2-O2	5.13	121.98	118.90
1	C2	275	C	N1-C2-O2	5.11	121.97	118.90
1	C2	617	U	C2-N1-C1'	5.07	123.78	117.70
2	SB	96	LEU	CA-CB-CG	5.06	126.93	115.30
1	C2	430	G	C4-C5-N7	-5.05	108.78	110.80
1	C2	610	G	O4'-C1'-N9	5.05	112.24	108.20
1	C2	795	U	C6-N1-C2	-5.03	117.98	121.00
1	C2	965	U	C6-N1-C1'	-5.03	114.16	121.20
1	C2	453	U	C5-C6-N1	5.02	125.21	122.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	SH	110	GLN	Peptide
5	SH	31	SER	Peptide
5	SH	64	VAL	Peptide
5	SH	9	LEU	Peptide
9	SN	21	ASN	Peptide
13	SY	48	TYR	Peptide
13	SY	51	GLU	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	C2	23575	0	11854	213	0
2	SB	1722	0	1793	29	0
3	SE	2068	0	2154	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	SG	1755	0	1846	31	0
5	SH	1486	0	1576	28	0
6	SI	1489	0	1525	28	0
7	SJ	1494	0	1573	29	0
8	SL	1168	0	1233	17	0
9	SN	1192	0	1255	13	0
10	SO	949	0	985	23	0
11	SW	1021	0	1060	10	0
12	SX	1121	0	1196	22	0
13	SY	1073	0	1132	17	0
14	Sb	610	0	632	0	0
15	Se	201	0	222	0	0
16	CA	1436	0	1515	21	0
17	JL	2262	0	2330	24	0
18	Sb	1	0	0	0	0
All	All	44623	0	33881	469	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 6.

All (469) 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)
1:C2:826:U:H3	1:C2:846:G:H1	1.09	0.96
1:C2:976:G:H1	1:C2:1023:A:HO2'	1.07	0.94
1:C2:895:G:H1	1:C2:917:U:H3	0.94	0.93
1:C2:564:G:H1	1:C2:578:U:H3	1.07	0.92
1:C2:868:G:H1	1:C2:960:U:H3	0.91	0.90
1:C2:486:G:H1	1:C2:501:U:H3	0.93	0.89
1:C2:34:G:H1	1:C2:474:A:H2	1.07	0.89
1:C2:34:G:N1	1:C2:474:A:C2	2.46	0.84
1:C2:34:G:N1	1:C2:474:A:H2	1.80	0.79
6:SI:62:THR:HA	6:SI:76:THR:O	1.84	0.77
10:SO:28:VAL:O	10:SO:41:ARG:HA	1.85	0.77
5:SH:150:GLN:HB3	5:SH:181:ILE:HG22	1.70	0.73
13:SY:45:ALA:HA	13:SY:50:ALA:HB3	1.73	0.70
1:C2:862:A:OP2	9:SN:64:ARG:NH2	2.25	0.70
12:SX:71:CYS:SG	12:SX:72:VAL:N	2.63	0.70
8:SL:14:GLN:HB3	8:SL:54:ILE:HG13	1.73	0.69
1:C2:1065:A:N3	2:SB:146:GLN:NE2	2.40	0.69
1:C2:228:G:N1	1:C2:236:A:N6	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:229:U:O4	1:C2:235:G:O6	2.11	0.68
1:C2:873:U:O4	1:C2:954:G:O6	2.11	0.68
4:SG:31:ARG:HH22	4:SG:68:LEU:HD11	1.58	0.68
2:SB:149:GLN:HE21	2:SB:151:LYS:HB3	1.59	0.67
1:C2:190:C:H41	6:SI:137:LYS:HD3	1.60	0.67
2:SB:89:ASP:OD2	2:SB:99:ASN:ND2	2.28	0.66
1:C2:1140:G:H2'	1:C2:1141:G:H8	1.61	0.65
1:C2:284:G:N7	4:SG:188:ARG:NH1	2.44	0.65
8:SL:26:LYS:NZ	8:SL:29:LYS:O	2.29	0.65
10:SO:137:LEU:HB2	16:CA:248:VAL:HG11	1.78	0.64
1:C2:231:U:C2	1:C2:234:G:O6	2.50	0.64
1:C2:564:G:N2	1:C2:578:U:O2	2.30	0.64
1:C2:336:G:O6	6:SI:5:ARG:NH1	2.30	0.64
1:C2:329:G:H5''	6:SI:98:LYS:HB3	1.80	0.64
11:SW:80:ASN:OD1	11:SW:124:LYS:NZ	2.31	0.63
4:SG:70:PRO:HB3	4:SG:101:ILE:HB	1.80	0.63
6:SI:61:GLU:HG2	6:SI:62:THR:HG22	1.80	0.63
9:SN:35:GLU:HA	9:SN:38:VAL:HG22	1.81	0.63
16:CA:220:THR:HG21	16:CA:243:ALA:HB2	1.80	0.63
1:C2:72:A:N7	4:SG:164:LYS:NZ	2.47	0.63
5:SH:85:PHE:HB3	5:SH:88:ARG:HD2	1.80	0.62
3:SE:128:LYS:HG2	3:SE:140:VAL:HG12	1.82	0.61
1:C2:189:C:N4	1:C2:197:A:N6	2.47	0.61
12:SX:109:ARG:HE	12:SX:114:LYS:HA	1.65	0.61
17:JL:75:LEU:HD11	17:JL:107:LEU:HB2	1.82	0.61
9:SN:16:ILE:O	11:SW:57:ARG:NH2	2.34	0.61
1:C2:218:A:H61	1:C2:844:A:H1'	1.64	0.61
3:SE:11:ARG:NH1	3:SE:21:ASP:O	2.33	0.61
2:SB:64:ARG:HH21	10:SO:36:LYS:HB3	1.66	0.61
1:C2:228:G:H1	1:C2:236:A:N6	1.98	0.61
1:C2:1135:U:OP1	12:SX:121:ARG:NH2	2.33	0.61
9:SN:5:HIS:HB3	9:SN:117:LEU:HD13	1.83	0.61
1:C2:816:G:H2'	1:C2:817:A:H8	1.66	0.60
11:SW:15:ASN:ND2	11:SW:72:CYS:O	2.34	0.60
10:SO:20:TYR:HB3	10:SO:27:PHE:HB2	1.84	0.60
1:C2:647:G:H21	1:C2:687:G:H1	1.49	0.60
10:SO:28:VAL:HG11	10:SO:67:VAL:HG11	1.83	0.60
1:C2:899:G:N1	1:C2:911:U:N3	2.50	0.60
5:SH:138:LYS:HD3	5:SH:150:GLN:HE21	1.65	0.60
1:C2:231:U:O2	1:C2:234:G:O6	2.20	0.60
2:SB:32:ILE:HG13	2:SB:96:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CA:125:LYS:HG2	16:CA:145:PHE:HD1	1.67	0.59
1:C2:231:U:O2	1:C2:234:G:C6	2.55	0.59
16:CA:191:LYS:HE2	16:CA:193:LEU:HD21	1.84	0.59
1:C2:689:G:H2'	1:C2:690:G:C8	2.38	0.59
1:C2:592:A:OP1	7:SJ:39:LYS:NZ	2.34	0.59
3:SE:72:VAL:HG22	3:SE:90:ILE:HG22	1.84	0.59
1:C2:328:A:N3	6:SI:86:SER:OG	2.33	0.59
2:SB:34:ALA:HB3	2:SB:41:ARG:HA	1.85	0.58
12:SX:95:PHE:O	12:SX:142:LYS:NZ	2.34	0.58
9:SN:55:ARG:NH1	9:SN:56:ASP:OD1	2.36	0.58
16:CA:242:MET:HG2	16:CA:266:VAL:HG21	1.84	0.58
1:C2:1081:A:O2'	1:C2:1083:G:N7	2.36	0.58
1:C2:689:G:H2'	1:C2:690:G:H8	1.68	0.58
3:SE:194:THR:OG1	3:SE:231:GLN:NE2	2.37	0.58
7:SJ:129:ILE:HG12	7:SJ:134:ILE:HG13	1.84	0.57
10:SO:111:ARG:NH1	16:CA:94:PHE:O	2.37	0.57
6:SI:99:ALA:N	6:SI:169:ILE:O	2.37	0.57
9:SN:142:GLU:HB2	9:SN:145:THR:HG22	1.85	0.57
17:JL:162:ARG:HH11	17:JL:171:LEU:HD22	1.67	0.57
12:SX:58:GLY:HA2	12:SX:70:LYS:HB3	1.85	0.57
1:C2:227:U:O2	1:C2:834:G:O6	2.22	0.57
1:C2:895:G:H4'	10:SO:37:GLU:HG2	1.87	0.57
4:SG:98:ARG:NH2	4:SG:105:ASP:OD1	2.37	0.57
1:C2:151:G:N3	4:SG:13:GLN:NE2	2.52	0.57
3:SE:170:THR:HG22	3:SE:171:ASP:H	1.70	0.57
3:SE:103:TYR:O	3:SE:182:TYR:OH	2.22	0.57
6:SI:69:SER:OG	6:SI:70:GLU:OE1	2.22	0.57
1:C2:1787:C:OP1	10:SO:127:ARG:NH2	2.37	0.57
11:SW:46:TYR:HB3	11:SW:69:LEU:HD13	1.87	0.57
5:SH:80:GLU:HG2	5:SH:83:LYS:HE3	1.86	0.56
12:SX:54:LEU:HD11	12:SX:75:GLN:HB3	1.87	0.56
1:C2:950:C:O2'	9:SN:104:ARG:NH2	2.38	0.56
3:SE:31:PRO:HB3	3:SE:43:PRO:HG3	1.87	0.56
3:SE:162:ILE:HG23	3:SE:167:GLY:HA2	1.87	0.56
1:C2:354:C:H5''	6:SI:16:ALA:HB2	1.86	0.56
1:C2:742:U:H5'	5:SH:105:THR:HG22	1.88	0.56
12:SX:53:VAL:HA	12:SX:74:VAL:HG22	1.86	0.56
17:JL:95:THR:O	17:JL:99:ARG:NH1	2.38	0.56
12:SX:135:LEU:HD11	12:SX:142:LYS:HB2	1.88	0.56
1:C2:1785:U:OP1	10:SO:133:ARG:NH2	2.39	0.56
6:SI:172:ARG:HE	6:SI:175:GLN:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SG:57:ASP:HA	4:SG:106:LEU:HA	1.88	0.56
4:SG:76:LEU:HD21	4:SG:92:ARG:HD2	1.87	0.56
1:C2:642:G:C2	1:C2:693:U:O2	2.59	0.56
1:C2:843:U:H2'	1:C2:844:A:H8	1.71	0.56
1:C2:903:U:OP1	10:SO:135:ARG:NH2	2.39	0.56
1:C2:1776:A:O2'	17:JL:233:ARG:NH1	2.39	0.56
7:SJ:119:ALA:O	7:SJ:124:HIS:ND1	2.35	0.56
12:SX:69:ARG:NH1	12:SX:116:ASP:OD1	2.31	0.56
8:SL:125:VAL:HG12	8:SL:139:VAL:HA	1.88	0.55
3:SE:21:ASP:OD1	3:SE:21:ASP:N	2.38	0.55
1:C2:228:G:C6	1:C2:236:A:N6	2.73	0.55
1:C2:235:G:H2'	1:C2:236:A:C8	2.41	0.55
1:C2:29:U:H2'	1:C2:30:G:H8	1.71	0.55
1:C2:127:G:N7	4:SG:202:ARG:NH2	2.51	0.55
1:C2:154:G:OP2	13:SY:131:ARG:NH2	2.39	0.55
1:C2:1082:C:H41	1:C2:1091:A:H62	1.53	0.55
3:SE:104:ASP:HB2	3:SE:110:ALA:HB2	1.88	0.55
4:SG:69:LEU:O	4:SG:71:THR:N	2.39	0.55
6:SI:42:ARG:HB3	6:SI:59:ARG:HG2	1.87	0.55
11:SW:122:SER:OG	11:SW:123:GLY:N	2.37	0.55
13:SY:59:GLY:O	13:SY:71:GLY:HA3	2.07	0.55
1:C2:900:A:H3'	1:C2:901:G:H21	1.71	0.55
2:SB:61:LEU:HD22	2:SB:64:ARG:HD2	1.89	0.55
3:SE:18:TRP:O	3:SE:51:ARG:NH2	2.40	0.55
9:SN:87:ASP:OD1	9:SN:87:ASP:N	2.40	0.55
17:JL:244:SER:HB2	17:JL:247:VAL:HG12	1.89	0.55
1:C2:629:U:OP1	9:SN:127:ARG:NH2	2.33	0.54
7:SJ:114:TYR:HA	7:SJ:119:ALA:HB3	1.88	0.54
1:C2:1032:G:H1	1:C2:1103:U:H3	1.54	0.54
1:C2:530:C:O2	13:SY:61:ARG:NH1	2.40	0.54
1:C2:474:A:H5''	7:SJ:144:PRO:HD2	1.88	0.54
13:SY:91:LEU:HD22	13:SY:96:LEU:HD23	1.89	0.54
1:C2:1008:G:OP1	10:SO:135:ARG:NH1	2.41	0.54
8:SL:10:GLU:HB2	8:SL:14:GLN:HE22	1.73	0.54
1:C2:763:G:OP1	7:SJ:78:ARG:NH2	2.38	0.54
9:SN:99:ARG:NH1	9:SN:143:SER:OG	2.40	0.54
1:C2:140:A:N6	1:C2:281:G:OP1	2.40	0.54
1:C2:936:G:OP1	1:C2:1074:G:N2	2.36	0.54
4:SG:7:TYR:HB2	4:SG:113:ILE:HD12	1.89	0.54
8:SL:77:SER:HB3	8:SL:85:VAL:HB	1.89	0.54
13:SY:35:VAL:HB	13:SY:40:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:JL:302:ASP:OD1	17:JL:305:ARG:NH1	2.40	0.54
1:C2:584:C:H2'	1:C2:585:A:H8	1.73	0.53
5:SH:47:ARG:HB3	5:SH:59:ALA:HB3	1.90	0.53
1:C2:65:A:H2	1:C2:84:A:H62	1.56	0.53
2:SB:46:THR:OG1	2:SB:64:ARG:NH1	2.41	0.53
3:SE:115:THR:OG1	3:SE:117:GLU:O	2.24	0.53
11:SW:81:VAL:O	11:SW:122:SER:OG	2.23	0.53
12:SX:103:LEU:HB3	12:SX:126:LYS:HB2	1.91	0.53
1:C2:205:U:O2	1:C2:263:C:N3	2.42	0.53
1:C2:152:U:O2	4:SG:4:ASN:ND2	2.42	0.52
1:C2:699:U:O2	1:C2:739:G:O6	2.27	0.52
2:SB:181:LEU:HA	2:SB:184:LEU:HB3	1.91	0.52
8:SL:132:SER:O	8:SL:132:SER:OG	2.24	0.52
3:SE:45:ILE:HB	3:SE:80:THR:HG22	1.92	0.52
4:SG:74:LYS:NZ	4:SG:96:SER:OG	2.42	0.52
1:C2:688:G:H2'	1:C2:689:G:C8	2.45	0.52
1:C2:854:U:O4	1:C2:855:A:N6	2.42	0.52
4:SG:67:VAL:HG13	4:SG:99:GLY:HA2	1.91	0.52
12:SX:71:CYS:SG	12:SX:87:VAL:N	2.78	0.52
4:SG:217:SER:OG	4:SG:218:GLU:OE2	2.27	0.52
1:C2:641:G:N2	5:SH:177:THR:O	2.42	0.52
13:SY:59:GLY:O	13:SY:71:GLY:CA	2.57	0.52
1:C2:836:U:H2'	1:C2:837:G:C8	2.45	0.52
1:C2:1057:U:N3	1:C2:1061:A:C6	2.78	0.52
12:SX:56:LYS:HA	12:SX:72:VAL:HA	1.91	0.52
1:C2:140:A:H1'	4:SG:179:VAL:HG11	1.92	0.52
1:C2:856:A:N6	5:SH:115:SER:O	2.42	0.52
5:SH:34:LEU:HD21	5:SH:38:LEU:HD13	1.92	0.52
1:C2:193:U:O4	6:SI:137:LYS:NZ	2.44	0.51
2:SB:208:GLN:HG3	2:SB:209:ASN:HB2	1.92	0.51
1:C2:4:C:H1'	7:SJ:17:ARG:HH21	1.75	0.51
1:C2:826:U:O2	1:C2:846:G:N2	2.33	0.51
3:SE:37:LYS:HB2	3:SE:40:GLU:HG2	1.90	0.51
7:SJ:66:ASP:HB3	7:SJ:69:ARG:HB3	1.91	0.51
13:SY:20:ARG:HD2	13:SY:74:LEU:HD13	1.92	0.51
1:C2:230:C:N4	1:C2:233:C:N3	2.58	0.51
5:SH:9:LEU:HG	5:SH:10:SER:H	1.74	0.51
1:C2:897:C:O2	10:SO:41:ARG:NH2	2.44	0.51
3:SE:71:LYS:HG2	3:SE:76:VAL:HG22	1.92	0.51
2:SB:190:PRO:HG2	2:SB:192:VAL:HG13	1.93	0.51
1:C2:115:G:C8	8:SL:129:ARG:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SB:117:TRP:HB3	2:SB:153:HIS:HA	1.93	0.51
1:C2:918:U:H2'	1:C2:919:A:H8	1.76	0.51
1:C2:538:A:H5'	1:C2:543:C:H41	1.75	0.51
1:C2:539:G:N3	1:C2:540:G:N2	2.59	0.51
1:C2:939:A:H2'	1:C2:940:A:C8	2.46	0.51
10:SO:128:LYS:NZ	16:CA:188:LYS:O	2.34	0.50
1:C2:953:G:H2'	1:C2:954:G:C8	2.46	0.50
4:SG:78:THR:OG1	4:SG:79:LYS:N	2.43	0.50
8:SL:29:LYS:NZ	8:SL:31:THR:O	2.40	0.50
1:C2:34:G:O6	1:C2:474:A:N1	2.44	0.50
1:C2:486:G:O6	1:C2:501:U:O4	2.30	0.50
1:C2:564:G:O6	1:C2:580:A:C6	2.65	0.50
17:JL:53:GLN:O	17:JL:55:ARG:NH1	2.44	0.50
1:C2:29:U:H2'	1:C2:30:G:C8	2.45	0.50
1:C2:985:G:N1	1:C2:1017:U:C2	2.80	0.50
5:SH:25:VAL:HA	5:SH:28:GLU:HB2	1.93	0.50
1:C2:564:G:C6	1:C2:580:A:N1	2.80	0.50
1:C2:191:C:O2'	1:C2:192:U:O4'	2.30	0.49
1:C2:331:A:N7	6:SI:172:ARG:NH2	2.59	0.49
1:C2:564:G:C6	1:C2:580:A:C6	3.00	0.49
3:SE:100:ARG:HB2	3:SE:114:ILE:HD13	1.93	0.49
7:SJ:87:SER:HB3	7:SJ:90:LYS:HB2	1.95	0.49
1:C2:151:G:H22	1:C2:163:G:H1	1.58	0.49
1:C2:307:G:OP1	8:SL:103:ARG:NH1	2.41	0.49
1:C2:742:U:H3	1:C2:745:U:H5''	1.77	0.49
1:C2:1041:G:H2'	1:C2:1042:G:C8	2.46	0.49
7:SJ:63:ASP:OD1	7:SJ:64:GLU:N	2.45	0.49
7:SJ:109:LEU:HB2	7:SJ:146:PHE:HB3	1.94	0.49
1:C2:107:C:OP1	1:C2:383:G:O2'	2.29	0.49
2:SB:33:LYS:HD3	2:SB:41:ARG:HH12	1.77	0.49
1:C2:325:G:OP1	8:SL:134:THR:OG1	2.27	0.49
1:C2:393:C:O2'	4:SG:92:ARG:NH2	2.45	0.49
2:SB:104:ASP:OD1	2:SB:105:PHE:N	2.45	0.49
1:C2:337:G:N2	1:C2:340:U:OP2	2.45	0.49
1:C2:146:U:H2'	1:C2:147:A:H8	1.77	0.49
1:C2:954:G:H2'	1:C2:955:A:C8	2.48	0.49
1:C2:1142:A:H2'	1:C2:1143:A:C8	2.47	0.49
17:JL:125:CYS:O	17:JL:151:SER:HA	2.13	0.49
5:SH:38:LEU:HG	5:SH:41:LEU:HD11	1.95	0.49
16:CA:181:TYR:O	16:CA:234:LEU:HA	2.12	0.49
1:C2:789:A:OP1	3:SE:108:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:954:G:H2'	1:C2:955:A:H8	1.78	0.49
13:SY:57:VAL:HG12	13:SY:73:GLY:HA3	1.95	0.49
1:C2:899:G:C6	1:C2:911:U:N3	2.81	0.48
3:SE:181:VAL:HG21	3:SE:195:ILE:HG13	1.95	0.48
10:SO:47:LYS:HZ3	10:SO:62:LEU:HB3	1.78	0.48
1:C2:25:C:HO2'	1:C2:366:A:HO2'	1.58	0.48
2:SB:35:PRO:HB3	2:SB:231:LEU:HD21	1.94	0.48
1:C2:868:G:O6	1:C2:960:U:O4	2.31	0.48
1:C2:800:U:H2'	1:C2:801:G:H8	1.79	0.48
1:C2:905:A:O3'	10:SO:52:ARG:NE	2.44	0.48
2:SB:26:ARG:HH12	2:SB:49:ASN:HA	1.78	0.48
16:CA:113:TRP:HA	16:CA:116:ILE:HG22	1.94	0.48
1:C2:241:U:H5'	4:SG:216:LEU:HD21	1.94	0.48
1:C2:780:A:C4	13:SY:8:ARG:HD2	2.49	0.48
2:SB:27:LYS:NZ	2:SB:49:ASN:OD1	2.34	0.48
2:SB:217:LEU:HD21	2:SB:220:GLN:HG3	1.95	0.48
1:C2:195:G:H2'	1:C2:196:G:C8	2.48	0.48
1:C2:472:U:O2'	1:C2:769:A:N3	2.41	0.48
3:SE:129:VAL:HG22	3:SE:139:VAL:HG12	1.95	0.48
12:SX:51:GLY:HA2	12:SX:77:ILE:HG12	1.95	0.48
1:C2:816:G:H2'	1:C2:817:A:C8	2.48	0.48
6:SI:83:TYR:HB3	6:SI:101:ILE:HB	1.94	0.48
7:SJ:59:LEU:HD22	7:SJ:69:ARG:HA	1.96	0.48
1:C2:1115:U:H2'	1:C2:1116:A:H8	1.79	0.47
2:SB:88:VAL:HG21	2:SB:96:LEU:HD12	1.94	0.47
7:SJ:15:PRO:HD3	7:SJ:43:TYR:CE1	2.48	0.47
1:C2:640:U:O2	5:SH:179:LYS:NZ	2.40	0.47
7:SJ:161:THR:HG22	7:SJ:162:SER:H	1.79	0.47
1:C2:262:U:H2'	1:C2:263:C:C6	2.49	0.47
2:SB:207:LEU:HB3	2:SB:210:ILE:HD11	1.96	0.47
2:SB:65:VAL:HA	2:SB:86:LEU:O	2.14	0.47
4:SG:46:LYS:N	4:SG:119:GLN:HE22	2.12	0.47
7:SJ:93:LEU:HA	7:SJ:96:VAL:HG12	1.97	0.47
5:SH:133:THR:HG21	5:SH:159:VAL:HA	1.96	0.47
6:SI:62:THR:HB	6:SI:77:ARG:HD2	1.95	0.47
1:C2:235:G:H2'	1:C2:236:A:H8	1.80	0.47
3:SE:24:SER:H	7:SJ:3:ARG:HH22	1.62	0.47
6:SI:138:ASN:HA	6:SI:141:ARG:HG2	1.97	0.47
12:SX:54:LEU:HD21	12:SX:75:GLN:HG2	1.96	0.47
10:SO:13:VAL:HG23	10:SO:76:ILE:HA	1.96	0.47
1:C2:220:A:C8	1:C2:832:U:C2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:539:G:H1'	1:C2:540:G:H21	1.80	0.47
1:C2:1140:G:H2'	1:C2:1141:G:C8	2.46	0.47
13:SY:37:LYS:HA	13:SY:40:LEU:HD13	1.97	0.47
1:C2:52:U:H2'	1:C2:53:G:C8	2.50	0.46
1:C2:139:C:O2'	1:C2:177:U:O2	2.29	0.46
1:C2:871:G:H2'	1:C2:872:G:C8	2.50	0.46
3:SE:139:VAL:HG13	3:SE:150:PRO:HG3	1.97	0.46
7:SJ:124:HIS:HA	7:SJ:127:VAL:HG12	1.97	0.46
1:C2:68:A:OP1	4:SG:160:ARG:NH2	2.39	0.46
3:SE:90:ILE:HG13	3:SE:99:PHE:HB2	1.97	0.46
16:CA:266:VAL:HA	16:CA:269:ARG:HG2	1.97	0.46
3:SE:147:ILE:HG21	3:SE:169:ILE:HG13	1.96	0.46
16:CA:174:LEU:HA	16:CA:180:LEU:HD12	1.98	0.46
16:CA:177:LEU:HD22	16:CA:180:LEU:HD21	1.97	0.46
4:SG:44:GLU:O	4:SG:119:GLN:NE2	2.40	0.46
8:SL:115:PHE:HB3	8:SL:142:VAL:HG21	1.97	0.46
16:CA:250:LEU:HD22	16:CA:259:VAL:HG11	1.97	0.46
1:C2:912:U:O2	1:C2:914:G:N1	2.49	0.46
7:SJ:162:SER:O	7:SJ:162:SER:OG	2.33	0.46
17:JL:75:LEU:HB3	17:JL:103:VAL:HG21	1.97	0.46
1:C2:688:G:H2'	1:C2:689:G:H8	1.80	0.46
17:JL:94:LEU:HD12	17:JL:97:ARG:HE	1.81	0.46
10:SO:30:VAL:HG13	10:SO:39:ILE:HB	1.98	0.46
12:SX:97:ASP:N	12:SX:100:ASP:OD1	2.43	0.46
17:JL:41:ASN:ND2	17:JL:195:ASN:OD1	2.41	0.46
1:C2:31:C:H5''	12:SX:134:ALA:HB2	1.98	0.46
1:C2:154:G:OP1	4:SG:2:LYS:NZ	2.35	0.46
1:C2:176:C:O2'	1:C2:177:U:O4'	2.31	0.46
1:C2:405:C:O2'	4:SG:92:ARG:O	2.32	0.46
1:C2:1057:U:C4	1:C2:1061:A:N1	2.84	0.46
5:SH:17:GLU:HA	5:SH:20:VAL:HG12	1.98	0.46
10:SO:18:ARG:HH12	10:SO:35:GLY:HA2	1.81	0.46
1:C2:177:U:O2'	4:SG:191:ARG:NH1	2.49	0.45
1:C2:1132:A:H2'	1:C2:1133:A:C8	2.51	0.45
2:SB:46:THR:OG1	10:SO:32:ASP:OD1	2.33	0.45
3:SE:211:LYS:HB2	3:SE:217:THR:HG22	1.97	0.45
7:SJ:162:SER:O	7:SJ:164:PHE:N	2.49	0.45
6:SI:121:LEU:O	6:SI:123:LYS:NZ	2.41	0.45
13:SY:130:ALA:O	13:SY:134:ALA:HB2	2.16	0.45
17:JL:159:PHE:HA	17:JL:162:ARG:HB2	1.99	0.45
17:JL:72:VAL:HG23	17:JL:73:ARG:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:230:C:H2'	1:C2:231:U:H6	1.82	0.45
1:C2:547:U:H1'	1:C2:596:C:H1'	1.98	0.45
1:C2:584:C:H2'	1:C2:585:A:C8	2.51	0.45
1:C2:985:G:C2	1:C2:1017:U:O2	2.69	0.45
1:C2:800:U:H2'	1:C2:801:G:C8	2.52	0.45
1:C2:788:A:H2'	3:SE:19:LEU:HD22	1.97	0.45
8:SL:26:LYS:HA	8:SL:26:LYS:HD2	1.84	0.45
5:SH:37:GLU:OE1	5:SH:72:LYS:NZ	2.42	0.45
12:SX:86:PHE:N	12:SX:122:PHE:O	2.49	0.45
1:C2:140:A:H61	1:C2:281:G:H5''	1.80	0.45
6:SI:40:ALA:O	6:SI:59:ARG:HG3	2.17	0.45
6:SI:83:TYR:HB2	6:SI:196:LEU:HD21	1.98	0.45
13:SY:43:LYS:HD3	13:SY:43:LYS:HA	1.85	0.45
1:C2:482:U:H2'	1:C2:483:A:C8	2.52	0.45
1:C2:895:G:O6	1:C2:917:U:O4	2.34	0.45
4:SG:32:ILE:HA	4:SG:52:ILE:HB	1.98	0.45
4:SG:50:PHE:HE1	4:SG:113:ILE:HG12	1.81	0.45
1:C2:1087:A:H2'	1:C2:1088:A:C8	2.53	0.44
10:SO:38:THR:OG1	10:SO:39:ILE:N	2.50	0.44
1:C2:1039:A:O2'	1:C2:1040:G:O5'	2.28	0.44
1:C2:1071:U:H2'	1:C2:1072:C:C6	2.52	0.44
4:SG:159:ARG:HH21	4:SG:170:THR:HG23	1.81	0.44
5:SH:22:GLN:HA	5:SH:25:VAL:HG22	2.00	0.44
6:SI:10:LYS:HE3	6:SI:10:LYS:HB3	1.75	0.44
1:C2:836:U:H2'	1:C2:837:G:H8	1.82	0.44
1:C2:873:U:H3	1:C2:954:G:H1	1.66	0.44
1:C2:899:G:N1	1:C2:911:U:C2	2.85	0.44
3:SE:18:TRP:HZ3	3:SE:29:PRO:HD2	1.82	0.44
1:C2:472:U:H2'	1:C2:473:A:H8	1.83	0.44
1:C2:642:G:H2'	1:C2:643:G:H8	1.82	0.44
3:SE:125:LYS:HA	3:SE:158:ASP:O	2.17	0.44
17:JL:73:ARG:O	17:JL:77:GLN:HG3	2.17	0.44
3:SE:51:ARG:HA	3:SE:51:ARG:HD3	1.85	0.44
1:C2:34:G:C6	1:C2:474:A:N1	2.86	0.44
1:C2:329:G:H2'	1:C2:330:G:H8	1.82	0.44
7:SJ:60:LEU:HD23	7:SJ:60:LEU:HA	1.88	0.44
1:C2:189:C:N3	1:C2:197:A:C6	2.85	0.44
1:C2:765:G:C6	7:SJ:149:ARG:HD3	2.53	0.44
16:CA:228:ASP:OD1	16:CA:228:ASP:N	2.50	0.44
1:C2:158:U:O2'	1:C2:160:C:OP2	2.28	0.44
1:C2:564:G:O6	1:C2:578:U:O4	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:590:C:H2'	1:C2:591:A:C8	2.53	0.44
1:C2:788:A:OP2	3:SE:108:ARG:NH2	2.50	0.44
1:C2:899:G:C2	1:C2:911:U:O2	2.71	0.44
3:SE:134:LYS:HE3	3:SE:134:LYS:HB3	1.79	0.44
10:SO:23:PHE:HE2	10:SO:90:ARG:HH11	1.65	0.44
16:CA:223:ARG:HB2	16:CA:234:LEU:HB3	2.00	0.44
3:SE:166:SER:OG	3:SE:168:LYS:HE2	2.17	0.44
3:SE:176:ASP:OD1	3:SE:179:LYS:NZ	2.40	0.44
17:JL:230:VAL:HG22	17:JL:295:ALA:HB2	2.00	0.44
1:C2:1793:G:C8	16:CA:200:ARG:HD2	2.53	0.43
17:JL:191:VAL:HB	17:JL:204:SER:HB2	2.00	0.43
6:SI:105:ASP:OD1	6:SI:106:ALA:N	2.51	0.43
16:CA:212:THR:O	16:CA:215:ALA:HB3	2.18	0.43
1:C2:482:U:H2'	1:C2:483:A:H8	1.82	0.43
1:C2:598:U:H2'	1:C2:599:A:H8	1.84	0.43
2:SB:167:VAL:HA	2:SB:170:GLU:HG2	2.00	0.43
3:SE:100:ARG:NH2	3:SE:121:TYR:O	2.51	0.43
1:C2:553:G:H3'	1:C2:554:C:H2'	2.01	0.43
6:SI:83:TYR:OH	8:SL:11:ARG:O	2.29	0.43
2:SB:166:LYS:HD2	2:SB:166:LYS:HA	1.77	0.43
16:CA:125:LYS:HD3	16:CA:146:THR:HG23	2.01	0.43
4:SG:113:ILE:HD11	4:SG:124:LEU:HD21	1.99	0.43
1:C2:532:U:OP1	7:SJ:132:ARG:NH2	2.52	0.43
5:SH:98:ILE:HG12	5:SH:121:VAL:HG11	2.00	0.43
6:SI:88:ASN:O	6:SI:91:VAL:HG12	2.19	0.43
17:JL:222:GLU:OE1	17:JL:317:PHE:N	2.49	0.43
1:C2:1793:G:H8	16:CA:200:ARG:HD2	1.84	0.43
7:SJ:85:VAL:HG11	7:SJ:104:PHE:HE1	1.84	0.43
12:SX:56:LYS:HB3	12:SX:72:VAL:HG12	1.99	0.43
1:C2:642:G:N1	1:C2:693:U:C2	2.87	0.43
11:SW:87:GLU:O	11:SW:90:THR:OG1	2.26	0.43
17:JL:87:ASP:HB2	17:JL:90:MET:HB2	2.01	0.43
1:C2:219:A:C8	1:C2:831:U:H1'	2.54	0.42
1:C2:1044:U:H5''	2:SB:153:HIS:HE1	1.84	0.42
1:C2:327:U:H2'	1:C2:328:A:C8	2.55	0.42
1:C2:444:C:OP2	13:SY:108:ARG:NH2	2.52	0.42
1:C2:510:G:H2'	1:C2:511:A:H8	1.84	0.42
1:C2:884:A:H2'	1:C2:885:G:C8	2.54	0.42
3:SE:45:ILE:HA	3:SE:61:VAL:HG11	2.02	0.42
5:SH:111:LYS:HE2	5:SH:111:LYS:HB3	1.73	0.42
1:C2:387:A:OP1	6:SI:23:LYS:NZ	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SH:84:LYS:HB2	5:SH:84:LYS:HE2	1.88	0.42
1:C2:417:A:H5'	1:C2:418:G:C8	2.54	0.42
1:C2:537:G:H3'	7:SJ:171:ARG:HH22	1.85	0.42
5:SH:15:GLU:HA	5:SH:18:LEU:HD12	2.01	0.42
17:JL:76:GLU:HA	17:JL:103:VAL:HG11	2.01	0.42
1:C2:340:U:H2'	1:C2:341:A:C8	2.55	0.42
1:C2:591:A:H2'	1:C2:592:A:C8	2.54	0.42
1:C2:1124:A:H2'	1:C2:1125:A:C8	2.54	0.42
7:SJ:64:GLU:OE1	7:SJ:69:ARG:NH2	2.53	0.42
8:SL:84:ILE:HD11	8:SL:139:VAL:HG21	2.02	0.42
9:SN:98:VAL:HG13	9:SN:115:LEU:HD13	2.01	0.42
17:JL:54:ILE:HD12	17:JL:77:GLN:HE22	1.85	0.42
1:C2:563:U:H2'	1:C2:564:G:H8	1.83	0.42
1:C2:1770:U:H2'	1:C2:1771:U:C6	2.55	0.42
3:SE:165:ALA:HB3	3:SE:168:LYS:NZ	2.35	0.42
4:SG:7:TYR:CZ	4:SG:9:VAL:HB	2.54	0.42
5:SH:14:THR:OG1	5:SH:15:GLU:N	2.51	0.42
5:SH:70:PHE:O	5:SH:74:GLN:HG2	2.19	0.42
7:SJ:163:PRO:HB3	7:SJ:169:PRO:HA	2.01	0.42
12:SX:137:LYS:HE3	12:SX:137:LYS:HB3	1.89	0.42
1:C2:209:U:H2'	1:C2:210:A:H8	1.85	0.42
1:C2:406:U:H2'	1:C2:407:A:C8	2.55	0.42
1:C2:424:C:O2	1:C2:427:C:N4	2.53	0.42
5:SH:11:GLN:HG3	5:SH:13:PRO:HD2	2.01	0.42
16:CA:178:ASP:N	16:CA:178:ASP:OD1	2.52	0.42
8:SL:26:LYS:NZ	8:SL:27:THR:O	2.43	0.42
1:C2:642:G:H2'	1:C2:643:G:C8	2.54	0.42
3:SE:207:LEU:HD12	3:SE:219:VAL:HG12	2.02	0.42
9:SN:29:SER:OG	9:SN:30:SER:N	2.53	0.42
1:C2:435:C:H5''	12:SX:50:LYS:HE2	2.01	0.41
1:C2:961:U:H2'	1:C2:962:C:C6	2.55	0.41
6:SI:36:THR:HG22	6:SI:57:ALA:O	2.19	0.41
7:SJ:90:LYS:HG2	7:SJ:95:TYR:HB3	2.02	0.41
1:C2:108:A:H2'	1:C2:109:G:C8	2.55	0.41
1:C2:861:U:O2'	11:SW:56:HIS:O	2.38	0.41
2:SB:59:ASP:OD1	2:SB:59:ASP:N	2.45	0.41
13:SY:49:LYS:HD3	13:SY:49:LYS:HA	1.80	0.41
1:C2:196:G:O2'	1:C2:197:A:H8	2.04	0.41
3:SE:163:ASP:OD1	3:SE:163:ASP:N	2.53	0.41
10:SO:22:SER:OG	10:SO:23:PHE:N	2.52	0.41
1:C2:248:U:H4'	8:SL:36:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SB:156:ALA:HB3	2:SB:161:ILE:HD11	2.02	0.41
1:C2:123:G:H21	3:SE:146:THR:HG21	1.85	0.41
1:C2:183:U:H2'	1:C2:184:C:C6	2.55	0.41
1:C2:472:U:H2'	1:C2:473:A:C8	2.56	0.41
6:SI:167:ALA:HA	6:SI:183:ILE:HA	2.03	0.41
8:SL:109:VAL:HG21	8:SL:125:VAL:HG11	2.03	0.41
12:SX:104:LEU:HD23	12:SX:124:VAL:HA	2.02	0.41
17:JL:75:LEU:HD22	17:JL:81:VAL:HG21	2.03	0.41
5:SH:28:GLU:HB3	5:SH:35:LYS:NZ	2.36	0.41
13:SY:78:SER:O	13:SY:78:SER:OG	2.32	0.41
1:C2:521:A:N3	13:SY:34:ASN:ND2	2.68	0.41
5:SH:30:SER:N	5:SH:31:SER:HA	2.35	0.41
5:SH:127:GLU:HG2	5:SH:135:ILE:HD12	2.02	0.41
1:C2:5:U:H2'	1:C2:6:G:H8	1.85	0.41
1:C2:189:C:H42	1:C2:197:A:N6	2.15	0.41
1:C2:804:A:N3	11:SW:105:THR:HG22	2.36	0.41
1:C2:891:A:H2'	1:C2:892:A:H8	1.85	0.41
2:SB:47:LEU:HD21	10:SO:39:ILE:HD11	2.03	0.41
3:SE:42:LEU:HB2	3:SE:109:PHE:HD2	1.85	0.41
4:SG:49:VAL:HG21	4:SG:115:LYS:HD3	2.02	0.41
6:SI:142:LYS:HE3	6:SI:142:LYS:HB2	1.63	0.41
12:SX:79:ASN:HB3	12:SX:81:LYS:HG2	2.02	0.41
17:JL:161:LEU:HD22	17:JL:171:LEU:HD12	2.02	0.41
1:C2:97:C:O2	1:C2:425:A:O2'	2.36	0.41
11:SW:86:ILE:HD11	11:SW:122:SER:HB2	2.02	0.41
1:C2:199:G:O2'	1:C2:200:A:H8	2.04	0.40
6:SI:60:ILE:HD13	6:SI:60:ILE:HA	1.93	0.40
16:CA:201:ALA:O	16:CA:205:ILE:HG12	2.21	0.40
17:JL:258:PHE:HA	17:JL:261:MET:HG3	2.03	0.40
1:C2:975:C:OP1	9:SN:112:LYS:NZ	2.53	0.40
1:C2:18:C:H2'	1:C2:19:A:H8	1.86	0.40
1:C2:220:A:N7	1:C2:832:U:N3	2.70	0.40
1:C2:393:C:H2'	1:C2:394:C:C6	2.56	0.40
1:C2:399:A:H4'	3:SE:3:ARG:HG2	2.03	0.40
1:C2:535:A:OP1	7:SJ:168:ARG:NH2	2.54	0.40
2:SB:125:VAL:HG12	2:SB:127:VAL:HG23	2.03	0.40
17:JL:201:GLN:HG2	17:JL:202:VAL:HG13	2.02	0.40
1:C2:175:G:H22	1:C2:266:A:P	2.45	0.40
1:C2:899:G:C2	1:C2:911:U:C2	3.10	0.40
5:SH:76:LYS:HA	5:SH:76:LYS:HD3	1.84	0.40
7:SJ:107:ARG:HA	7:SJ:107:ARG:HD2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SB	214/255 (84%)	199 (93%)	15 (7%)	0	100	100
3	SE	258/261 (99%)	237 (92%)	21 (8%)	0	100	100
4	SG	216/236 (92%)	206 (95%)	10 (5%)	0	100	100
5	SH	183/190 (96%)	163 (89%)	19 (10%)	1 (0%)	29	68
6	SI	184/200 (92%)	178 (97%)	6 (3%)	0	100	100
7	SJ	183/197 (93%)	172 (94%)	11 (6%)	0	100	100
8	SL	144/156 (92%)	131 (91%)	13 (9%)	0	100	100
9	SN	148/151 (98%)	136 (92%)	12 (8%)	0	100	100
10	SO	126/137 (92%)	109 (86%)	17 (14%)	0	100	100
11	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
12	SX	142/145 (98%)	120 (84%)	22 (16%)	0	100	100
13	SY	132/135 (98%)	116 (88%)	15 (11%)	1 (1%)	19	58
14	Sb	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
15	Se	21/63 (33%)	19 (90%)	2 (10%)	0	100	100
16	CA	179/274 (65%)	174 (97%)	5 (3%)	0	100	100
17	JL	281/318 (88%)	270 (96%)	11 (4%)	0	100	100
All	All	2617/2930 (89%)	2417 (92%)	198 (8%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	SY	32	ARG
5	SH	74	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SB	192/224 (86%)	191 (100%)	1 (0%)	88	94
3	SE	221/222 (100%)	221 (100%)	0	100	100
4	SG	187/201 (93%)	186 (100%)	1 (0%)	88	94
5	SH	165/170 (97%)	163 (99%)	2 (1%)	71	87
6	SI	150/161 (93%)	150 (100%)	0	100	100
7	SJ	158/166 (95%)	158 (100%)	0	100	100
8	SL	129/137 (94%)	128 (99%)	1 (1%)	81	91
9	SN	127/128 (99%)	127 (100%)	0	100	100
10	SO	97/105 (92%)	96 (99%)	1 (1%)	76	88
11	SW	110/111 (99%)	110 (100%)	0	100	100
12	SX	119/120 (99%)	119 (100%)	0	100	100
13	SY	112/113 (99%)	112 (100%)	0	100	100
14	Sb	70/71 (99%)	70 (100%)	0	100	100
15	Se	21/54 (39%)	20 (95%)	1 (5%)	25	60
16	CA	158/238 (66%)	158 (100%)	0	100	100
17	JL	255/283 (90%)	254 (100%)	1 (0%)	91	96
All	All	2271/2504 (91%)	2263 (100%)	8 (0%)	91	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	222	LYS
4	SG	98	ARG
5	SH	7	LYS
5	SH	72	LYS
8	SL	67	ARG
10	SO	107	ARG
15	Se	29	LYS
17	JL	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	99	ASN
2	SB	149	GLN
5	SH	150	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C2	1100/1800 (61%)	245 (22%)	10 (0%)

All (245) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C2	2	A
1	C2	4	C
1	C2	8	U
1	C2	9	U
1	C2	10	G
1	C2	11	A
1	C2	25	C
1	C2	26	A
1	C2	27	U
1	C2	34	G
1	C2	43	A
1	C2	46	A
1	C2	47	A
1	C2	57	G
1	C2	60	U
1	C2	63	G
1	C2	65	A
1	C2	67	A
1	C2	68	A
1	C2	72	A
1	C2	77	U
1	C2	103	A
1	C2	104	A
1	C2	105	A
1	C2	114	C
1	C2	127	G
1	C2	132	U
1	C2	137	U

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Mol	Chain	Res	Type
1	C2	140	A
1	C2	145	A
1	C2	146	U
1	C2	153	G
1	C2	158	U
1	C2	166	C
1	C2	176	C
1	C2	178	U
1	C2	184	C
1	C2	185	U
1	C2	189	C
1	C2	190	C
1	C2	192	U
1	C2	193	U
1	C2	196	G
1	C2	197	A
1	C2	200	A
1	C2	215	A
1	C2	216	U
1	C2	217	A
1	C2	218	A
1	C2	220	A
1	C2	223	U
1	C2	227	U
1	C2	229	U
1	C2	230	C
1	C2	233	C
1	C2	235	G
1	C2	240	U
1	C2	241	U
1	C2	261	U
1	C2	262	U
1	C2	265	A
1	C2	273	G
1	C2	276	C
1	C2	277	U
1	C2	278	U
1	C2	280	U
1	C2	299	A
1	C2	316	A
1	C2	319	U
1	C2	321	C

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Mol	Chain	Res	Type
1	C2	322	G
1	C2	333	A
1	C2	337	G
1	C2	338	C
1	C2	344	A
1	C2	352	A
1	C2	359	A
1	C2	360	A
1	C2	361	C
1	C2	369	A
1	C2	371	G
1	C2	399	A
1	C2	400	A
1	C2	401	A
1	C2	402	C
1	C2	404	G
1	C2	417	A
1	C2	418	G
1	C2	423	G
1	C2	424	C
1	C2	426	G
1	C2	434	G
1	C2	437	A
1	C2	439	U
1	C2	444	C
1	C2	445	A
1	C2	448	C
1	C2	454	U
1	C2	459	G
1	C2	460	A
1	C2	461	G
1	C2	464	A
1	C2	468	A
1	C2	475	A
1	C2	477	A
1	C2	480	G
1	C2	484	C
1	C2	488	G
1	C2	501	U
1	C2	506	A
1	C2	507	U
1	C2	510	G

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Mol	Chain	Res	Type
1	C2	511	A
1	C2	514	G
1	C2	519	C
1	C2	527	A
1	C2	539	G
1	C2	540	G
1	C2	542	A
1	C2	543	C
1	C2	544	A
1	C2	554	C
1	C2	555	A
1	C2	556	A
1	C2	557	G
1	C2	559	C
1	C2	568	G
1	C2	569	C
1	C2	574	G
1	C2	579	A
1	C2	581	U
1	C2	582	U
1	C2	583	C
1	C2	594	A
1	C2	595	G
1	C2	606	A
1	C2	610	G
1	C2	611	U
1	C2	619	A
1	C2	620	A
1	C2	623	A
1	C2	624	G
1	C2	635	A
1	C2	639	U
1	C2	645	C
1	C2	685	A
1	C2	691	C
1	C2	696	C
1	C2	701	U
1	C2	703	G
1	C2	705	U
1	C2	734	A
1	C2	738	G
1	C2	743	U

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Mol	Chain	Res	Type
1	C2	752	A
1	C2	755	A
1	C2	756	A
1	C2	765	G
1	C2	766	U
1	C2	767	U
1	C2	774	A
1	C2	775	G
1	C2	779	U
1	C2	780	A
1	C2	781	U
1	C2	782	U
1	C2	783	G
1	C2	787	G
1	C2	789	A
1	C2	794	U
1	C2	811	A
1	C2	812	A
1	C2	818	C
1	C2	820	U
1	C2	821	U
1	C2	823	G
1	C2	826	U
1	C2	829	A
1	C2	830	U
1	C2	831	U
1	C2	833	U
1	C2	835	U
1	C2	850	A
1	C2	852	C
1	C2	853	G
1	C2	854	U
1	C2	863	A
1	C2	873	U
1	C2	876	G
1	C2	886	U
1	C2	898	A
1	C2	906	A
1	C2	913	G
1	C2	914	G
1	C2	933	A
1	C2	935	U

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Mol	Chain	Res	Type
1	C2	942	G
1	C2	944	A
1	C2	945	U
1	C2	959	U
1	C2	962	C
1	C2	966	A
1	C2	969	C
1	C2	970	A
1	C2	992	A
1	C2	993	A
1	C2	998	A
1	C2	1000	C
1	C2	1001	A
1	C2	1002	G
1	C2	1006	C
1	C2	1007	C
1	C2	1021	C
1	C2	1026	A
1	C2	1028	C
1	C2	1031	U
1	C2	1039	A
1	C2	1040	G
1	C2	1052	U
1	C2	1053	G
1	C2	1058	U
1	C2	1059	U
1	C2	1060	U
1	C2	1070	C
1	C2	1076	A
1	C2	1082	C
1	C2	1092	A
1	C2	1093	A
1	C2	1096	C
1	C2	1097	U
1	C2	1098	U
1	C2	1100	G
1	C2	1109	G
1	C2	1113	A
1	C2	1126	G
1	C2	1138	A
1	C2	1769	U
1	C2	1770	U

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Mol	Chain	Res	Type
1	C2	1772	C
1	C2	1780	G
1	C2	1781	A
1	C2	1783	C
1	C2	1792	G
1	C2	1793	G
1	C2	1795	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C2	136	C
1	C2	139	C
1	C2	272	U
1	C2	417	A
1	C2	555	A
1	C2	755	A
1	C2	817	A
1	C2	997	G
1	C2	1051	G
1	C2	1097	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32791. These allow visual inspection of the internal detail of the map and identification of artifacts.

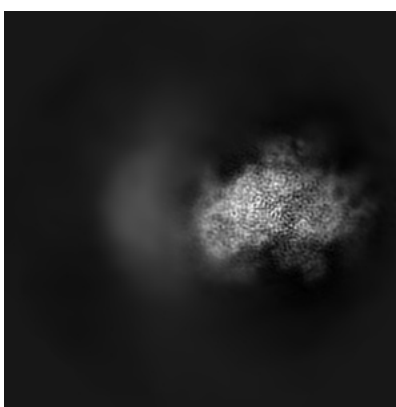
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

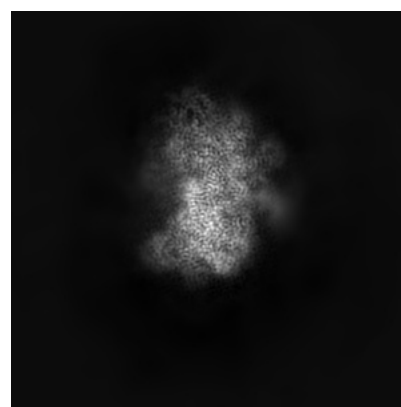
6.1.1 Primary map



X



Y

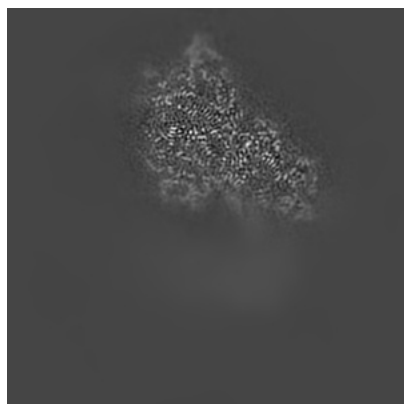


Z

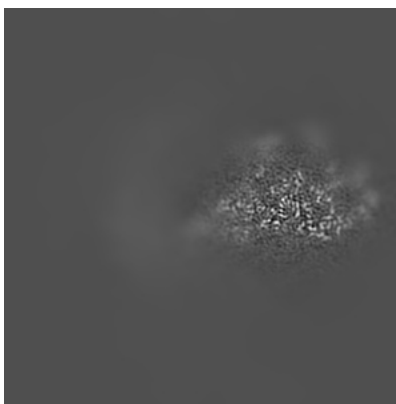
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

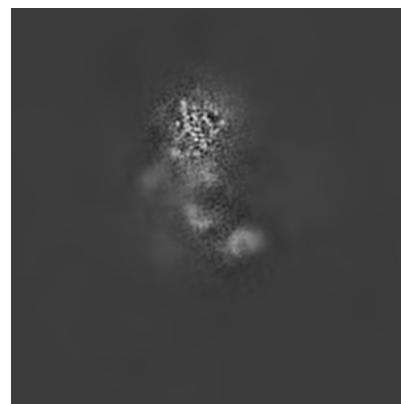
6.2.1 Primary map



X Index: 180



Y Index: 180

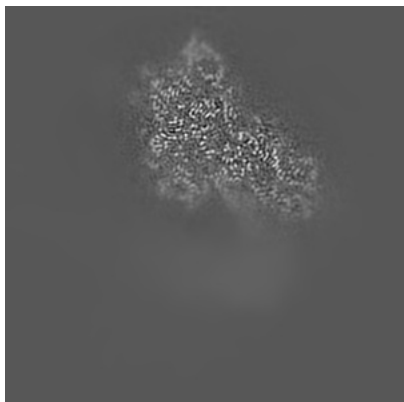


Z Index: 180

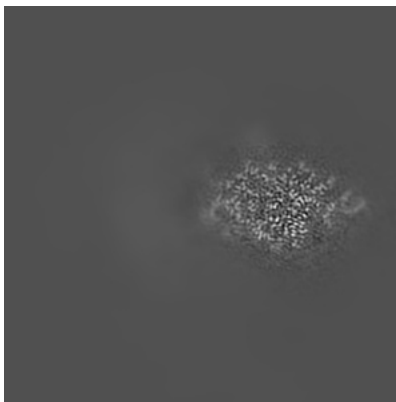
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

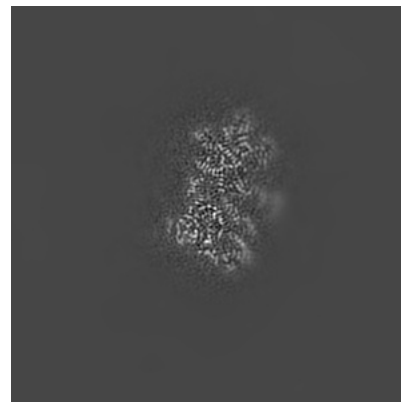
6.3.1 Primary map



X Index: 178



Y Index: 163

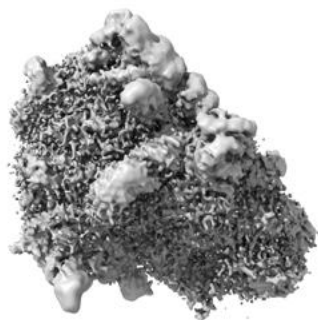


Z Index: 241

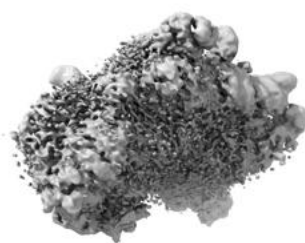
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

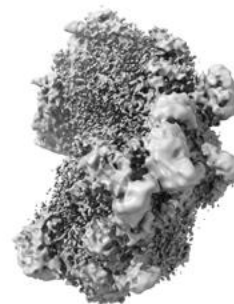
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

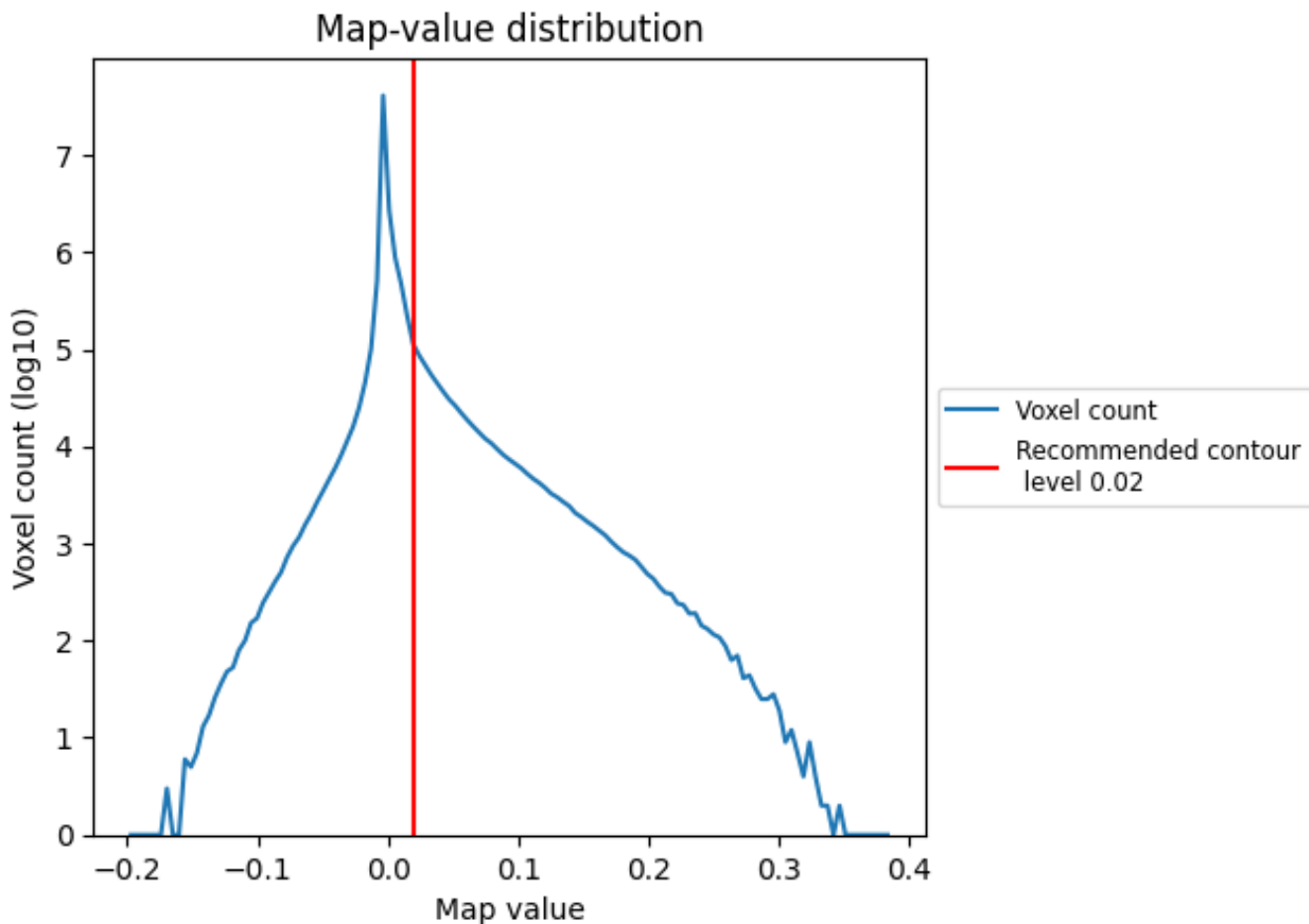
6.5 Mask visualisation

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

7 Map analysis [i](#)

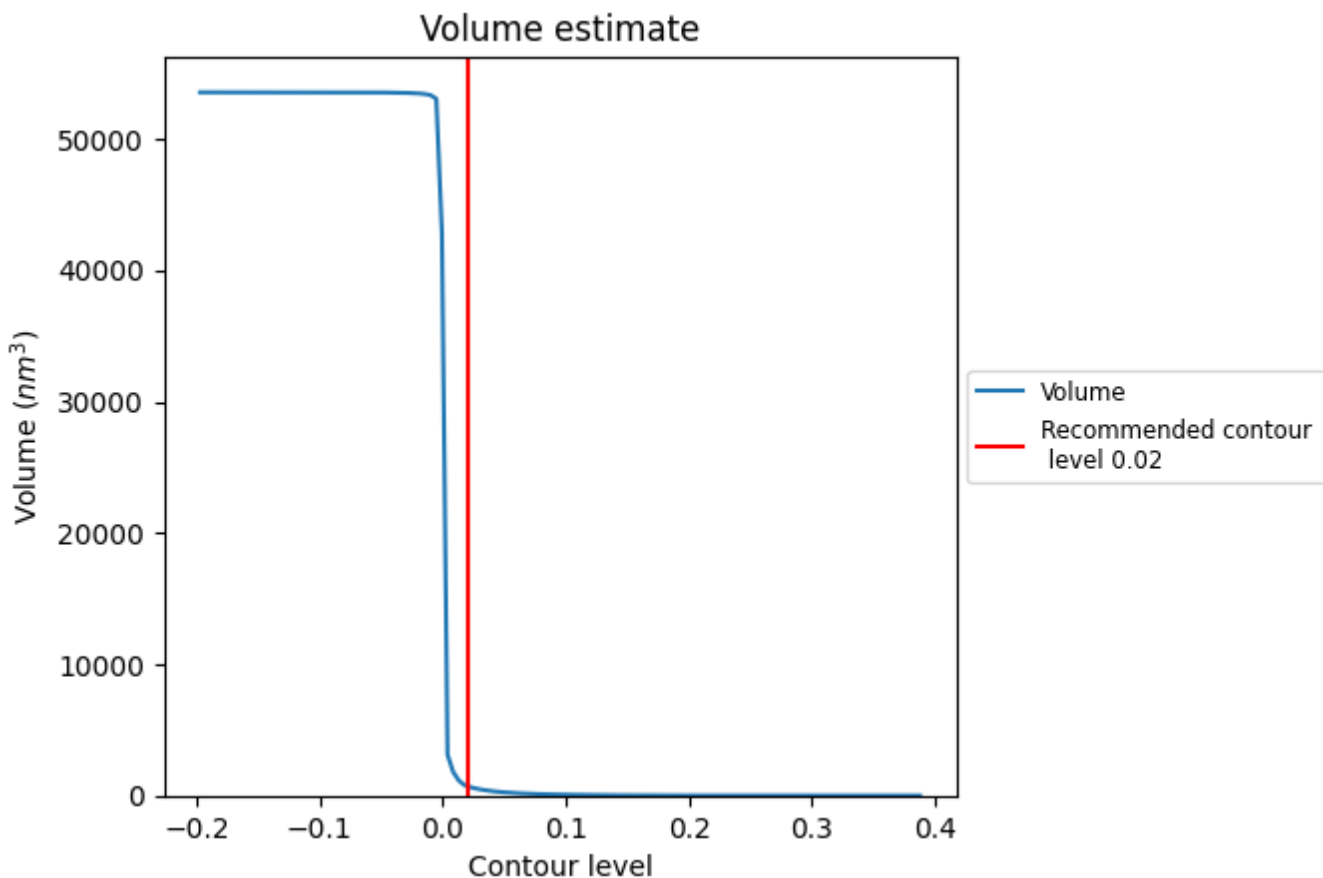
This section contains the results of statistical analysis of the map.

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.

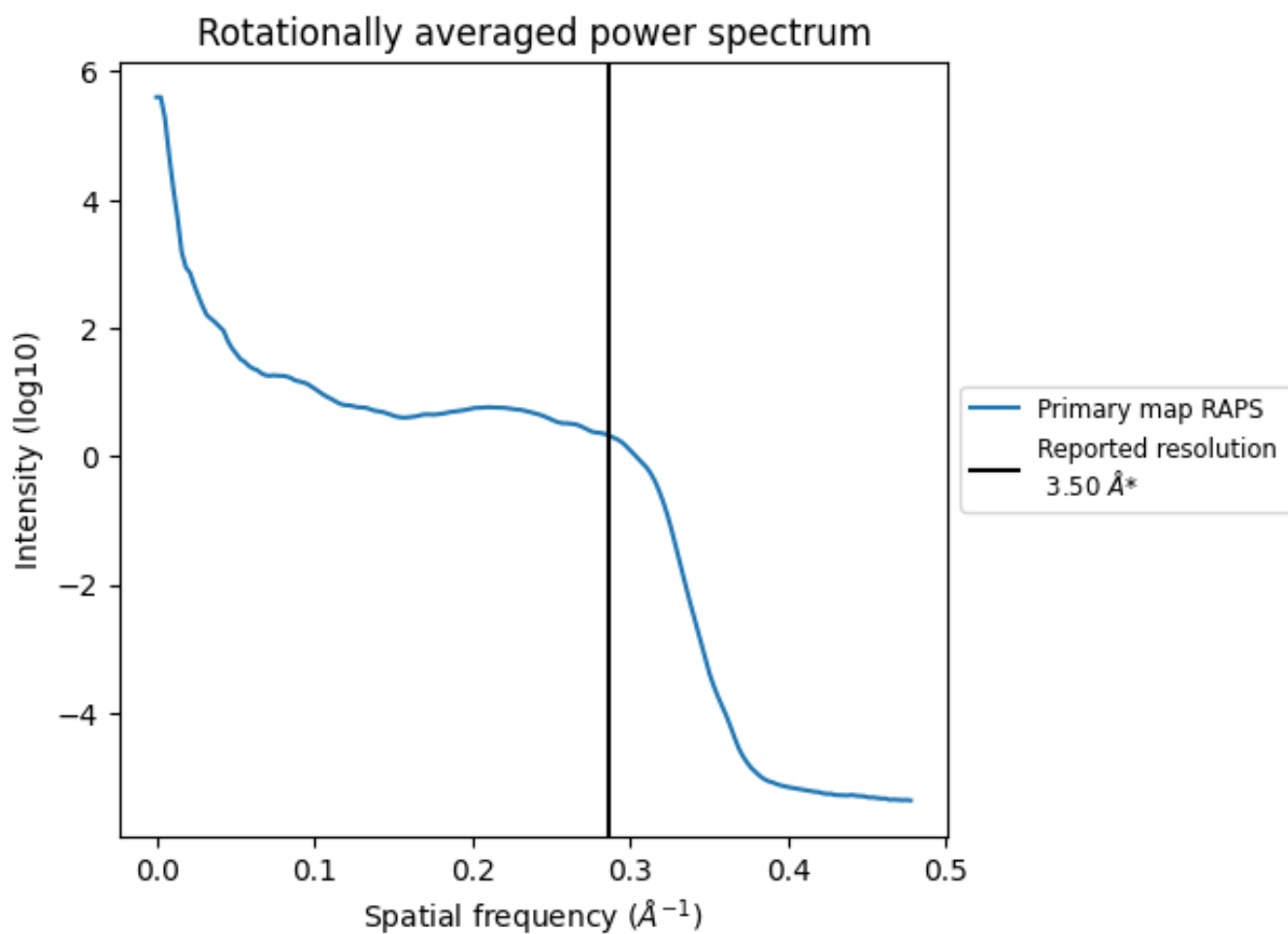
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 721 nm³; this corresponds to an approximate mass of 651 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 i

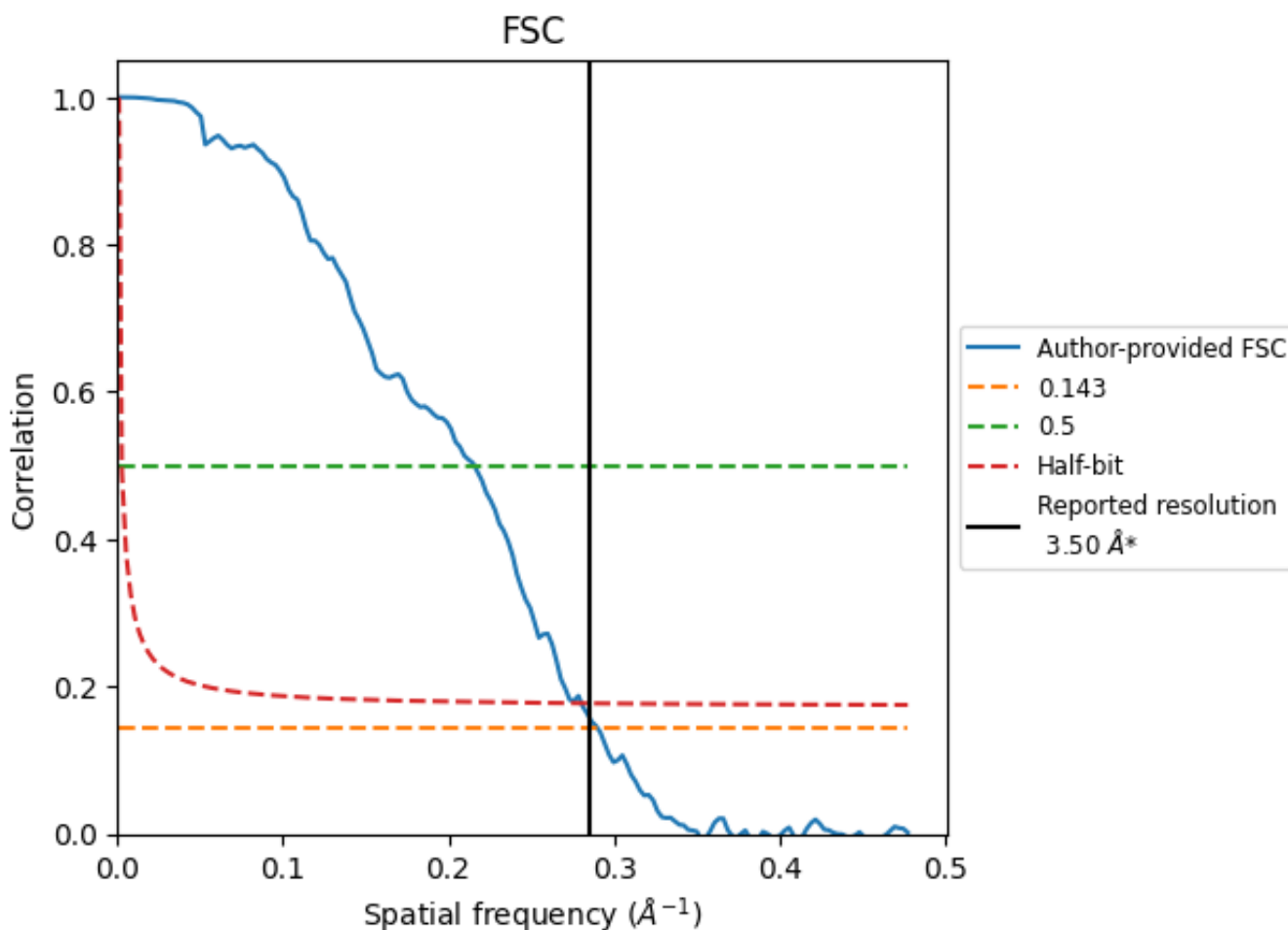


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

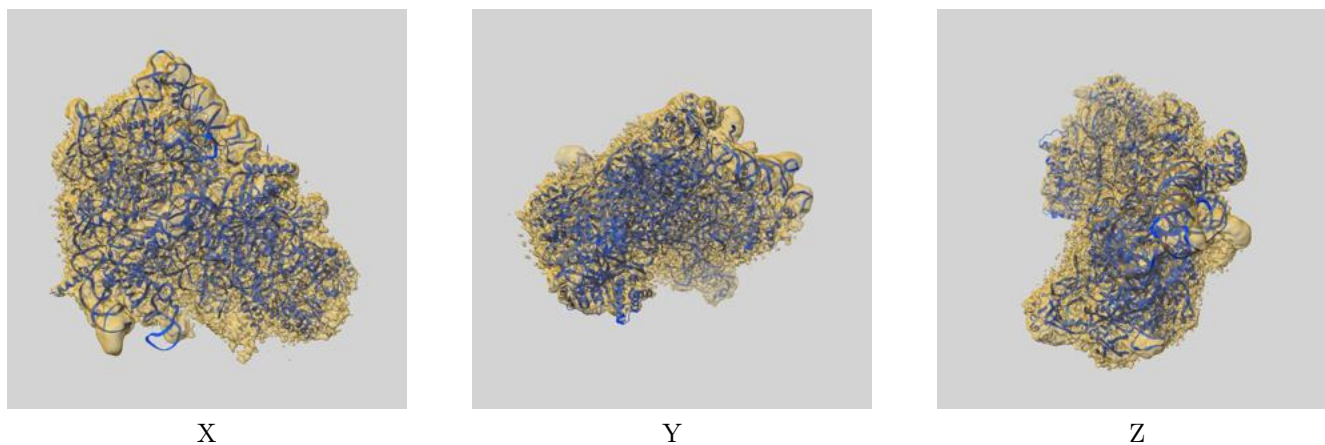
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.45	4.64	3.57
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

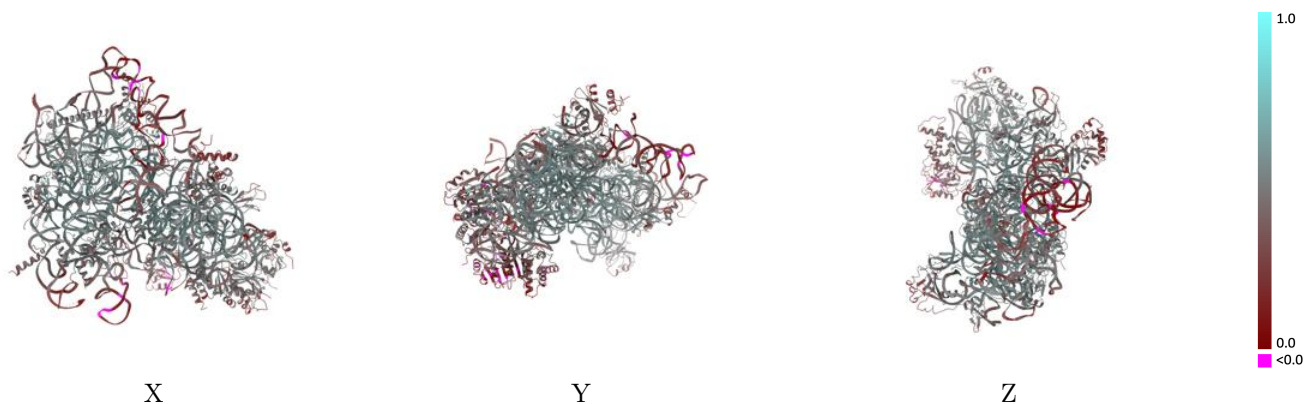
This section contains information regarding the fit between EMDB map EMD-32791 and PDB model 7WTM. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



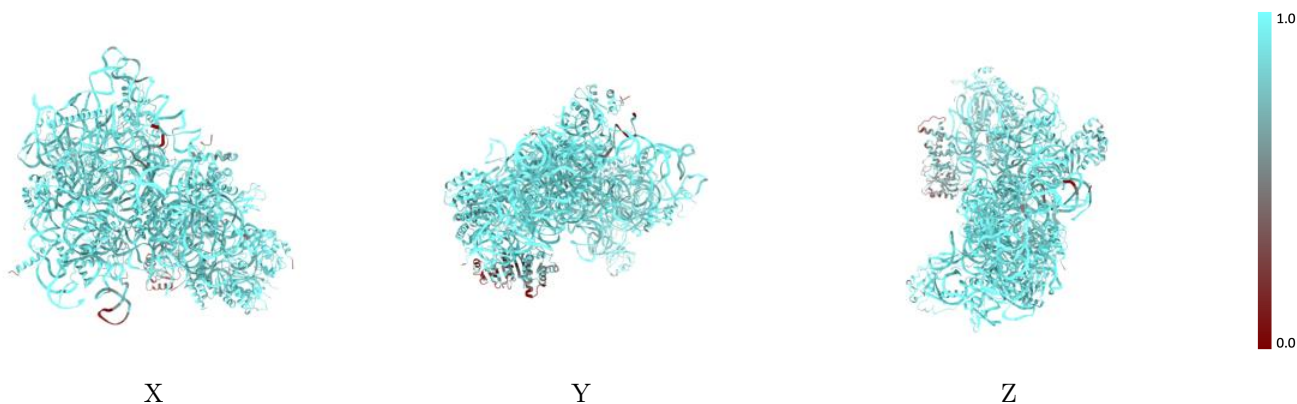
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



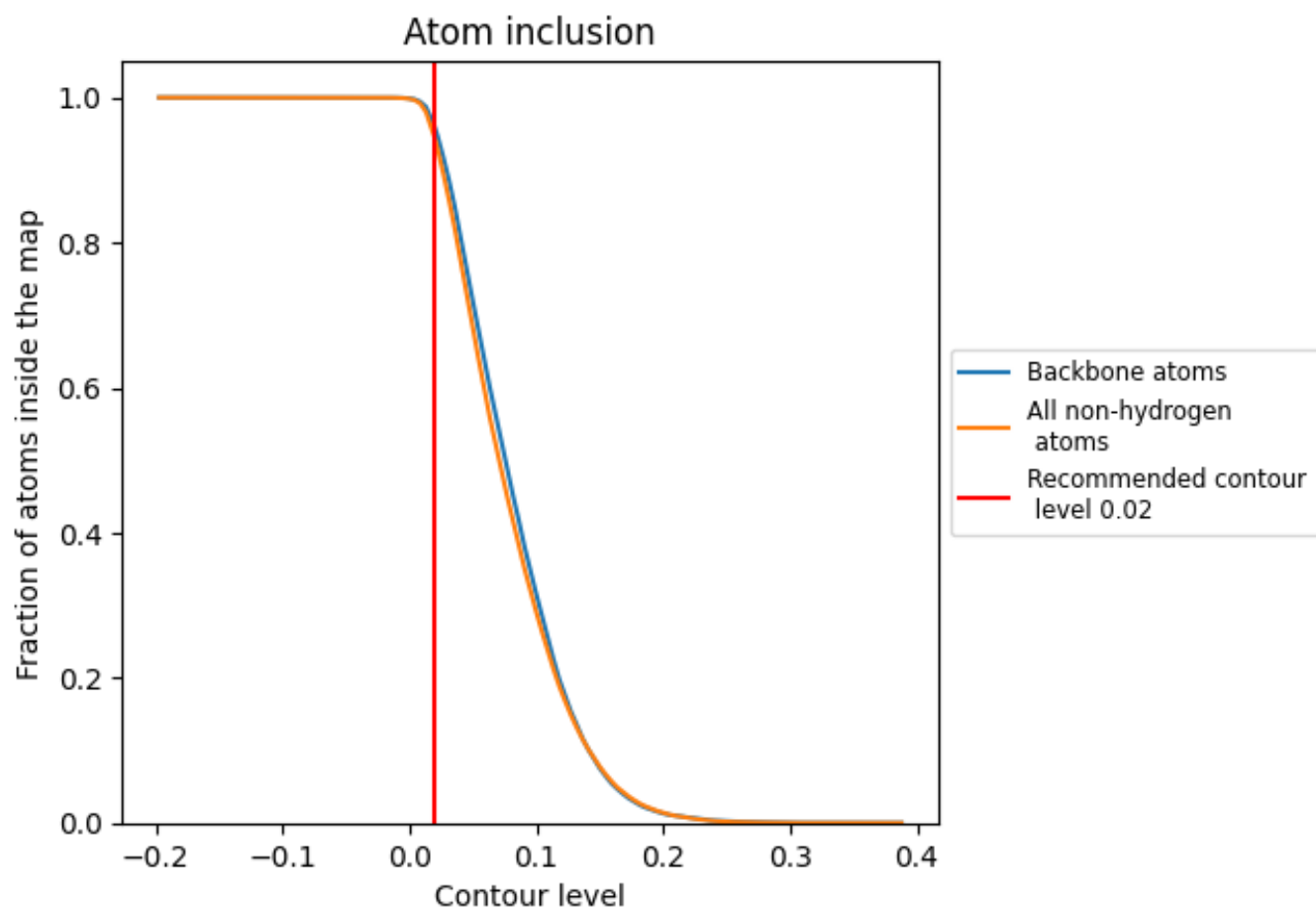
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9442	 0.4510
C2	 0.9693	 0.4580
CA	 0.9479	 0.4060
JL	 0.6124	 0.2340
SB	 0.9486	 0.4530
SE	 0.9777	 0.5370
SG	 0.9548	 0.4370
SH	 0.8868	 0.3760
SI	 0.9714	 0.4880
SJ	 0.9653	 0.4790
SL	 0.9692	 0.5270
SN	 0.9688	 0.5040
SO	 0.9565	 0.4600
SW	 0.9790	 0.5400
SX	 0.8949	 0.4000
SY	 0.9625	 0.4910
Sb	 0.9336	 0.4520
Se	 0.9319	 0.4110

