Full wwPDB EM Validation Report

Jun 20, 2024 – 08:23 AM JST

PDB ID	:	7WTQ
EMDB ID	:	EMD-32795
Title	:	Cryo-EM structure of a yeast pre-40S ribosomal subunit - State Tsr1-2 (without Rps2)
Authors	:	Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on	:	2022-02-05
Resolution	:	3.70 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 (i) 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 (i)) were used in the production of this report:

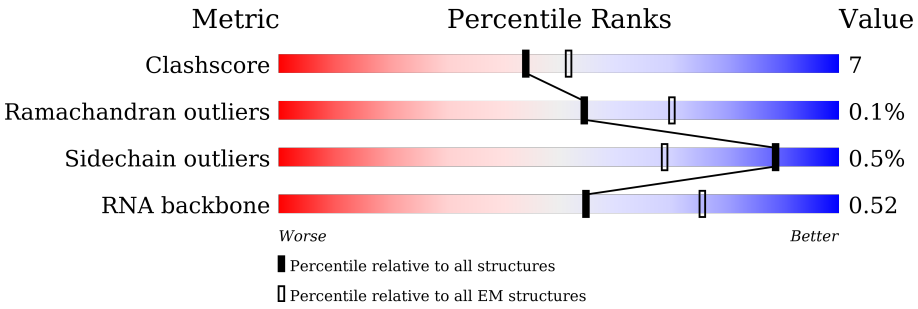
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.70 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.



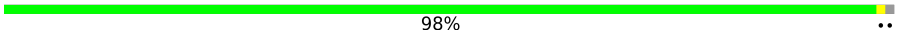
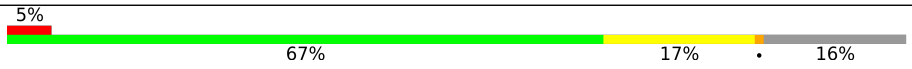
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	37% 26% 6% 30%
2	SB	255	68% 16% 15%
3	SE	261	82% 18%
4	SG	236	70% 22% 8%
5	SH	190	73% 23%
6	SI	200	74% 20% 6%
7	SJ	197	75% 19% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	SL	156	
9	SN	151	
10	SO	137	
11	SW	130	
12	SX	145	
13	SY	135	
14	Sb	82	
15	Se	63	
16	CA	274	
17	CB	275	
18	CC	788	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 51309 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
1	C2	1255	Total	C	N	O	P	0	0
			26763	11971	4765	8772	1255		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Se	38	Total	C	N	O	S	0	0
			313	198	65	49	1		

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

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

- Molecule 17 is a protein called 18S rRNA (guanine(1575)-N(7))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CB	35	Total	C	N	O	S	0	0
			302	189	69	43	1		

- Molecule 18 is a protein called Ribosome biogenesis protein TSR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CC	661	Total	C	N	O	S	0	0
			5346	3413	933	986	14		

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

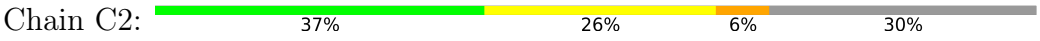
Mol	Chain	Residues	Atoms		AltConf
19	Sb	1	Total	Zn	0
			1	1	

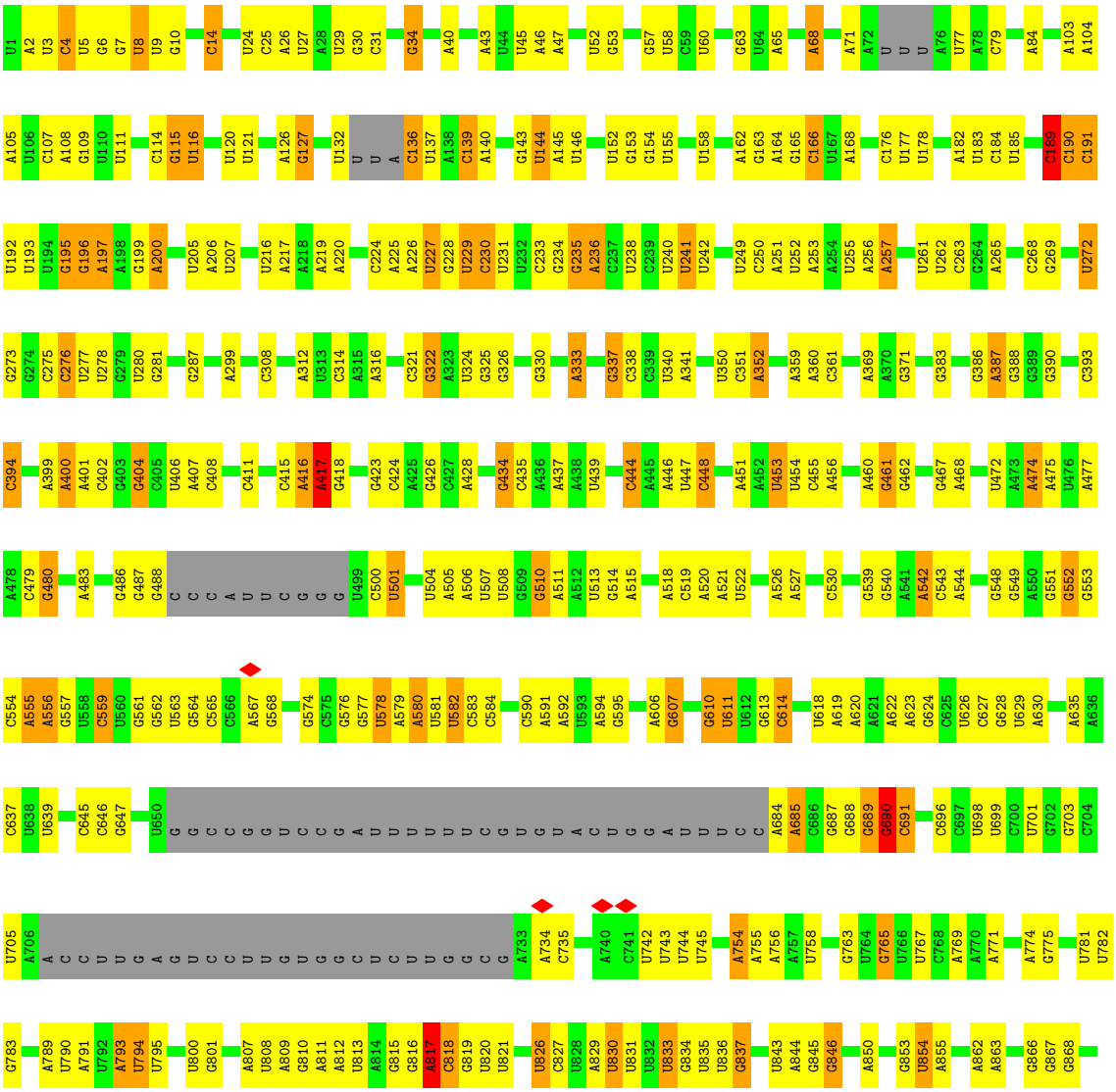
3 Residue-property plots (i)

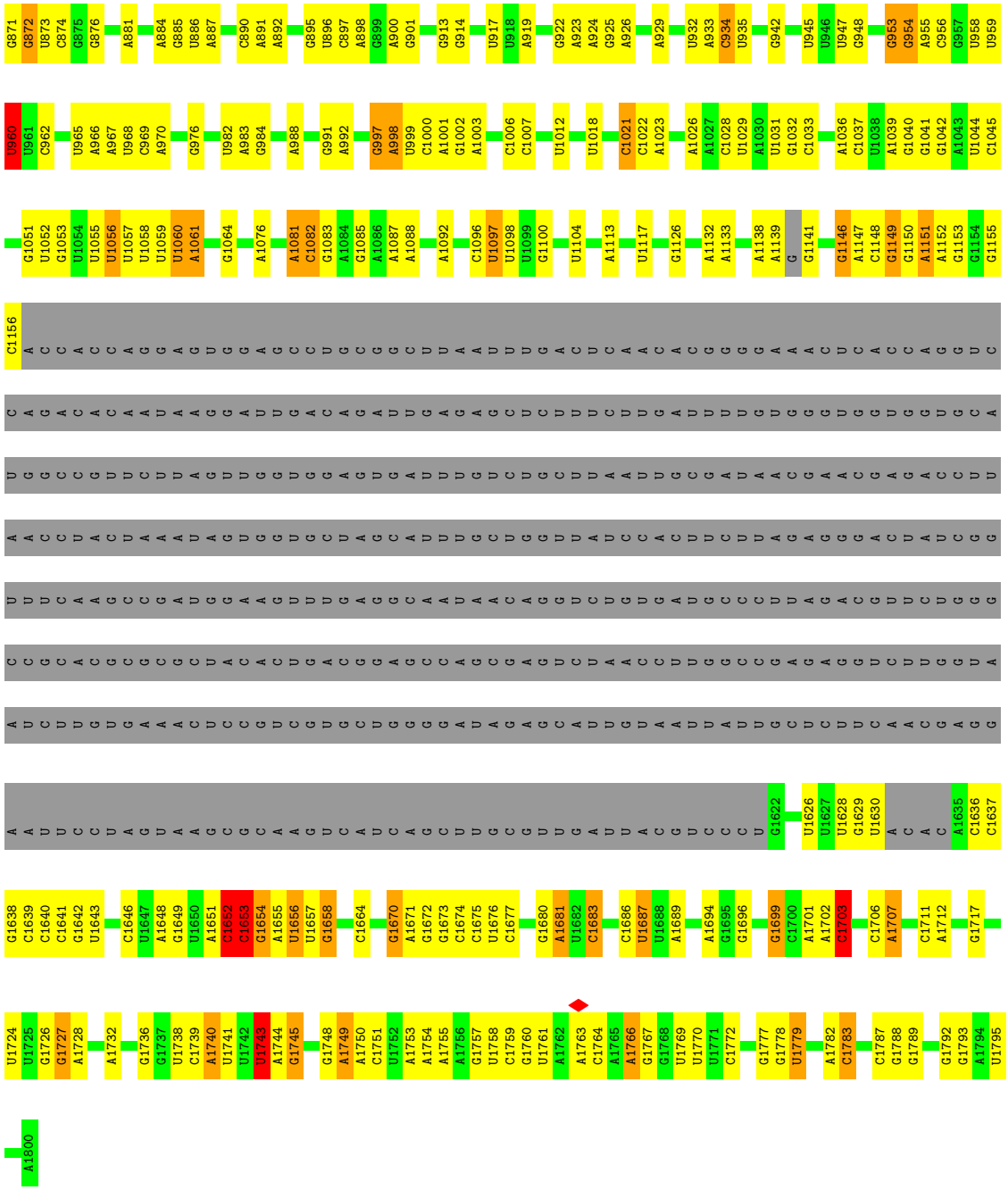
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S rRNA

Chain C2:

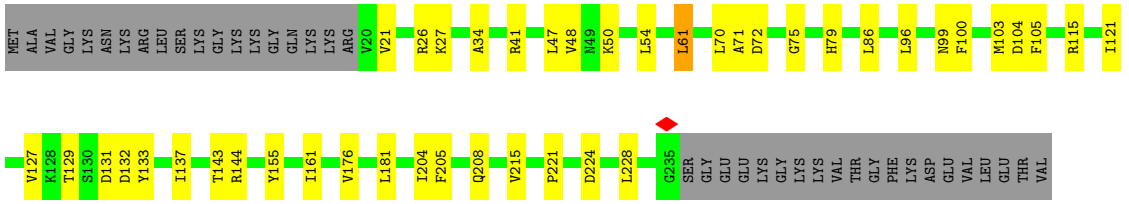






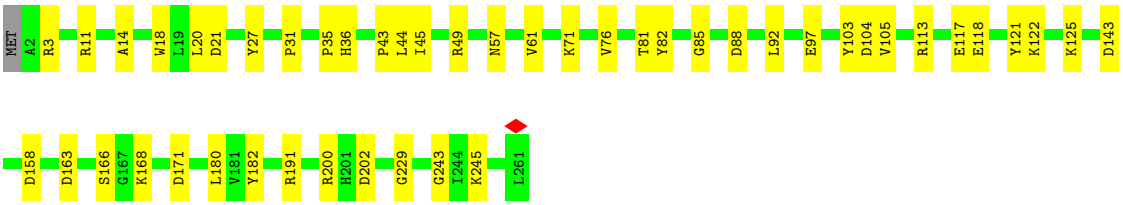
• Molecule 2: 40S ribosomal protein S1-A

Chain SB:



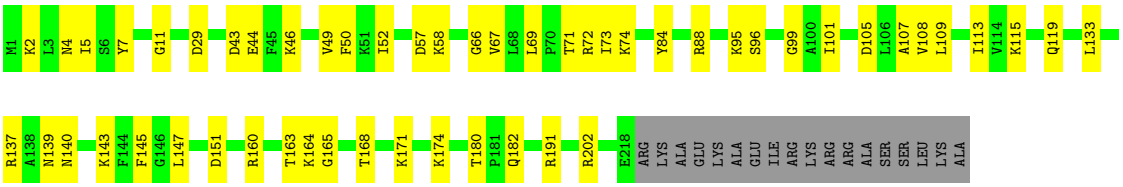
• Molecule 3: 40S ribosomal protein S4-A

Chain SE:



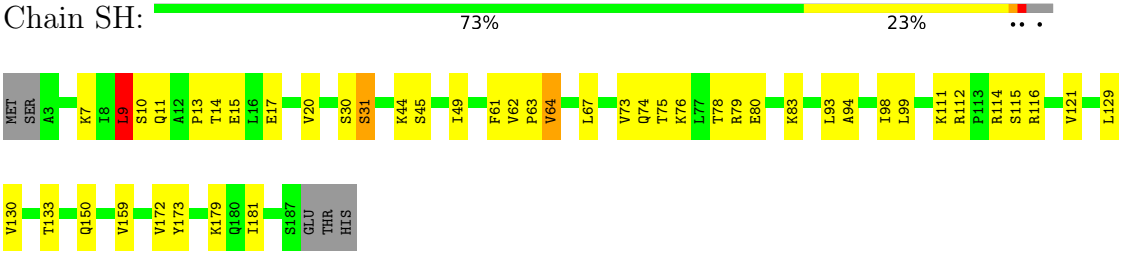
• Molecule 4: 40S ribosomal protein S6-A

Chain SG:



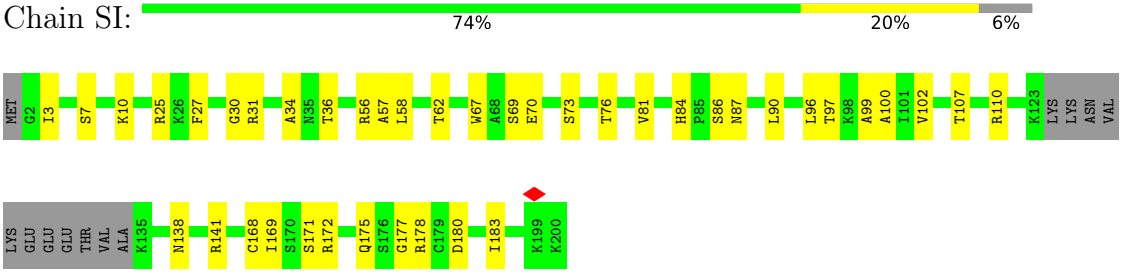
• Molecule 5: 40S ribosomal protein S7-A

Chain SH:



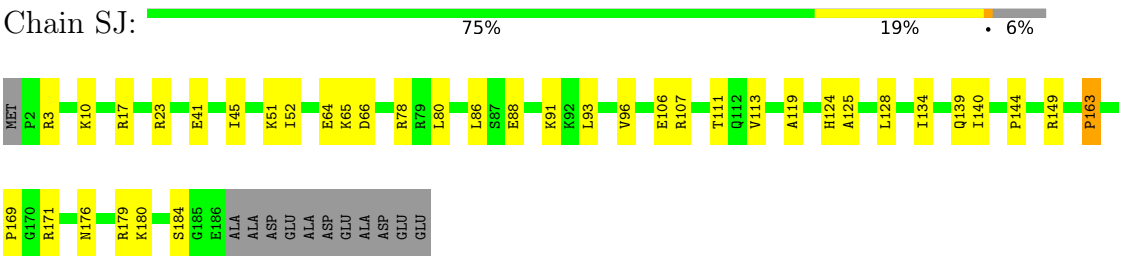
• Molecule 6: 40S ribosomal protein S8-A

Chain SI:



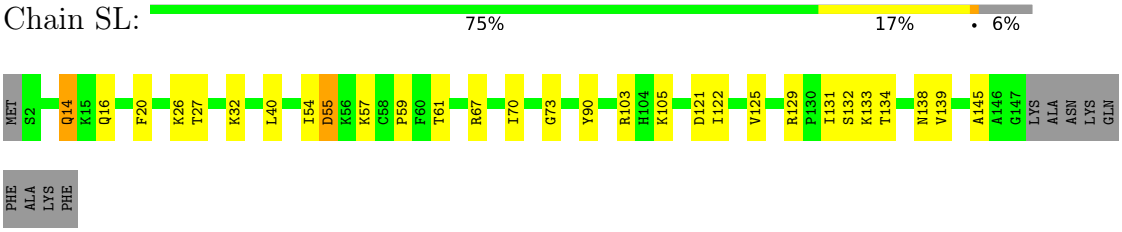
• Molecule 7: 40S ribosomal protein S9-A

Chain SJ:



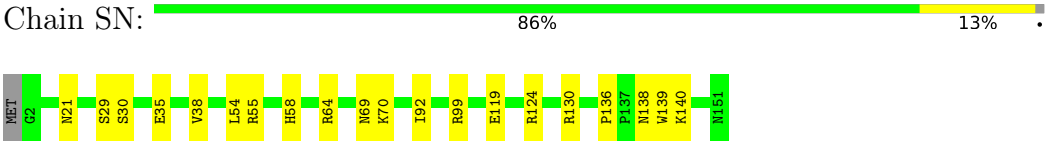
• Molecule 8: 40S ribosomal protein S11-A

Chain SL:



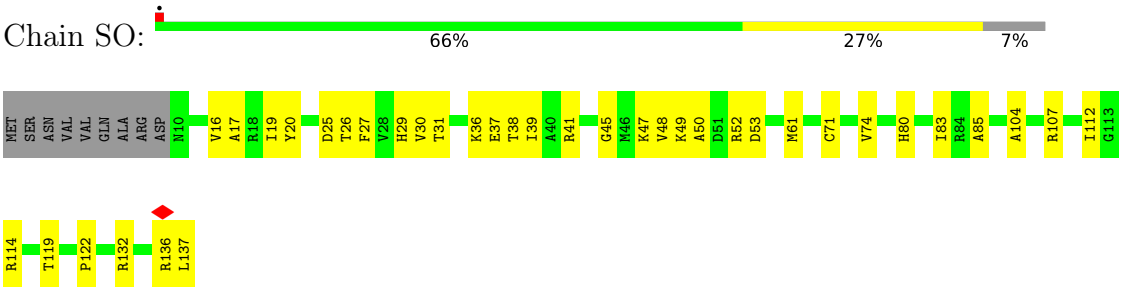
• Molecule 9: 40S ribosomal protein S13

Chain SN:



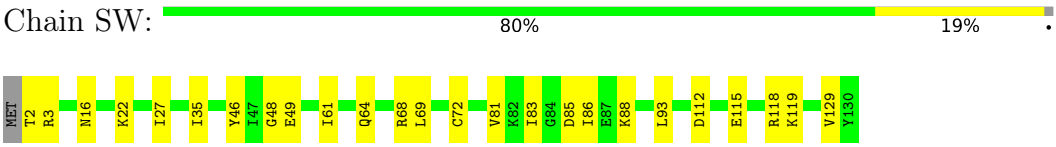
• Molecule 10: 40S ribosomal protein S14-A

Chain SO:



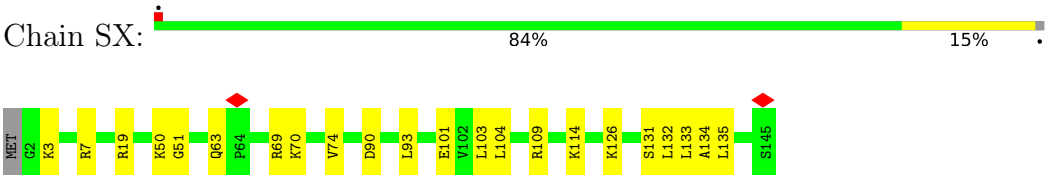
• Molecule 11: 40S ribosomal protein S22-A

Chain SW:



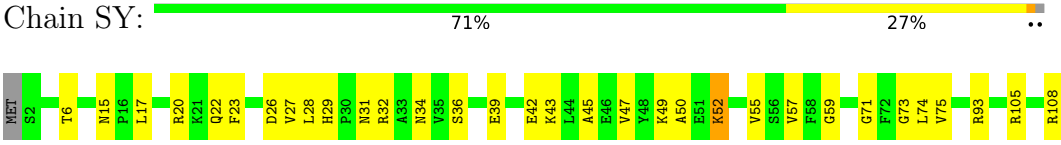
• Molecule 12: 40S ribosomal protein S23-A

Chain SX:



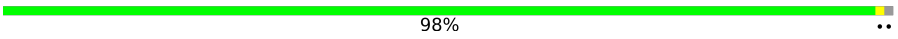
• Molecule 13: 40S ribosomal protein S24-A

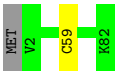
Chain SY:



• Molecule 14: 40S ribosomal protein S27-A

Chain Sb:



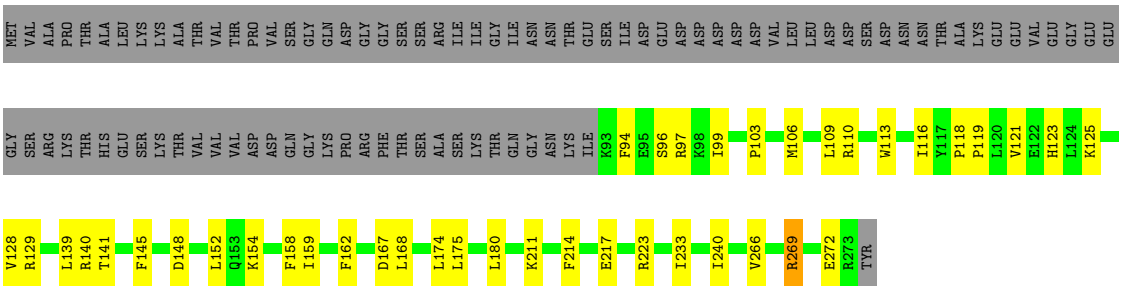


• Molecule 15: 40S ribosomal protein S30-A

Chain Se:

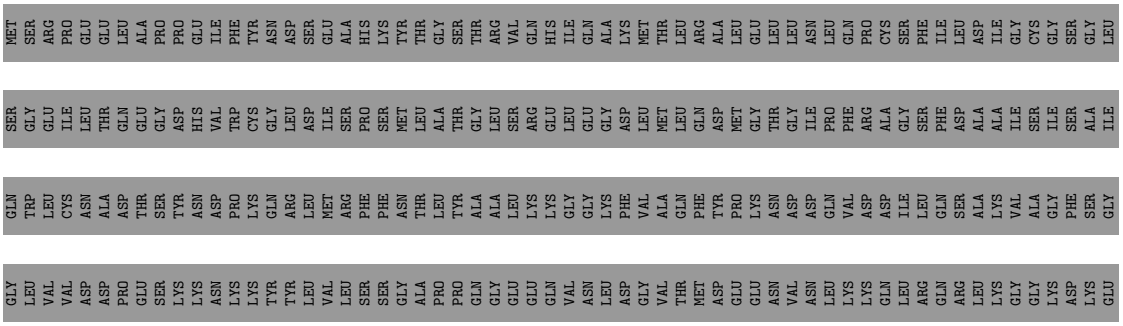
• Molecule 16: Pre-rRNA-processing protein PNO1

Chain CA:



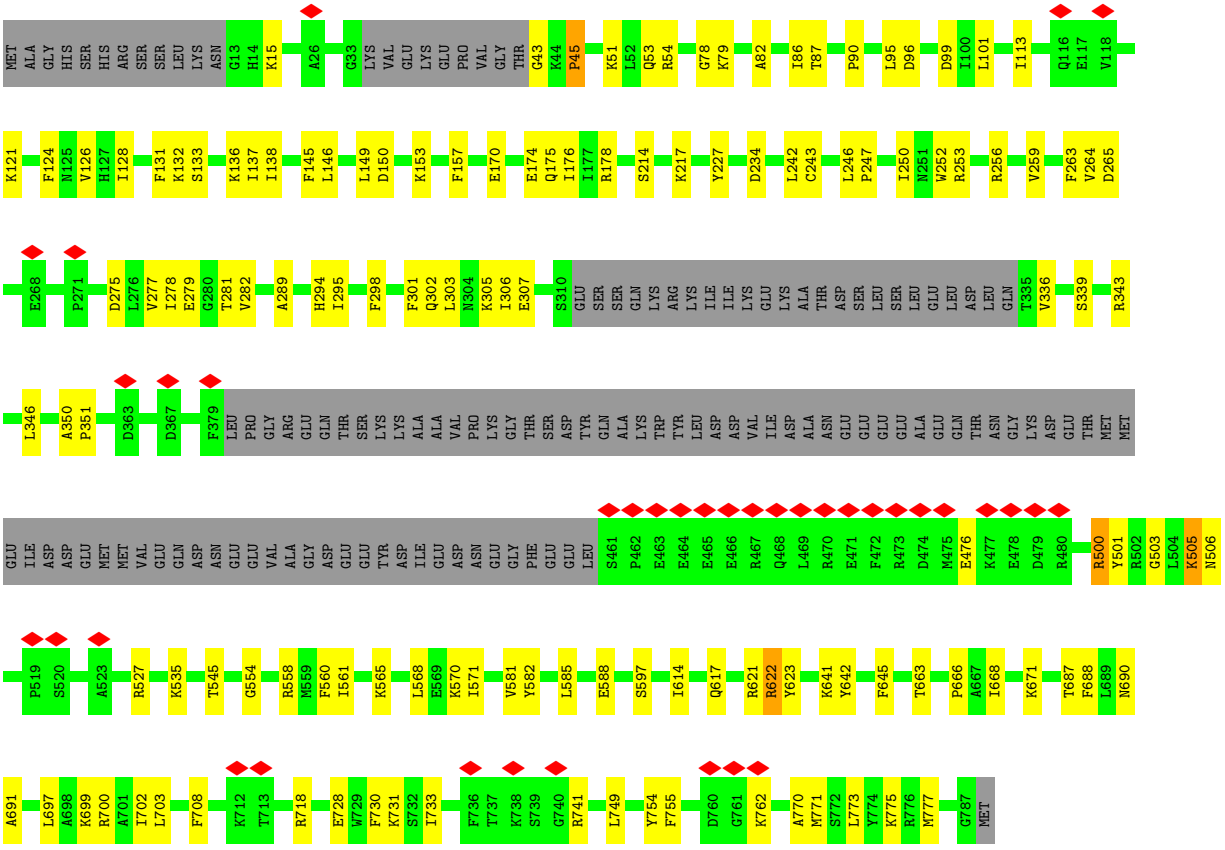
• Molecule 17: 18S rRNA (guanine(1575)-N(7))-methyltransferase

Chain CB:



• Molecule 18: Ribosome biogenesis protein TSR1

Chain CC:


MET ALA GLY HIS SER HIS ARG SER SER LEU LYS ASN G13 H14 K15 A26 G33 LYS VAL GLU LYS GLU PRO VAL GLY THR G43 K44 P45 K51 L52 Q53 R54 G78 K79 A82 I86 T87 P90 L95 D96 D99 I100 L101 I113 Q116 E117 V118
K121 F124 N125 V126 H127 I128 F131 K132 S133 K136 I137 I138 F145 L146 L149 D150 K153 F157 E170 E174 Q175 I176 I177 R178 S214 K217 Y227 D234 L242 C243 L246 P247 I250 N251 W252 R253 R256 V259 F263 V264 D265
E268 P271 D275 L276 V277 I278 E279 G280 T281 V282 A289 H294 I295 F298 F301 Q302 L303 N304 K305 I306 E307 S310 GLU SER SER GLN LYS ARG LYS ILE ILE LYS GLU LYS ALA THR ASP SER LEU SER LEU GLU LEU ASP LEU GLN T335 V336 S339 R343
L346 A350 P351 D363 D367 F379 LEU PRO GLY ARG GLU GLN THR SER LYS LYS ALA ALA VAL PRO LYS GLY THR SER ASP TYR GLN ALA LYS TRP TYR LEU ASP ASP VAL ILE ASP ALA ASN GLU GLU GLU GLU ALA GLU GLN THR ASN GLY LYS ASP GLU THR MET MET
GLU ILE ASP ASP GLU MET MET VAL GLU GLN ASP ASN GLU GLU VAL ALA GLY ASP GLU GLU TYR ASP ILE GLU ASP ASN GLU GLY PHE GLU GLU LEU S461 P462 E463 E464 E465 E466 R467 Q468 L469 R470 E471 F472 R473 D474 M475 E476 K477 E478 D479 R480 R500 Y501 R502 G503 L504 K505 N506
P519 S520 A523 R527 K535 T545 G554 R558 M559 F560 I561 K565 L568 E569 K570 I571 V581 Y582 L585 E588 S597 I614 Q617 R621 R622 Y623 K641 Y642 F645 T663 P666 A667 I668 K671 T687 F688 L689 N690
A691 L697 A698 K699 R700 A701 I702 L703 F708 K712 T713 R718 E728 W729 F730 K731 S732 I733 F736 T737 K738 S739 G740 R741 L749 Y754 F755 D760 G761 K762 A770 M771 S772 L773 Y774 K775 R776 M777 G787 MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39865	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 ($e^-/Å^2$)	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	0.290	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	0.50	1/29940 (0.0%)	1.04	109/46636 (0.2%)
2	SB	0.33	0/1748	0.71	3/2352 (0.1%)
3	SE	0.33	0/2109	0.64	0/2839
4	SG	0.30	0/1779	0.64	1/2379 (0.0%)
5	SH	0.30	0/1511	0.70	1/2036 (0.0%)
6	SI	0.32	0/1514	0.66	0/2021
7	SJ	0.32	0/1519	0.69	1/2035 (0.0%)
8	SL	0.37	0/1194	0.66	1/1610 (0.1%)
9	SN	0.33	0/1215	0.64	0/1638
10	SO	0.31	0/960	0.71	0/1290
11	SW	0.34	0/1038	0.71	2/1395 (0.1%)
12	SX	0.34	0/1139	0.70	1/1518 (0.1%)
13	SY	0.34	0/1087	0.71	1/1449 (0.1%)
14	Sb	0.31	0/620	0.70	0/838
15	Se	0.31	0/319	0.80	0/425
16	CA	0.30	0/1462	0.69	0/1969
17	CB	0.28	0/305	0.70	0/394
18	CC	0.32	1/5469 (0.0%)	0.59	4/7383 (0.1%)
All	All	0.43	2/54928 (0.0%)	0.90	124/80207 (0.2%)

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	3
9	SN	0	1
11	SW	0	1
12	SX	0	1
13	SY	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
14	Sb	0	1
15	Se	0	1
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	CC	45	PRO	CG-CD	-12.51	1.09	1.50
1	C2	474	A	N9-C4	-5.11	1.34	1.37

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	CC	45	PRO	N-CD-CG	-15.32	80.22	103.20
1	C2	190	C	N3-C2-O2	-11.98	113.51	121.90
1	C2	1699	G	C5-C6-O6	11.62	135.57	128.60
1	C2	1699	G	N1-C6-O6	-11.11	113.23	119.90
1	C2	645	C	N3-C2-O2	-10.91	114.26	121.90
1	C2	646	C	N3-C2-O2	-8.92	115.66	121.90
1	C2	191	C	O4'-C1'-N1	8.78	115.22	108.20
1	C2	956	C	N3-C2-O2	-8.54	115.92	121.90
1	C2	1652	C	N1-C2-O2	8.50	124.00	118.90
1	C2	1675	C	N3-C2-O2	-8.24	116.14	121.90
1	C2	14	C	N3-C2-O2	-8.15	116.19	121.90
1	C2	190	C	N1-C2-O2	8.07	123.74	118.90
1	C2	224	C	N3-C2-O2	-8.02	116.29	121.90
18	CC	45	PRO	CA-CB-CG	-7.93	88.93	104.00
1	C2	874	C	N3-C2-O2	-7.92	116.35	121.90
1	C2	189	C	N1-C2-O2	7.77	123.56	118.90
1	C2	191	C	C2-N1-C1'	-7.73	110.30	118.80
1	C2	1653	C	N3-C2-O2	-7.36	116.75	121.90
1	C2	646	C	C6-N1-C2	-7.26	117.40	120.30
1	C2	190	C	C6-N1-C2	-7.23	117.41	120.30
1	C2	1652	C	N3-C2-O2	-7.22	116.84	121.90
1	C2	1653	C	C6-N1-C2	-7.18	117.43	120.30
1	C2	854	U	C5-C6-N1	7.16	126.28	122.70
1	C2	1021	C	C2-N1-C1'	7.07	126.58	118.80
1	C2	4	C	N1-C2-O2	7.07	123.14	118.90
1	C2	184	C	N1-C2-O2	6.99	123.09	118.90
1	C2	191	C	C6-N1-C1'	6.99	129.19	120.80
1	C2	1703	C	N3-C4-N4	-6.98	113.11	118.00
1	C2	645	C	N1-C2-O2	6.97	123.08	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C2	954	G	C5-C6-O6	6.97	132.78	128.60
1	C2	1674	C	N1-C2-O2	6.96	123.08	118.90
1	C2	1703	C	N3-C4-C5	6.89	124.66	121.90
1	C2	14	C	C6-N1-C2	-6.89	117.54	120.30
1	C2	954	G	C8-N9-C4	-6.87	103.65	106.40
5	SH	9	LEU	CA-CB-CG	6.84	131.03	115.30
1	C2	953	G	N3-C4-N9	6.62	129.97	126.00
1	C2	956	C	N1-C2-O2	6.57	122.84	118.90
1	C2	144	U	C2-N1-C1'	6.52	125.53	117.70
18	CC	45	PRO	CA-N-CD	-6.52	102.37	111.50
1	C2	236	A	N7-C8-N9	6.47	117.04	113.80
1	C2	645	C	C6-N1-C2	-6.46	117.72	120.30
1	C2	698	U	C2-N1-C1'	6.43	125.42	117.70
1	C2	1643	U	N1-C2-O2	6.35	127.24	122.80
1	C2	758	U	N1-C2-O2	6.30	127.21	122.80
1	C2	272	U	P-O3'-C3'	6.25	127.20	119.70
4	SG	105	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C2	1021	C	C6-N1-C2	-6.21	117.82	120.30
1	C2	1643	U	C2-N1-C1'	6.20	125.14	117.70
1	C2	4	C	N3-C2-O2	-6.18	117.57	121.90
1	C2	184	C	N3-C2-O2	-6.18	117.58	121.90
1	C2	229	U	C2-N1-C1'	6.11	125.04	117.70
1	C2	954	G	N7-C8-N9	6.08	116.14	113.10
1	C2	1683	C	C2-N1-C1'	6.04	125.44	118.80
1	C2	276	C	N3-C2-O2	-6.04	117.67	121.90
1	C2	530	C	N1-C2-O2	5.95	122.47	118.90
1	C2	1646	C	N1-C2-O2	5.93	122.46	118.90
2	SB	54	LEU	CA-CB-CG	5.91	128.88	115.30
1	C2	758	U	N3-C2-O2	-5.90	118.07	122.20
1	C2	691	C	C2-N1-C1'	5.90	125.28	118.80
7	SJ	66	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C2	116	U	N3-C2-O2	-5.86	118.10	122.20
1	C2	1674	C	C2-N1-C1'	5.83	125.22	118.80
18	CC	777	MET	C-N-CA	5.83	136.28	121.70
11	SW	112	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C2	837	G	N3-C4-N9	5.76	129.46	126.00
1	C2	4	C	C2-N1-C1'	5.75	125.13	118.80
1	C2	184	C	C2-N1-C1'	5.74	125.11	118.80
12	SX	135	LEU	CA-CB-CG	5.72	128.45	115.30
1	C2	953	G	N3-C4-C5	-5.71	125.75	128.60
1	C2	690	G	C8-N9-C4	-5.69	104.12	106.40
1	C2	1097	U	P-O3'-C3'	5.67	126.51	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C2	196	G	N1-C6-O6	-5.63	116.52	119.90
1	C2	698	U	N1-C2-O2	5.61	126.73	122.80
1	C2	411	C	C2-N1-C1'	5.61	124.97	118.80
1	C2	1664	C	C2-N1-C1'	5.60	124.96	118.80
1	C2	767	U	C2-N1-C1'	5.60	124.42	117.70
1	C2	196	G	C5-C6-O6	5.58	131.95	128.60
1	C2	1643	U	N3-C2-O2	-5.57	118.30	122.20
1	C2	698	U	N3-C2-O2	-5.56	118.31	122.20
1	C2	1711	C	N3-C2-O2	-5.55	118.02	121.90
1	C2	1675	C	C6-N1-C2	-5.54	118.08	120.30
1	C2	1022	C	C2-N1-C1'	5.49	124.84	118.80
1	C2	1686	C	C2-N1-C1'	5.49	124.84	118.80
13	SY	26	ASP	CB-CG-OD1	5.48	123.23	118.30
1	C2	689	G	N1-C6-O6	-5.44	116.64	119.90
1	C2	1021	C	N1-C2-O2	5.44	122.16	118.90
1	C2	1141	G	N1-C6-O6	-5.43	116.64	119.90
1	C2	417	A	P-O3'-C3'	5.38	126.16	119.70
1	C2	542	A	N7-C8-N9	5.38	116.49	113.80
1	C2	965	U	C2-N1-C1'	5.32	124.09	117.70
1	C2	275	C	N1-C2-O2	5.32	122.09	118.90
8	SL	55	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C2	394	C	C5-C6-N1	5.32	123.66	121.00
1	C2	281	G	N1-C2-N2	-5.31	111.42	116.20
1	C2	224	C	N1-C2-O2	5.31	122.09	118.90
1	C2	10	G	C4-N9-C1'	5.30	133.40	126.50
1	C2	189	C	N3-C2-O2	-5.30	118.19	121.90
1	C2	1687	U	N1-C2-O2	5.28	126.50	122.80
1	C2	1743	U	C2-N1-C1'	5.27	124.03	117.70
1	C2	767	U	N3-C2-O2	-5.27	118.51	122.20
1	C2	136	C	P-O3'-C3'	5.25	126.00	119.70
1	C2	872	G	C5-C6-O6	5.24	131.75	128.60
1	C2	1687	U	C2-N1-C1'	5.23	123.98	117.70
2	SB	61	LEU	CA-CB-CG	5.21	127.29	115.30
1	C2	817	A	P-O3'-C3'	5.17	125.91	119.70
1	C2	10	G	N3-C4-C5	-5.17	126.02	128.60
1	C2	1657	U	N1-C2-O2	5.16	126.41	122.80
1	C2	139	C	P-O3'-C3'	5.16	125.89	119.70
1	C2	874	C	N1-C2-O2	5.15	121.99	118.90
1	C2	14	C	C5-C4-N4	5.14	123.80	120.20
1	C2	1629	G	P-O3'-C3'	5.14	125.86	119.70
1	C2	542	A	C5-N7-C8	-5.13	101.33	103.90
1	C2	960	U	C2-N1-C1'	5.13	123.86	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	SB	224	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C2	453	U	N1-C2-O2	5.11	126.37	122.80
1	C2	522	U	N3-C2-O2	-5.10	118.63	122.20
1	C2	1141	G	C5-C6-O6	5.10	131.66	128.60
1	C2	689	G	C8-N9-C4	-5.09	104.36	106.40
1	C2	795	U	C2-N1-C1'	5.07	123.78	117.70
1	C2	934	C	C2-N1-C1'	5.06	124.37	118.80
1	C2	195	G	N1-C6-O6	-5.06	116.87	119.90
1	C2	559	C	C2-N1-C1'	5.04	124.35	118.80
1	C2	610	G	C4-N9-C1'	5.03	133.03	126.50
11	SW	93	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	SH	31	SER	Peptide
5	SH	64	VAL	Peptide
5	SH	9	LEU	Peptide
9	SN	21	ASN	Peptide
11	SW	68	ARG	Sidechain
12	SX	63	GLN	Peptide
13	SY	31	ASN	Peptide
14	Sb	59	CYS	Peptide
15	Se	46	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C2	26763	0	13462	270	0
2	SB	1722	0	1793	27	0
3	SE	2068	0	2154	29	0
4	SG	1755	0	1846	37	0
5	SH	1486	0	1576	28	0
6	SI	1489	0	1525	30	0
7	SJ	1494	0	1573	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	SL	1168	0	1233	18	0
9	SN	1192	0	1255	14	0
10	SO	949	0	985	25	0
11	SW	1021	0	1060	16	0
12	SX	1121	0	1196	12	0
13	SY	1073	0	1132	26	0
14	Sb	610	0	633	0	0
15	Se	313	0	343	0	0
16	CA	1436	0	1515	25	0
17	CB	302	0	340	7	0
18	CC	5346	0	5247	84	0
19	Sb	1	0	0	0	0
All	All	51309	0	38868	597	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 7.

All (597) 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)
18:CC:264:VAL:HA	18:CC:277:VAL:O	1.46	1.12
1:C2:486:G:H1	1:C2:501:U:H3	1.00	0.95
1:C2:1677:C:H42	1:C2:1724:U:H3	1.15	0.90
1:C2:1658:G:H1	1:C2:1743:U:H3	0.88	0.87
1:C2:1656:U:H3	1:C2:1745:G:H1	0.85	0.81
1:C2:984:G:C6	1:C2:1018:U:N3	2.51	0.78
1:C2:578:U:C4	1:C2:580:A:N6	2.53	0.76
18:CC:275:ASP:HA	18:CC:561:ILE:O	1.85	0.76
5:SH:9:LEU:HD12	5:SH:10:SER:H	1.51	0.75
13:SY:45:ALA:HA	13:SY:50:ALA:HB3	1.71	0.73
1:C2:34:G:H1	1:C2:474:A:H2	1.35	0.73
10:SO:20:TYR:HB3	10:SO:27:PHE:HB2	1.70	0.72
1:C2:565:C:N3	1:C2:578:U:O2	2.22	0.72
1:C2:984:G:C2	1:C2:1018:U:O2	2.43	0.71
1:C2:219:A:N7	1:C2:830:U:O4	2.23	0.71
3:SE:31:PRO:HG3	3:SE:43:PRO:HG3	1.73	0.71
18:CC:699:LYS:HB2	18:CC:775:LYS:HB3	1.72	0.71
1:C2:105:A:H62	1:C2:308:C:N4	1.89	0.70
1:C2:152:U:O2	1:C2:163:G:N2	2.24	0.70
3:SE:191:ARG:HH11	3:SE:245:LYS:HB3	1.57	0.70
7:SJ:163:PRO:HB3	7:SJ:169:PRO:HA	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:984:G:N1	1:C2:1018:U:C2	2.61	0.69
1:C2:984:G:C2	1:C2:1018:U:C2	2.80	0.69
18:CC:282:VAL:O	18:CC:554:GLY:N	2.25	0.69
1:C2:1652:C:N4	1:C2:1749:A:N6	2.41	0.68
1:C2:1779:U:H3	1:C2:1783:C:H42	1.42	0.68
7:SJ:17:ARG:O	7:SJ:23:ARG:NH2	2.26	0.68
1:C2:1779:U:H3	1:C2:1783:C:N4	1.93	0.67
18:CC:128:ILE:O	18:CC:132:LYS:HA	1.95	0.67
6:SI:99:ALA:N	6:SI:169:ILE:O	2.29	0.66
1:C2:154:G:O6	13:SY:128:LYS:NZ	2.28	0.66
18:CC:703:LEU:O	18:CC:770:ALA:HA	1.94	0.66
1:C2:115:G:H5'	8:SL:129:ARG:HH11	1.61	0.65
9:SN:64:ARG:HD3	9:SN:70:LYS:HE2	1.77	0.65
1:C2:826:U:H3	1:C2:846:G:H1	0.78	0.65
1:C2:1151:A:N7	1:C2:1628:U:O2	2.29	0.65
1:C2:1656:U:O4	1:C2:1745:G:O6	2.15	0.65
11:SW:49:GLU:H	11:SW:64:GLN:HB2	1.61	0.65
1:C2:229:U:O4	1:C2:235:G:O6	2.15	0.65
1:C2:127:G:N7	4:SG:202:ARG:NH2	2.44	0.64
13:SY:15:ASN:HD22	13:SY:22:GLN:HE22	1.45	0.64
1:C2:105:A:H62	1:C2:308:C:H42	1.43	0.64
1:C2:984:G:N1	1:C2:1018:U:N3	2.45	0.64
18:CC:597:SER:HG	18:CC:687:THR:H	1.44	0.64
1:C2:231:U:C2	1:C2:234:G:O6	2.51	0.64
1:C2:953:G:H2'	1:C2:954:G:C8	2.33	0.64
10:SO:16:VAL:HG12	10:SO:80:HIS:HB2	1.79	0.64
5:SH:150:GLN:O	5:SH:181:ILE:HA	1.97	0.63
1:C2:873:U:O4	1:C2:954:G:O6	2.16	0.63
9:SN:136:PRO:HD2	9:SN:139:TRP:HD1	1.63	0.63
11:SW:115:GLU:HB3	11:SW:118:ARG:HH21	1.63	0.63
1:C2:564:G:C6	1:C2:580:A:N1	2.67	0.62
1:C2:1658:G:N2	1:C2:1743:U:O2	2.30	0.62
1:C2:189:C:N4	1:C2:197:A:N6	2.48	0.62
1:C2:954:G:H2'	1:C2:955:A:H8	1.64	0.62
2:SB:121:ILE:HG12	2:SB:161:ILE:HG23	1.82	0.62
8:SL:16:GLN:NE2	8:SL:61:THR:OG1	2.32	0.62
17:CB:266:PHE:HB2	17:CB:271:ARG:HH22	1.65	0.62
1:C2:231:U:O2	1:C2:234:G:C6	2.53	0.61
1:C2:900:A:H3'	1:C2:901:G:H21	1.65	0.61
1:C2:1064:G:O2'	2:SB:204:ILE:O	2.19	0.61
1:C2:154:G:OP2	13:SY:131:ARG:NH1	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SX:70:LYS:HD2	12:SX:93:LEU:HG	1.82	0.61
10:SO:17:ALA:HA	10:SO:29:HIS:O	2.01	0.61
18:CC:303:LEU:HD21	18:CC:306:ILE:HG13	1.82	0.61
1:C2:793:A:H3'	1:C2:794:U:H5'	1.82	0.61
1:C2:227:U:O2	1:C2:834:G:O6	2.18	0.60
1:C2:816:G:H2'	1:C2:817:A:H8	1.64	0.60
1:C2:687:G:H5"	11:SW:119:LYS:HE3	1.84	0.60
1:C2:163:G:N2	4:SG:4:ASN:OD1	2.33	0.60
1:C2:578:U:O4	1:C2:580:A:N6	2.34	0.60
1:C2:958:U:O2'	9:SN:55:ARG:NH1	2.35	0.60
4:SG:7:TYR:HB2	4:SG:113:ILE:HD12	1.83	0.60
1:C2:1151:A:N7	1:C2:1628:U:C2	2.69	0.60
1:C2:1670:G:C2	1:C2:1732:A:N6	2.70	0.60
1:C2:1696:G:C2	1:C2:1706:C:C2	2.90	0.60
1:C2:205:U:O2	1:C2:263:C:N3	2.35	0.60
2:SB:48:VAL:HG21	2:SB:61:LEU:HD12	1.82	0.60
18:CC:259:VAL:HB	18:CC:581:VAL:HB	1.84	0.60
1:C2:325:G:OP1	8:SL:134:THR:OG1	2.20	0.59
1:C2:1694:A:H61	1:C2:1707:A:H62	1.49	0.59
10:SO:50:ALA:O	10:SO:52:ARG:NH1	2.36	0.59
10:SO:107:ARG:NH1	16:CA:148:ASP:OD1	2.35	0.59
1:C2:34:G:N1	1:C2:474:A:C2	2.67	0.59
1:C2:1673:G:H1	1:C2:1728:A:H61	1.51	0.59
11:SW:48:GLY:HA3	11:SW:64:GLN:O	2.02	0.59
1:C2:868:G:H1	1:C2:960:U:H3	1.51	0.59
18:CC:145:PHE:HD2	18:CC:176:ILE:HD11	1.67	0.59
18:CC:87:THR:HG22	18:CC:138:ILE:HB	1.85	0.58
1:C2:1057:U:N3	1:C2:1061:A:C6	2.71	0.58
6:SI:62:THR:HA	6:SI:76:THR:O	2.04	0.58
18:CC:264:VAL:CA	18:CC:277:VAL:O	2.36	0.58
1:C2:967:A:OP2	9:SN:124:ARG:NH2	2.34	0.58
1:C2:1081:A:O2'	1:C2:1083:G:N7	2.36	0.58
2:SB:132:ASP:HB3	2:SB:221:PRO:HB3	1.85	0.58
18:CC:565:LYS:O	18:CC:568:LEU:HB2	2.04	0.58
1:C2:582:U:H5'	17:CB:270:LYS:HG3	1.86	0.58
1:C2:895:G:H1	1:C2:917:U:H3	1.52	0.58
6:SI:172:ARG:HE	6:SI:175:GLN:HG3	1.69	0.58
4:SG:163:THR:HG22	4:SG:168:THR:HG22	1.85	0.57
11:SW:46:TYR:HB3	11:SW:69:LEU:HD13	1.86	0.57
5:SH:93:LEU:HD21	5:SH:129:LEU:HB3	1.85	0.57
2:SB:34:ALA:HB3	2:SB:41:ARG:HA	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SX:69:ARG:NH1	12:SX:90:ASP:OD1	2.37	0.57
18:CC:641:LYS:NZ	18:CC:642:TYR:O	2.34	0.57
1:C2:521:A:N3	13:SY:34:ASN:ND2	2.52	0.57
1:C2:1117:U:OP1	18:CC:43:GLY:N	2.37	0.57
2:SB:47:LEU:HD21	10:SO:39:ILE:HD11	1.87	0.57
1:C2:446:A:H5"	3:SE:57:ASN:HD22	1.70	0.57
2:SB:61:LEU:HD21	2:SB:96:LEU:HD22	1.87	0.57
4:SG:44:GLU:O	4:SG:119:GLN:NE2	2.37	0.57
2:SB:27:LYS:NZ	10:SO:37:GLU:OE1	2.35	0.56
1:C2:34:G:N1	1:C2:474:A:H2	2.02	0.56
3:SE:45:ILE:HG13	3:SE:61:VAL:HG11	1.87	0.56
5:SH:62:VAL:HG12	5:SH:64:VAL:H	1.70	0.56
10:SO:85:ALA:H	10:SO:119:THR:HG22	1.70	0.56
1:C2:1681:A:H1'	4:SG:66:GLY:HA2	1.88	0.56
1:C2:231:U:O2	1:C2:234:G:O6	2.24	0.56
1:C2:235:G:H2'	1:C2:236:A:C8	2.40	0.56
1:C2:897:C:O2	10:SO:41:ARG:NH2	2.37	0.56
3:SE:44:LEU:HD23	3:SE:82:TYR:HB3	1.87	0.56
7:SJ:80:LEU:HB3	7:SJ:86:LEU:HD23	1.87	0.56
1:C2:340:U:H2'	1:C2:341:A:H8	1.71	0.56
18:CC:350:ALA:O	18:CC:527:ARG:NH1	2.38	0.56
1:C2:513:U:O4	7:SJ:171:ARG:NH2	2.39	0.56
1:C2:610:G:O2'	1:C2:613:G:O2'	2.23	0.56
1:C2:1151:A:C5	1:C2:1628:U:O2	2.59	0.55
18:CC:749:LEU:H	18:CC:755:PHE:HA	1.71	0.55
1:C2:1696:G:N2	1:C2:1706:C:C2	2.74	0.55
3:SE:31:PRO:HA	3:SE:81:THR:HB	1.88	0.55
7:SJ:128:LEU:HD23	7:SJ:134:ILE:HD11	1.88	0.55
10:SO:30:VAL:HG23	10:SO:39:ILE:HB	1.88	0.55
1:C2:836:U:H2'	1:C2:837:G:H8	1.72	0.55
1:C2:689:G:H2'	1:C2:690:G:C8	2.42	0.55
9:SN:99:ARG:NH2	9:SN:119:GLU:OE2	2.40	0.55
16:CA:266:VAL:HA	16:CA:269:ARG:HD3	1.89	0.55
18:CC:741:ARG:NH1	18:CC:762:LYS:O	2.40	0.55
1:C2:337:G:N2	1:C2:340:U:OP2	2.39	0.55
1:C2:1653:C:O2'	1:C2:1654:G:O4'	2.22	0.55
2:SB:127:VAL:HG21	2:SB:176:VAL:HG11	1.89	0.54
1:C2:330:G:OP2	6:SI:172:ARG:NH1	2.40	0.54
1:C2:1696:G:N1	1:C2:1706:C:N3	2.56	0.54
18:CC:708:PHE:HB2	18:CC:718:ARG:HB2	1.88	0.54
1:C2:143:G:OP2	4:SG:139:ASN:ND2	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SI:87:ASN:HB3	6:SI:90:LEU:HD13	1.88	0.54
1:C2:448:C:OP2	3:SE:49:ARG:NH1	2.37	0.54
1:C2:826:U:O4	1:C2:846:G:O6	2.24	0.54
1:C2:1658:G:O6	1:C2:1743:U:O4	2.26	0.54
12:SX:74:VAL:HG11	12:SX:104:LEU:HD11	1.90	0.54
13:SY:20:ARG:HE	13:SY:22:GLN:NE2	2.06	0.54
18:CC:302:GLN:HG3	18:CC:346:LEU:HG	1.90	0.54
8:SL:125:VAL:HG12	8:SL:139:VAL:HA	1.88	0.54
18:CC:289:ALA:HA	18:CC:303:LEU:HD22	1.88	0.54
1:C2:255:U:H2'	1:C2:256:A:H8	1.72	0.54
4:SG:2:LYS:HB3	4:SG:108:VAL:HG22	1.88	0.54
1:C2:564:G:O6	1:C2:580:A:N6	2.41	0.54
3:SE:200:ARG:NH2	3:SE:202:ASP:OD1	2.41	0.54
1:C2:564:G:C6	1:C2:580:A:C6	2.96	0.54
1:C2:451:A:N6	1:C2:453:U:O2	2.41	0.53
10:SO:31:THR:HG22	10:SO:38:THR:HA	1.89	0.53
18:CC:90:PRO:HB3	18:CC:95:LEU:HD22	1.90	0.53
1:C2:177:U:O2'	4:SG:191:ARG:NH1	2.42	0.53
5:SH:73:VAL:HG13	5:SH:74:GLN:H	1.74	0.53
18:CC:617:GLN:HB2	18:CC:622:ARG:HG3	1.91	0.53
13:SY:112:LYS:NZ	13:SY:113:ASN:OD1	2.36	0.53
1:C2:333:A:OP1	6:SI:31:ARG:NH2	2.42	0.53
1:C2:919:A:N3	10:SO:36:LYS:NZ	2.55	0.53
10:SO:61:MET:HG3	10:SO:104:ALA:HB2	1.91	0.53
1:C2:1789:G:N7	10:SO:132:ARG:NH2	2.57	0.53
1:C2:1037:C:O2	11:SW:16:ASN:ND2	2.41	0.53
1:C2:1787:C:H2'	1:C2:1788:G:H8	1.74	0.53
3:SE:97:GLU:HG2	3:SE:113:ARG:HH21	1.74	0.53
7:SJ:119:ALA:O	7:SJ:124:HIS:ND1	2.36	0.53
9:SN:35:GLU:HA	9:SN:38:VAL:HG22	1.90	0.53
11:SW:48:GLY:CA	11:SW:64:GLN:O	2.57	0.53
2:SB:72:ASP:OD1	10:SO:114:ARG:NH2	2.42	0.53
1:C2:1041:G:H2'	1:C2:1042:G:C8	2.44	0.53
1:C2:207:U:O2	6:SI:178:ARG:NH1	2.32	0.53
2:SB:103:MET:HB3	2:SB:215:VAL:HG22	1.91	0.53
13:SY:59:GLY:O	13:SY:71:GLY:CA	2.57	0.53
1:C2:52:U:H2'	1:C2:53:G:H8	1.73	0.52
1:C2:862:A:OP2	9:SN:64:ARG:NH1	2.42	0.52
4:SG:43:ASP:HA	4:SG:46:LYS:HE3	1.91	0.52
18:CC:535:LYS:NZ	18:CC:690:ASN:OD1	2.40	0.52
1:C2:688:G:H2'	1:C2:689:G:C8	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:1673:G:H1	1:C2:1728:A:N6	2.07	0.52
18:CC:339:SER:HB2	18:CC:343:ARG:HE	1.74	0.52
1:C2:813:U:O2'	1:C2:815:G:OP1	2.26	0.52
1:C2:8:U:O2'	1:C2:1139:A:OP2	2.26	0.52
1:C2:1676:U:H5"	6:SI:58:LEU:HD21	1.92	0.52
3:SE:171:ASP:OD1	3:SE:171:ASP:N	2.42	0.52
8:SL:54:ILE:HG23	8:SL:55:ASP:H	1.74	0.52
1:C2:29:U:H2'	1:C2:30:G:H8	1.75	0.52
1:C2:790:U:H2'	1:C2:791:A:H8	1.74	0.52
1:C2:925:G:H2'	1:C2:926:A:H8	1.74	0.52
1:C2:810:G:C2	5:SH:111:LYS:HB3	2.45	0.52
6:SI:69:SER:OG	6:SI:70:GLU:OE1	2.27	0.52
13:SY:59:GLY:O	13:SY:71:GLY:HA3	2.10	0.52
1:C2:1677:C:N4	1:C2:1724:U:H3	1.95	0.52
3:SE:122:LYS:NZ	3:SE:143:ASP:OD2	2.35	0.52
1:C2:486:G:O6	1:C2:501:U:O4	2.28	0.51
1:C2:1699:G:O6	1:C2:1703:C:N4	2.42	0.51
18:CC:86:ILE:HG13	18:CC:157:PHE:HB2	1.91	0.51
1:C2:68:A:OP2	4:SG:171:LYS:NZ	2.43	0.51
7:SJ:139:GLN:NE2	7:SJ:140:ILE:O	2.43	0.51
4:SG:58:LYS:HD2	4:SG:107:ALA:HB2	1.91	0.51
9:SN:130:ARG:NH2	9:SN:138:ASN:O	2.39	0.51
16:CA:110:ARG:HA	16:CA:113:TRP:HB2	1.93	0.51
1:C2:976:G:N1	1:C2:1023:A:O2'	2.35	0.51
13:SY:42:GLU:HG3	13:SY:52:LYS:HD2	1.91	0.51
1:C2:168:A:H5'	4:SG:137:ARG:HG3	1.92	0.51
1:C2:765:G:N7	7:SJ:149:ARG:NH1	2.59	0.51
8:SL:14:GLN:HB3	8:SL:54:ILE:HG21	1.93	0.51
10:SO:48:VAL:HG11	10:SO:53:ASP:HB2	1.91	0.51
18:CC:256:ARG:NH2	18:CC:588:GLU:OE2	2.44	0.51
1:C2:406:U:H2'	1:C2:407:A:H8	1.76	0.51
1:C2:474:A:H5"	7:SJ:144:PRO:HD2	1.93	0.51
1:C2:52:U:H2'	1:C2:53:G:C8	2.46	0.51
1:C2:867:G:O6	1:C2:962:C:N4	2.44	0.51
4:SG:180:THR:HG22	4:SG:182:GLN:H	1.76	0.51
10:SO:19:ILE:HB	10:SO:83:ILE:HG22	1.92	0.51
16:CA:141:THR:HG21	16:CA:152:LEU:HB2	1.92	0.51
1:C2:844:A:H2'	1:C2:845:G:H8	1.76	0.50
3:SE:105:VAL:HG12	3:SE:243:GLY:HA2	1.93	0.50
8:SL:40:LEU:HD13	8:SL:70:ILE:HD11	1.93	0.50
8:SL:57:LYS:O	8:SL:138:ASN:ND2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CA:94:PHE:HA	16:CA:141:THR:O	2.11	0.50
1:C2:325:G:H2'	1:C2:326:G:H8	1.76	0.50
2:SB:143:THR:HB	2:SB:205:PHE:HE2	1.75	0.50
6:SI:84:HIS:NE2	6:SI:97:THR:OG1	2.36	0.50
6:SI:99:ALA:CA	6:SI:169:ILE:O	2.60	0.50
16:CA:129:ARG:HE	16:CA:140:ARG:HH22	1.57	0.50
18:CC:227:TYR:HB3	18:CC:234:ASP:HB3	1.93	0.50
1:C2:58:U:OP1	1:C2:456:A:O2'	2.27	0.50
1:C2:1152:A:H2'	1:C2:1153:G:H8	1.75	0.50
3:SE:180:LEU:N	3:SE:229:GLY:O	2.44	0.50
1:C2:268:C:H2'	1:C2:269:G:H8	1.77	0.50
1:C2:647:G:H22	1:C2:687:G:H1	1.59	0.50
1:C2:800:U:H2'	1:C2:801:G:H8	1.76	0.50
10:SO:136:ARG:NH1	10:SO:137:LEU:O	2.44	0.50
12:SX:103:LEU:HB3	12:SX:126:LYS:HB2	1.93	0.50
1:C2:618:U:O2'	18:CC:15:LYS:NZ	2.44	0.50
3:SE:92:LEU:HD23	13:SY:17:LEU:HD11	1.93	0.50
1:C2:1726:G:H2'	1:C2:1727:G:C8	2.47	0.50
2:SB:115:ARG:HH12	16:CA:103:PRO:HG3	1.77	0.50
6:SI:99:ALA:HA	6:SI:169:ILE:O	2.12	0.50
11:SW:27:ILE:HB	11:SW:61:ILE:HB	1.93	0.50
2:SB:133:TYR:HE2	2:SB:181:LEU:HD22	1.76	0.50
4:SG:67:VAL:HG13	4:SG:99:GLY:HA2	1.94	0.50
1:C2:836:U:H2'	1:C2:837:G:C8	2.46	0.49
1:C2:322:G:O3'	6:SI:10:LYS:NZ	2.44	0.49
6:SI:107:THR:HA	6:SI:110:ARG:HG2	1.93	0.49
18:CC:301:PHE:HB2	18:CC:561:ILE:HD11	1.94	0.49
3:SE:85:GLY:N	3:SE:88:ASP:OD2	2.39	0.49
1:C2:312:A:N6	1:C2:352:A:N3	2.60	0.49
1:C2:891:A:H2'	1:C2:892:A:H8	1.77	0.49
1:C2:954:G:H2'	1:C2:955:A:C8	2.44	0.49
1:C2:1081:A:H2	1:C2:1082:C:H41	1.59	0.49
1:C2:1085:G:N2	1:C2:1088:A:OP2	2.41	0.49
1:C2:1699:G:C6	1:C2:1703:C:N3	2.81	0.49
5:SH:99:LEU:O	5:SH:112:ARG:NH1	2.41	0.49
5:SH:115:SER:OG	5:SH:116:ARG:NH1	2.44	0.49
7:SJ:88:GLU:O	7:SJ:91:LYS:NZ	2.38	0.49
7:SJ:93:LEU:HA	7:SJ:96:VAL:HG12	1.93	0.49
18:CC:545:THR:HG21	18:CC:585:LEU:HD22	1.95	0.49
18:CC:730:PHE:HE1	18:CC:773:LEU:HD21	1.77	0.49
1:C2:896:U:O2	10:SO:41:ARG:NH1	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SX:3:LYS:HB2	12:SX:7:ARG:HH22	1.78	0.49
18:CC:150:ASP:HA	18:CC:153:LYS:HG2	1.95	0.49
1:C2:444:C:H6	13:SY:105:ARG:HH12	1.61	0.49
1:C2:434:G:N1	1:C2:437:A:OP2	2.38	0.49
6:SI:36:THR:HG23	6:SI:96:LEU:HB2	1.95	0.49
1:C2:486:G:N2	1:C2:501:U:O2	2.35	0.49
1:C2:563:U:H2'	1:C2:564:G:C8	2.47	0.49
1:C2:871:G:H2'	1:C2:872:G:C8	2.46	0.49
18:CC:246:LEU:HD12	18:CC:247:PRO:HD2	1.95	0.49
18:CC:642:TYR:HA	18:CC:697:LEU:HD23	1.95	0.49
1:C2:763:G:H5"	7:SJ:78:ARG:HH22	1.78	0.49
10:SO:112:ILE:HG22	16:CA:97:ARG:HH12	1.78	0.48
13:SY:20:ARG:HD2	13:SY:74:LEU:HD12	1.95	0.48
18:CC:282:VAL:O	18:CC:554:GLY:CA	2.61	0.48
2:SB:70:LEU:HD23	2:SB:79:HIS:HB3	1.95	0.48
4:SG:84:TYR:HD1	4:SG:95:LYS:HE3	1.79	0.48
7:SJ:176:ASN:OD1	7:SJ:179:ARG:NH2	2.40	0.48
9:SN:29:SER:OG	9:SN:30:SER:N	2.46	0.48
13:SY:57:VAL:HG12	13:SY:73:GLY:HA3	1.94	0.48
18:CC:305:LYS:HB3	18:CC:560:PHE:HB2	1.95	0.48
18:CC:351:PRO:HA	18:CC:527:ARG:HH12	1.77	0.48
1:C2:107:C:OP1	1:C2:383:G:O2'	2.31	0.48
18:CC:305:LYS:HE2	18:CC:336:VAL:HG13	1.95	0.48
1:C2:65:A:H2	1:C2:84:A:H62	1.61	0.48
1:C2:162:A:H2'	1:C2:163:G:C8	2.48	0.48
1:C2:818:C:H2'	1:C2:819:G:C8	2.48	0.48
7:SJ:41:GLU:O	7:SJ:45:ILE:HG12	2.13	0.48
18:CC:307:GLU:HB3	18:CC:558:ARG:HB2	1.95	0.48
7:SJ:64:GLU:HG3	7:SJ:65:LYS:HG2	1.95	0.48
13:SY:20:ARG:HE	13:SY:22:GLN:HE21	1.61	0.48
1:C2:205:U:H2'	1:C2:206:A:H8	1.79	0.48
1:C2:590:C:H2'	1:C2:591:A:H8	1.79	0.48
6:SI:34:ALA:HB2	6:SI:56:ARG:HD3	1.95	0.48
6:SI:57:ALA:HB2	6:SI:177:GLY:HA2	1.95	0.48
16:CA:269:ARG:HA	16:CA:272:GLU:HG2	1.95	0.48
17:CB:266:PHE:O	17:CB:271:ARG:NH2	2.47	0.48
1:C2:1766:A:H2'	1:C2:1767:G:C8	2.49	0.48
6:SI:3:ILE:O	6:SI:30:GLY:N	2.44	0.48
18:CC:128:ILE:O	18:CC:132:LYS:CA	2.62	0.48
1:C2:189:C:N3	1:C2:197:A:C6	2.82	0.48
1:C2:564:G:O6	1:C2:580:A:C6	2.67	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CC:264:VAL:HG22	18:CC:278:ILE:HA	1.96	0.48
13:SY:27:VAL:HG13	13:SY:29:HIS:HD2	1.78	0.47
18:CC:666:PRO:HA	18:CC:687:THR:HA	1.96	0.47
10:SO:45:GLY:O	10:SO:49:LYS:NZ	2.42	0.47
11:SW:85:ASP:HB2	11:SW:88:LYS:HD3	1.95	0.47
16:CA:211:LYS:O	16:CA:214:PHE:HB3	2.13	0.47
1:C2:308:C:OP2	8:SL:103:ARG:NH1	2.42	0.47
4:SG:74:LYS:NZ	4:SG:96:SER:OG	2.39	0.47
4:SG:145:PHE:HB3	4:SG:147:LEU:HD13	1.95	0.47
4:SG:147:LEU:HD23	4:SG:151:ASP:HB2	1.95	0.47
2:SB:71:ALA:O	2:SB:75:GLY:N	2.45	0.47
5:SH:75:THR:O	5:SH:78:THR:OG1	2.28	0.47
12:SX:131:SER:OG	12:SX:132:LEU:N	2.48	0.47
18:CC:295:ILE:HB	18:CC:298:PHE:HB2	1.96	0.47
1:C2:40:A:H62	1:C2:467:G:H21	1.61	0.47
1:C2:844:A:H2'	1:C2:845:G:C8	2.50	0.47
1:C2:1672:G:H2'	1:C2:1673:G:C8	2.50	0.47
1:C2:1787:C:H2'	1:C2:1788:G:C8	2.49	0.47
3:SE:104:ASP:OD1	3:SE:105:VAL:N	2.44	0.47
4:SG:57:ASP:OD2	4:SG:72:ARG:NH1	2.47	0.47
16:CA:128:VAL:HG12	16:CA:139:LEU:HG	1.96	0.47
1:C2:607:G:N2	1:C2:614:C:H5"	2.30	0.47
1:C2:1740:A:O2'	18:CC:53:GLN:OE1	2.33	0.47
16:CA:109:LEU:HD13	16:CA:162:PHE:HE2	1.80	0.47
1:C2:5:U:H2'	1:C2:6:G:H8	1.80	0.47
3:SE:11:ARG:NH1	3:SE:21:ASP:O	2.48	0.47
1:C2:340:U:H2'	1:C2:341:A:C8	2.50	0.47
1:C2:393:C:H2'	1:C2:394:C:C6	2.50	0.47
1:C2:406:U:H2'	1:C2:407:A:C8	2.50	0.47
1:C2:144:U:H5	4:SG:137:ARG:HH22	1.63	0.46
1:C2:255:U:H2'	1:C2:256:A:C8	2.49	0.46
1:C2:922:G:H2'	1:C2:923:A:H8	1.79	0.46
1:C2:982:U:H2'	1:C2:983:A:H8	1.81	0.46
18:CC:702:ILE:HA	18:CC:771:MET:O	2.15	0.46
1:C2:590:C:H2'	1:C2:591:A:C8	2.50	0.46
2:SB:99:ASN:OD1	2:SB:100:PHE:N	2.47	0.46
8:SL:20:PHE:O	8:SL:32:LYS:NZ	2.39	0.46
10:SO:71:CYS:HA	10:SO:74:VAL:HG12	1.97	0.46
5:SH:67:LEU:HD22	5:SH:94:ALA:HB2	1.97	0.46
17:CB:243:LYS:HD2	17:CB:268:GLY:HA3	1.97	0.46
1:C2:155:U:OP2	13:SY:132:ARG:NH1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:166:C:O2'	4:SG:133:LEU:O	2.32	0.46
1:C2:399:A:H4'	3:SE:3:ARG:HG2	1.97	0.46
5:SH:129:LEU:HD12	5:SH:130:VAL:HB	1.97	0.46
18:CC:113:ILE:HG21	18:CC:126:VAL:HG13	1.97	0.46
5:SH:111:LYS:HG3	5:SH:112:ARG:H	1.80	0.46
9:SN:54:LEU:HD13	9:SN:58:HIS:HD2	1.80	0.46
18:CC:174:GLU:OE2	18:CC:178:ARG:NH2	2.48	0.46
1:C2:68:A:OP1	4:SG:160:ARG:NH2	2.35	0.46
1:C2:1652:C:H42	1:C2:1749:A:N6	2.12	0.46
6:SI:67:TRP:CG	6:SI:183:ILE:HD11	2.50	0.46
1:C2:591:A:H2'	1:C2:592:A:C8	2.51	0.46
1:C2:628:G:OP1	9:SN:124:ARG:NH1	2.41	0.46
1:C2:925:G:H2'	1:C2:926:A:C8	2.51	0.46
2:SB:104:ASP:OD1	2:SB:105:PHE:N	2.49	0.46
1:C2:108:A:H2'	1:C2:109:G:C8	2.51	0.46
1:C2:480:G:H1	1:C2:508:U:H3	1.64	0.46
1:C2:866:G:H2'	1:C2:867:G:H8	1.81	0.46
5:SH:133:THR:HG21	5:SH:159:VAL:HG12	1.98	0.46
1:C2:333:A:N6	6:SI:27:PHE:O	2.47	0.46
1:C2:472:U:O2'	1:C2:769:A:N3	2.38	0.46
1:C2:884:A:H2'	1:C2:885:G:C8	2.50	0.46
6:SI:7:SER:O	6:SI:7:SER:OG	2.31	0.46
8:SL:59:PRO:HD3	8:SL:138:ASN:ND2	2.31	0.46
1:C2:168:A:OP1	4:SG:140:ASN:ND2	2.47	0.45
1:C2:250:C:H2'	1:C2:251:A:H8	1.81	0.45
1:C2:513:U:H2'	1:C2:514:G:C8	2.51	0.45
1:C2:611:U:OP1	12:SX:19:ARG:NH2	2.35	0.45
18:CC:728:GLU:HA	18:CC:731:LYS:HG3	1.97	0.45
1:C2:29:U:H2'	1:C2:30:G:C8	2.50	0.45
1:C2:526:A:P	13:SY:93:ARG:HH21	2.40	0.45
10:SO:47:LYS:HA	10:SO:47:LYS:HD3	1.72	0.45
1:C2:968:U:OP1	1:C2:1033:C:O2'	2.34	0.45
3:SE:71:LYS:HG2	3:SE:76:VAL:HG22	1.99	0.45
1:C2:400:A:H5"	6:SI:25:ARG:HA	1.99	0.45
1:C2:982:U:H2'	1:C2:983:A:C8	2.52	0.45
1:C2:1152:A:H2'	1:C2:1153:G:C8	2.51	0.45
7:SJ:51:LYS:HB3	7:SJ:51:LYS:HE2	1.74	0.45
1:C2:455:C:H3'	1:C2:456:A:H8	1.81	0.45
1:C2:833:U:H5'	1:C2:834:G:H5"	1.98	0.45
2:SB:144:ARG:HB3	2:SB:208:GLN:HB3	1.99	0.45
13:SY:20:ARG:HH21	13:SY:22:GLN:HE21	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CC:214:SER:HA	18:CC:217:LYS:HG2	1.99	0.45
1:C2:1087:A:H2'	1:C2:1088:A:C8	2.51	0.45
1:C2:1149:G:N2	1:C2:1628:U:O2	2.50	0.45
11:SW:2:THR:OG1	11:SW:3:ARG:N	2.50	0.45
1:C2:688:G:H2'	1:C2:689:G:H8	1.82	0.45
1:C2:997:G:O2'	1:C2:998:A:O5'	2.35	0.45
4:SG:5:ILE:HD11	4:SG:50:PHE:CE1	2.52	0.45
1:C2:241:U:O2'	1:C2:242:U:O4'	2.29	0.45
5:SH:30:SER:N	5:SH:31:SER:HA	2.32	0.45
10:SO:25:ASP:OD1	10:SO:26:THR:N	2.49	0.45
1:C2:79:C:H1'	4:SG:174:LYS:HG3	1.99	0.45
6:SI:171:SER:OG	6:SI:180:ASP:N	2.40	0.45
1:C2:923:A:H2'	1:C2:924:A:C8	2.52	0.44
2:SB:129:THR:OG1	2:SB:131:ASP:OD1	2.32	0.44
5:SH:14:THR:OG1	5:SH:15:GLU:OE1	2.33	0.44
18:CC:505:LYS:HD2	18:CC:506:ASN:HB2	1.98	0.44
1:C2:576:G:H2'	1:C2:577:G:C8	2.52	0.44
1:C2:435:C:H5"	12:SX:50:LYS:HE2	1.98	0.44
3:SE:166:SER:OG	3:SE:168:LYS:NZ	2.47	0.44
4:SG:7:TYR:O	4:SG:11:GLY:CA	2.66	0.44
8:SL:26:LYS:NZ	8:SL:27:THR:O	2.47	0.44
13:SY:6:THR:HB	13:SY:28:LEU:HB2	1.98	0.44
18:CC:568:LEU:HD23	18:CC:571:ILE:HD12	1.99	0.44
18:CC:170:GLU:O	18:CC:175:GLN:NE2	2.35	0.44
18:CC:250:ILE:HB	18:CC:253:ARG:HG2	1.98	0.44
1:C2:24:U:OP1	7:SJ:10:LYS:NZ	2.38	0.44
1:C2:189:C:C4	1:C2:197:A:C6	3.06	0.44
1:C2:997:G:O2'	1:C2:998:A:O4'	2.32	0.44
5:SH:173:TYR:HE2	5:SH:179:LYS:HB2	1.83	0.44
8:SL:121:ASP:H	8:SL:145:ALA:HB2	1.83	0.44
13:SY:105:ARG:HD2	13:SY:108:ARG:HH12	1.83	0.44
16:CA:116:ILE:HG23	16:CA:158:PHE:HE2	1.81	0.44
3:SE:103:TYR:O	3:SE:182:TYR:OH	2.35	0.44
8:SL:57:LYS:HD3	8:SL:131:ILE:HD12	2.00	0.44
16:CA:118:PRO:HA	16:CA:121:VAL:HG22	2.00	0.44
18:CC:78:GLY:HA2	18:CC:82:ALA:HB2	1.99	0.44
18:CC:153:LYS:HD3	18:CC:252:TRP:HH2	1.83	0.44
18:CC:264:VAL:HG13	18:CC:278:ILE:HG13	2.00	0.44
18:CC:500:ARG:HD2	18:CC:775:LYS:HE3	2.00	0.44
1:C2:555:A:H2'	1:C2:556:A:C8	2.53	0.44
1:C2:754:A:N6	1:C2:793:A:N7	2.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:890:C:H2'	1:C2:891:A:H8	1.82	0.44
5:SH:61:PHE:HA	5:SH:93:LEU:O	2.17	0.44
16:CA:154:LYS:HB3	16:CA:175:LEU:HD12	2.00	0.44
18:CC:718:ARG:NE	18:CC:754:TYR:OH	2.49	0.44
1:C2:31:C:H5"	12:SX:134:ALA:HB2	2.00	0.43
1:C2:607:G:H21	1:C2:614:C:H5"	1.83	0.43
1:C2:947:U:H2'	1:C2:948:G:H8	1.83	0.43
2:SB:21:VAL:HB	2:SB:26:ARG:HH22	1.82	0.43
4:SG:2:LYS:O	4:SG:108:VAL:HA	2.18	0.43
8:SL:90:TYR:HE1	8:SL:105:LYS:HG3	1.83	0.43
9:SN:69:ASN:OD1	9:SN:70:LYS:N	2.51	0.43
18:CC:259:VAL:HA	18:CC:281:THR:O	2.18	0.43
1:C2:826:U:H2'	1:C2:827:C:C6	2.53	0.43
1:C2:932:U:OP2	2:SB:155:TYR:OH	2.29	0.43
16:CA:103:PRO:HA	16:CA:106:MET:HB3	1.99	0.43
18:CC:263:PHE:HB2	18:CC:279:GLU:HB3	2.00	0.43
18:CC:265:ASP:O	18:CC:277:VAL:N	2.50	0.43
4:SG:57:ASP:OD1	4:SG:57:ASP:N	2.46	0.43
16:CA:99:ILE:HD11	16:CA:159:ILE:HB	2.00	0.43
18:CC:256:ARG:NH1	18:CC:663:THR:OG1	2.51	0.43
1:C2:843:U:H2'	1:C2:844:A:C8	2.54	0.43
9:SN:92:ILE:HD11	9:SN:139:TRP:HH2	1.83	0.43
16:CA:214:PHE:HA	16:CA:217:GLU:HB2	2.00	0.43
18:CC:503:GLY:HA3	18:CC:733:ILE:HG12	2.00	0.43
1:C2:225:A:H2'	1:C2:226:A:C8	2.54	0.43
4:SG:29:ASP:HA	4:SG:101:ILE:HG23	2.00	0.43
4:SG:52:ILE:HG23	4:SG:109:LEU:HD11	2.00	0.43
5:SH:11:GLN:HG3	5:SH:13:PRO:HD2	2.01	0.43
5:SH:44:LYS:HE2	5:SH:63:PRO:HG3	2.00	0.43
16:CA:174:LEU:HA	16:CA:180:LEU:HD12	1.99	0.43
1:C2:404:G:O4'	4:SG:88:ARG:NH1	2.51	0.43
1:C2:487:G:C2	1:C2:501:U:C2	3.06	0.43
1:C2:808:U:H2'	1:C2:809:A:C8	2.54	0.43
1:C2:984:G:O6	1:C2:1018:U:C4	2.72	0.43
2:SB:133:TYR:CE2	2:SB:181:LEU:HD22	2.53	0.43
5:SH:13:PRO:HA	5:SH:14:THR:HA	1.64	0.43
5:SH:79:ARG:O	5:SH:83:LYS:HG2	2.18	0.43
18:CC:501:TYR:HB3	18:CC:773:LEU:HB3	2.00	0.43
1:C2:446:A:N1	1:C2:461:G:O2'	2.46	0.43
1:C2:479:C:O2	1:C2:510:G:N2	2.51	0.43
16:CA:223:ARG:HA	16:CA:223:ARG:HD3	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CC:617:GLN:HB3	18:CC:668:ILE:HG22	2.00	0.43
1:C2:34:G:O6	1:C2:474:A:N1	2.52	0.43
1:C2:552:G:H2'	1:C2:553:G:C8	2.53	0.43
1:C2:637:C:O2	5:SH:114:ARG:NH2	2.46	0.43
5:SH:75:THR:HB	5:SH:79:ARG:HH22	1.84	0.43
7:SJ:52:ILE:HD13	7:SJ:80:LEU:HD11	1.99	0.43
7:SJ:107:ARG:HA	7:SJ:107:ARG:HD2	1.77	0.43
12:SX:51:GLY:O	12:SX:101:GLU:HA	2.19	0.43
3:SE:121:TYR:HA	3:SE:163:ASP:HA	2.01	0.43
4:SG:49:VAL:HB	4:SG:115:LYS:HB3	2.01	0.43
5:SH:49:ILE:HD11	5:SH:172:VAL:HG22	2.00	0.43
6:SI:100:ALA:O	6:SI:168:CYS:HA	2.18	0.43
16:CA:233:ILE:HG22	16:CA:240:ILE:HG22	2.00	0.43
3:SE:163:ASP:OD1	3:SE:163:ASP:N	2.51	0.42
4:SG:7:TYR:O	4:SG:11:GLY:N	2.52	0.42
18:CC:642:TYR:HB2	18:CC:697:LEU:HB3	2.01	0.42
1:C2:626:U:H2'	1:C2:627:C:H6	1.83	0.42
7:SJ:180:LYS:O	7:SJ:184:SER:OG	2.28	0.42
18:CC:700:ARG:HH21	18:CC:702:ILE:HD11	1.84	0.42
1:C2:1057:U:C4	1:C2:1061:A:N1	2.87	0.42
3:SE:11:ARG:NH1	3:SE:20:LEU:HB3	2.34	0.42
1:C2:800:U:H2'	1:C2:801:G:C8	2.55	0.42
11:SW:81:VAL:HG11	11:SW:86:ILE:HD13	2.01	0.42
1:C2:324:U:OP1	8:SL:133:LYS:NZ	2.39	0.42
1:C2:1044:U:H2'	1:C2:1045:C:C6	2.55	0.42
3:SE:35:PRO:HB2	3:SE:36:HIS:CE1	2.54	0.42
3:SE:125:LYS:HA	3:SE:158:ASP:O	2.20	0.42
1:C2:407:A:O2'	1:C2:1671:A:N3	2.44	0.42
1:C2:968:U:O3'	1:C2:1032:G:N2	2.52	0.42
1:C2:1057:U:N3	1:C2:1061:A:N6	2.67	0.42
8:SL:73:GLY:O	8:SL:122:ILE:HA	2.20	0.42
18:CC:51:LYS:HA	18:CC:54:ARG:HH11	1.83	0.42
18:CC:294:HIS:N	18:CC:582:TYR:O	2.46	0.42
1:C2:250:C:H2'	1:C2:251:A:C8	2.55	0.42
1:C2:629:U:H2'	1:C2:630:A:H8	1.85	0.42
18:CC:688:PHE:HZ	18:CC:691:ALA:HB2	1.83	0.42
1:C2:561:G:H2'	1:C2:562:G:C8	2.55	0.42
11:SW:48:GLY:N	11:SW:64:GLN:O	2.52	0.42
18:CC:621:ARG:HE	18:CC:623:TYR:HE1	1.66	0.42
1:C2:407:A:H2'	1:C2:408:C:C6	2.55	0.42
2:SB:137:ILE:HG22	2:SB:215:VAL:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CC:124:PHE:O	18:CC:136:LYS:HA	2.20	0.42
1:C2:447:U:O2'	3:SE:27:TYR:O	2.37	0.42
1:C2:504:U:H2'	1:C2:505:A:C8	2.55	0.42
1:C2:1779:U:O2	1:C2:1783:C:N3	2.53	0.42
2:SB:86:LEU:HD23	2:SB:100:PHE:HA	2.02	0.42
13:SY:55:VAL:HG12	13:SY:75:VAL:HG23	2.02	0.42
16:CA:167:ASP:OD1	16:CA:168:LEU:N	2.53	0.42
1:C2:7:G:H5"	17:CB:249:LYS:NZ	2.35	0.41
4:SG:69:LEU:O	4:SG:71:THR:N	2.44	0.41
5:SH:45:SER:HB3	5:SH:61:PHE:HB2	2.02	0.41
11:SW:35:ILE:HD13	11:SW:35:ILE:HA	1.86	0.41
16:CA:96:SER:HA	16:CA:139:LEU:O	2.20	0.41
1:C2:199:G:O2'	1:C2:200:A:H8	2.03	0.41
1:C2:230:C:H2'	1:C2:231:U:H6	1.84	0.41
1:C2:887:A:H1'	10:SO:122:PRO:HB3	2.01	0.41
12:SX:109:ARG:HE	12:SX:114:LYS:HD3	1.85	0.41
18:CC:86:ILE:HG12	18:CC:242:LEU:HD22	2.00	0.41
1:C2:563:U:H2'	1:C2:564:G:H8	1.84	0.41
1:C2:684:A:H2'	1:C2:685:A:H8	1.85	0.41
2:SB:100:PHE:HB3	2:SB:181:LEU:HD21	2.02	0.41
13:SY:123:LYS:HA	13:SY:123:LYS:HD3	1.68	0.41
18:CC:96:ASP:OD2	18:CC:99:ASP:N	2.53	0.41
1:C2:107:C:H2'	1:C2:108:A:H8	1.84	0.41
1:C2:1057:U:C4	1:C2:1061:A:C6	3.09	0.41
11:SW:83:ILE:O	11:SW:86:ILE:HG22	2.19	0.41
18:CC:146:LEU:HD23	18:CC:149:LEU:HD12	2.01	0.41
1:C2:462:G:H5"	7:SJ:3:ARG:HH21	1.86	0.41
12:SX:133:LEU:HD13	17:CB:275:PHE:HD1	1.85	0.41
1:C2:1766:A:H2'	1:C2:1767:G:H8	1.86	0.41
11:SW:72:CYS:HB3	11:SW:129:VAL:HG23	2.02	0.41
13:SY:43:LYS:O	13:SY:47:VAL:HG23	2.21	0.41
18:CC:501:TYR:HE1	18:CC:775:LYS:HD2	1.84	0.41
1:C2:991:G:N1	1:C2:1012:U:OP2	2.40	0.41
3:SE:117:GLU:O	3:SE:118:GLU:HG3	2.21	0.41
7:SJ:106:GLU:O	7:SJ:111:THR:OG1	2.38	0.41
8:SL:132:SER:O	8:SL:134:THR:N	2.42	0.41
18:CC:614:ILE:HA	18:CC:671:LYS:HD3	2.02	0.41
1:C2:922:G:H2'	1:C2:923:A:C8	2.55	0.41
1:C2:1777:G:H2'	1:C2:1778:G:C8	2.56	0.41
18:CC:101:LEU:HD13	18:CC:137:ILE:HG21	2.02	0.41
18:CC:121:LYS:HB2	18:CC:121:LYS:HE2	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CC:128:ILE:HG22	18:CC:131:PHE:H	1.85	0.41
1:C2:120:U:H2'	1:C2:121:U:H6	1.86	0.41
1:C2:164:A:H2'	1:C2:165:G:H8	1.86	0.41
1:C2:252:U:H2'	1:C2:253:A:H8	1.86	0.41
1:C2:386:G:H2'	1:C2:387:A:C8	2.56	0.41
1:C2:386:G:OP2	6:SI:25:ARG:NH2	2.39	0.41
1:C2:584:C:OP2	17:CB:270:LYS:NZ	2.32	0.41
1:C2:924:A:H2'	1:C2:925:G:C8	2.56	0.41
1:C2:984:G:C6	1:C2:1018:U:C4	3.08	0.41
1:C2:1036:A:H2'	1:C2:1037:C:C6	2.56	0.41
1:C2:1057:U:H5	1:C2:1060:U:H1'	1.86	0.41
5:SH:17:GLU:HA	5:SH:20:VAL:HG12	2.02	0.41
6:SI:86:SER:OG	6:SI:87:ASN:N	2.54	0.41
7:SJ:113:VAL:HG13	7:SJ:125:ALA:HB1	2.02	0.41
13:SY:36:SER:O	13:SY:39:GLU:HG2	2.21	0.41
18:CC:259:VAL:HG22	18:CC:282:VAL:HG22	2.03	0.41
18:CC:476:GLU:HG3	18:CC:645:PHE:CG	2.56	0.41
1:C2:182:A:H2'	1:C2:183:U:C6	2.55	0.41
1:C2:1055:U:H2'	1:C2:1056:U:C6	2.55	0.41
1:C2:1132:A:H2'	1:C2:1133:A:H8	1.85	0.41
2:SB:228:LEU:HD12	2:SB:228:LEU:HA	1.91	0.41
4:SG:164:LYS:HG3	4:SG:165:GLY:H	1.85	0.41
6:SI:81:VAL:HG22	6:SI:102:VAL:HG12	2.02	0.41
1:C2:257:A:H1'	6:SI:73:SER:HB2	2.03	0.40
16:CA:125:LYS:HG2	16:CA:145:PHE:HB3	2.02	0.40
1:C2:520:A:H2'	1:C2:521:A:C8	2.57	0.40
3:SE:14:ALA:HB1	3:SE:18:TRP:CE3	2.57	0.40
9:SN:140:LYS:HD2	9:SN:140:LYS:HA	1.92	0.40
13:SY:23:PHE:HE1	13:SY:75:VAL:HG12	1.86	0.40
1:C2:891:A:H2'	1:C2:892:A:C8	2.55	0.40
1:C2:1146:G:H2'	1:C2:1147:A:N3	2.36	0.40
5:SH:98:ILE:HD11	5:SH:121:VAL:HG11	2.04	0.40
16:CA:119:PRO:O	16:CA:123:HIS:N	2.48	0.40
1:C2:227:U:O2	1:C2:834:G:C6	2.74	0.40
1:C2:1689:A:H61	1:C2:1712:A:N6	2.20	0.40
6:SI:178:ARG:H	6:SI:178:ARG:HG2	1.65	0.40
1:C2:416:A:H5"	1:C2:417:A:C8	2.57	0.40
1:C2:1132:A:H2'	1:C2:1133:A:C8	2.56	0.40
4:SG:73:ILE:HD12	4:SG:73:ILE:HA	2.00	0.40
5:SH:76:LYS:O	5:SH:80:GLU:HG2	2.22	0.40
6:SI:138:ASN:HA	6:SI:141:ARG:HE	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SW:22:LYS:HA	11:SW:22:LYS:HD2	1.94	0.40
18:CC:133:SER:OG	18:CC:243:CYS:SG	2.70	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%)	196 (92%)	18 (8%)	0	100	100
3	SE	258/261 (99%)	237 (92%)	21 (8%)	0	100	100
4	SG	216/236 (92%)	202 (94%)	14 (6%)	0	100	100
5	SH	183/190 (96%)	163 (89%)	20 (11%)	0	100	100
6	SI	184/200 (92%)	177 (96%)	7 (4%)	0	100	100
7	SJ	183/197 (93%)	165 (90%)	17 (9%)	1 (0%)	29	66
8	SL	144/156 (92%)	128 (89%)	16 (11%)	0	100	100
9	SN	148/151 (98%)	134 (90%)	14 (10%)	0	100	100
10	SO	126/137 (92%)	110 (87%)	16 (13%)	0	100	100
11	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
12	SX	142/145 (98%)	121 (85%)	21 (15%)	0	100	100
13	SY	132/135 (98%)	116 (88%)	14 (11%)	2 (2%)	10	44
14	Sb	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
15	Se	36/63 (57%)	29 (81%)	7 (19%)	0	100	100
16	CA	179/274 (65%)	172 (96%)	7 (4%)	0	100	100
17	CB	33/275 (12%)	30 (91%)	3 (9%)	0	100	100
18	CC	653/788 (83%)	622 (95%)	30 (5%)	1 (0%)	47	78
All	All	3037/3675 (83%)	2789 (92%)	244 (8%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	SY	52	LYS
13	SY	32	ARG
18	CC	79	LYS
7	SJ	163	PRO

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%)	164 (99%)	1 (1%)	86 93
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%)	127 (98%)	2 (2%)	62 80
9	SN	127/128 (99%)	127 (100%)	0	100 100
10	SO	97/105 (92%)	97 (100%)	0	100 100
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%)	111 (99%)	1 (1%)	78 88
14	Sb	70/71 (99%)	70 (100%)	0	100 100
15	Se	34/54 (63%)	34 (100%)	0	100 100
16	CA	158/238 (66%)	157 (99%)	1 (1%)	86 93
17	CB	31/233 (13%)	30 (97%)	1 (3%)	39 65
18	CC	575/703 (82%)	570 (99%)	5 (1%)	78 88
All	All	2635/3157 (84%)	2622 (100%)	13 (0%)	89 94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	50	LYS
4	SG	143	LYS
5	SH	7	LYS
8	SL	14	GLN
8	SL	67	ARG
13	SY	49	LYS
16	CA	269	ARG
17	CB	259	LYS
18	CC	45	PRO
18	CC	500	ARG
18	CC	505	LYS
18	CC	570	LYS
18	CC	622	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
8	SL	14	GLN
8	SL	16	GLN
11	SW	80	ASN
13	SY	22	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C2	1247/1800 (69%)	324 (25%)	13 (1%)

All (324) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C2	2	A
1	C2	3	U
1	C2	4	C
1	C2	8	U
1	C2	9	U
1	C2	14	C
1	C2	25	C
1	C2	26	A
1	C2	27	U
1	C2	34	G
1	C2	43	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C2	45	U
1	C2	46	A
1	C2	47	A
1	C2	57	G
1	C2	60	U
1	C2	63	G
1	C2	68	A
1	C2	71	A
1	C2	77	U
1	C2	104	A
1	C2	111	U
1	C2	114	C
1	C2	115	G
1	C2	116	U
1	C2	126	A
1	C2	127	G
1	C2	132	U
1	C2	137	U
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	185	U
1	C2	189	C
1	C2	190	C
1	C2	191	C
1	C2	192	U
1	C2	193	U
1	C2	195	G
1	C2	196	G
1	C2	197	A
1	C2	200	A
1	C2	216	U
1	C2	217	A
1	C2	220	A
1	C2	227	U
1	C2	228	G
1	C2	230	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C2	233	C
1	C2	235	G
1	C2	238	U
1	C2	240	U
1	C2	241	U
1	C2	249	U
1	C2	257	A
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	287	G
1	C2	299	A
1	C2	314	C
1	C2	316	A
1	C2	321	C
1	C2	322	G
1	C2	333	A
1	C2	337	G
1	C2	338	C
1	C2	350	U
1	C2	351	C
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	387	A
1	C2	388	G
1	C2	390	G
1	C2	400	A
1	C2	401	A
1	C2	402	C
1	C2	404	G
1	C2	415	C
1	C2	416	A
1	C2	418	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C2	423	G
1	C2	424	C
1	C2	426	G
1	C2	428	A
1	C2	434	G
1	C2	439	U
1	C2	444	C
1	C2	448	C
1	C2	454	U
1	C2	460	A
1	C2	461	G
1	C2	468	A
1	C2	475	A
1	C2	477	A
1	C2	480	G
1	C2	483	A
1	C2	488	G
1	C2	500	C
1	C2	501	U
1	C2	506	A
1	C2	507	U
1	C2	510	G
1	C2	511	A
1	C2	515	A
1	C2	518	A
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	548	G
1	C2	549	G
1	C2	551	G
1	C2	552	G
1	C2	554	C
1	C2	555	A
1	C2	556	A
1	C2	557	G
1	C2	559	C
1	C2	567	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C2	568	G
1	C2	574	G
1	C2	578	U
1	C2	579	A
1	C2	580	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	607	G
1	C2	611	U
1	C2	614	C
1	C2	619	A
1	C2	620	A
1	C2	622	A
1	C2	623	A
1	C2	624	G
1	C2	635	A
1	C2	639	U
1	C2	685	A
1	C2	690	G
1	C2	691	C
1	C2	696	C
1	C2	699	U
1	C2	701	U
1	C2	703	G
1	C2	705	U
1	C2	734	A
1	C2	735	C
1	C2	742	U
1	C2	743	U
1	C2	744	U
1	C2	745	U
1	C2	754	A
1	C2	755	A
1	C2	756	A
1	C2	765	G
1	C2	771	A
1	C2	774	A
1	C2	775	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C2	781	U
1	C2	782	U
1	C2	783	G
1	C2	789	A
1	C2	793	A
1	C2	794	U
1	C2	807	A
1	C2	811	A
1	C2	812	A
1	C2	818	C
1	C2	820	U
1	C2	821	U
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	846	G
1	C2	850	A
1	C2	853	G
1	C2	854	U
1	C2	855	A
1	C2	863	A
1	C2	876	G
1	C2	881	A
1	C2	886	U
1	C2	898	A
1	C2	913	G
1	C2	914	G
1	C2	929	A
1	C2	933	A
1	C2	934	C
1	C2	935	U
1	C2	942	G
1	C2	945	U
1	C2	959	U
1	C2	960	U
1	C2	966	A
1	C2	969	C
1	C2	970	A
1	C2	988	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C2	992	A
1	C2	998	A
1	C2	999	U
1	C2	1000	C
1	C2	1001	A
1	C2	1002	G
1	C2	1003	A
1	C2	1006	C
1	C2	1007	C
1	C2	1021	C
1	C2	1026	A
1	C2	1028	C
1	C2	1029	U
1	C2	1031	U
1	C2	1039	A
1	C2	1040	G
1	C2	1052	U
1	C2	1053	G
1	C2	1056	U
1	C2	1058	U
1	C2	1059	U
1	C2	1060	U
1	C2	1061	A
1	C2	1076	A
1	C2	1081	A
1	C2	1082	C
1	C2	1092	A
1	C2	1096	C
1	C2	1097	U
1	C2	1098	U
1	C2	1100	G
1	C2	1104	U
1	C2	1113	A
1	C2	1126	G
1	C2	1138	A
1	C2	1146	G
1	C2	1148	C
1	C2	1149	G
1	C2	1150	G
1	C2	1151	A
1	C2	1155	G
1	C2	1156	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C2	1626	U
1	C2	1630	U
1	C2	1636	C
1	C2	1637	C
1	C2	1638	G
1	C2	1639	C
1	C2	1640	C
1	C2	1641	C
1	C2	1642	G
1	C2	1648	A
1	C2	1649	G
1	C2	1651	A
1	C2	1652	C
1	C2	1653	C
1	C2	1654	G
1	C2	1655	A
1	C2	1656	U
1	C2	1658	G
1	C2	1670	G
1	C2	1680	G
1	C2	1681	A
1	C2	1683	C
1	C2	1687	U
1	C2	1701	A
1	C2	1702	A
1	C2	1703	C
1	C2	1707	A
1	C2	1717	G
1	C2	1727	G
1	C2	1736	G
1	C2	1738	U
1	C2	1739	C
1	C2	1740	A
1	C2	1741	U
1	C2	1743	U
1	C2	1744	A
1	C2	1745	G
1	C2	1748	G
1	C2	1749	A
1	C2	1750	A
1	C2	1751	C
1	C2	1753	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C2	1754	A
1	C2	1755	A
1	C2	1757	G
1	C2	1758	U
1	C2	1759	C
1	C2	1760	G
1	C2	1761	U
1	C2	1763	A
1	C2	1764	C
1	C2	1766	A
1	C2	1769	U
1	C2	1770	U
1	C2	1772	C
1	C2	1779	U
1	C2	1782	A
1	C2	1783	C
1	C2	1792	G
1	C2	1793	G
1	C2	1795	U

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C2	25	C
1	C2	103	A
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
1	C2	1652	C

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

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

5.5 Carbohydrates (i)

There are no 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.

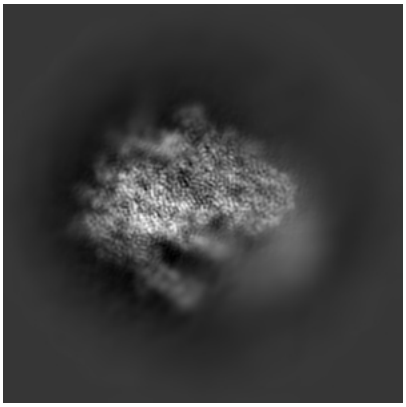
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32795. These allow visual inspection of the internal detail of the map and identification of artifacts.

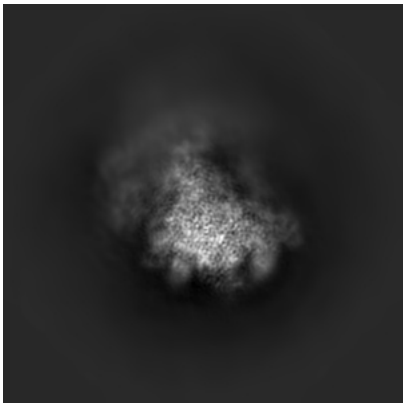
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

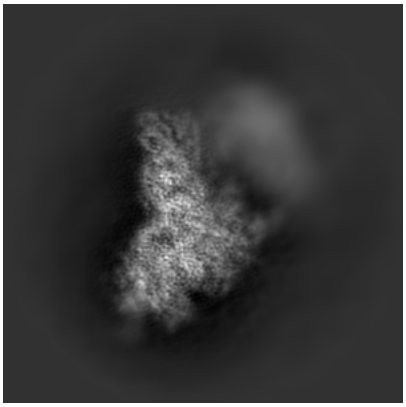
6.1.1 Primary map



X



Y

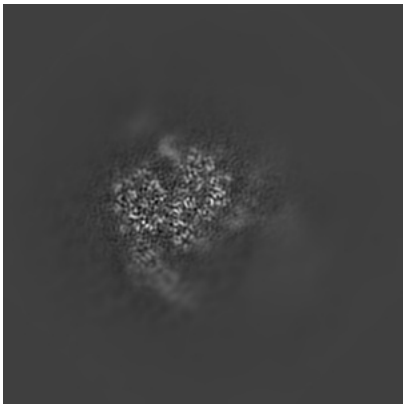


Z

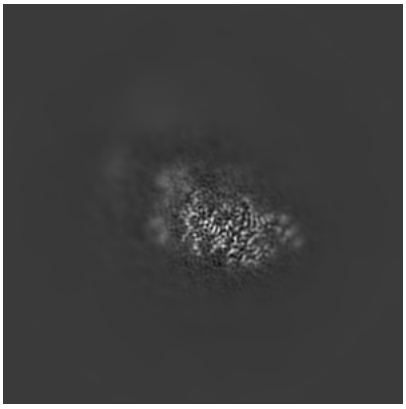
The images above show the map projected in three orthogonal directions.

6.2 Central slices

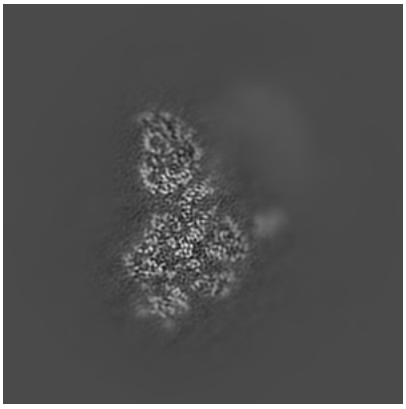
6.2.1 Primary map



X Index: 180



Y Index: 180

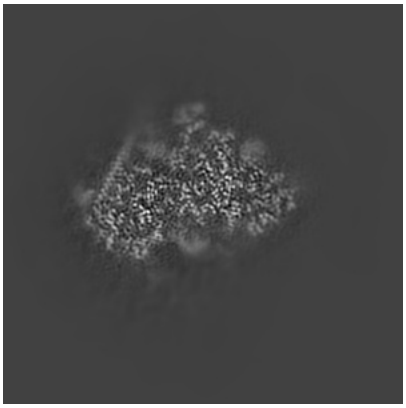


Z Index: 180

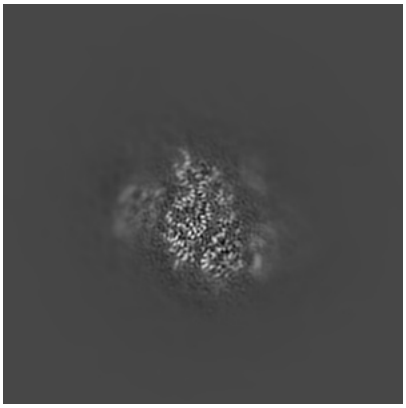
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

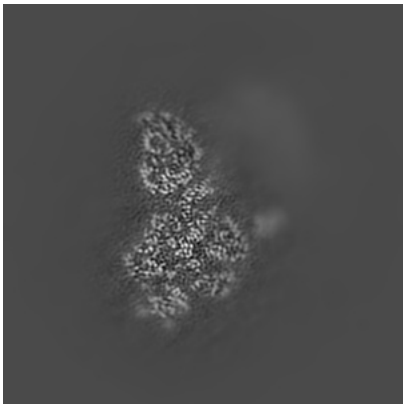
6.3.1 Primary map



X Index: 147



Y Index: 137

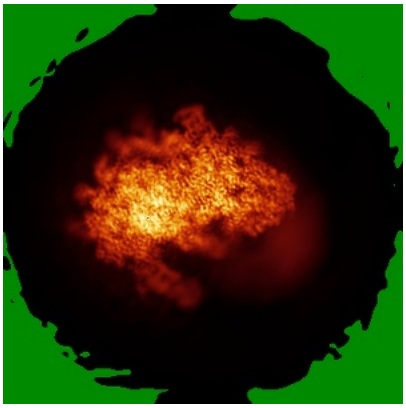


Z Index: 180

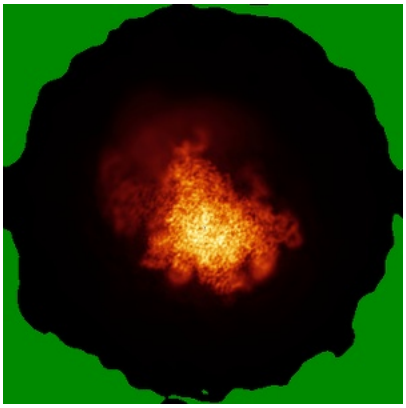
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

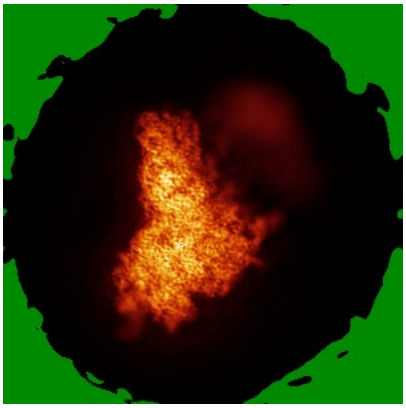
6.4.1 Primary map



X



Y

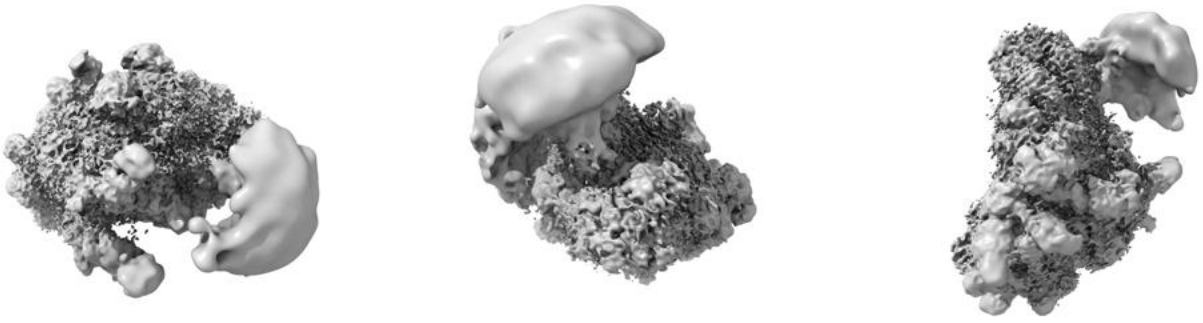


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

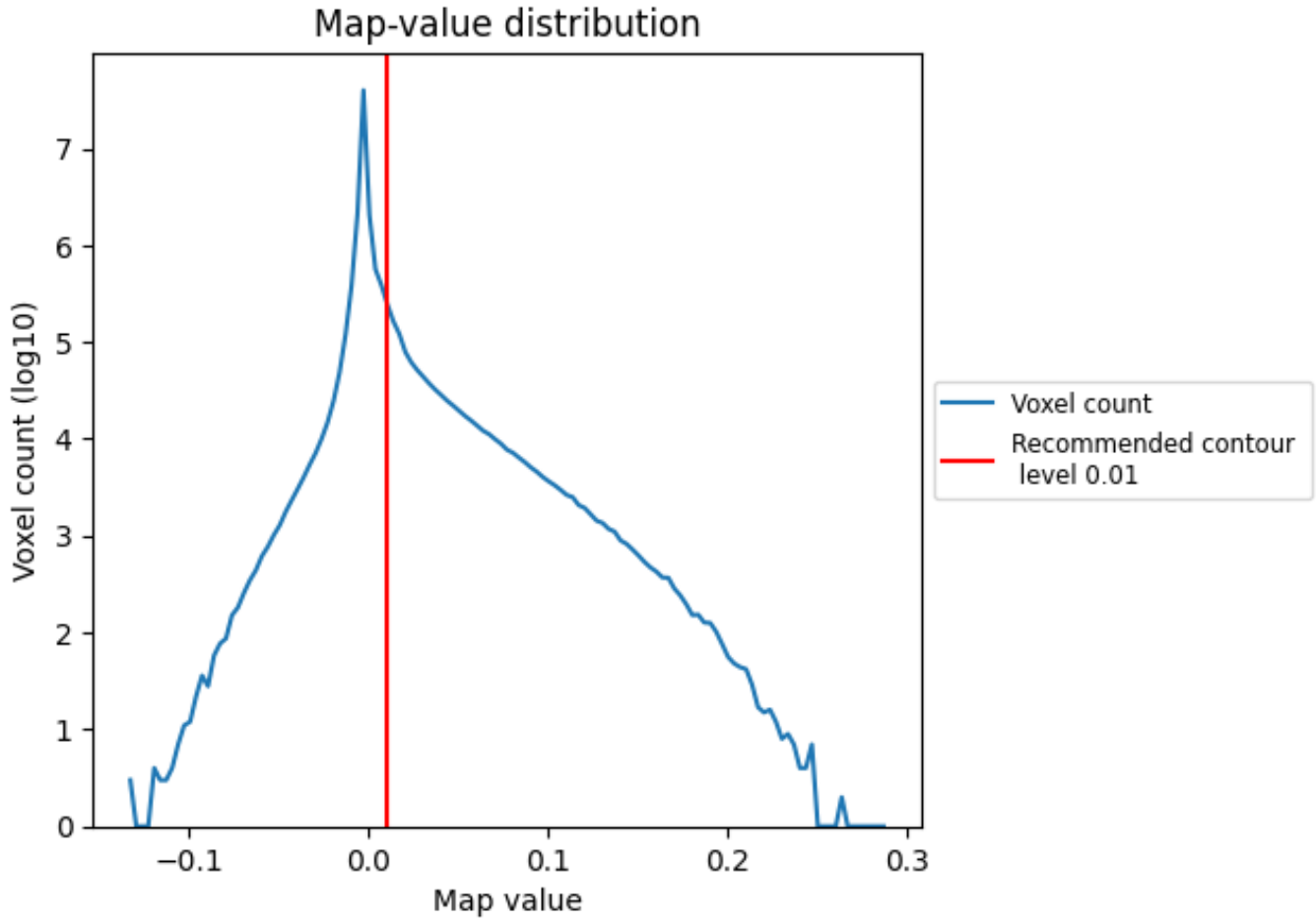
6.6 Mask visualisation (i)

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

7 Map analysis

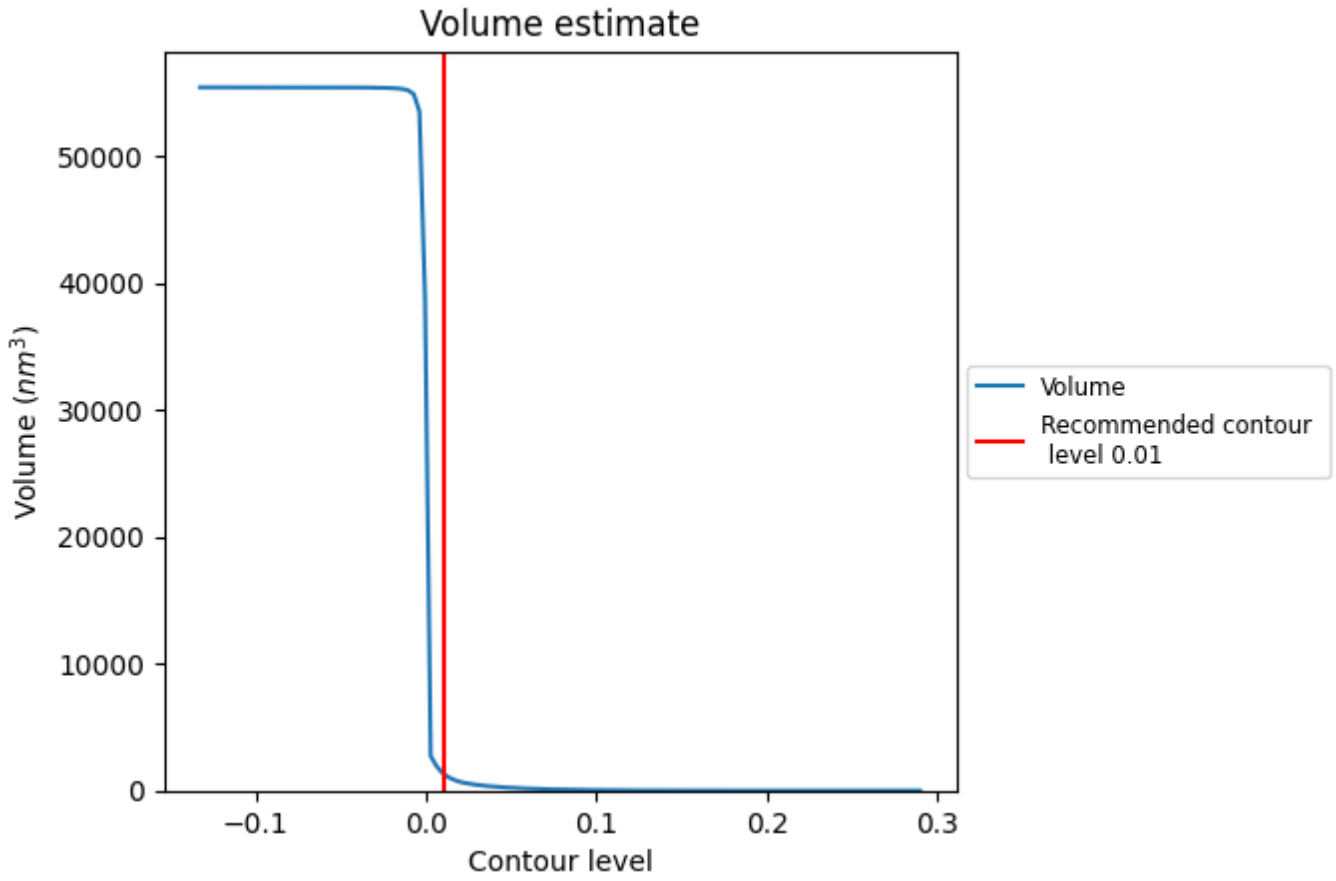
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

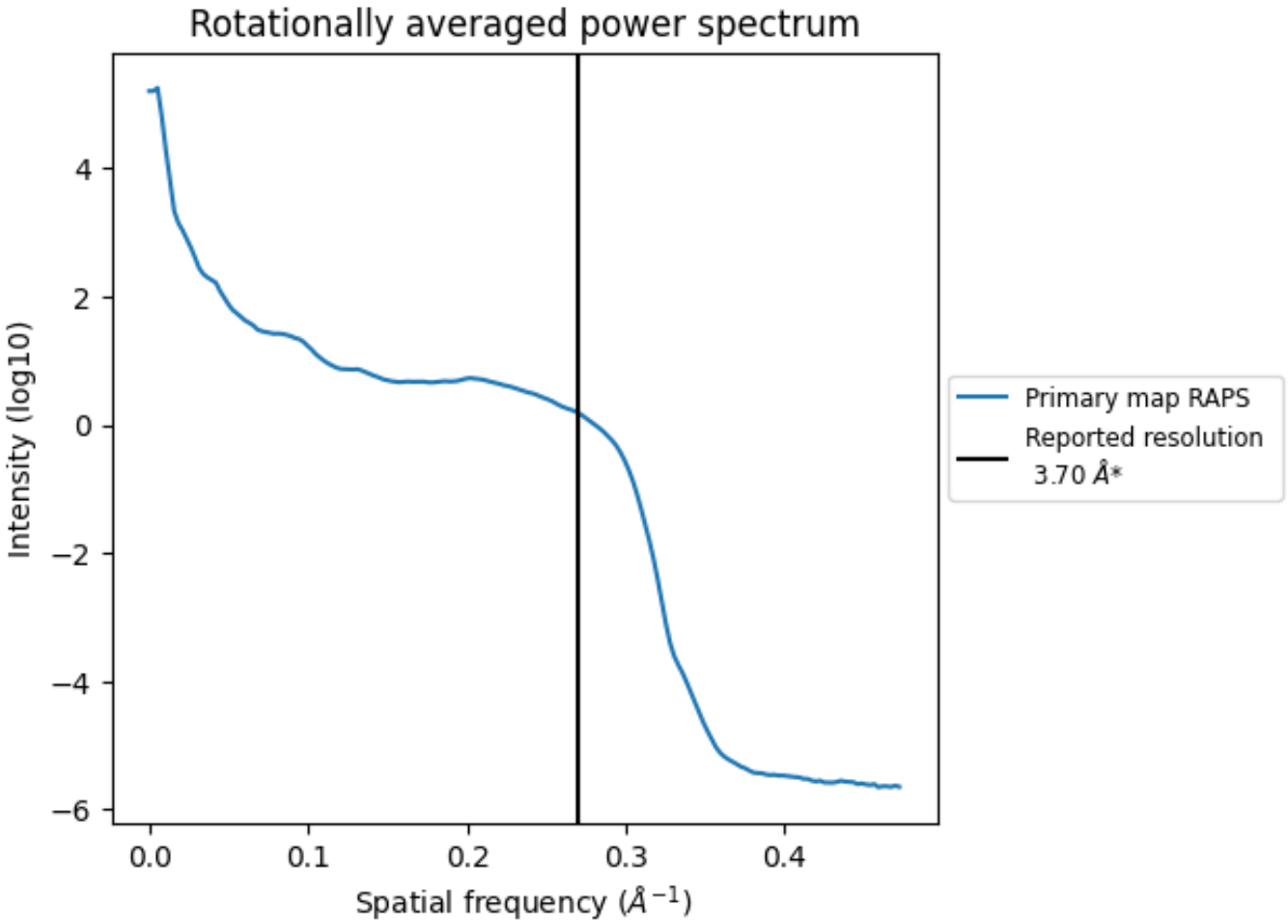
7.2 Volume estimate



The volume at the recommended contour level is 1347 nm^3; this corresponds to an approximate mass of 1217 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)

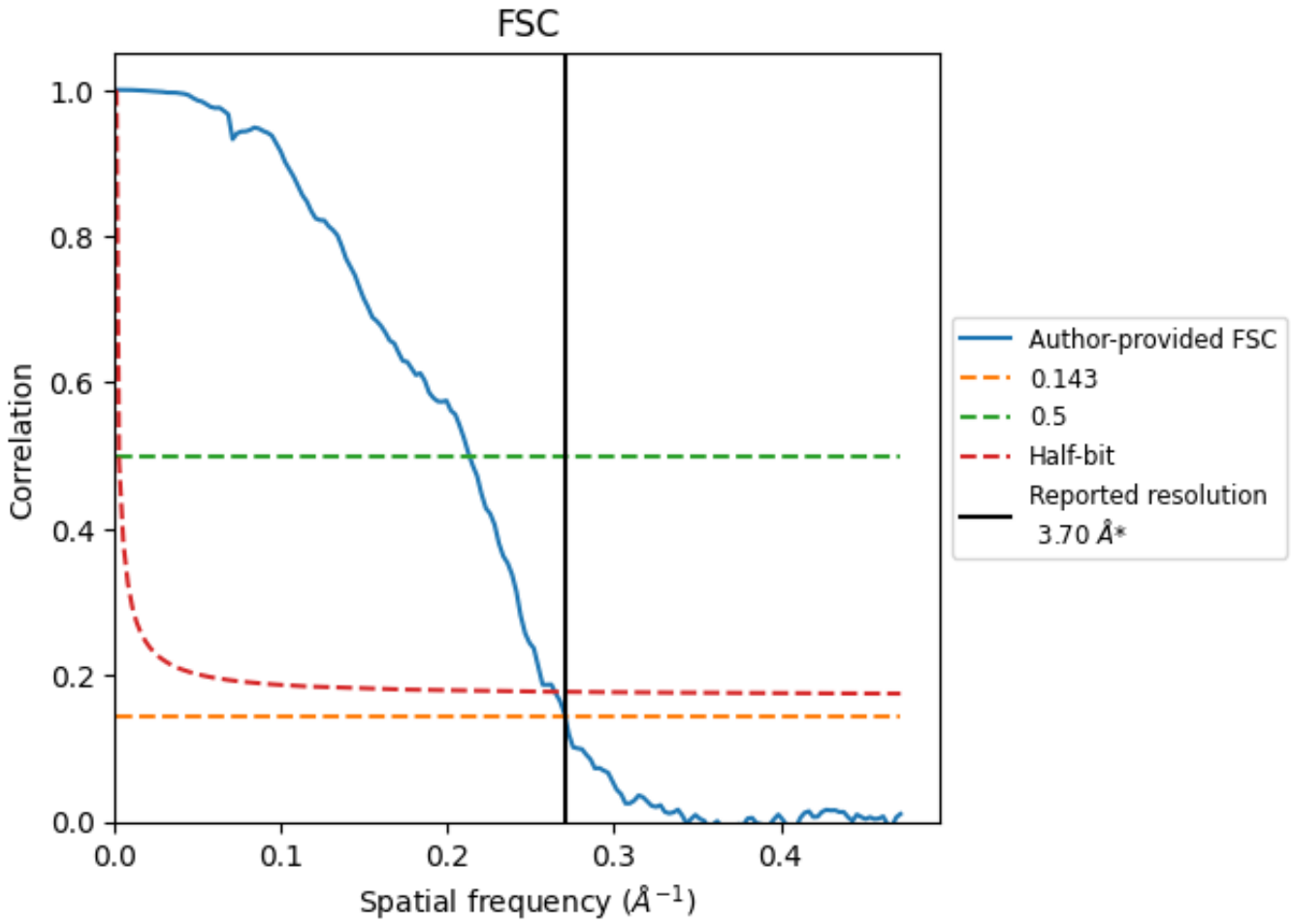


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

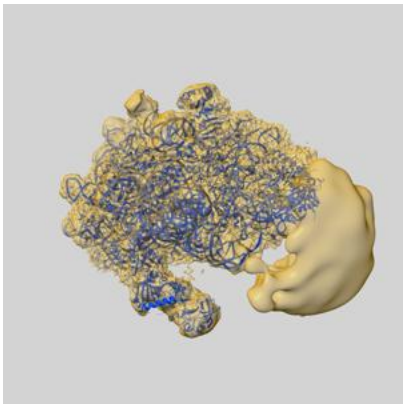
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.69	3.78
Unmasked-calculated*	-	-	-

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

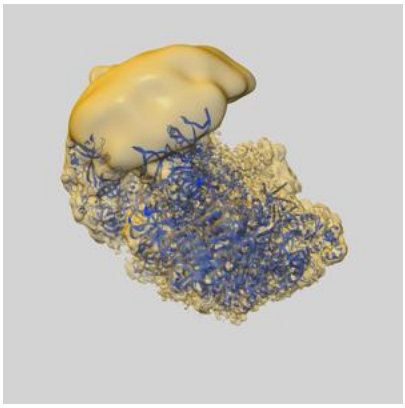
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32795 and PDB model 7WTQ. Per-residue inclusion information can be found in section 3 on page 7.

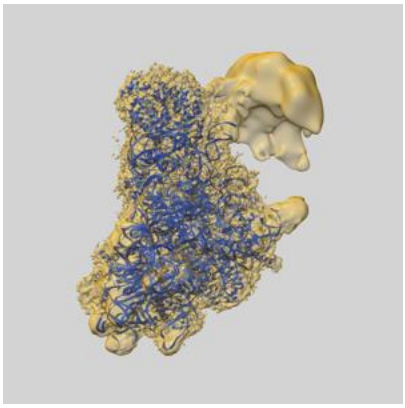
9.1 Map-model overlay



X



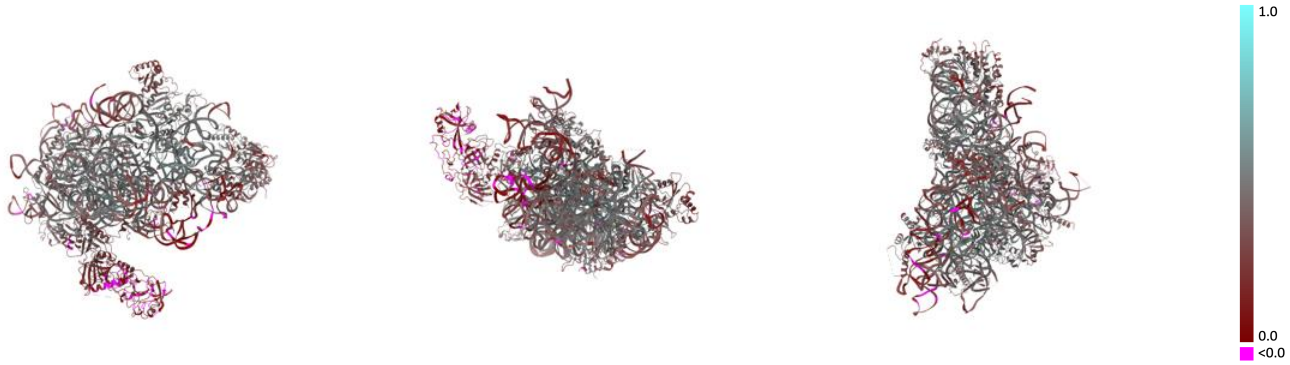
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

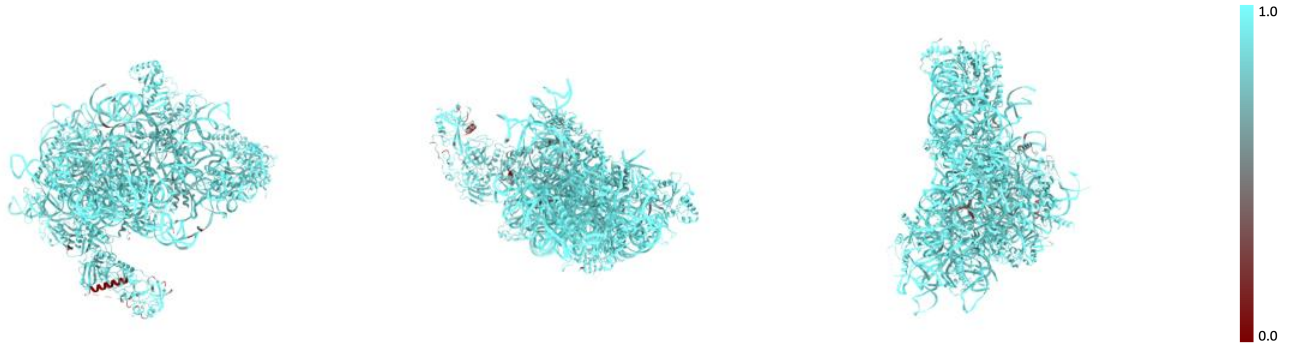
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

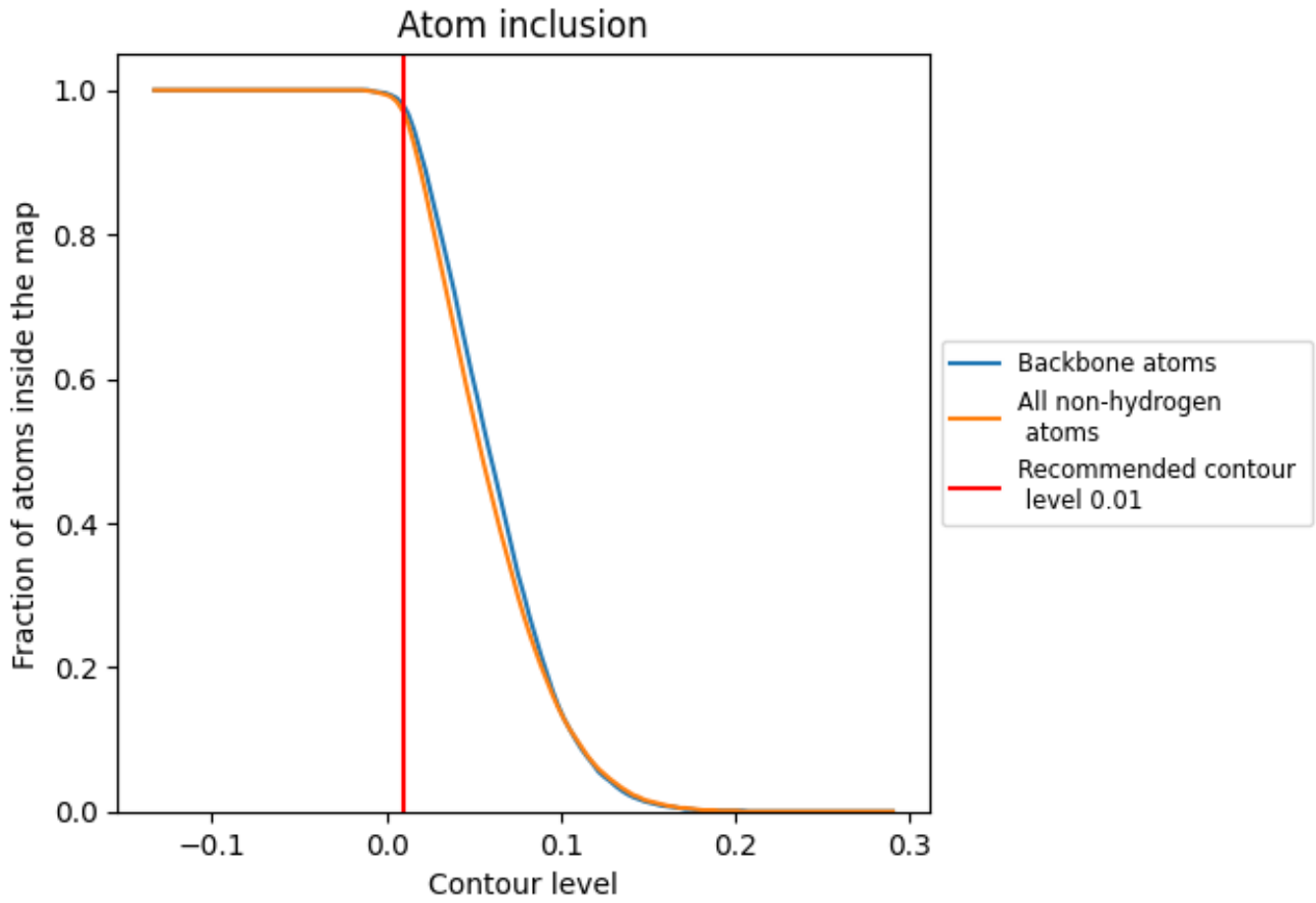
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9690	0.3820
C2	0.9830	0.3920
CA	0.9600	0.3670
CB	0.8040	0.2660
CC	0.8760	0.1900
SB	0.9680	0.4140
SE	0.9860	0.4800
SG	0.9890	0.4060
SH	0.9750	0.3300
SI	0.9850	0.4480
SJ	0.9860	0.4250
SL	0.9770	0.4880
SN	0.9900	0.4610
SO	0.9540	0.4060
SW	0.9860	0.4720
SX	0.9580	0.4330
SY	0.9840	0.4300
Sb	0.9800	0.4330
Se	0.9230	0.3280