



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 9GUU / pdb_00009guu
EMDB ID : EMD-51620
Title : 30S mRNA delivery complex (consensus)
Authors : Rahil, H.; Weixlbaumer, A.; Webster, M.W.
Deposited on : 2024-09-20
Resolution : 2.50 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:

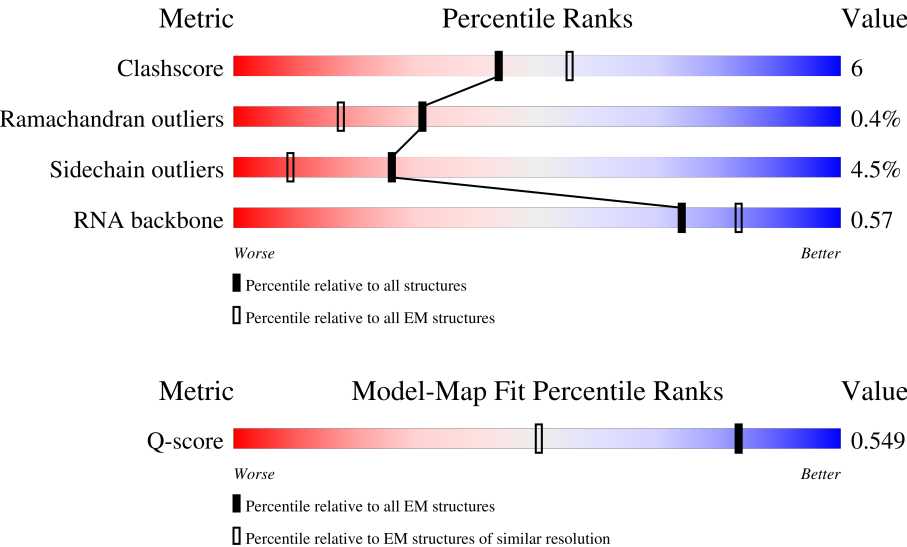
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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.



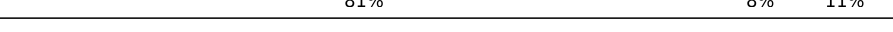
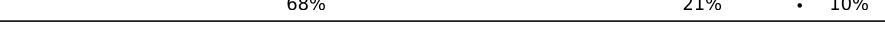
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	A	1541	
2	B	557	
3	C	241	

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Mol	Chain	Length	Quality of chain
4	D	233	 78%12%9%
5	E	206	 89%10%
6	F	156	 83%16%
7	G	131	 63%16%21%
8	H	156	 85%13%..
9	I	130	 84%14%..
10	J	130	 78%18%..
11	K	103	 76%22%.
12	L	129	 73%18%9%
13	M	124	 79%17%..
14	N	118	 80%17%..
15	O	101	 36%48%14%..
16	P	89	 96%...
17	Q	82	 91%9%
18	R	84	 82%13%5%
19	S	75	 81%8%11%
20	T	92	 68%21%10%
21	U	87	 87%11%.
22	V	71	 87%10%..
23	W	77	 5%47%47%6%
24	X	53	 17%9%6%68%

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 55336 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1539	Total	C	N	O	P	0	0
			33023	14736	6046	10702	1539		

- Molecule 2 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1089	668	193	227	1		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

- Molecule 4 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 7 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 9 is a protein called 30S ribosomal protein S8.

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

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

- Molecule 11 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			808	504	155	148	1		

- Molecule 12 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 14 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 15 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 17 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 18 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 19 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	67	Total	C	N	O	S	0	0
			554	350	104	99	1		

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 21 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 22 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	17	Total	C	N	O	P	0	0
			365	163	65	120	17		

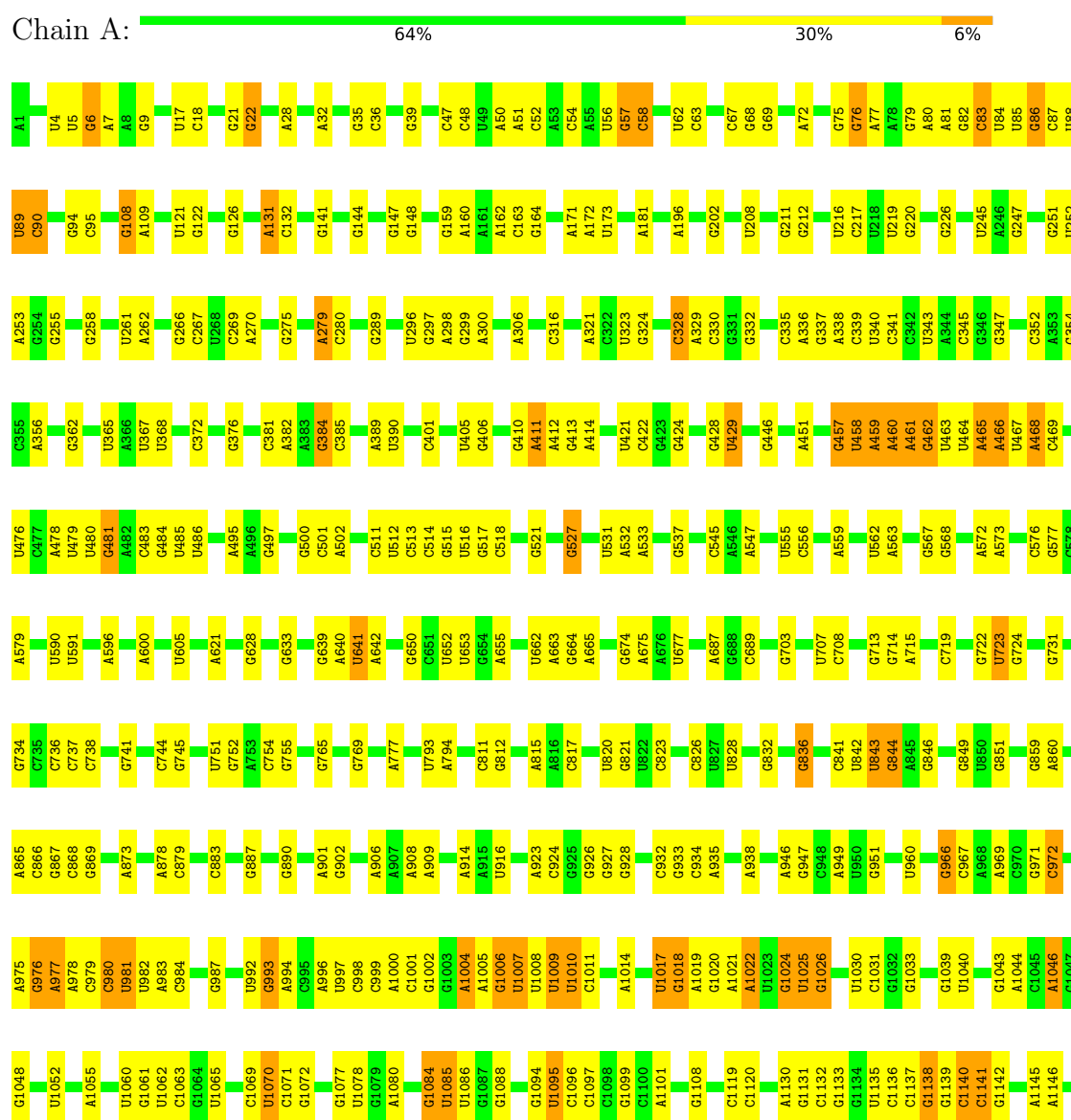
- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

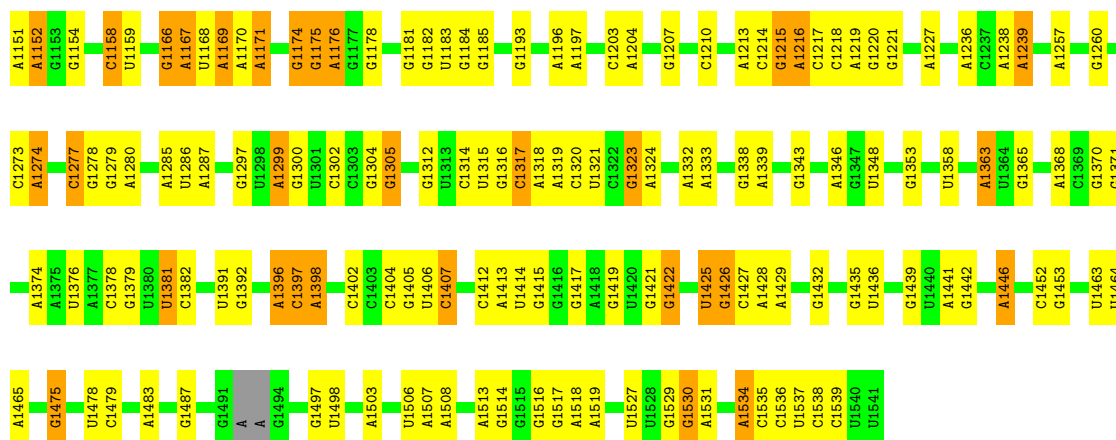
Mol	Chain	Residues	Atoms		AltConf
25	A	120	Total	Mg	0
			120	120	

3 Residue-property plots

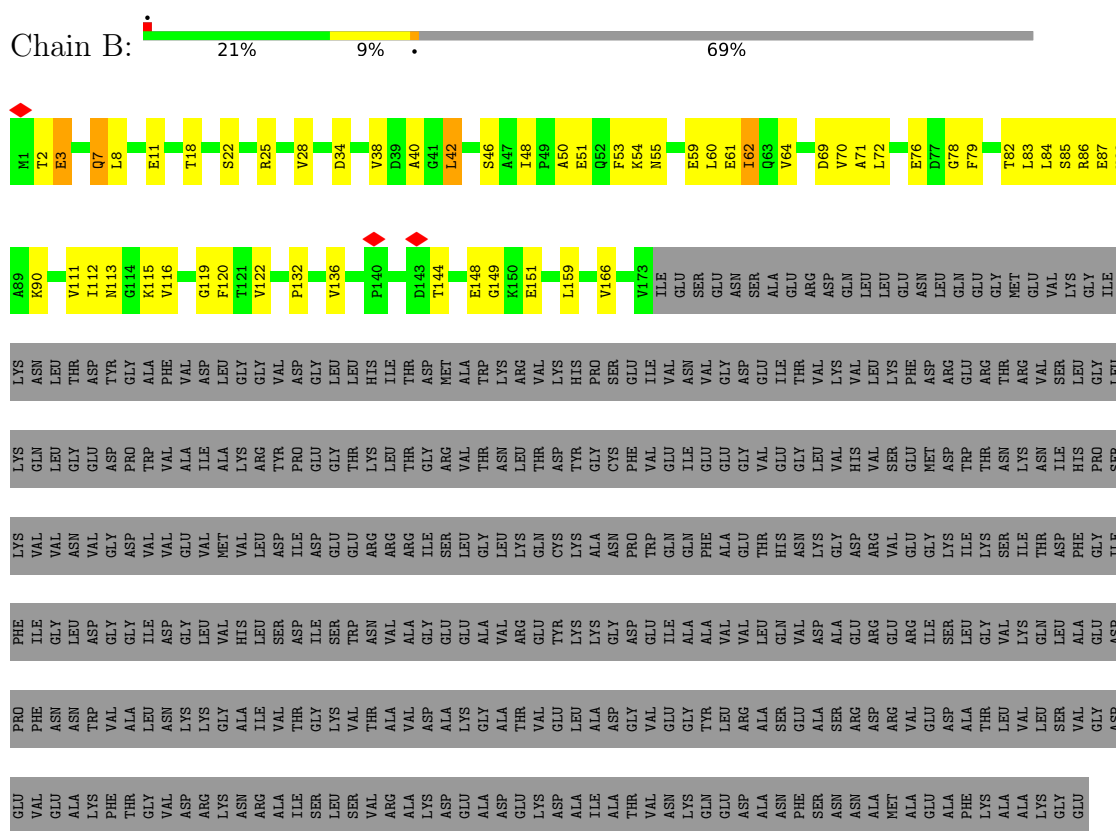
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

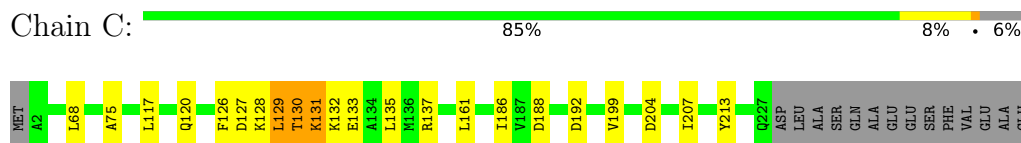




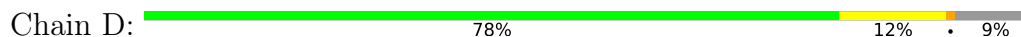
• Molecule 2: 30S ribosomal protein S1

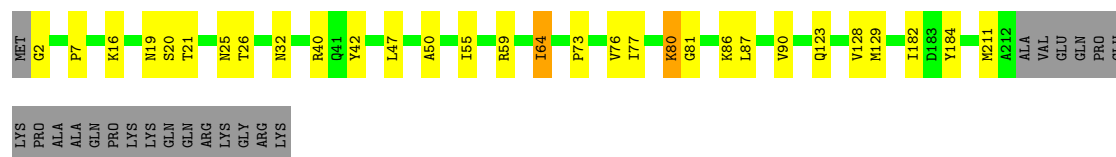


• Molecule 3: 30S ribosomal protein S2



• Molecule 4: Small ribosomal subunit protein uS3





- Molecule 5: Small ribosomal subunit protein uS4

Chain E: 89% 10%



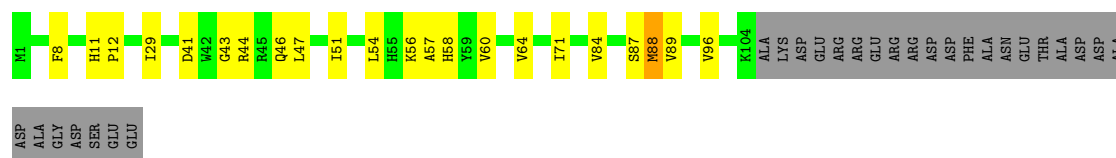
- Molecule 6: 30S ribosomal protein S5

Chain F: 83% 16%



- Molecule 7: Small ribosomal subunit protein bS6

Chain G: 63% 16% 21%



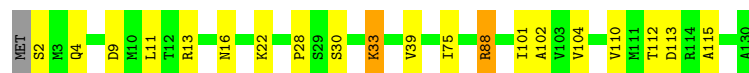
- Molecule 8: 30S ribosomal protein S7

Chain H: 85% 13%



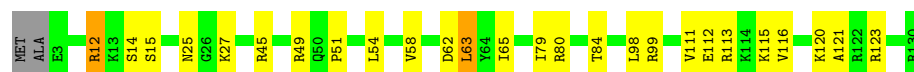
- Molecule 9: 30S ribosomal protein S8

Chain I: 84% 14%



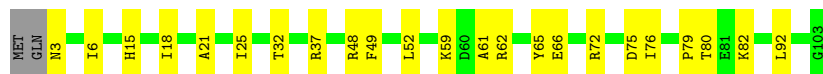
- Molecule 10: 30S ribosomal protein S9

Chain J: 78% 18%



- Molecule 11: 30S ribosomal protein S10

Chain K:  76% 22%



- Molecule 12: 30S ribosomal protein S11

Chain L:  73% 18% 9%



- Molecule 13: 30S ribosomal protein S12

Chain M:  79% 17%

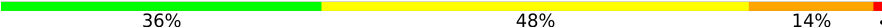


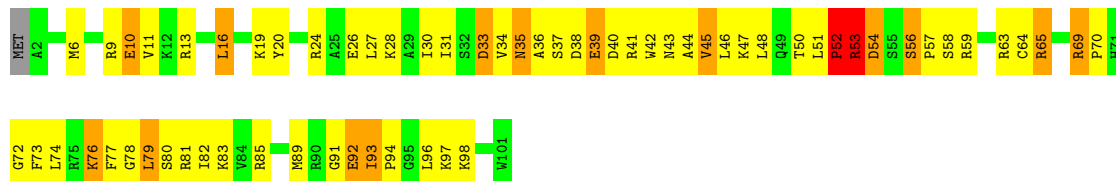
- Molecule 14: 30S ribosomal protein S13

Chain N:  80% 17%



- Molecule 15: 30S ribosomal protein S14

Chain O:  36% 48% 14%



- Molecule 16: Small ribosomal subunit protein uS15

Chain P:  96%



- Molecule 17: 30S ribosomal protein S16

Chain Q:  91% 9%



- Molecule 18: 30S ribosomal protein S17

Chain R: 82% 13% 5%



- Molecule 19: 30S ribosomal protein S18

Chain S: 81% 8% 11%



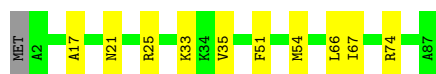
- Molecule 20: 30S ribosomal protein S19

Chain T: 68% 21% 10%



- Molecule 21: 30S ribosomal protein S20

Chain U: 87% 11% 2%



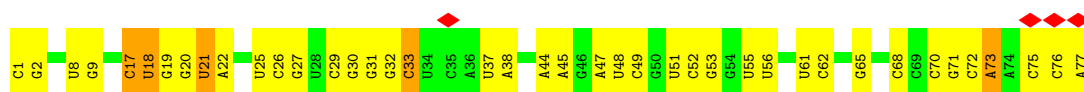
- Molecule 22: 30S ribosomal protein S21

Chain V: 87% 10% 3%



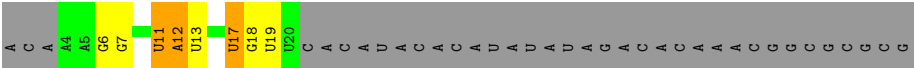
- Molecule 23: tRNA(fmet) P-site

Chain W: 5% 47% 47% 6%



- Molecule 24: mRNA

Chain X: 17% 9% 6% 68%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	256024	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.95	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	11.756	Depositor
Minimum map value	-6.593	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.175	Depositor
Recommended contour level	0.248	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, UR3, MG, MA6, 4SU, OMC, PSU, 5MC, H2U, D2T, 2MG, 4OC, G7M

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	A	0.18	3/36692 (0.0%)	0.31	4/57230 (0.0%)
2	B	0.09	0/1094	0.30	0/1491
3	C	0.10	0/1796	0.27	0/2420
4	D	0.10	0/1680	0.29	0/2263
5	E	0.12	0/1665	0.27	0/2227
6	F	0.13	0/1165	0.31	0/1568
7	G	0.13	0/867	0.35	0/1171
8	H	0.09	0/1219	0.29	0/1635
9	I	0.11	0/989	0.24	0/1326
10	J	0.12	0/1043	0.36	0/1387
11	K	0.19	0/818	0.39	0/1105
12	L	0.09	0/893	0.27	0/1205
13	M	0.29	0/954	0.44	2/1279 (0.2%)
14	N	0.09	0/900	0.28	0/1204
15	O	0.87	5/817 (0.6%)	1.23	11/1088 (1.0%)
16	P	0.09	0/722	0.25	0/964
17	Q	0.09	0/659	0.25	0/884
18	R	0.09	0/657	0.27	0/881
19	S	0.10	0/563	0.28	0/754
20	T	0.37	0/680	0.63	1/915 (0.1%)
21	U	0.08	0/676	0.20	0/895
22	V	0.09	0/598	0.23	0/792
23	W	0.15	0/1725	0.25	0/2687
24	X	0.12	0/408	0.30	0/634
All	All	0.19	8/59280 (0.0%)	0.34	18/88005 (0.0%)

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
10	J	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	980	C	O3'-P	-8.68	1.48	1.61
1	A	562	U	O3'-P	-7.57	1.49	1.61
15	O	52	PRO	N-CA	5.96	1.54	1.47
15	O	57	PRO	N-CA	5.80	1.55	1.47
15	O	53	ARG	N-CA	5.59	1.53	1.46
15	O	93	ILE	C-O	-5.57	1.17	1.24
15	O	69	ARG	C-N	5.56	1.40	1.34
1	A	527	G7M	O3'-P	5.43	1.61	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	51	LEU	O-C-N	-8.69	111.75	121.66
1	A	1274	A	C2'-C3'-O3'	-8.55	100.87	113.70
15	O	56	SER	CA-C-N	8.03	127.96	119.05
15	O	56	SER	C-N-CA	8.03	127.96	119.05
1	A	563	A	C1'-C2'-O2'	-6.91	98.03	108.40
15	O	69	ARG	CA-C-N	6.75	127.33	120.04
15	O	69	ARG	C-N-CA	6.75	127.33	120.04
13	M	44	LYS	CA-C-N	6.71	126.85	119.87
13	M	44	LYS	C-N-CA	6.71	126.85	119.87
20	T	12	ASP	N-CA-C	6.17	119.41	110.28
15	O	52	PRO	N-CA-C	5.72	124.26	112.47
15	O	54	ASP	CB-CA-C	5.71	121.35	110.27
15	O	54	ASP	N-CA-C	-5.62	106.51	113.19
15	O	52	PRO	CA-C-O	-5.57	110.47	120.60
15	O	93	ILE	CA-C-N	5.56	126.80	119.84
15	O	93	ILE	C-N-CA	5.56	126.80	119.84
1	A	1084	G	C4'-C3'-O3'	-5.30	105.05	113.00
1	A	563	A	C3'-C2'-O2'	5.04	118.27	110.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	12	ARG	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	A	33023	0	16641	329	0
2	B	1089	0	867	32	0
3	C	1765	0	1792	9	0
4	D	1653	0	1727	17	0
5	E	1643	0	1707	13	0
6	F	1152	0	1196	12	0
7	G	848	0	846	11	0
8	H	1203	0	1254	14	0
9	I	979	0	1031	11	0
10	J	1031	0	1076	17	0
11	K	808	0	845	17	0
12	L	877	0	887	16	0
13	M	951	0	1012	12	0
14	N	891	0	952	12	0
15	O	805	0	844	57	0
16	P	714	0	734	3	0
17	Q	649	0	666	4	0
18	R	648	0	691	6	0
19	S	554	0	573	5	0
20	T	663	0	688	17	0
21	U	670	0	719	6	0
22	V	590	0	629	5	0
23	W	1645	0	842	16	0
24	X	365	0	182	5	0
25	A	120	0	0	0	0
All	All	55336	0	38401	579	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 (579) 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:A:458:U:C6	1:A:458:U:H5''	1.91	1.04
1:A:458:U:H5''	1:A:458:U:H6	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:G:C8	1:A:462:G:H5''	2.06	0.90
1:A:1018:G:H8	1:A:1018:G:H5''	1.36	0.87
1:A:466:A:H2'	1:A:468:A:C2	2.15	0.82
1:A:464:U:H6	1:A:464:U:O5'	1.65	0.78
1:A:1381:U:C2	1:A:1382:C:C5	2.72	0.77
1:A:1138:G:H3'	1:A:1138:G:N3	2.00	0.76
1:A:466:A:O5'	1:A:466:A:H8	1.68	0.76
2:B:76:GLU:HG2	2:B:78:GLY:H	1.51	0.75
2:B:86:ARG:HH21	2:B:90:LYS:HE3	1.52	0.75
1:A:1381:U:C2	1:A:1382:C:C6	2.75	0.74
1:A:993:G:O2'	1:A:994:A:N7	2.20	0.73
1:A:500:G:H5''	13:M:121:ARG:HH12	1.54	0.73
1:A:823:C:HO2'	9:I:2:SER:N	1.86	0.73
1:A:1305:G:H21	1:A:1332:A:H2	1.32	0.73
1:A:1218:C:H2'	1:A:1219:A:C8	2.24	0.73
1:A:462:G:C8	1:A:462:G:C5'	2.72	0.73
20:T:11:ILE:HG13	20:T:38:SER:HB2	1.70	0.73
1:A:462:G:H4'	1:A:462:G:OP1	1.89	0.72
1:A:1007:U:O4	1:A:1022:A:N1	2.23	0.71
1:A:1158:C:H42	1:A:1181:G:H1	1.36	0.71
1:A:1381:U:H2'	1:A:1382:C:H6	1.55	0.71
1:A:1018:G:H5''	1:A:1018:G:C8	2.23	0.71
20:T:50:ALA:HB1	20:T:57:HIS:HB3	1.71	0.71
1:A:6:G:H3'	1:A:6:G:N3	2.07	0.70
1:A:216:U:H4'	1:A:464:U:H4'	1.74	0.69
1:A:1422:G:H1	1:A:1478:U:H3	1.40	0.69
10:J:84:THR:HG23	10:J:98:LEU:HD13	1.74	0.69
1:A:1006:G:C6	1:A:1007:U:C4	2.80	0.69
8:H:27:VAL:HG22	8:H:43:VAL:HG11	1.75	0.69
1:A:568:G:N2	1:A:883:C:O2	2.26	0.69
1:A:1397:C:OP1	6:F:29:ARG:NH1	2.26	0.69
8:H:5:ARG:NH1	8:H:7:ILE:O	2.25	0.69
1:A:1279:G:N3	1:A:1279:G:H3'	2.08	0.68
12:L:88:GLY:H	12:L:114:THR:HG22	1.59	0.68
5:E:100:ASN:OD1	5:E:111:ARG:NH1	2.24	0.67
15:O:36:ALA:HB3	15:O:41:ARG:NH1	2.10	0.67
21:U:17:ALA:O	21:U:21:ASN:ND2	2.27	0.67
23:W:51:U:H3	23:W:65:G:H1	1.42	0.67
1:A:458:U:C6	1:A:458:U:C5'	2.76	0.67
1:A:1527:U:H5	22:V:42:THR:HG21	1.59	0.67
1:A:600:A:OP2	9:I:88:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:A:N7	14:N:105:ASN:ND2	2.43	0.66
1:A:1215:G:H2'	1:A:1216:A:H5'	1.76	0.66
15:O:33:ASP:OD2	15:O:35:ASN:N	2.29	0.66
1:A:1077:G:N2	1:A:1080:A:OP2	2.25	0.65
9:I:28:PRO:O	9:I:33:LYS:NZ	2.29	0.65
1:A:983:A:OP1	15:O:6:MET:HE1	1.97	0.65
15:O:10:GLU:OE1	15:O:13:ARG:HD2	1.96	0.65
15:O:72:GLY:O	15:O:80:SER:HA	1.98	0.64
1:A:1317:C:N3	20:T:37:ARG:NH1	2.42	0.64
18:R:79:VAL:HG22	18:R:80:GLU:HG3	1.78	0.64
15:O:33:ASP:O	15:O:41:ARG:NH1	2.31	0.64
1:A:1006:G:C6	1:A:1007:U:C5	2.86	0.64
15:O:92:GLU:O	15:O:94:PRO:HD3	1.97	0.64
1:A:1316:G:N1	1:A:1319:A:OP2	2.29	0.63
2:B:25:ARG:H	2:B:25:ARG:HE	1.44	0.63
2:B:111:VAL:HA	2:B:151:GLU:HA	1.81	0.63
15:O:24:ARG:NH2	15:O:56:SER:HB2	2.13	0.63
1:A:1158:C:N4	1:A:1181:G:H1	1.96	0.63
1:A:1381:U:N3	1:A:1382:C:C5	2.67	0.63
1:A:1018:G:C8	1:A:1018:G:C5'	2.82	0.62
2:B:42:LEU:HB2	2:B:82:THR:HG21	1.81	0.62
1:A:976:G:H5''	1:A:1358:U:O2'	2.00	0.62
1:A:56:U:H2'	1:A:57:G:C8	2.34	0.62
6:F:80:THR:HA	6:F:120:VAL:HG13	1.82	0.62
6:F:88:VAL:HG23	6:F:93:ARG:HG2	1.81	0.61
1:A:765:G:H1	1:A:812:G:HO2'	1.47	0.61
1:A:859:G:H2'	1:A:860:A:C8	2.36	0.61
15:O:77:PHE:C	15:O:79:LEU:N	2.56	0.61
2:B:48:ILE:HB	2:B:53:PHE:HE1	1.65	0.61
12:L:46:THR:HG23	12:L:49:GLY:H	1.66	0.61
1:A:1006:G:N1	1:A:1007:U:C4	2.69	0.61
2:B:25:ARG:HA	2:B:69:ASP:HA	1.81	0.61
1:A:1277:C:O2'	1:A:1279:G:H8	1.83	0.60
15:O:65:ARG:HG3	15:O:65:ARG:HH11	1.65	0.60
20:T:3:ARG:HH21	20:T:7:LYS:HB3	1.66	0.60
1:A:1215:G:C6	1:A:1216:A:N7	2.70	0.60
15:O:39:GLU:O	15:O:43:ASN:OD1	2.20	0.60
2:B:112:ILE:HA	2:B:122:VAL:HA	1.84	0.60
15:O:65:ARG:HG3	15:O:65:ARG:NH1	2.17	0.60
1:A:261:U:OP2	21:U:74:ARG:NH1	2.31	0.60
8:H:113:ASP:HB3	8:H:119:ARG:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:9:ASP:OD1	9:I:13:ARG:NH1	2.35	0.59
9:I:11:LEU:HD22	9:I:75:ILE:HD11	1.83	0.59
1:A:1317:C:C5'	15:O:24:ARG:HH22	2.16	0.59
1:A:1018:G:H8	1:A:1018:G:C5'	2.11	0.59
2:B:144:THR:O	2:B:148:GLU:N	2.35	0.59
1:A:83:C:O2'	1:A:85:U:O2	2.20	0.59
7:G:12:PRO:O	7:G:44:ARG:NH2	2.36	0.59
1:A:677:U:H3	1:A:713:G:H22	1.51	0.59
12:L:87:LYS:HB2	12:L:113:VAL:HG23	1.85	0.59
6:F:38:VAL:HG11	6:F:114:VAL:HG22	1.84	0.58
1:A:890:G:O2'	1:A:906:A:N6	2.36	0.58
7:G:11:HIS:HD2	7:G:12:PRO:HD2	1.69	0.58
16:P:18:ASP:OD1	16:P:18:ASP:N	2.37	0.58
20:T:9:PRO:HB3	20:T:39:THR:HG21	1.86	0.58
1:A:1404:C:H2'	1:A:1405:G:C8	2.39	0.57
13:M:46:ASN:OD1	13:M:46:ASN:N	2.36	0.57
1:A:1006:G:C5	1:A:1007:U:C5	2.92	0.57
7:G:47:LEU:HD21	7:G:57:ALA:HB3	1.85	0.57
1:A:1239:A:H62	1:A:1299:A:H62	1.53	0.57
1:A:859:G:H2'	1:A:860:A:H8	1.70	0.57
15:O:42:TRP:CE2	15:O:46:LEU:HD11	2.40	0.57
8:H:5:ARG:HD2	8:H:7:ILE:H	1.70	0.56
15:O:38:ASP:N	15:O:38:ASP:OD1	2.38	0.56
1:A:977:A:O2'	1:A:980:C:N4	2.38	0.56
1:A:1014:A:C2	1:A:1219:A:H1'	2.40	0.56
1:A:279:A:H5''	1:A:280:C:H3'	1.88	0.56
1:A:466:A:O5'	1:A:466:A:C8	2.55	0.56
1:A:1025:U:H4'	1:A:1026:G:H5'	1.87	0.56
14:N:89:LEU:HD23	14:N:92:ARG:HE	1.70	0.56
1:A:83:C:O2'	1:A:85:U:C2	2.57	0.55
1:A:275:G:H5'	18:R:16:LYS:HD2	1.88	0.55
15:O:42:TRP:O	15:O:46:LEU:HG	2.06	0.55
9:I:30:SER:HB2	9:I:33:LYS:HG3	1.87	0.55
1:A:979:C:C6	1:A:1318:A:N1	2.75	0.55
4:D:80:LYS:HZ3	4:D:81:GLY:H	1.53	0.55
1:A:1374:A:OP1	8:H:36:LYS:NZ	2.39	0.55
11:K:21:ALA:HB1	11:K:92:LEU:HD23	1.89	0.55
15:O:63:ARG:HG2	15:O:70:PRO:HA	1.89	0.55
1:A:83:C:O2'	1:A:85:U:N3	2.40	0.55
1:A:362:G:N2	1:A:365:U:OP2	2.35	0.55
6:F:99:ALA:HB2	6:F:124:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:120:LYS:HB2	10:J:123:ARG:HB3	1.88	0.55
4:D:47:LEU:HB3	4:D:50:ALA:HB3	1.89	0.55
1:A:83:C:O2'	1:A:86:G:N2	2.40	0.54
1:A:983:A:H5'	1:A:984:C:OP2	2.08	0.54
23:W:17:C:H5''	23:W:18:U:C6	2.42	0.54
1:A:451:A:H61	1:A:481:G:H5'	1.73	0.54
1:A:464:U:H2'	1:A:465:A:H3'	1.90	0.54
1:A:1530:G:H2'	1:A:1531:A:C8	2.42	0.54
18:R:17:MET:HG3	18:R:20:SER:HB2	1.88	0.54
14:N:54:ASP:OD1	14:N:57:ARG:NH1	2.41	0.54
2:B:115:LYS:HA	2:B:120:PHE:HA	1.88	0.54
6:F:89:HIS:CE1	6:F:138:ARG:HD2	2.42	0.54
1:A:736:C:OP1	19:S:61:ARG:NH1	2.40	0.54
1:A:1166:G:O2'	1:A:1167:A:OP1	2.24	0.54
1:A:1239:A:H62	1:A:1299:A:N6	2.05	0.54
4:D:47:LEU:HD21	4:D:87:LEU:HD11	1.90	0.54
7:G:47:LEU:HD13	7:G:51:ILE:HD12	1.90	0.54
23:W:72:C:H2'	23:W:73:A:H5'	1.90	0.54
1:A:17:U:H2'	1:A:18:C:C6	2.43	0.54
1:A:978:A:C6	1:A:1318:A:C6	2.96	0.54
6:F:105:ILE:HD11	6:F:112:ARG:HA	1.88	0.54
15:O:77:PHE:O	15:O:79:LEU:N	2.40	0.54
1:A:979:C:H1'	1:A:1317:C:H41	1.73	0.53
1:A:1007:U:H2'	1:A:1007:U:O2	2.06	0.53
1:A:1412:C:H2'	1:A:1413:A:C8	2.42	0.53
2:B:3:GLU:HB3	2:B:7:GLN:HE21	1.72	0.53
1:A:1088:G:H21	1:A:1167:A:H62	1.56	0.53
5:E:170:TRP:CD2	5:E:186:PRO:HB3	2.43	0.53
15:O:64:CYS:SG	15:O:79:LEU:HD12	2.48	0.53
15:O:73:PHE:C	15:O:73:PHE:CD2	2.86	0.53
1:A:87:C:H2'	1:A:88:U:C6	2.44	0.53
1:A:1007:U:C4	1:A:1022:A:N1	2.77	0.53
1:A:1381:U:O2	1:A:1382:C:C6	2.62	0.53
1:A:1317:C:C5'	15:O:24:ARG:NH2	2.72	0.53
5:E:56:ARG:HH22	5:E:63:ARG:HH21	1.55	0.53
1:A:947:G:P	14:N:107:ARG:HE	2.33	0.52
2:B:159:LEU:HA	2:B:166:VAL:HA	1.91	0.52
12:L:88:GLY:O	12:L:93:ARG:NH1	2.43	0.52
15:O:20:TYR:CE2	15:O:52:PRO:HG2	2.43	0.52
3:C:192:ASP:OD1	3:C:192:ASP:N	2.43	0.52
1:A:1382:C:H2'	1:A:1382:C:O2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:ARG:HE	4:D:64:ILE:HD13	1.74	0.52
24:X:17:U:H2'	24:X:18:G:O4'	2.10	0.52
1:A:299:G:H2'	1:A:300:A:C8	2.45	0.52
1:A:58:C:O5'	1:A:58:C:H6	1.93	0.52
1:A:1215:G:C2'	1:A:1216:A:H5'	2.38	0.52
20:T:9:PRO:CB	20:T:39:THR:HG21	2.39	0.52
2:B:51:GLU:HA	2:B:54:LYS:HD3	1.90	0.52
20:T:36:ARG:NH2	20:T:75:ALA:O	2.41	0.52
2:B:40:ALA:HB3	2:B:42:LEU:HD11	1.92	0.52
23:W:70:C:H2'	23:W:71:G:H8	1.75	0.52
1:A:6:G:H4'	1:A:298:A:H4'	1.92	0.52
1:A:462:G:OP1	1:A:462:G:C4'	2.58	0.52
1:A:1096:C:H2'	1:A:1097:C:H6	1.75	0.52
1:A:1439:G:OP1	21:U:33:LYS:NZ	2.42	0.52
7:G:29:ILE:HD13	7:G:64:VAL:HG11	1.92	0.52
1:A:362:G:OP1	13:M:58:THR:OG1	2.26	0.52
1:A:1507:A:H2'	1:A:1508:A:C8	2.44	0.52
1:A:58:C:C5'	1:A:58:C:C6	2.93	0.51
1:A:457:G:H5''	1:A:457:G:H8	1.75	0.51
1:A:980:C:C5	1:A:981:U:C4	2.98	0.51
1:A:1279:G:N3	1:A:1279:G:C3'	2.73	0.51
14:N:65:VAL:O	14:N:66:GLU:HB2	2.11	0.51
1:A:1215:G:C2	1:A:1216:A:C8	2.98	0.51
11:K:52:LEU:HB2	15:O:81:ARG:HD2	1.92	0.51
15:O:33:ASP:OD1	15:O:36:ALA:HB2	2.10	0.51
1:A:1096:C:H2'	1:A:1097:C:C6	2.45	0.51
5:E:56:ARG:HA	5:E:56:ARG:NE	2.24	0.51
1:A:458:U:H2'	1:A:459:A:C8	2.46	0.51
11:K:65:TYR:OH	15:O:85:ARG:HG3	2.09	0.51
1:A:979:C:OP2	1:A:980:C:H5	1.93	0.51
1:A:1138:G:N3	1:A:1138:G:C3'	2.73	0.51
12:L:111:THR:HG23	22:V:3:VAL:HG22	1.93	0.51
23:W:70:C:H2'	23:W:71:G:C8	2.46	0.51
1:A:997:U:H2'	1:A:998:C:H6	1.75	0.51
8:H:68:ASN:ND2	8:H:130:ASN:OD1	2.43	0.51
1:A:85:U:C2	1:A:86:G:N2	2.79	0.51
17:Q:12:LYS:HG2	17:Q:13:LYS:HG2	1.92	0.51
8:H:106:GLU:OE1	8:H:110:LYS:NZ	2.44	0.51
1:A:713:G:H2'	1:A:714:G:C8	2.46	0.51
1:A:1279:G:N3	1:A:1279:G:C2'	2.74	0.51
17:Q:39:PHE:HD1	17:Q:50:THR:HG22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:64:CYS:SG	18:R:74:THR:OG1	2.59	0.51
1:A:769:G:H4'	1:A:1513:A:H4'	1.93	0.50
1:A:1513:A:H2'	1:A:1514:G:C8	2.46	0.50
13:M:53:CYS:SG	13:M:67:ILE:HD11	2.50	0.50
1:A:328:C:H2'	1:A:328:C:O2	2.10	0.50
1:A:867:G:O2'	1:A:873:A:N1	2.36	0.50
1:A:978:A:C8	1:A:979:C:H5	2.29	0.50
1:A:979:C:H2'	1:A:979:C:O2	2.11	0.50
1:A:1425:U:H3	1:A:1475:G:H1	1.58	0.50
1:A:1005:A:N6	1:A:1024:G:O2'	2.41	0.50
10:J:51:PRO:HD3	10:J:80:ARG:HG3	1.93	0.50
11:K:65:TYR:HB3	15:O:96:LEU:HD11	1.94	0.50
12:L:52:PHE:HE1	12:L:65:VAL:HG11	1.75	0.50
24:X:6:G:H2'	24:X:7:G:H8	1.77	0.50
1:A:868:C:H2'	1:A:869:G:O4'	2.12	0.50
1:A:951:G:OP2	14:N:101:ARG:NH2	2.44	0.50
1:A:545:C:H5'	5:E:69:GLU:HB2	1.93	0.50
1:A:1017:U:H5''	1:A:1017:U:H6	1.77	0.50
3:C:186:ILE:HD13	3:C:213:TYR:CD2	2.47	0.50
1:A:67:C:H2'	1:A:68:G:C8	2.47	0.49
2:B:116:VAL:N	2:B:119:GLY:O	2.45	0.49
7:G:46:GLN:H	7:G:56:LYS:HA	1.77	0.49
15:O:27:LEU:O	15:O:31:ILE:HG13	2.12	0.49
15:O:31:ILE:HD11	15:O:44:ALA:O	2.12	0.49
1:A:28:A:O2'	1:A:296:U:OP1	2.24	0.49
1:A:744:C:H2'	1:A:745:G:C8	2.47	0.49
4:D:16:LYS:NZ	4:D:182:ILE:O	2.45	0.49
15:O:73:PHE:CZ	15:O:78:GLY:HA2	2.47	0.49
3:C:129:LEU:O	3:C:133:GLU:HB2	2.11	0.49
1:A:481:G:O2'	1:A:483:C:N4	2.45	0.49
1:A:662:U:H2'	1:A:663:A:C8	2.47	0.49
9:I:112:THR:HG23	9:I:115:ALA:H	1.78	0.49
1:A:6:G:O2'	1:A:7:A:H8	1.95	0.49
1:A:1174:G:H2'	1:A:1175:G:H5'	1.93	0.49
1:A:35:G:N3	13:M:115:SER:OG	2.45	0.49
1:A:461:A:H4'	1:A:461:A:OP1	2.13	0.49
1:A:1273:C:H2'	1:A:1274:A:O4'	2.12	0.49
7:G:41:ASP:OD1	7:G:58:HIS:NE2	2.45	0.49
1:A:982:U:H4'	1:A:983:A:O4'	2.13	0.49
1:A:1203:C:H2'	1:A:1204:A:C8	2.48	0.49
1:A:1539:C:OP2	22:V:21:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:A:H4'	1:A:412:A:H5'	1.95	0.48
1:A:674:G:H2'	1:A:675:A:C8	2.48	0.48
1:A:1084:G:H2'	1:A:1085:U:C5	2.48	0.48
1:A:1317:C:O2	20:T:37:ARG:NH2	2.47	0.48
3:C:130:THR:O	3:C:132:LYS:N	2.46	0.48
15:O:31:ILE:HG12	15:O:45:VAL:HG23	1.93	0.48
1:A:171:A:H2'	1:A:172:A:C8	2.48	0.48
1:A:811:C:O2'	1:A:901:A:N1	2.46	0.48
5:E:118:VAL:HG22	5:E:123:ILE:HG13	1.95	0.48
1:A:1406:U:H5''	1:A:1407:5MC:HM53	1.95	0.48
4:D:19:ASN:HB2	15:O:91:GLY:O	2.14	0.48
1:A:1478:U:H2'	1:A:1479:C:C6	2.49	0.48
3:C:120:GLN:OE1	3:C:137:ARG:NH1	2.46	0.48
1:A:1323:G:H2'	1:A:1324:A:C8	2.49	0.48
1:A:1425:U:H2'	1:A:1426:G:H8	1.79	0.48
3:C:120:GLN:HB2	3:C:126:PHE:HE2	1.79	0.48
10:J:65:ILE:HD13	10:J:79:ILE:HG23	1.95	0.48
1:A:744:C:H2'	1:A:745:G:H8	1.79	0.48
24:X:18:G:H2'	24:X:19:U:O4'	2.13	0.48
1:A:1175:G:HO2'	1:A:1176:A:H8	1.61	0.48
23:W:27:G:H22	23:W:45:A:H2	1.61	0.48
1:A:501:C:H2'	1:A:502:A:C8	2.49	0.47
1:A:1321:U:O2'	20:T:78:ARG:NH1	2.47	0.47
15:O:76:LYS:O	15:O:76:LYS:HG3	2.14	0.47
15:O:77:PHE:O	15:O:79:LEU:HB2	2.14	0.47
1:A:932:C:OP1	8:H:4:ARG:HB2	2.14	0.47
1:A:1368:A:OP1	10:J:113:ARG:NH2	2.48	0.47
10:J:45:ARG:O	10:J:49:ARG:HG2	2.14	0.47
13:M:110:ARG:HB2	13:M:119:VAL:HG21	1.94	0.47
1:A:459:A:OP2	1:A:459:A:H3'	2.15	0.47
5:E:139:PRO:HA	5:E:182:PHE:HD1	1.79	0.47
14:N:4:ILE:HD13	14:N:9:ILE:HD12	1.94	0.47
1:A:500:G:H2'	1:A:501:C:C6	2.49	0.47
1:A:652:U:O4	1:A:752:G:O2'	2.29	0.47
1:A:1183:U:O2'	1:A:1185:G:OP2	2.32	0.47
7:G:43:GLY:HA2	7:G:58:HIS:CE1	2.50	0.47
1:A:590:U:H2'	1:A:591:U:C6	2.49	0.47
1:A:1203:C:H2'	1:A:1204:A:H8	1.79	0.47
1:A:1215:G:C5	1:A:1216:A:N7	2.82	0.47
1:A:878:A:O4'	9:I:4:GLN:HG3	2.14	0.47
2:B:113:ASN:HA	2:B:149:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:A:C2	1:A:754:C:N4	2.82	0.47
1:A:859:G:OP2	1:A:869:G:N1	2.39	0.47
1:A:1004:A:C6	1:A:1026:G:H1'	2.50	0.47
1:A:1297:G:H21	8:H:114:LYS:HB3	1.80	0.47
3:C:75:ALA:HB1	3:C:207:ILE:HG12	1.97	0.47
15:O:73:PHE:CE1	15:O:78:GLY:HA2	2.50	0.47
15:O:77:PHE:O	15:O:78:GLY:C	2.57	0.47
1:A:6:G:N3	1:A:6:G:C3'	2.76	0.47
14:N:83:LEU:HD11	20:T:65:GLU:HB3	1.96	0.47
1:A:1317:C:H5''	15:O:24:ARG:NH2	2.29	0.47
15:O:24:ARG:HG3	15:O:48:LEU:HD11	1.96	0.47
21:U:51:PHE:HA	21:U:54:MET:HG2	1.97	0.47
22:V:13:ASP:OD1	22:V:13:ASP:N	2.40	0.47
1:A:500:G:H5''	13:M:121:ARG:NH1	2.28	0.47
1:A:1534:A:H2'	1:A:1535:C:C6	2.50	0.47
1:A:401:C:O2'	1:A:621:A:N3	2.46	0.46
1:A:908:A:H2'	1:A:909:A:C8	2.50	0.46
1:A:1363:A:O2'	1:A:1365:G:N7	2.43	0.46
12:L:16:VAL:HG12	12:L:18:ASP:OD1	2.14	0.46
1:A:1217:C:H2'	1:A:1218:C:C6	2.50	0.46
2:B:7:GLN:HG3	2:B:8:LEU:N	2.29	0.46
4:D:40:ARG:NH1	4:D:55:ILE:O	2.43	0.46
1:A:1006:G:C2	1:A:1007:U:C6	3.03	0.46
1:A:1017:U:H5''	1:A:1017:U:C6	2.50	0.46
4:D:20:SER:HB2	15:O:94:PRO:HD3	1.98	0.46
21:U:25:ARG:HG3	21:U:66:LEU:HD11	1.97	0.46
1:A:1217:C:H2'	1:A:1218:C:H6	1.80	0.46
15:O:72:GLY:O	15:O:80:SER:CA	2.63	0.46
23:W:1:C:H2'	23:W:2:G:H8	1.81	0.46
23:W:29:C:H2'	23:W:30:G:C8	2.50	0.46
1:A:464:U:O5'	1:A:464:U:C6	2.56	0.46
2:B:112:ILE:O	2:B:149:GLY:N	2.32	0.46
18:R:26:GLU:HA	18:R:41:THR:HA	1.97	0.46
1:A:1071:C:H2'	1:A:1072:G:C8	2.51	0.46
1:A:1332:A:H2'	1:A:1333:A:O4'	2.14	0.46
1:A:75:G:H2'	1:A:76:G:O4'	2.15	0.46
1:A:88:U:H2'	1:A:89:U:H5'	1.97	0.46
1:A:108:G:H5'	1:A:109:A:H5''	1.98	0.46
1:A:1348:U:OP1	10:J:112:GLU:N	2.46	0.46
2:B:85:SER:OG	2:B:87:GLU:HG3	2.16	0.46
1:A:219:U:H2'	1:A:220:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:C:H2'	1:A:270:A:C8	2.51	0.46
2:B:72:LEU:HA	2:B:84:LEU:HD22	1.97	0.46
1:A:979:C:OP2	1:A:980:C:C5	2.69	0.46
1:A:1166:G:O2'	1:A:1169:A:N6	2.44	0.46
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.46
6:F:37:THR:HG21	6:F:64:MET:SD	2.56	0.46
1:A:640:A:C2'	1:A:641:U:H5'	2.46	0.46
1:A:1277:C:O2'	1:A:1279:G:C8	2.68	0.46
14:N:97:VAL:HG23	14:N:109:ARG:HH12	1.81	0.46
10:J:27:LYS:HB3	10:J:62:ASP:OD1	2.17	0.45
2:B:28:VAL:HG22	2:B:38:VAL:HG22	1.98	0.45
1:A:1095:U:H2'	1:A:1096:C:C6	2.52	0.45
22:V:55:ARG:O	22:V:59:LYS:HG2	2.16	0.45
1:A:58:C:H6	1:A:58:C:C5'	2.29	0.45
1:A:459:A:OP2	1:A:459:A:H8	1.99	0.45
10:J:12:ARG:O	10:J:15:SER:N	2.50	0.45
1:A:384:G:H2'	1:A:385:C:C6	2.51	0.45
1:A:714:G:H2'	1:A:715:A:C8	2.52	0.45
24:X:11:U:H1'	24:X:12:A:OP2	2.17	0.45
10:J:115:LYS:NZ	10:J:121:ALA:O	2.45	0.45
1:A:1084:G:O5'	1:A:1084:G:H8	1.99	0.45
1:A:1193:G:O6	4:D:2:GLY:N	2.50	0.45
1:A:1371:G:OP1	10:J:14:SER:OG	2.25	0.45
6:F:111:MET:HE2	6:F:111:MET:HB3	1.89	0.45
11:K:59:LYS:HE2	11:K:62:ARG:NH2	2.31	0.45
1:A:1119:C:H2'	1:A:1120:C:H6	1.82	0.45
15:O:19:LYS:HD3	15:O:20:TYR:CE2	2.51	0.45
1:A:81:A:N6	1:A:82:G:O6	2.50	0.45
1:A:405:U:O4	5:E:2:ALA:N	2.49	0.45
1:A:1215:G:C6	1:A:1216:A:C5	3.05	0.45
15:O:77:PHE:C	15:O:79:LEU:H	2.25	0.45
1:A:466:A:H2'	1:A:468:A:H2	1.73	0.44
1:A:994:A:N6	1:A:1046:A:H2	2.14	0.44
1:A:1317:C:H5''	15:O:24:ARG:HH22	1.80	0.44
19:S:32:TYR:HB3	19:S:55:LEU:HD21	1.99	0.44
1:A:83:C:HO2'	1:A:85:U:H3	1.66	0.44
1:A:1060:U:OP1	15:O:85:ARG:NH2	2.39	0.44
1:A:1396:A:H4'	1:A:1397:C:O5'	2.17	0.44
1:A:297:G:N2	1:A:300:A:OP2	2.35	0.44
1:A:736:C:H2'	1:A:737:C:C6	2.51	0.44
1:A:512:U:H2'	1:A:513:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:A:H2'	1:A:924:C:C6	2.52	0.44
1:A:946:A:H2'	1:A:947:G:C8	2.52	0.44
1:A:1318:A:H5''	20:T:3:ARG:NH1	2.32	0.44
1:A:1317:C:OP1	15:O:24:ARG:NH2	2.42	0.44
1:A:1343:G:H1'	10:J:123:ARG:NH1	2.32	0.44
2:B:50:ALA:O	2:B:54:LYS:N	2.47	0.44
5:E:9:LEU:HD13	5:E:32:CYS:HB3	1.99	0.44
12:L:34:ILE:HB	12:L:74:VAL:HG21	1.99	0.44
1:A:461:A:OP1	1:A:461:A:C4'	2.65	0.44
1:A:752:G:OP1	16:P:73:LYS:NZ	2.51	0.44
1:A:1130:A:H2'	1:A:1131:G:C8	2.52	0.44
1:A:1219:A:H2'	1:A:1220:G:C8	2.52	0.44
1:A:1417:G:O2'	1:A:1483:A:N6	2.47	0.44
2:B:55:ASN:HD21	2:B:59:GLU:HB3	1.83	0.44
14:N:86:TYR:O	14:N:90:ARG:HG2	2.18	0.44
1:A:1071:C:H2'	1:A:1072:G:H8	1.83	0.44
1:A:1463:U:H2'	1:A:1464:U:C6	2.53	0.44
2:B:25:ARG:H	2:B:25:ARG:NE	2.14	0.44
12:L:34:ILE:HG12	12:L:70:CYS:SG	2.57	0.44
15:O:73:PHE:CD2	15:O:73:PHE:O	2.70	0.44
24:X:11:U:H4'	24:X:12:A:O5'	2.16	0.44
1:A:62:U:H2'	1:A:63:C:C6	2.53	0.44
1:A:335:C:H2'	1:A:336:A:C8	2.53	0.44
1:A:999:C:H2'	1:A:1000:A:C8	2.53	0.44
23:W:32:G:H2'	23:W:33:OMC:O4'	2.18	0.43
1:A:1007:U:O4	1:A:1022:A:C6	2.69	0.43
1:A:1014:A:H4'	20:T:14:HIS:CD2	2.53	0.43
5:E:72:PHE:HE1	5:E:94:LEU:HD11	1.83	0.43
9:I:102:ALA:HB3	9:I:113:ASP:HB3	2.00	0.43
11:K:52:LEU:HD23	11:K:62:ARG:HG2	2.00	0.43
15:O:11:VAL:O	15:O:11:VAL:HG12	2.16	0.43
1:A:1039:G:H2'	1:A:1040:U:C6	2.53	0.43
1:A:1048:G:C6	1:A:1210:C:N4	2.86	0.43
1:A:1219:A:H2'	1:A:1220:G:H8	1.84	0.43
12:L:25:ALA:HB1	12:L:90:GLY:HA3	2.01	0.43
23:W:17:C:OP2	23:W:61:U:O2'	2.30	0.43
1:A:980:C:C4	1:A:981:U:C2	3.07	0.43
15:O:46:LEU:O	15:O:50:THR:HG23	2.18	0.43
1:A:1391:U:H2'	1:A:1392:G:C8	2.53	0.43
1:A:126:G:OP1	1:A:605:U:O2'	2.26	0.43
1:A:1004:A:H2'	1:A:1005:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:U:H2'	1:A:1063:C:C6	2.53	0.43
1:A:1427:C:H2'	1:A:1428:A:H8	1.83	0.43
1:A:147:G:H2'	1:A:148:G:C8	2.53	0.43
1:A:381:C:H2'	1:A:382:A:O4'	2.19	0.43
1:A:1435:G:H2'	1:A:1436:U:C6	2.53	0.43
23:W:30:G:H2'	23:W:31:G:C8	2.54	0.43
1:A:707:U:H2'	1:A:708:C:C6	2.53	0.43
1:A:978:A:C8	1:A:979:C:C5	3.07	0.43
1:A:1169:A:H2'	1:A:1170:A:C8	2.54	0.43
12:L:70:CYS:O	12:L:74:VAL:HG23	2.19	0.43
13:M:68:GLY:O	13:M:99:ARG:NH1	2.49	0.43
1:A:18:C:H4'	1:A:1078:U:O2	2.19	0.43
1:A:1001:C:H2'	1:A:1002:G:C8	2.54	0.43
4:D:7:PRO:HD2	4:D:184:TYR:CD2	2.54	0.43
1:A:21:G:H2'	1:A:22:G:C8	2.53	0.43
1:A:457:G:H5''	1:A:457:G:C8	2.53	0.43
1:A:1158:C:H3'	1:A:1158:C:O2	2.19	0.43
10:J:54:LEU:HD23	10:J:98:LEU:HD23	2.01	0.43
15:O:24:ARG:HH21	15:O:56:SER:HB2	1.84	0.43
1:A:159:G:N2	1:A:162:A:OP2	2.50	0.42
1:A:664:G:H22	1:A:741:G:H1	1.67	0.42
1:A:1069:C:H2'	1:A:1070:U:O4'	2.19	0.42
6:F:42:GLY:O	6:F:119:GLY:HA3	2.17	0.42
1:A:689:C:OP1	12:L:29:ASN:ND2	2.51	0.42
1:A:933:G:O6	8:H:3:ARG:NH2	2.31	0.42
1:A:1220:G:H1'	20:T:52:HIS:CE1	2.53	0.42
1:A:1464:U:H2'	1:A:1465:A:H8	1.83	0.42
1:A:1537:U:H2'	1:A:1538:C:C6	2.53	0.42
11:K:15:HIS:O	11:K:18:ILE:HG22	2.19	0.42
11:K:82:LYS:HB2	11:K:82:LYS:HE2	1.82	0.42
15:O:73:PHE:HA	15:O:80:SER:HA	2.01	0.42
23:W:52:C:H2'	23:W:53:G:O4'	2.20	0.42
1:A:335:C:H2'	1:A:336:A:H8	1.84	0.42
1:A:826:C:O2	9:I:16:ASN:ND2	2.53	0.42
1:A:1006:G:N2	1:A:1007:U:C2	2.87	0.42
1:A:1174:G:C2'	1:A:1175:G:H5'	2.48	0.42
3:C:68:LEU:HB3	3:C:161:LEU:HD12	2.00	0.42
4:D:73:PRO:HA	4:D:76:VAL:HG12	2.01	0.42
2:B:70:VAL:CG1	2:B:84:LEU:HB3	2.49	0.42
5:E:19:LEU:HB2	5:E:21:LEU:HG	2.00	0.42
11:K:3:ASN:HB3	11:K:79:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:21:LYS:HE3	20:T:21:LYS:HB2	1.81	0.42
1:A:89:U:H2'	1:A:90:C:C6	2.55	0.42
1:A:252:U:O4	1:A:253:A:N6	2.49	0.42
1:A:410:G:H2'	1:A:429:U:C5	2.54	0.42
1:A:751:U:H5'	16:P:21:ASP:OD1	2.20	0.42
1:A:1010:U:H2'	1:A:1011:C:C6	2.54	0.42
2:B:53:PHE:HB3	2:B:62:ILE:HG12	2.01	0.42
13:M:44:LYS:HB3	13:M:45:PRO:HD3	2.01	0.42
1:A:79:G:H2'	1:A:80:A:O4'	2.18	0.42
1:A:148:G:O2'	1:A:1446:A:N3	2.48	0.42
1:A:337:G:H2'	1:A:338:A:C8	2.54	0.42
1:A:514:C:H2'	1:A:515:G:H8	1.85	0.42
1:A:1170:A:H2'	1:A:1171:A:O4'	2.20	0.42
2:B:132:PRO:O	2:B:136:VAL:N	2.52	0.42
4:D:25:ASN:OD1	4:D:26:THR:N	2.50	0.42
8:H:65:ALA:O	8:H:69:VAL:HG23	2.19	0.42
11:K:49:PHE:O	11:K:65:TYR:N	2.51	0.42
1:A:458:U:H3'	1:A:459:A:H8	1.85	0.42
1:A:754:C:H3'	1:A:754:C:O2	2.19	0.42
1:A:1152:A:P	11:K:72:ARG:HH22	2.43	0.42
1:A:1297:G:N2	8:H:114:LYS:HB3	2.35	0.42
15:O:69:ARG:HD3	15:O:80:SER:HB2	2.01	0.42
1:A:219:U:H2'	1:A:220:G:C8	2.55	0.42
1:A:459:A:H2'	1:A:460:A:C8	2.55	0.42
1:A:1061:G:H5'	11:K:61:ALA:HB2	2.02	0.42
1:A:1218:C:H2'	1:A:1219:A:H8	1.80	0.42
1:A:1343:G:H1'	10:J:123:ARG:HH11	1.84	0.42
7:G:8:PHE:HA	7:G:87:SER:HA	2.00	0.42
1:A:216:U:H2'	1:A:217:C:C6	2.55	0.42
1:A:376:G:H5''	17:Q:5:ARG:HB2	2.02	0.42
1:A:429:U:H5'	5:E:9:LEU:HD12	2.02	0.42
1:A:1048:G:O6	1:A:1210:C:N4	2.53	0.42
2:B:60:LEU:HD22	2:B:62:ILE:HD11	2.02	0.42
10:J:25:ASN:HD21	10:J:27:LYS:HB2	1.85	0.42
15:O:52:PRO:O	15:O:54:ASP:N	2.50	0.42
1:A:339:C:H2'	1:A:340:U:C6	2.55	0.42
1:A:389:A:H3'	1:A:390:U:H6	1.85	0.42
1:A:843:U:OP1	1:A:844:G:N2	2.53	0.42
1:A:1175:G:O2'	1:A:1176:A:H8	2.03	0.42
4:D:123:GLN:HB3	4:D:128:VAL:HG21	2.02	0.42
13:M:79:VAL:O	13:M:103:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:G:H5'	1:A:723:U:OP1	2.20	0.41
1:A:878:A:H2'	1:A:879:C:C6	2.55	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.54	0.41
1:A:1535:C:H2'	1:A:1536:C:C6	2.54	0.41
13:M:66:TYR:HB2	13:M:87:VAL:HG21	2.02	0.41
23:W:71:G:C6	23:W:72:C:C4	3.08	0.41
1:A:737:C:H2'	1:A:738:C:C6	2.55	0.41
3:C:188:ASP:HB2	3:C:204:ASP:OD2	2.20	0.41
4:D:86:LYS:O	4:D:90:VAL:HG23	2.20	0.41
13:M:6:GLN:HA	13:M:9:ARG:HH11	1.85	0.41
15:O:16:LEU:HD12	15:O:16:LEU:HA	1.74	0.41
15:O:63:ARG:O	15:O:64:CYS:C	2.63	0.41
1:A:1178:G:H3'	10:J:99:ARG:NH2	2.35	0.41
2:B:53:PHE:HD2	2:B:62:ILE:HG21	1.84	0.41
14:N:66:GLU:HB3	14:N:67:GLY:H	1.62	0.41
21:U:35:VAL:HG21	21:U:54:MET:SD	2.61	0.41
12:L:45:ALA:HB3	12:L:70:CYS:HB2	2.01	0.41
1:A:664:G:OP1	19:S:57:ARG:NH2	2.44	0.41
12:L:92:GLY:C	12:L:94:GLU:H	2.29	0.41
15:O:93:ILE:HD12	15:O:96:LEU:HD23	2.02	0.41
1:A:131:A:H2'	1:A:132:C:C6	2.56	0.41
1:A:356:A:N3	1:A:368:U:O2'	2.41	0.41
1:A:1006:G:C4	1:A:1007:U:C6	3.08	0.41
1:A:1008:U:H2'	1:A:1009:U:O4'	2.20	0.41
1:A:1220:G:H1'	20:T:52:HIS:ND1	2.35	0.41
4:D:73:PRO:O	4:D:77:ILE:HG13	2.20	0.41
11:K:25:ILE:HG13	11:K:92:LEU:HD21	2.03	0.41
1:A:35:G:H2'	1:A:36:C:C6	2.55	0.41
1:A:340:U:H2'	1:A:341:C:H6	1.85	0.41
8:H:26:PHE:HZ	8:H:120:LEU:HD21	1.86	0.41
19:S:26:ILE:HD13	19:S:26:ILE:HA	1.89	0.41
1:A:464:U:C6	1:A:464:U:C3'	3.04	0.41
1:A:663:A:H5'	1:A:836:G:OP1	2.21	0.41
1:A:978:A:C5	1:A:1318:A:C6	3.09	0.41
1:A:1052:U:O2'	1:A:1055:A:OP2	2.21	0.41
1:A:1181:G:O2'	1:A:1182:G:N7	2.48	0.41
1:A:1338:G:H2'	1:A:1339:A:C8	2.56	0.41
11:K:48:ARG:HG2	11:K:66:GLU:HB3	2.01	0.41
15:O:9:ARG:O	15:O:13:ARG:HG3	2.20	0.41
15:O:38:ASP:O	15:O:42:TRP:HB3	2.21	0.41
1:A:255:G:P	18:R:71:LYS:HZ1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:U:H2'	1:A:324:G:O4'	2.20	0.41
1:A:719:C:O2'	19:S:38:LYS:HB2	2.20	0.41
1:A:1317:C:C4'	15:O:24:ARG:HH22	2.33	0.41
1:A:1537:U:H2'	1:A:1538:C:H6	1.86	0.41
2:B:62:ILE:H	2:B:62:ILE:HG13	1.61	0.41
4:D:42:TYR:CZ	4:D:90:VAL:HG11	2.56	0.41
6:F:153:VAL:HA	6:F:156:LYS:HE3	2.02	0.41
7:G:11:HIS:CD2	7:G:54:LEU:HD13	2.55	0.41
7:G:88:MET:HE3	7:G:88:MET:HB2	2.00	0.41
10:J:63:LEU:HD13	10:J:65:ILE:HD11	2.01	0.41
11:K:37:ARG:HB2	11:K:75:ASP:HB3	2.02	0.41
1:A:343:U:H2'	1:A:345:C:C5	2.56	0.41
1:A:865:A:H2'	1:A:866:C:O4'	2.21	0.41
1:A:1140:C:O2'	1:A:1141:C:H6	2.04	0.41
1:A:1318:A:H5''	20:T:3:ARG:HH12	1.86	0.41
1:A:1397:C:H5''	1:A:1398:A:C8	2.56	0.41
2:B:71:ALA:HB3	2:B:88:LYS:HB2	2.03	0.41
23:W:37:U:H2'	23:W:38:A:O4'	2.21	0.41
1:A:410:G:H2'	1:A:429:U:C4	2.56	0.40
1:A:1132:C:H2'	1:A:1132:C:O2	2.21	0.40
1:A:1279:G:N3	1:A:1279:G:H2'	2.35	0.40
2:B:70:VAL:HG11	2:B:84:LEU:HB3	2.04	0.40
8:H:11:LYS:HE3	8:H:11:LYS:HB3	1.92	0.40
12:L:17:SER:HA	12:L:79:ILE:HA	2.02	0.40
20:T:47:LEU:O	20:T:62:VAL:HG12	2.22	0.40
1:A:555:U:H2'	1:A:556:C:C6	2.56	0.40
1:A:567:G:H2'	1:A:568:G:O4'	2.22	0.40
1:A:820:U:H4'	1:A:821:G:OP2	2.20	0.40
1:A:938:A:N3	1:A:1376:U:O2'	2.47	0.40
4:D:32:ASN:HA	4:D:59:ARG:HH12	1.86	0.40
6:F:77:ASN:HB2	6:F:82:GLN:HG3	2.02	0.40
9:I:39:VAL:HG21	9:I:110:VAL:HG12	2.03	0.40
11:K:6:ILE:HG13	11:K:76:ILE:HB	2.03	0.40
1:A:689:C:OP1	12:L:46:THR:OG1	2.33	0.40
1:A:1425:U:H2'	1:A:1426:G:C8	2.56	0.40
14:N:19:LEU:HD23	14:N:19:LEU:HA	1.93	0.40
1:A:1220:G:H2'	1:A:1221:G:O4'	2.22	0.40
1:A:1427:C:H2'	1:A:1428:A:C8	2.57	0.40
1:A:972:C:OP2	11:K:59:LYS:NZ	2.43	0.40
1:A:1236:A:H4'	1:A:1304:G:H4'	2.04	0.40
5:E:15:GLU:CD	5:E:60:LYS:HB2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:40:ASN:HB3	17:Q:43:ALA:HB2	2.03	0.40
23:W:25:U:H2'	23:W:26:C:H6	1.87	0.40
23:W:29:C:H2'	23:W:30:G:H8	1.86	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	B	171/557 (31%)	159 (93%)	12 (7%)	0	100	100
3	C	224/241 (93%)	213 (95%)	9 (4%)	2 (1%)	14	27
4	D	209/233 (90%)	204 (98%)	4 (2%)	1 (0%)	24	43
5	E	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
6	F	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
7	G	102/131 (78%)	98 (96%)	3 (3%)	1 (1%)	12	24
8	H	151/156 (97%)	145 (96%)	6 (4%)	0	100	100
9	I	127/130 (98%)	127 (100%)	0	0	100	100
10	J	126/130 (97%)	117 (93%)	9 (7%)	0	100	100
11	K	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
12	L	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
13	M	119/124 (96%)	114 (96%)	3 (2%)	2 (2%)	7	13
14	N	113/118 (96%)	111 (98%)	1 (1%)	1 (1%)	14	27
15	O	98/101 (97%)	86 (88%)	10 (10%)	2 (2%)	6	10
16	P	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
17	Q	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
18	R	78/84 (93%)	75 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	65/75 (87%)	61 (94%)	4 (6%)	0	100	100
20	T	81/92 (88%)	81 (100%)	0	0	100	100
21	U	84/87 (97%)	84 (100%)	0	0	100	100
22	V	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	2553/3095 (82%)	2459 (96%)	85 (3%)	9 (0%)	31	49

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	80	LYS
14	N	66	GLU
15	O	53	ARG
3	C	131	LYS
3	C	127	ASP
15	O	52	PRO
13	M	48	ALA
7	G	60	VAL
13	M	88	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	74/461 (16%)	60 (81%)	14 (19%)	1	3
3	C	187/199 (94%)	180 (96%)	7 (4%)	30	57
4	D	172/190 (90%)	168 (98%)	4 (2%)	44	72
5	E	172/173 (99%)	170 (99%)	2 (1%)	63	83
6	F	119/119 (100%)	114 (96%)	5 (4%)	26	52
7	G	91/112 (81%)	86 (94%)	5 (6%)	19	40
8	H	126/129 (98%)	123 (98%)	3 (2%)	43	70
9	I	104/105 (99%)	99 (95%)	5 (5%)	23	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	106/107 (99%)	102 (96%)	4 (4%)	29	56
11	K	88/90 (98%)	86 (98%)	2 (2%)	44	72
12	L	90/99 (91%)	90 (100%)	0	100	100
13	M	102/103 (99%)	97 (95%)	5 (5%)	22	45
14	N	93/96 (97%)	90 (97%)	3 (3%)	34	62
15	O	83/84 (99%)	57 (69%)	26 (31%)	0	0
16	P	76/77 (99%)	75 (99%)	1 (1%)	61	82
17	Q	65/65 (100%)	65 (100%)	0	100	100
18	R	74/78 (95%)	73 (99%)	1 (1%)	59	81
19	S	58/65 (89%)	58 (100%)	0	100	100
20	T	72/79 (91%)	70 (97%)	2 (3%)	38	66
21	U	65/66 (98%)	64 (98%)	1 (2%)	57	80
22	V	60/61 (98%)	57 (95%)	3 (5%)	22	44
All	All	2077/2558 (81%)	1984 (96%)	93 (4%)	26	49

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

Mol	Chain	Res	Type
2	B	2	THR
2	B	3	GLU
2	B	7	GLN
2	B	11	GLU
2	B	18	THR
2	B	22	SER
2	B	34	ASP
2	B	42	LEU
2	B	46	SER
2	B	61	GLU
2	B	62	ILE
2	B	64	VAL
2	B	79	PHE
2	B	83	LEU
3	C	117	LEU
3	C	128	LYS
3	C	129	LEU
3	C	130	THR
3	C	131	LYS

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Mol	Chain	Res	Type
3	C	135	LEU
3	C	199	VAL
4	D	21	THR
4	D	64	ILE
4	D	129	MET
4	D	211	MET
5	E	56	ARG
5	E	129	VAL
6	F	68	ARG
6	F	72	ILE
6	F	94	VAL
6	F	105	ILE
6	F	123	VAL
7	G	71	ILE
7	G	84	VAL
7	G	88	MET
7	G	89	VAL
7	G	96	VAL
8	H	6	VAL
8	H	120	LEU
8	H	144	MET
9	I	22	LYS
9	I	33	LYS
9	I	88	ARG
9	I	101	ILE
9	I	104	VAL
10	J	58	VAL
10	J	63	LEU
10	J	111	VAL
10	J	116	VAL
11	K	32	THR
11	K	80	THR
13	M	16	VAL
13	M	21	VAL
13	M	43	LYS
13	M	46	ASN
13	M	87	VAL
14	N	16	VAL
14	N	46	SER
14	N	102	THR
15	O	10	GLU
15	O	16	LEU

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Mol	Chain	Res	Type
15	O	26	GLU
15	O	28	LYS
15	O	30	ILE
15	O	33	ASP
15	O	34	VAL
15	O	35	ASN
15	O	37	SER
15	O	39	GLU
15	O	40	ASP
15	O	45	VAL
15	O	47	LYS
15	O	53	ARG
15	O	58	SER
15	O	59	ARG
15	O	65	ARG
15	O	74	LEU
15	O	76	LYS
15	O	79	LEU
15	O	82	ILE
15	O	83	LYS
15	O	89	MET
15	O	92	GLU
15	O	97	LYS
15	O	98	LYS
16	P	18	ASP
18	R	25	ILE
20	T	62	VAL
20	T	79	THR
21	U	67	ILE
22	V	4	ILE
22	V	13	ASP
22	V	44	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	7	GLN
3	C	42	ASN
3	C	122	GLN
4	D	41	GLN
4	D	69	HIS
4	D	123	GLN

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Mol	Chain	Res	Type
5	E	36	GLN
5	E	40	GLN
5	E	59	GLN
5	E	74	ASN
5	E	116	GLN
5	E	131	ASN
5	E	136	GLN
5	E	198	HIS
6	F	77	ASN
7	G	11	HIS
7	G	46	GLN
8	H	68	ASN
11	K	56	HIS
12	L	81	ASN
14	N	52	GLN
15	O	49	GLN
15	O	62	ASN
16	P	80	GLN
17	Q	18	GLN
17	Q	59	HIS
19	S	54	GLN
19	S	75	GLN
20	T	14	HIS
21	U	3	ASN
21	U	61	GLN
21	U	70	ASN
21	U	75	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1537/1541 (99%)	273 (17%)	9 (0%)
23	W	76/77 (98%)	17 (22%)	2 (2%)
24	X	16/53 (30%)	3 (18%)	1 (6%)
All	All	1629/1671 (97%)	293 (17%)	12 (0%)

All (293) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U

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Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	52	C
1	A	54	C
1	A	57	G
1	A	58	C
1	A	69	G
1	A	72	A
1	A	76	G
1	A	77	A
1	A	83	C
1	A	84	U
1	A	86	G
1	A	89	U
1	A	90	C
1	A	94	G
1	A	95	C
1	A	108	G
1	A	121	U
1	A	122	G
1	A	131	A
1	A	141	G
1	A	144	G
1	A	160	A
1	A	163	C
1	A	164	G
1	A	173	U
1	A	181	A
1	A	196	A
1	A	202	G
1	A	208	U
1	A	211	G
1	A	212	G
1	A	226	G
1	A	245	U

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Mol	Chain	Res	Type
1	A	247	G
1	A	251	G
1	A	258	G
1	A	262	A
1	A	266	G
1	A	267	C
1	A	279	A
1	A	289	G
1	A	306	A
1	A	316	C
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	384	G
1	A	406	G
1	A	411	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	446	G
1	A	457	G
1	A	458	U
1	A	459	A
1	A	460	A
1	A	461	A
1	A	462	G
1	A	463	U
1	A	465	A
1	A	466	A
1	A	467	U
1	A	468	A
1	A	469	C

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Mol	Chain	Res	Type
1	A	476	U
1	A	478	A
1	A	479	U
1	A	480	U
1	A	481	G
1	A	484	G
1	A	485	U
1	A	486	U
1	A	495	A
1	A	497	G
1	A	511	C
1	A	517	G
1	A	518	C
1	A	521	G
1	A	527	G7M
1	A	531	U
1	A	532	A
1	A	533	A
1	A	537	G
1	A	547	A
1	A	559	A
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	596	A
1	A	628	G
1	A	633	G
1	A	639	G
1	A	641	U
1	A	642	A
1	A	650	G
1	A	653	U
1	A	665	A
1	A	687	A
1	A	703	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	755	G

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Mol	Chain	Res	Type
1	A	777	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	828	U
1	A	832	G
1	A	836	G
1	A	841	C
1	A	842	U
1	A	843	U
1	A	844	G
1	A	846	G
1	A	849	G
1	A	851	G
1	A	887	G
1	A	902	G
1	A	914	A
1	A	916	U
1	A	926	G
1	A	927	G
1	A	928	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	971	G
1	A	972	C
1	A	975	A
1	A	976	G
1	A	977	A
1	A	981	U
1	A	987	G
1	A	992	U
1	A	993	G
1	A	996	A
1	A	1004	A
1	A	1006	G
1	A	1007	U
1	A	1009	U
1	A	1010	U

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Mol	Chain	Res	Type
1	A	1017	U
1	A	1018	G
1	A	1019	A
1	A	1020	G
1	A	1021	A
1	A	1022	A
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1043	G
1	A	1044	A
1	A	1046	A
1	A	1065	U
1	A	1070	U
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1099	G
1	A	1101	A
1	A	1108	G
1	A	1133	G
1	A	1135	U
1	A	1136	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1145	A
1	A	1146	A
1	A	1151	A
1	A	1152	A
1	A	1154	G
1	A	1158	C
1	A	1159	U
1	A	1167	A
1	A	1168	U

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Mol	Chain	Res	Type
1	A	1169	A
1	A	1171	A
1	A	1174	G
1	A	1175	G
1	A	1176	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1216	A
1	A	1227	A
1	A	1238	A
1	A	1239	A
1	A	1257	A
1	A	1260	G
1	A	1277	C
1	A	1278	G
1	A	1280	A
1	A	1285	A
1	A	1286	U
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1320	C
1	A	1323	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1419	G
1	A	1421	G

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Mol	Chain	Res	Type
1	A	1422	G
1	A	1425	U
1	A	1426	G
1	A	1429	A
1	A	1432	G
1	A	1441	A
1	A	1442	G
1	A	1446	A
1	A	1452	C
1	A	1453	G
1	A	1475	G
1	A	1487	G
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1534	A
23	W	9	G
23	W	17	C
23	W	18	U
23	W	19	G
23	W	20	G
23	W	21	H2U
23	W	22	A
23	W	44	A
23	W	47	A
23	W	48	U
23	W	49	C
23	W	62	C
23	W	68	C
23	W	73	A
23	W	75	C
23	W	76	C
23	W	77	A
24	X	12	A
24	X	13	U
24	X	17	U

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	428	G
1	A	458	U
1	A	461	A
1	A	462	G
1	A	843	U
1	A	1018	G
1	A	1166	G
1	A	1214	C
1	A	1396	A
23	W	21	H2U
23	W	48	U
24	X	11	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	D2T	M	89	13	8,9,10	1.12	0	6,11,13	2.23	2 (33%)
23	OMC	W	33	23	19,22,23	3.08	8 (42%)	25,31,34	0.72	0
23	5MU	W	55	23	19,22,23	1.41	6 (31%)	27,32,35	2.03	6 (22%)
23	PSU	W	56	23	18,21,22	1.10	1 (5%)	21,30,33	1.93	5 (23%)
1	2MG	A	1207	1	23,26,27	2.89	9 (39%)	33,38,41	2.92	13 (39%)
1	4OC	A	1402	1	20,23,24	3.59	9 (45%)	25,32,35	0.92	1 (4%)
1	5MC	A	967	1	19,22,23	4.41	8 (42%)	26,32,35	1.00	2 (7%)
1	5MC	A	1407	1	19,22,23	4.40	8 (42%)	26,32,35	0.95	1 (3%)
1	2MG	A	1516	1	23,26,27	1.28	4 (17%)	33,38,41	2.17	7 (21%)
1	MA6	A	1519	1	23,26,27	1.56	5 (21%)	33,38,41	3.91	12 (36%)
23	H2U	W	21	23	18,21,22	3.16	5 (27%)	19,30,33	1.44	4 (21%)
1	2MG	A	966	1	23,26,27	2.94	8 (34%)	33,38,41	3.04	12 (36%)
23	4SU	W	8	23	18,21,22	4.39	8 (44%)	25,30,33	2.28	4 (16%)
1	UR3	A	1498	1	19,22,23	2.83	8 (42%)	26,32,35	1.60	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G7M	A	527	1	23,26,27	2.61	9 (39%)	34,39,42	2.59	11 (32%)
1	MA6	A	1518	1	23,26,27	1.57	6 (26%)	33,38,41	3.76	12 (36%)
1	PSU	A	516	25,1	18,21,22	1.17	2 (11%)	21,30,33	1.99	6 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	D2T	M	89	13	-	1/7/12/14	-
23	OMC	W	33	23	-	1/9/27/28	0/2/2/2
23	5MU	W	55	23	-	0/7/25/26	0/2/2/2
23	PSU	W	56	23	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
1	MA6	A	1519	1	-	5/11/29/30	0/3/3/3
23	H2U	W	21	23	-	5/7/38/39	0/2/2/2
1	2MG	A	966	1	-	2/9/27/28	0/3/3/3
23	4SU	W	8	23	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	3/7/25/26	0/3/3/3
1	MA6	A	1518	1	-	3/11/29/30	0/3/3/3
1	PSU	A	516	25,1	-	0/7/25/26	0/2/2/2

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	5MC	C6-C5	10.32	1.51	1.34
1	A	967	5MC	C6-C5	10.30	1.51	1.34
23	W	8	4SU	C4-N3	10.00	1.48	1.37
23	W	21	H2U	C2-N1	9.71	1.49	1.35
1	A	966	2MG	C2-N3	8.77	1.48	1.32
1	A	1207	2MG	C2-N3	8.35	1.47	1.32
23	W	8	4SU	C2-N1	8.21	1.51	1.38
1	A	967	5MC	C4-N3	7.91	1.46	1.34
1	A	1407	5MC	C4-N3	7.87	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C4-N3	7.73	1.45	1.32
1	A	967	5MC	C5-C4	7.52	1.49	1.44
1	A	1498	UR3	C2-N1	7.46	1.48	1.38
1	A	1407	5MC	C5-C4	7.43	1.49	1.44
1	A	967	5MC	C2-N3	7.02	1.50	1.36
1	A	1407	5MC	C2-N3	6.98	1.50	1.36
23	W	8	4SU	C2-N3	6.81	1.49	1.38
23	W	21	H2U	C2-N3	6.68	1.49	1.38
23	W	33	OMC	C2-N3	6.62	1.49	1.36
1	A	1402	4OC	C6-C5	6.58	1.50	1.35
1	A	527	G7M	C4-N3	6.45	1.49	1.34
1	A	1402	4OC	C2-N3	6.40	1.49	1.36
23	W	8	4SU	C5-C4	6.29	1.50	1.42
1	A	1498	UR3	C6-C5	6.20	1.49	1.35
23	W	8	4SU	C6-C5	6.17	1.49	1.35
23	W	33	OMC	C6-C5	6.12	1.49	1.35
1	A	966	2MG	C4-N3	6.04	1.48	1.34
23	W	8	4SU	C4-S4	-5.82	1.58	1.68
1	A	1207	2MG	C4-N3	5.74	1.47	1.34
1	A	1407	5MC	C6-N1	5.55	1.47	1.38
1	A	967	5MC	C4-N4	5.54	1.48	1.34
1	A	1407	5MC	C4-N4	5.54	1.48	1.34
1	A	967	5MC	C6-N1	5.45	1.47	1.38
23	W	33	OMC	C4-N3	5.35	1.45	1.34
1	A	527	G7M	C2-N3	5.21	1.45	1.33
23	W	21	H2U	C4-N3	5.14	1.46	1.37
1	A	967	5MC	C2-N1	5.10	1.50	1.40
1	A	966	2MG	C2-N2	5.10	1.44	1.33
1	A	1498	UR3	C2-N3	5.08	1.49	1.39
1	A	1207	2MG	C2-N2	5.06	1.44	1.33
1	A	1407	5MC	C2-N1	5.05	1.50	1.40
1	A	1402	4OC	C4-N4	5.03	1.46	1.36
23	W	33	OMC	C4-N4	4.80	1.45	1.33
1	A	527	G7M	C2-N2	4.77	1.45	1.34
1	A	1402	4OC	C2-N1	4.67	1.49	1.40
1	A	527	G7M	C5-N7	-4.65	1.33	1.39
1	A	1402	4OC	O2-C2	-4.62	1.15	1.23
23	W	33	OMC	C2-N1	4.60	1.49	1.40
1	A	1402	4OC	C5-C4	4.37	1.50	1.41
1	A	1207	2MG	C2-N1	4.31	1.43	1.36
1	A	966	2MG	C2-N1	4.22	1.43	1.36
1	A	1518	MA6	C6-N6	4.16	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1519	MA6	C6-N6	4.11	1.48	1.36
1	A	516	PSU	C6-C5	3.71	1.39	1.35
1	A	1402	4OC	CM4-N4	3.69	1.52	1.45
1	A	527	G7M	C5-C6	3.65	1.53	1.43
23	W	56	PSU	C6-C5	3.58	1.39	1.35
1	A	1207	2MG	O6-C6	-3.56	1.16	1.23
1	A	966	2MG	O6-C6	-3.48	1.17	1.23
1	A	1402	4OC	C6-N1	3.38	1.46	1.38
23	W	33	OMC	C6-N1	3.37	1.46	1.38
23	W	8	4SU	C6-N1	3.30	1.46	1.38
1	A	1518	MA6	C10-N6	3.23	1.52	1.45
1	A	1519	MA6	C10-N6	3.18	1.52	1.45
1	A	966	2MG	C5-N7	-3.13	1.32	1.39
1	A	1516	2MG	C5-C4	3.11	1.47	1.38
23	W	8	4SU	O2-C2	-3.06	1.17	1.23
1	A	1498	UR3	C6-N1	3.06	1.45	1.38
1	A	1207	2MG	C5-N7	-3.02	1.33	1.39
1	A	1207	2MG	C6-N1	2.96	1.44	1.38
1	A	527	G7M	C2-N1	2.83	1.44	1.37
1	A	966	2MG	C6-N1	2.77	1.44	1.38
1	A	1519	MA6	C5-C4	-2.76	1.34	1.39
23	W	55	5MU	C6-C5	2.72	1.39	1.34
23	W	33	OMC	O2-C2	-2.71	1.18	1.23
1	A	1518	MA6	C5-C4	-2.71	1.34	1.39
23	W	55	5MU	C4-N3	-2.60	1.34	1.38
1	A	1498	UR3	C4-N3	2.57	1.45	1.40
1	A	1207	2MG	C5-C6	2.54	1.53	1.44
23	W	33	OMC	C5-C4	2.54	1.48	1.42
1	A	527	G7M	O6-C6	-2.51	1.18	1.23
1	A	966	2MG	C5-C6	2.49	1.53	1.44
1	A	1519	MA6	C8-N7	2.46	1.36	1.31
1	A	527	G7M	C6-N1	2.45	1.43	1.38
1	A	1516	2MG	C6-N1	-2.44	1.34	1.38
1	A	527	G7M	C4-N9	-2.40	1.32	1.38
23	W	21	H2U	O2-C2	-2.39	1.18	1.23
1	A	1498	UR3	C5-C4	2.33	1.49	1.43
1	A	1518	MA6	C8-N7	2.32	1.36	1.31
23	W	55	5MU	C6-N1	-2.32	1.34	1.38
1	A	1519	MA6	C8-N9	-2.32	1.33	1.37
1	A	1407	5MC	O2-C2	-2.31	1.19	1.23
23	W	55	5MU	C4-C5	2.30	1.48	1.44
1	A	967	5MC	O2-C2	-2.30	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1518	MA6	C8-N9	-2.29	1.33	1.37
1	A	1516	2MG	C2-N3	2.20	1.36	1.32
23	W	21	H2U	O4-C4	-2.19	1.18	1.23
23	W	55	5MU	C2-N1	2.19	1.41	1.38
1	A	1207	2MG	C4-N9	-2.19	1.32	1.38
1	A	516	PSU	O4'-C1'	-2.16	1.40	1.43
1	A	1498	UR3	O4-C4	-2.15	1.19	1.23
23	W	55	5MU	C2-N3	-2.09	1.34	1.38
1	A	1498	UR3	O2-C2	-2.06	1.18	1.22
1	A	1516	2MG	C5-N7	-2.06	1.34	1.39
1	A	1518	MA6	C2-N3	2.04	1.37	1.33

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	N1-C6-N6	-15.46	98.02	116.86
1	A	1518	MA6	N1-C6-N6	-14.61	99.06	116.86
1	A	1519	MA6	C5-C6-N6	10.48	141.92	125.33
1	A	1518	MA6	C5-C6-N6	9.94	141.06	125.33
1	A	966	2MG	C1'-N9-C8	-9.18	100.66	126.73
1	A	966	2MG	C1'-N9-C4	8.57	151.79	126.49
1	A	1207	2MG	C1'-N9-C8	-7.93	104.20	126.73
23	W	8	4SU	C4-N3-C2	-7.86	119.78	127.31
1	A	1207	2MG	C1'-N9-C4	7.26	147.94	126.49
1	A	1516	2MG	C2-N3-C4	6.99	120.74	112.00
1	A	527	G7M	C1'-N9-C8	-6.52	104.74	126.74
1	A	966	2MG	C2-N3-C4	6.43	120.05	112.00
1	A	1207	2MG	C2-N3-C4	6.43	120.05	112.00
1	A	527	G7M	C1'-N9-C4	6.23	144.90	126.49
1	A	1516	2MG	C5-C4-N3	-5.87	119.05	128.39
1	A	1519	MA6	N1-C2-N3	-5.76	119.86	128.58
1	A	1498	UR3	C4-N3-C2	-5.66	120.02	124.58
1	A	1518	MA6	N1-C2-N3	-5.58	120.14	128.58
1	A	527	G7M	CN7-N7-C5	5.53	133.70	126.80
23	W	8	4SU	C5-C4-N3	5.46	119.83	114.75
1	A	966	2MG	C5-C4-N3	-5.24	120.05	128.39
1	A	1207	2MG	N1-C2-N2	5.12	121.79	116.56
1	A	516	PSU	N1-C2-N3	4.98	120.42	115.17
23	W	55	5MU	C4-N3-C2	-4.90	120.91	127.34
1	A	1518	MA6	C5-C4-N3	-4.86	120.03	126.72
23	W	56	PSU	C4-N3-C2	-4.85	119.69	126.37
23	W	55	5MU	N3-C2-N1	4.82	121.16	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	C4-N3-C2	-4.81	119.75	126.37
23	W	56	PSU	N1-C2-N3	4.78	120.21	115.17
1	A	1519	MA6	C5-C4-N3	-4.73	120.20	126.72
1	A	527	G7M	CN7-N7-C8	-4.68	117.71	124.79
1	A	1519	MA6	N9-C8-N7	-4.59	107.43	113.94
1	A	1207	2MG	C5-C4-N3	-4.56	121.13	128.39
1	A	1518	MA6	N9-C8-N7	-4.48	107.57	113.94
1	A	1516	2MG	N9-C4-N3	4.38	134.70	125.95
23	W	55	5MU	C5-C4-N3	4.25	119.02	115.32
1	A	1207	2MG	C2-N1-C6	-4.15	119.53	124.55
1	A	966	2MG	C2-N1-C6	-4.15	119.54	124.55
1	A	527	G7M	C2-N3-C4	4.14	119.43	112.30
13	M	89	D2T	CB1-SB-CB	4.08	109.70	102.36
1	A	1518	MA6	C4-C5-C6	3.98	120.03	115.91
23	W	55	5MU	O4-C4-C5	-3.92	120.43	124.92
1	A	527	G7M	C5-C6-N1	3.87	119.85	111.84
23	W	8	4SU	N3-C2-N1	3.82	119.86	114.89
23	W	8	4SU	C5-C4-S4	-3.62	120.17	124.31
1	A	1498	UR3	C5-C4-N3	3.59	119.77	115.04
1	A	527	G7M	O6-C6-C5	-3.56	120.07	128.01
1	A	1519	MA6	C4-C5-C6	3.54	119.58	115.91
1	A	527	G7M	C5-C4-N3	-3.46	121.61	128.15
1	A	1519	MA6	C2-N1-C6	3.44	120.24	111.83
1	A	1516	2MG	C6-C5-N7	3.38	136.45	130.29
1	A	1518	MA6	C2-N1-C6	3.38	120.08	111.83
1	A	1519	MA6	C2-N3-C4	3.37	120.06	111.83
23	W	55	5MU	C5-C6-N1	-3.33	119.70	123.31
1	A	966	2MG	N1-C2-N2	3.31	119.94	116.56
1	A	1518	MA6	C2-N3-C4	3.28	119.85	111.83
23	W	21	H2U	N3-C2-N1	3.24	119.90	116.65
1	A	967	5MC	C5-C6-N1	-3.16	119.88	123.31
1	A	1518	MA6	N3-C4-N9	3.15	132.52	127.17
1	A	1207	2MG	N9-C8-N7	-3.02	107.80	113.40
23	W	21	H2U	C5-C6-N1	3.02	120.65	111.52
1	A	1519	MA6	N3-C4-N9	2.98	132.23	127.17
1	A	1519	MA6	C5-N7-C8	2.97	108.11	103.45
1	A	966	2MG	N9-C4-N3	2.94	131.83	125.95
1	A	1518	MA6	C5-N7-C8	2.94	108.06	103.45
1	A	1407	5MC	C5-C6-N1	-2.93	120.14	123.31
1	A	1519	MA6	C4-N9-C8	2.92	108.81	105.74
1	A	1518	MA6	C4-N9-C8	2.85	108.73	105.74
1	A	527	G7M	C2-N1-C6	-2.80	120.03	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	21	H2U	C5-C4-N3	2.78	119.64	116.69
1	A	1516	2MG	C2'-C1'-N9	-2.75	105.59	113.25
1	A	527	G7M	N9-C4-N3	2.70	131.35	125.95
23	W	56	PSU	O2-C2-N1	-2.69	120.01	122.79
1	A	1207	2MG	C5-C6-N1	2.69	120.10	113.25
1	A	516	PSU	O2-C2-N1	-2.68	120.03	122.79
1	A	966	2MG	N9-C8-N7	-2.67	108.44	113.40
1	A	966	2MG	C5-C6-N1	2.62	119.93	113.25
13	M	89	D2T	OD2-CG-CB	2.62	118.81	113.15
1	A	527	G7M	N9-C8-N7	-2.61	106.15	112.48
1	A	1516	2MG	C4-C5-N7	-2.56	106.62	110.67
1	A	516	PSU	C6-N1-C2	-2.53	120.34	122.69
1	A	966	2MG	O6-C6-C5	-2.44	120.09	126.53
1	A	1207	2MG	O6-C6-C5	-2.43	120.12	126.53
23	W	21	H2U	O2-C2-N1	-2.37	120.25	123.10
1	A	516	PSU	C6-C5-C4	2.33	119.75	118.17
1	A	1498	UR3	C6-N1-C2	-2.32	119.90	121.80
1	A	1207	2MG	CM2-N2-C2	-2.31	118.69	123.65
23	W	56	PSU	C6-C5-C4	2.30	119.72	118.17
1	A	516	PSU	O4'-C1'-C2'	2.28	108.30	105.15
1	A	1402	4OC	C6-C5-C4	2.25	119.71	117.00
1	A	1207	2MG	N1-C2-N3	-2.23	119.92	123.68
23	W	56	PSU	C6-N1-C2	-2.19	120.66	122.69
1	A	1519	MA6	C4-C5-N7	-2.19	108.08	110.58
23	W	55	5MU	O2-C2-N1	-2.14	120.01	122.80
1	A	1207	2MG	C8-N7-C5	2.14	108.07	104.26
1	A	1518	MA6	C4-C5-N7	-2.11	108.17	110.58
1	A	967	5MC	CM5-C5-C6	-2.11	120.00	122.85
1	A	966	2MG	N1-C2-N3	-2.10	120.15	123.68
1	A	1207	2MG	N9-C4-N3	2.08	130.12	125.95
1	A	1516	2MG	O6-C6-C5	-2.05	121.13	126.53
1	A	966	2MG	C8-N7-C5	2.03	107.87	104.26

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	C5-C6-N6-C10
1	A	1519	MA6	C5-C6-N6-C10
23	W	21	H2U	O4'-C1'-N1-C6
23	W	33	OMC	C1'-C2'-O2'-CM2
1	A	966	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	966	2MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1518	MA6	N1-C6-N6-C10
1	A	1519	MA6	N1-C6-N6-C10
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
23	W	21	H2U	O4'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
23	W	21	H2U	O4'-C1'-N1-C2
23	W	21	H2U	C3'-C4'-C5'-O5'
1	A	527	G7M	C4'-C5'-O5'-P
1	A	1519	MA6	C5-C6-N6-C9
13	M	89	D2T	CG-CB-SB-CB1
23	W	21	H2U	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	W	33	OMC	1	0
1	A	1407	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 120 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

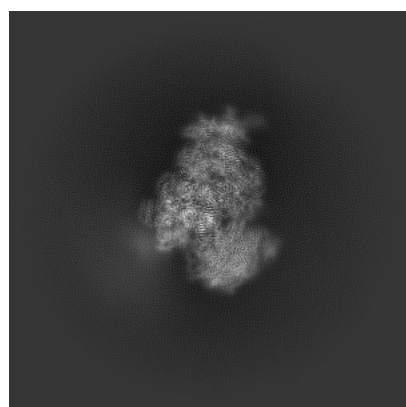
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51620. These allow visual inspection of the internal detail of the map and identification of artifacts.

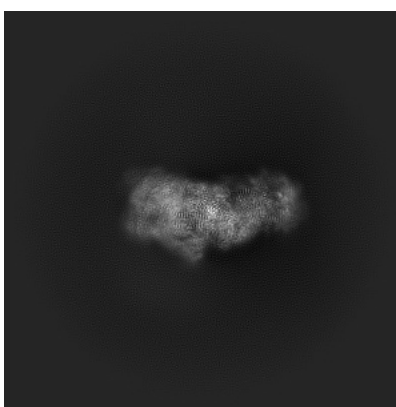
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

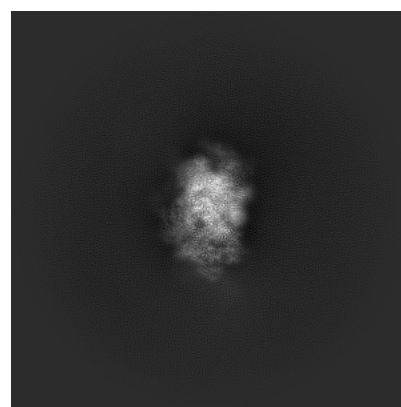
6.1.1 Primary map



X



Y

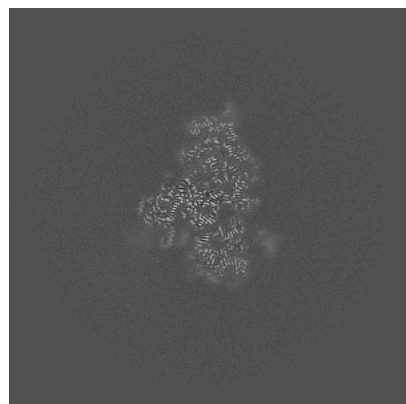


Z

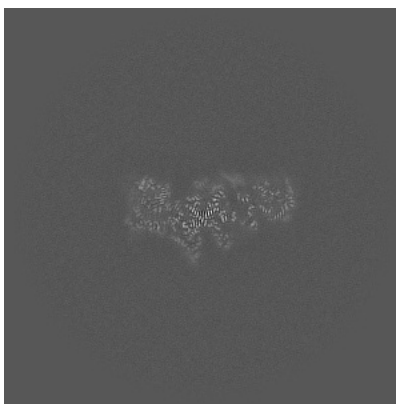
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

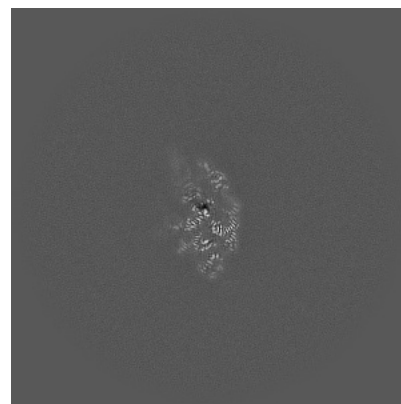
6.2.1 Primary map



X Index: 300



Y Index: 300

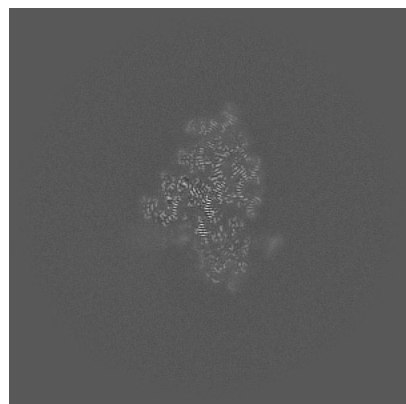


Z Index: 300

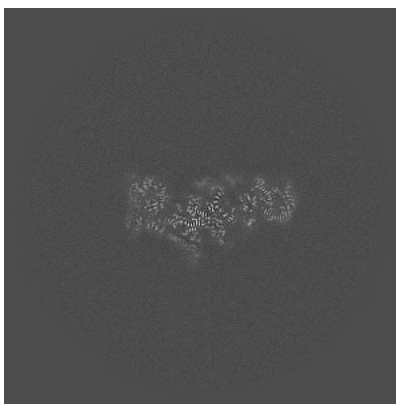
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

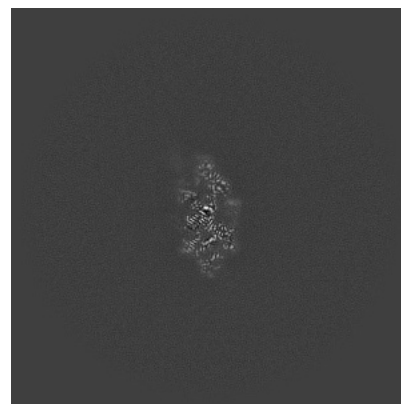
6.3.1 Primary map



X Index: 293



Y Index: 303

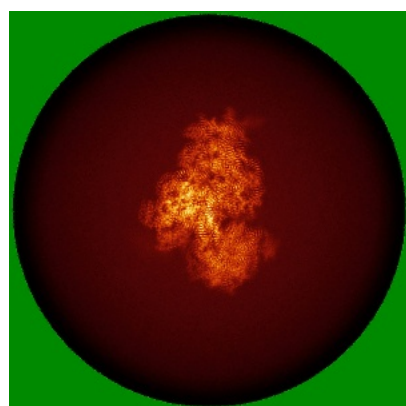


Z Index: 306

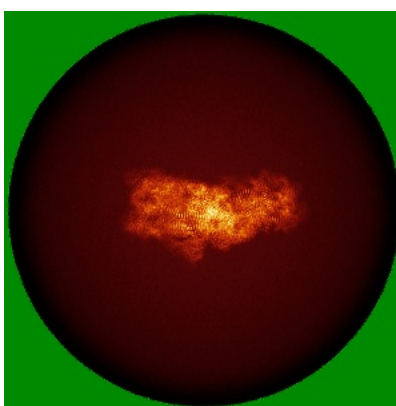
The images above show the largest variance slices of the map in three orthogonal directions.

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

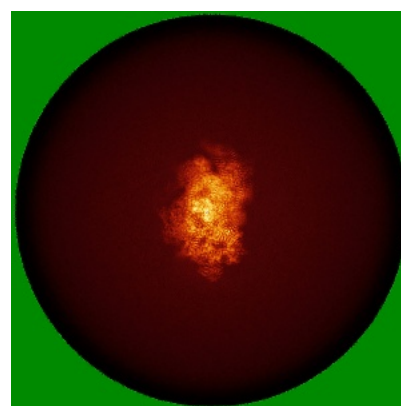
6.4.1 Primary map



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

This section was not generated.

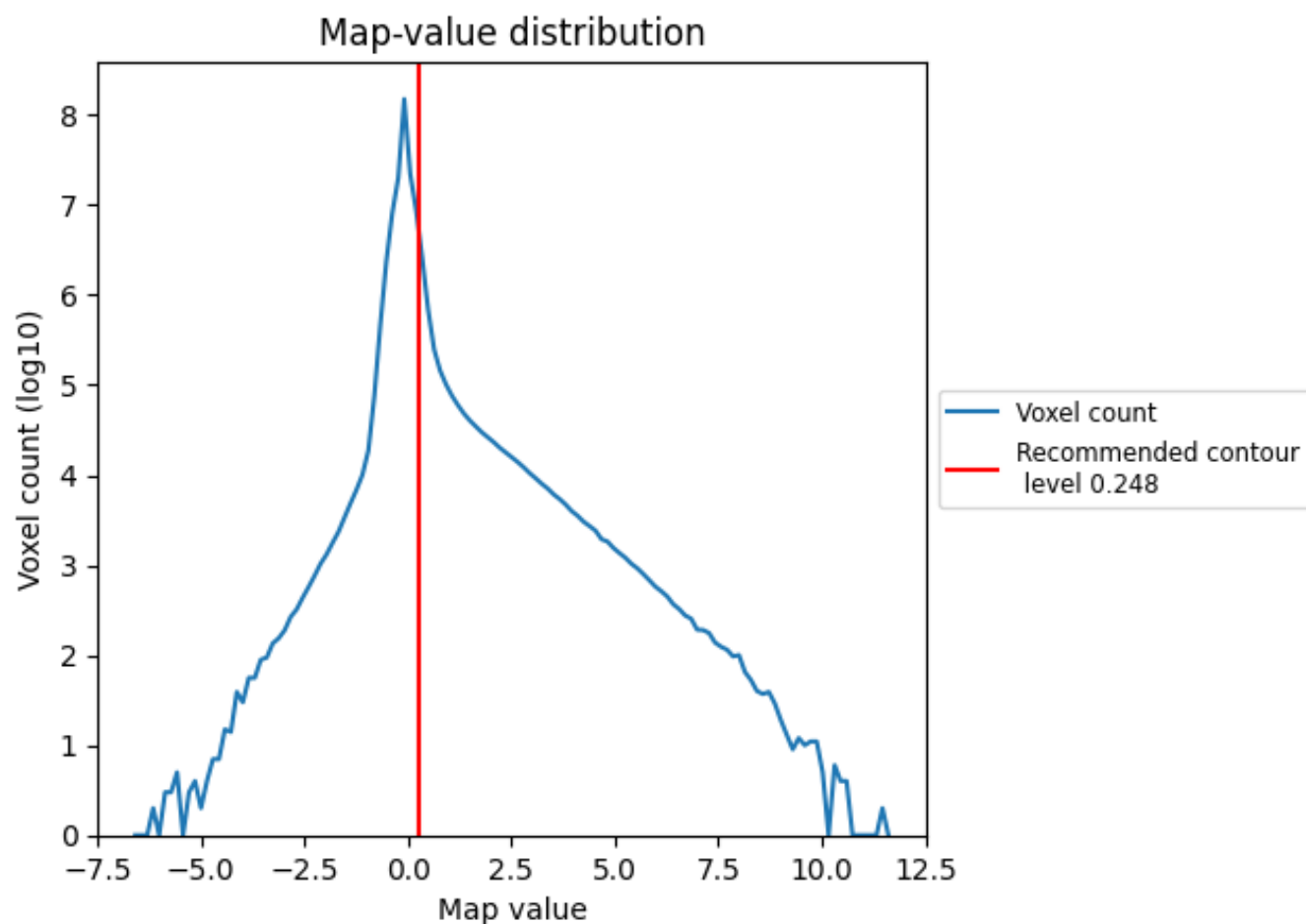
6.6 Mask visualisation

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

7 Map analysis [i](#)

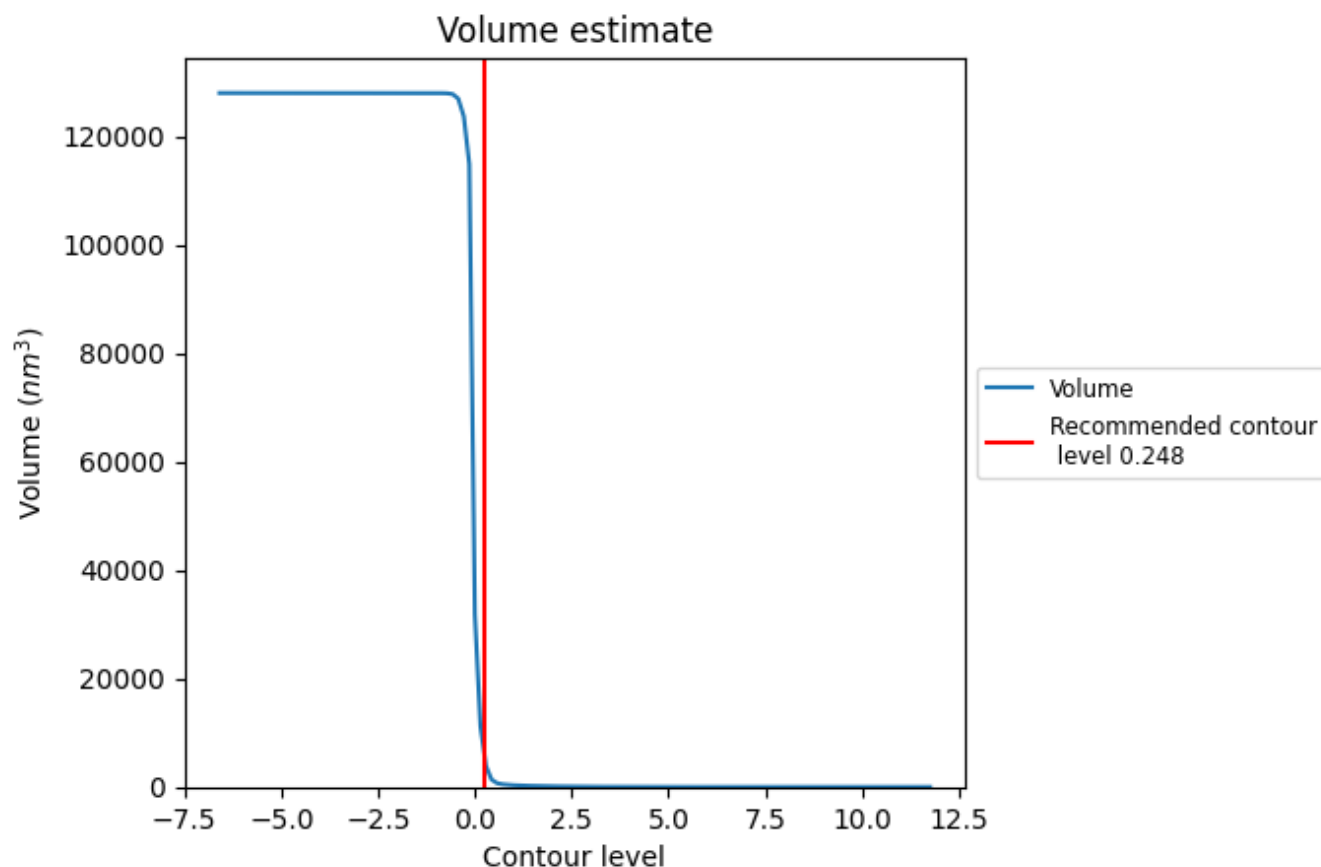
This section contains the results of statistical analysis of the map.

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.

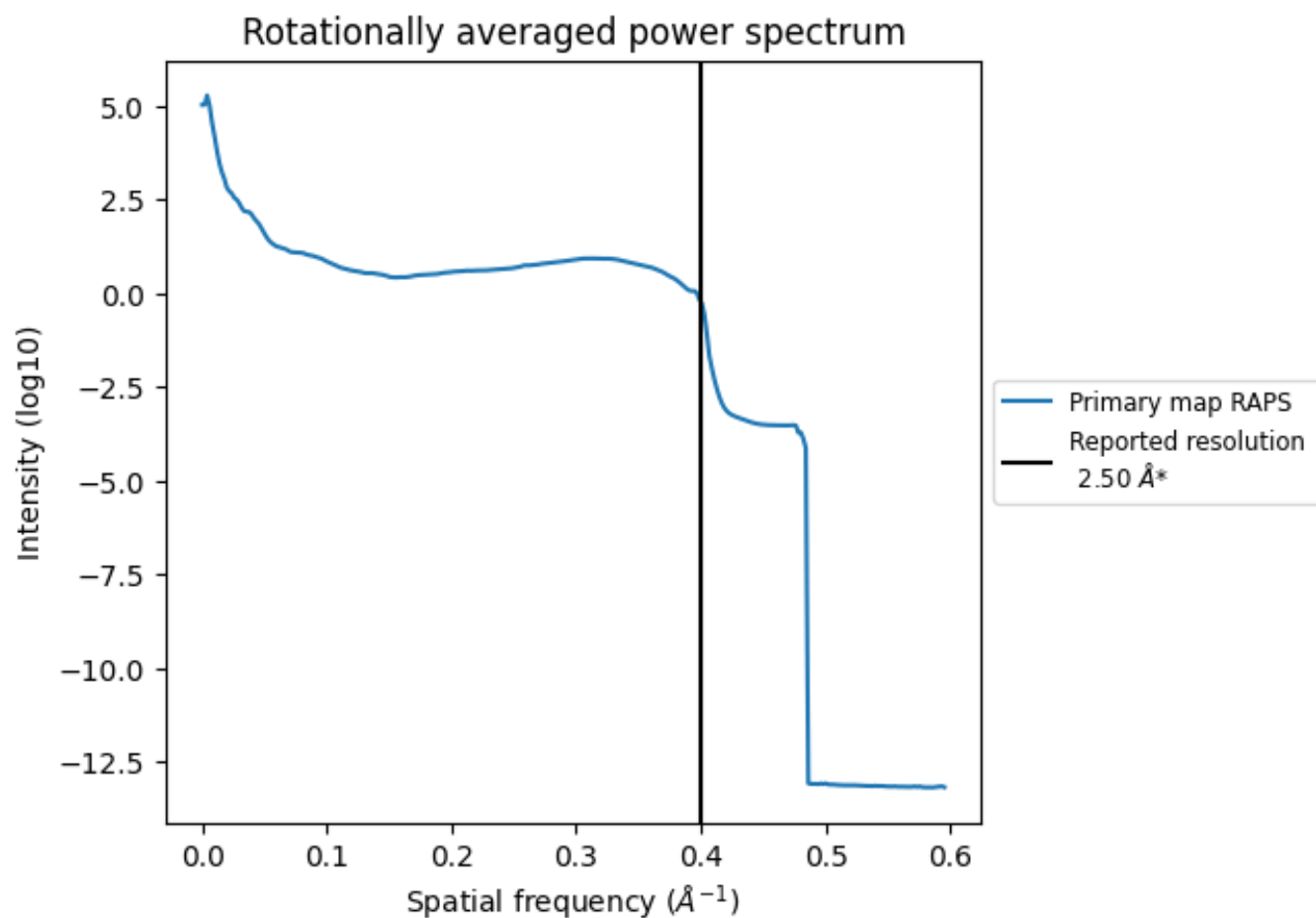
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5907 nm³; this corresponds to an approximate mass of 5336 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

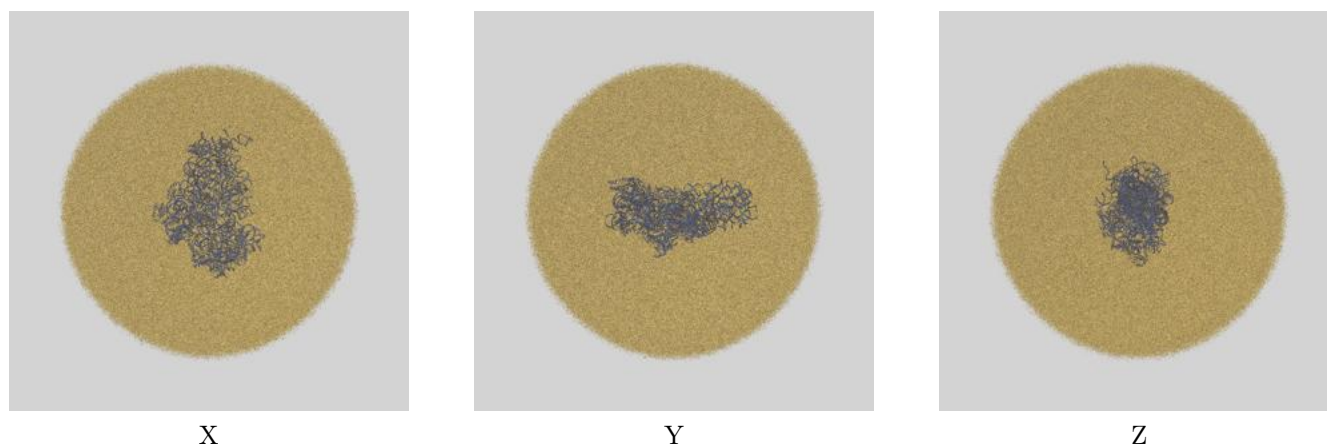
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

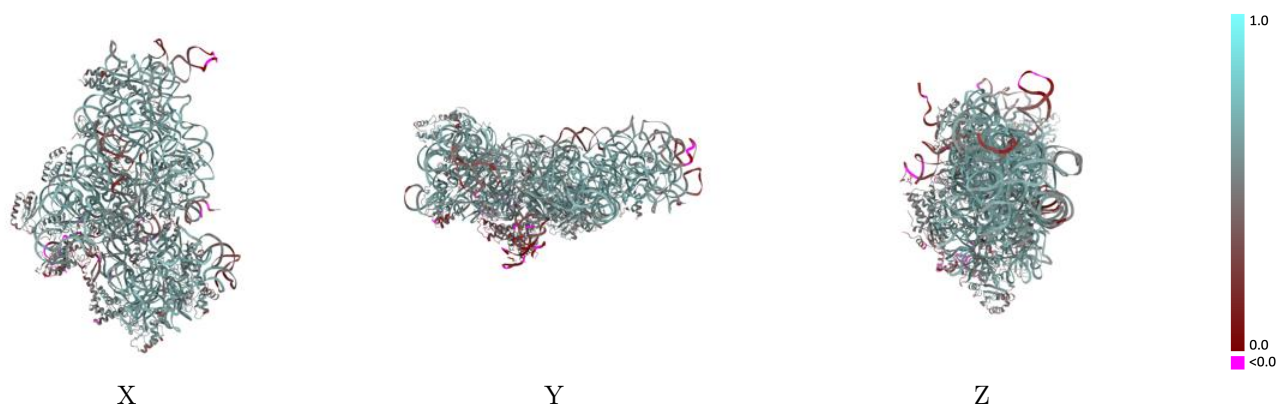
This section contains information regarding the fit between EMDB map EMD-51620 and PDB model 9GUU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



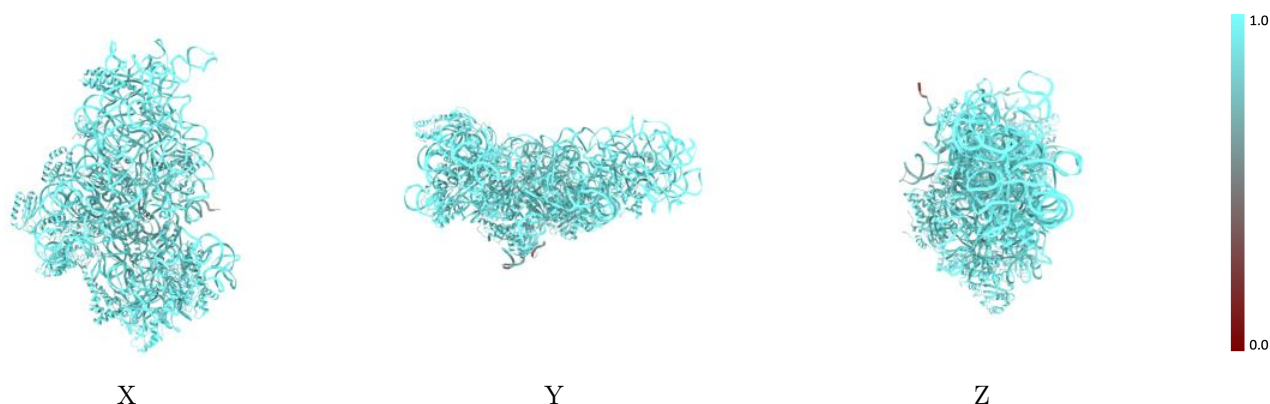
The images above show the 3D surface view of the map at the recommended contour level 0.248 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



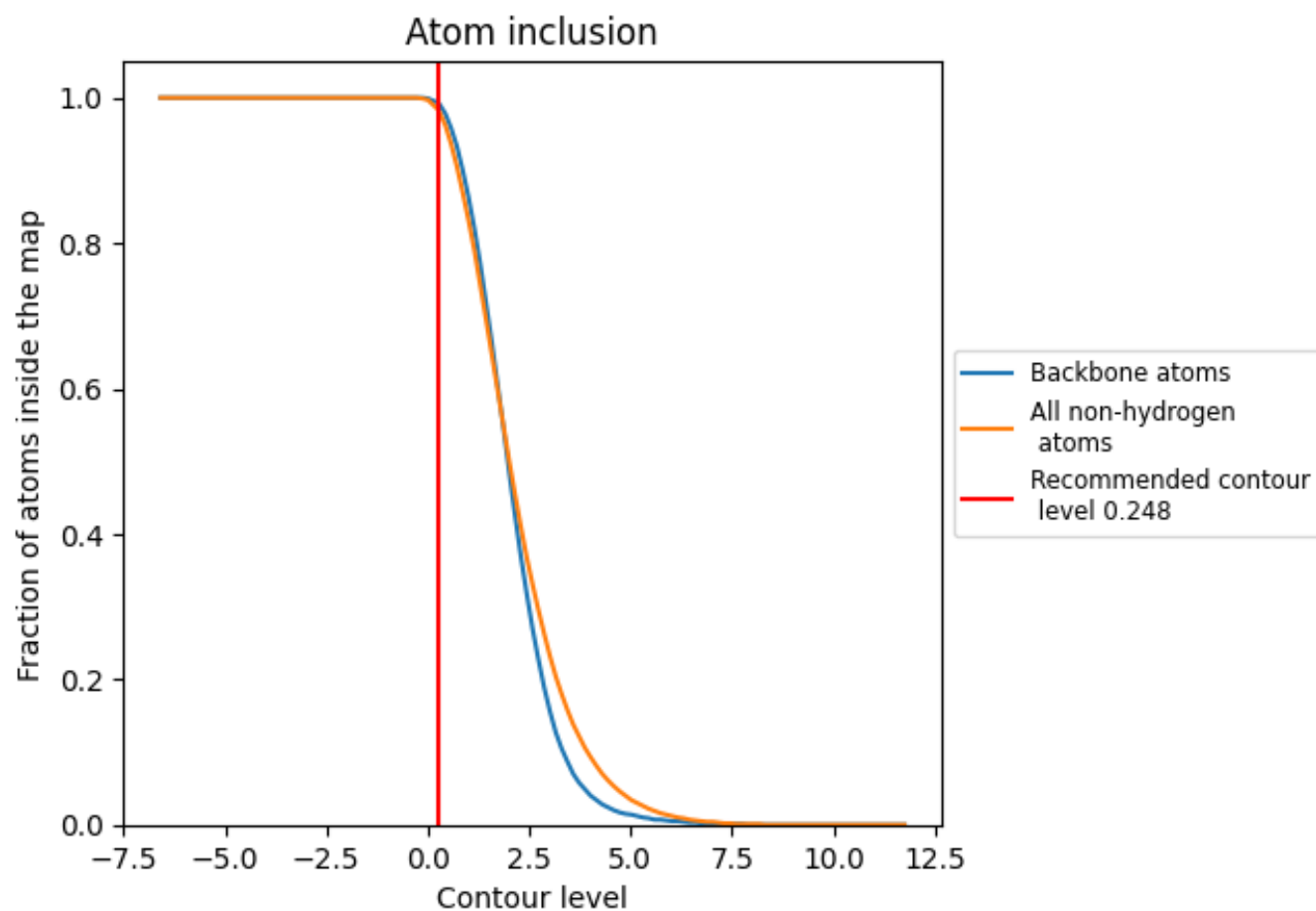
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.248).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.248) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9840	 0.5490
A	 0.9980	 0.5890
B	 0.9410	 0.2130
C	 0.9630	 0.4850
D	 0.9700	 0.5600
E	 0.9820	 0.5600
F	 0.9750	 0.5690
G	 0.9630	 0.4900
H	 0.9640	 0.4420
I	 0.9740	 0.5840
J	 0.9750	 0.5540
K	 0.9830	 0.4840
L	 0.9750	 0.4940
M	 0.9780	 0.5660
N	 0.9770	 0.5430
O	 0.9960	 0.6050
P	 0.9680	 0.5330
Q	 0.9810	 0.5910
R	 0.9750	 0.5390
S	 0.9680	 0.5260
T	 0.9770	 0.5650
U	 0.9830	 0.5590
V	 0.9480	 0.4420
W	 0.8530	 0.2240
X	 0.9430	 0.0730

