



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 01:47 PM UTC

PDB ID : 9GUV / pdb_00009guv
EMDB ID : EMD-51621
Title : 30S mRNA delivery complex (closed-head)
Authors : Rahil, H.; Webster, M.W.; Weixlbaumer, A.
Deposited on : 2024-09-20
Resolution : 3.00 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:

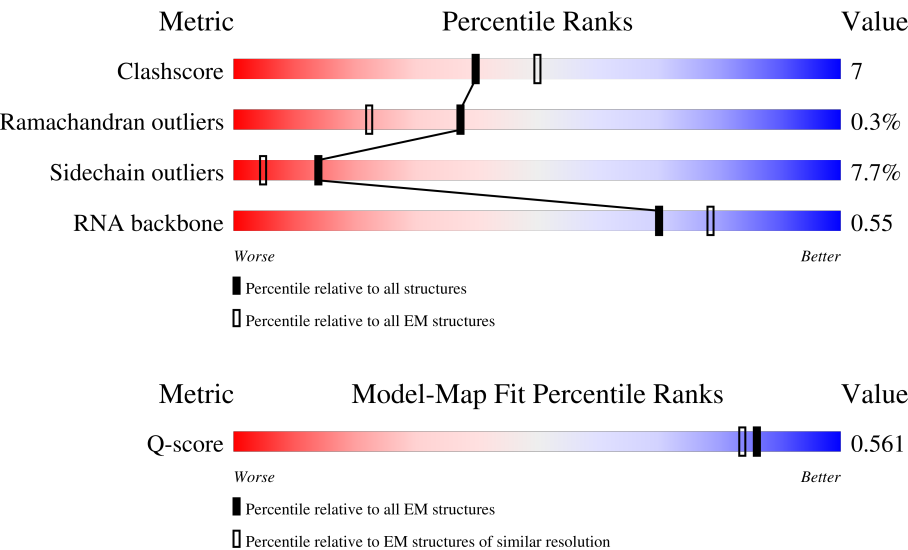
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 3.00 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.



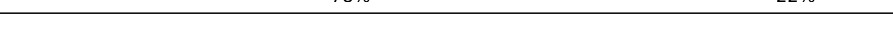
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	233	
5	E	206	
6	F	165	
7	G	131	
8	H	156	
9	I	130	
10	J	130	
11	K	103	
12	L	129	
13	M	124	
14	N	118	
15	O	101	
16	P	89	
17	Q	82	
18	R	84	
19	S	75	
20	T	92	
21	U	87	
22	V	71	
23	W	77	
24	X	53	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 55998 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	352	Total	C	N	O	S	0	0
			1797	1001	379	416	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 Small ribosomal subunit protein uS5.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	9	CYS	GLY	conflict	UNP C3SR27

- 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	152	Total	C	N	O	S	0	0
			1191	741	230	216	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		

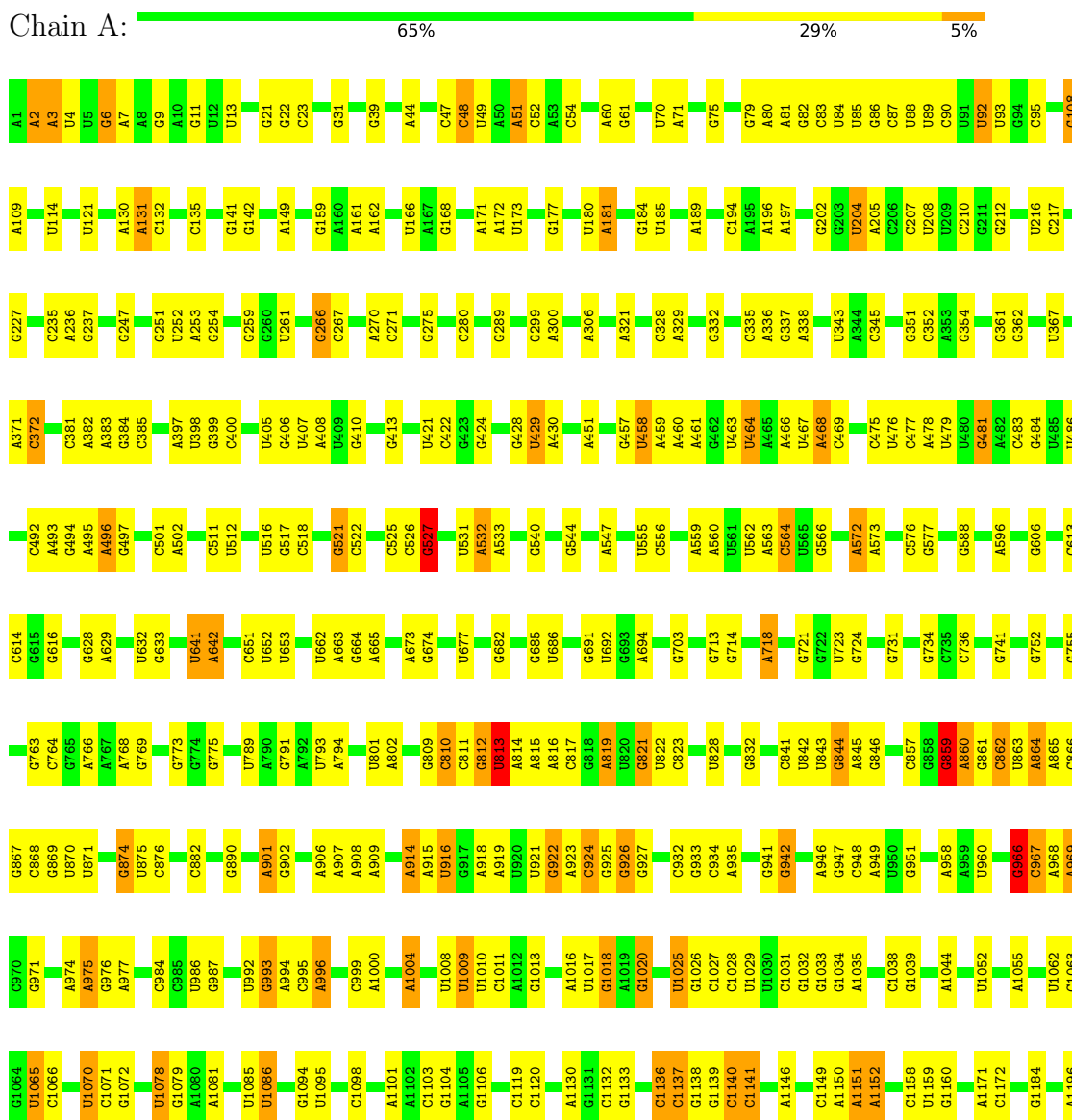
- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

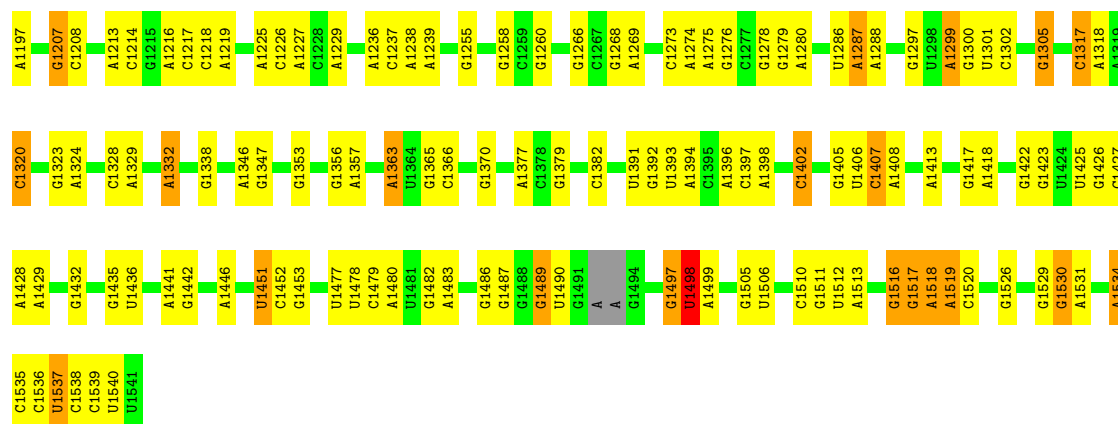
Mol	Chain	Residues	Atoms		AltConf
25	A	85	Total	Mg	0
			85	85	
25	O	1	Total	Mg	0
			1	1	

3 Residue-property plots

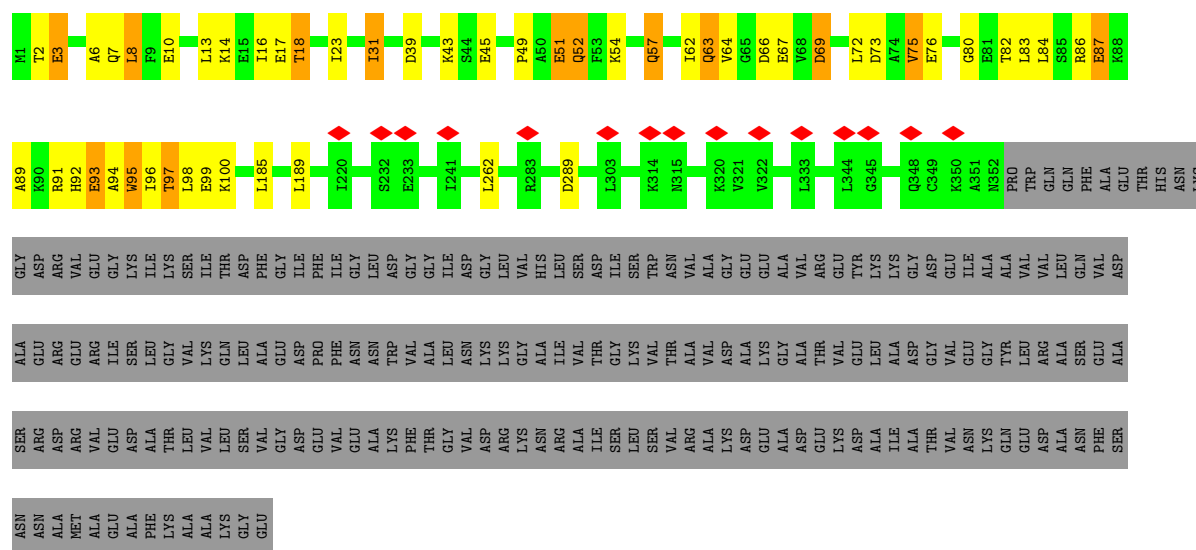
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

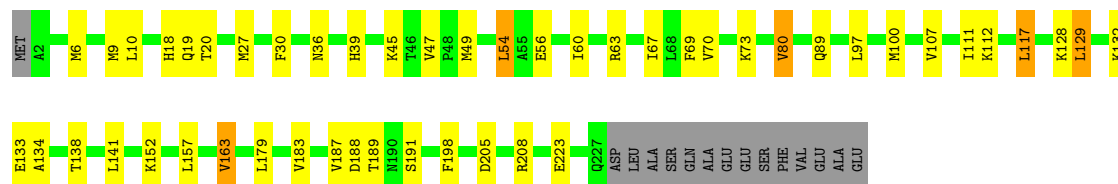




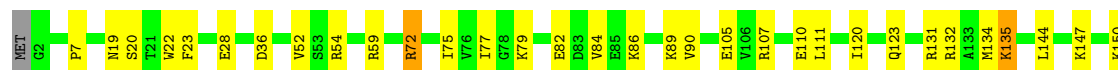
- Molecule 2: 30S ribosomal protein S1



- Molecule 3: 30S ribosomal protein S2



- Molecule 4: Small ribosomal subunit protein uS3

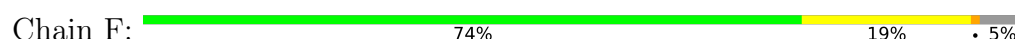




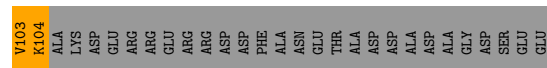
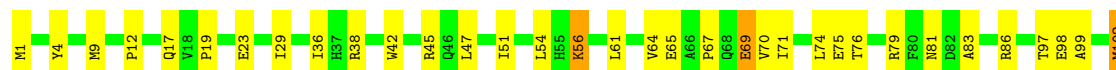
- Molecule 5: Small ribosomal subunit protein uS4



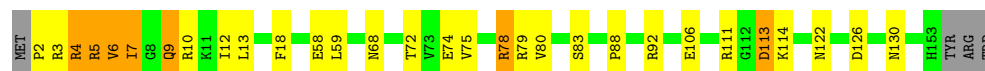
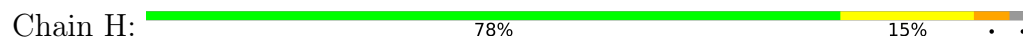
- Molecule 6: Small ribosomal subunit protein uS5



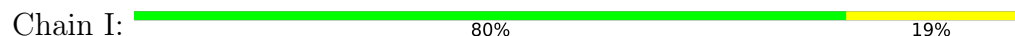
- Molecule 7: Small ribosomal subunit protein bS6



- Molecule 8: 30S ribosomal protein S7

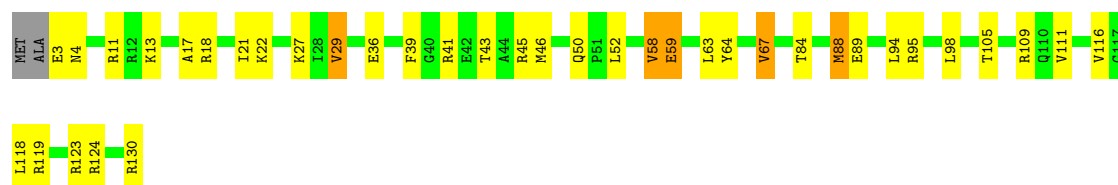


- Molecule 9: 30S ribosomal protein S8



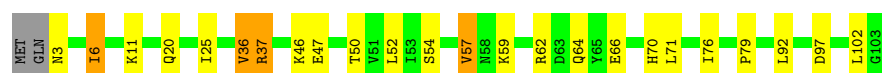
- Molecule 10: 30S ribosomal protein S9

Chain J:  69% 25% . .



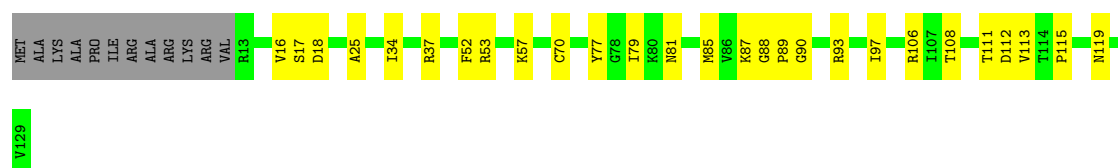
- Molecule 11: 30S ribosomal protein S10

Chain K:  75% 19% . .



- Molecule 12: 30S ribosomal protein S11

Chain L:  70% 21% 9%



- Molecule 13: 30S ribosomal protein S12

Chain M:  74% 21% . . .



- Molecule 14: 30S ribosomal protein S13

Chain N:  81% 13% . .



- Molecule 15: 30S ribosomal protein S14

Chain O:  89% 10% .

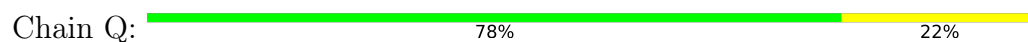


- Molecule 16: Small ribosomal subunit protein uS15

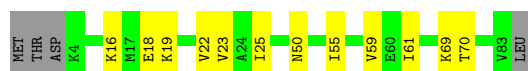
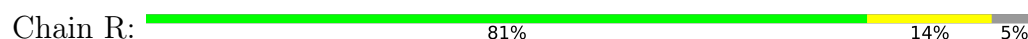
Chain P:  87% 12% .



- Molecule 17: 30S ribosomal protein S16



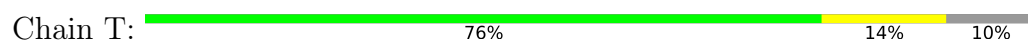
- Molecule 18: 30S ribosomal protein S17



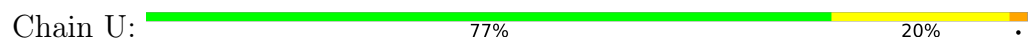
- Molecule 19: 30S ribosomal protein S18



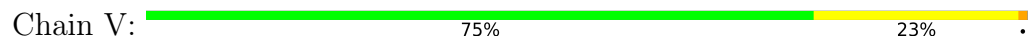
- Molecule 20: 30S ribosomal protein S19



- Molecule 21: 30S ribosomal protein S20

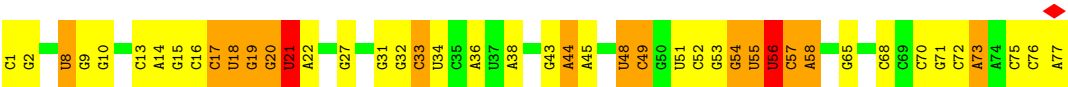


- Molecule 22: 30S ribosomal protein S21



- Molecule 23: tRNA(fmet) P-site





● Molecule 24: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112399	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	10.643	Depositor
Minimum map value	-4.354	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.179	Depositor
Recommended contour level	0.193	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	2/36692 (0.0%)	0.39	11/57230 (0.0%)
2	B	0.12	0/1806	0.39	0/2338
3	C	0.25	0/1796	0.40	0/2420
4	D	0.31	0/1680	0.43	0/2263
5	E	0.25	0/1665	0.41	0/2227
6	F	0.36	0/1165	0.47	0/1568
7	G	0.25	0/867	0.43	0/1171
8	H	0.33	0/1206	0.53	0/1617
9	I	0.31	0/989	0.42	0/1326
10	J	0.26	0/1043	0.45	0/1387
11	K	0.34	0/818	0.51	0/1105
12	L	0.26	0/893	0.43	0/1205
13	M	0.32	0/954	0.47	0/1279
14	N	0.22	0/900	0.52	0/1204
15	O	0.28	0/817	0.38	0/1088
16	P	0.27	0/722	0.44	0/964
17	Q	0.28	0/659	0.37	0/884
18	R	0.26	0/657	0.43	0/881
19	S	0.30	0/563	0.42	0/754
20	T	0.23	0/680	0.38	0/915
21	U	0.22	0/676	0.35	0/895
22	V	0.24	0/598	0.39	0/792
23	W	0.23	0/1725	0.39	0/2687
24	X	0.17	0/408	0.40	0/634
All	All	0.33	2/59979 (0.0%)	0.40	11/88834 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	A	O3'-P	-5.75	1.52	1.61
1	A	907	A	O3'-P	-5.04	1.53	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1065	U	C2'-C3'-O3'	12.88	128.82	109.50
1	A	6	G	C1'-C2'-O2'	-6.95	97.97	108.40
1	A	1078	U	C2'-C3'-O3'	6.88	124.03	113.70
1	A	1065	U	C4'-C3'-O3'	6.64	119.36	109.40
1	A	859	G	C1'-C2'-O2'	-5.75	99.78	108.40
1	A	3	A	C4'-C3'-O3'	-5.54	104.70	113.00
1	A	857	C	C4'-C3'-O3'	-5.50	104.75	113.00
1	A	641	U	C4'-C3'-O3'	5.25	117.28	109.40
1	A	901	A	C1'-C2'-O2'	-5.14	100.68	108.40
1	A	813	U	C4'-C3'-O3'	-5.05	105.42	113.00
1	A	860	A	C2'-C3'-O3'	-5.04	106.15	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33023	0	16643	283	0
2	B	1797	0	1082	34	0
3	C	1765	0	1792	31	0
4	D	1653	0	1727	27	0
5	E	1643	0	1707	40	0
6	F	1152	0	1196	24	0
7	G	848	0	846	18	0
8	H	1191	0	1245	26	0
9	I	979	0	1031	14	0
10	J	1031	0	1076	22	0
11	K	808	0	845	17	0
12	L	877	0	887	20	0
13	M	951	0	1012	18	0
14	N	891	0	952	14	0
15	O	805	0	844	9	0
16	P	714	0	734	5	0
17	Q	649	0	666	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	648	0	691	7	0
19	S	554	0	573	11	0
20	T	663	0	688	7	0
21	U	670	0	719	13	0
22	V	590	0	629	10	0
23	W	1645	0	842	32	0
24	X	365	0	182	12	0
25	A	85	0	0	0	0
25	O	1	0	0	0	0
All	All	55998	0	38609	621	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 (621) 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)
8:H:2:PRO:HG2	8:H:5:ARG:HA	1.42	1.00
23:W:33:OMC:HM22	23:W:34:U:H5'	1.45	0.99
8:H:5:ARG:HG2	8:H:6:VAL:N	1.91	0.84
8:H:79:ARG:HA	8:H:83:SER:HA	1.64	0.79
8:H:5:ARG:HG2	8:H:6:VAL:H	1.47	0.78
2:B:49:PRO:HG2	2:B:52:GLN:HE21	1.49	0.77
1:A:736:C:OP1	19:S:61:ARG:NH1	2.18	0.76
21:U:3:ASN:N	21:U:3:ASN:OD1	2.19	0.75
6:F:52:LYS:HB2	6:F:52:LYS:NZ	2.00	0.75
1:A:823:C:HO2'	9:I:2:SER:N	1.84	0.74
13:M:43:LYS:HE3	13:M:91:PRO:HG3	1.69	0.74
1:A:1530:G:H2'	1:A:1531:A:C8	2.23	0.74
14:N:16:VAL:HG13	14:N:17:ILE:HD12	1.69	0.73
2:B:73:ASP:HB2	2:B:83:LEU:HB3	1.69	0.73
4:D:79:LYS:HG2	4:D:82:GLU:HG2	1.70	0.73
1:A:407:U:O2'	5:E:113:GLU:OE1	2.07	0.73
3:C:27:MET:HG2	3:C:189:THR:HA	1.72	0.72
15:O:41:ARG:NH2	20:T:6:LYS:O	2.23	0.72
4:D:36:ASP:OD1	4:D:59:ARG:NH1	2.23	0.71
1:A:677:U:H3	1:A:713:G:H22	1.37	0.71
2:B:43:LYS:NZ	3:C:205:ASP:OD2	2.24	0.71
1:A:664:G:H22	1:A:741:G:H1	1.37	0.70
3:C:73:LYS:NZ	3:C:205:ASP:OD1	2.24	0.70
23:W:57:C:H6	23:W:57:C:H5'	1.55	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:113:ASP:OD2	8:H:122:ASN:ND2	2.25	0.70
4:D:179:ARG:HG3	4:D:206:GLU:HG2	1.74	0.69
2:B:87:GLU:OE1	2:B:91:ARG:NH2	2.26	0.69
1:A:845:A:H8	19:S:10:PHE:HB2	1.57	0.69
1:A:1130:A:OP1	10:J:18:ARG:NH2	2.23	0.69
1:A:933:G:N7	8:H:3:ARG:NH1	2.40	0.69
10:J:52:LEU:HD11	10:J:63:LEU:HD11	1.74	0.68
1:A:1239:A:H62	1:A:1299:A:H62	1.41	0.68
9:I:11:LEU:HD22	9:I:75:ILE:HD11	1.76	0.68
13:M:44:LYS:H	13:M:45:PRO:HD2	1.59	0.68
1:A:254:G:N2	18:R:18:GLU:OE2	2.22	0.67
1:A:974:A:OP1	15:O:69:ARG:NH2	2.27	0.67
4:D:19:ASN:OD1	4:D:54:ARG:NH1	2.26	0.67
4:D:77:ILE:HA	4:D:84:VAL:HG23	1.76	0.67
5:E:100:ASN:OD1	5:E:111:ARG:NH1	2.28	0.67
1:A:261:U:OP2	21:U:74:ARG:NH2	2.27	0.67
1:A:1422:G:H1	1:A:1478:U:H3	1.43	0.67
5:E:131:ASN:O	5:E:131:ASN:ND2	2.27	0.67
1:A:1363:A:O2'	1:A:1365:G:N7	2.27	0.66
2:B:3:GLU:HB2	2:B:8:LEU:HD23	1.76	0.66
1:A:512:U:OP1	5:E:44:ARG:NH2	2.29	0.66
1:A:874:G:H5'	1:A:874:G:C8	2.30	0.66
2:B:51:GLU:HA	2:B:54:LYS:HG3	1.78	0.66
5:E:85:ASN:ND2	6:F:101:GLU:OE2	2.29	0.66
6:F:52:LYS:HB2	6:F:52:LYS:HZ3	1.59	0.66
6:F:114:VAL:HG11	6:F:140:THR:HG21	1.78	0.66
11:K:3:ASN:HB3	11:K:79:PRO:HD2	1.76	0.66
5:E:102:VAL:HG13	5:E:114:ALA:HB1	1.76	0.66
1:A:1266:G:N2	1:A:1269:A:OP2	2.23	0.65
10:J:88:MET:HE1	10:J:94:LEU:HB2	1.78	0.65
1:A:908:A:H2'	1:A:909:A:C8	2.32	0.65
6:F:68:ARG:HH12	23:W:21:H2U:C4	2.10	0.65
8:H:113:ASP:N	8:H:113:ASP:OD1	2.27	0.65
15:O:24:ARG:NH1	15:O:55:SER:OG	2.29	0.65
20:T:36:ARG:NH2	20:T:75:ALA:O	2.30	0.65
8:H:111:ARG:NH2	8:H:126:ASP:OD2	2.29	0.64
1:A:874:G:H5'	1:A:874:G:H8	1.62	0.64
11:K:59:LYS:HE2	11:K:62:ARG:NH2	2.13	0.64
1:A:1119:C:OP2	10:J:11:ARG:NH2	2.31	0.64
8:H:4:ARG:NH1	8:H:4:ARG:HG3	2.13	0.64
1:A:1052:U:O2'	1:A:1055:A:OP2	2.10	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:88:MET:HE3	10:J:88:MET:HA	1.79	0.64
1:A:908:A:H2'	1:A:909:A:H8	1.63	0.64
5:E:196:ASN:HB3	5:E:199:LEU:HD13	1.78	0.63
8:H:5:ARG:CG	8:H:6:VAL:H	2.08	0.63
23:W:56:PSU:H2'	23:W:58:A:OP2	1.99	0.63
2:B:185:LEU:O	2:B:189:LEU:N	2.32	0.62
5:E:101:VAL:HG21	5:E:137:VAL:HG21	1.81	0.62
5:E:202:GLU:OE2	6:F:112:ARG:NH1	2.32	0.62
1:A:810:C:H5''	1:A:810:C:H6	1.62	0.62
1:A:874:G:H8	1:A:874:G:C5'	2.13	0.62
1:A:405:U:O4	5:E:2:ALA:N	2.33	0.62
6:F:60:ILE:HD12	6:F:61:GLN:N	2.15	0.61
1:A:477:C:H2'	1:A:478:A:C8	2.35	0.61
1:A:993:G:H2'	1:A:993:G:N3	2.15	0.61
5:E:194:ASP:OD1	5:E:194:ASP:N	2.28	0.61
1:A:1517:G:H3'	1:A:1518:MA6:H8	1.82	0.60
22:V:62:ARG:NH1	24:X:11:U:O4	2.34	0.60
1:A:1305:G:H1'	1:A:1332:A:H61	1.66	0.60
6:F:38:VAL:HG12	6:F:117:VAL:HG11	1.83	0.60
1:A:159:G:N2	1:A:162:A:OP2	2.30	0.60
12:L:97:ILE:HG22	22:V:12:PHE:HZ	1.66	0.60
1:A:949:A:N7	14:N:105:ASN:ND2	2.49	0.60
7:G:99:ALA:HB1	7:G:103:VAL:HG11	1.84	0.60
8:H:5:ARG:CG	8:H:6:VAL:N	2.57	0.60
1:A:1013:G:N2	1:A:1016:A:OP2	2.32	0.60
4:D:164:ARG:NE	4:D:166:GLU:OE2	2.31	0.60
8:H:78:ARG:HA	8:H:78:ARG:HH11	1.65	0.60
3:C:30:PHE:HE1	3:C:49:MET:HE1	1.67	0.60
13:M:99:ARG:NH1	13:M:105:SER:O	2.35	0.60
8:H:4:ARG:HG3	8:H:4:ARG:HH11	1.66	0.60
1:A:1305:G:H1'	1:A:1332:A:N6	2.17	0.59
9:I:77:ARG:NH1	9:I:79:SER:O	2.35	0.59
18:R:25:ILE:HD11	18:R:61:ILE:HD11	1.84	0.59
22:V:31:GLU:OE2	22:V:34:ARG:NH2	2.31	0.59
23:W:33:OMC:H6	23:W:33:OMC:O5'	1.86	0.59
13:M:34:CYS:HA	13:M:55:VAL:HG12	1.85	0.59
2:B:39:ASP:HB2	2:B:45:GLU:HG3	1.85	0.58
6:F:34:THR:HG22	6:F:52:LYS:HG3	1.84	0.58
10:J:39:PHE:O	10:J:45:ARG:NH1	2.36	0.58
24:X:15:C:H5''	24:X:16:A:H5'	1.85	0.58
3:C:128:LYS:H	3:C:128:LYS:HD2	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:U:HO2'	1:A:1018:G:H8	1.51	0.58
3:C:129:LEU:HB2	3:C:133:GLU:HB2	1.86	0.58
21:U:15:GLU:OE2	21:U:19:LYS:NZ	2.37	0.58
1:A:652:U:O4	1:A:752:G:O2'	2.19	0.58
1:A:1106:G:O2'	4:D:169:ARG:NH1	2.30	0.57
22:V:39:GLU:OE2	22:V:47:ARG:NH2	2.36	0.57
6:F:115:LEU:HD13	6:F:123:VAL:HG11	1.86	0.57
1:A:1025:U:H4'	1:A:1026:G:H5'	1.86	0.57
1:A:31:G:O2'	1:A:48:C:N4	2.36	0.57
1:A:259:G:OP1	21:U:36:TYR:OH	2.19	0.57
1:A:918:A:H2'	1:A:919:A:C8	2.39	0.57
1:A:1004:A:C6	1:A:1026:G:H1'	2.39	0.57
1:A:1413:A:H2	1:A:1487:G:H22	1.52	0.57
2:B:96:ILE:HG22	2:B:100:LYS:HE3	1.87	0.57
10:J:58:VAL:HG13	10:J:59:GLU:HG3	1.85	0.57
23:W:70:C:H2'	23:W:71:G:C8	2.40	0.57
1:A:1423:G:H1	1:A:1477:U:H3	1.51	0.57
1:A:1477:U:H2'	1:A:1478:U:C6	2.40	0.57
11:K:52:LEU:HD23	11:K:62:ARG:HG2	1.87	0.57
2:B:76:GLU:HG2	2:B:80:GLY:HA2	1.85	0.56
2:B:63:GLN:NE2	2:B:66:ASP:OD2	2.38	0.56
1:A:458:U:H5''	1:A:458:U:H6	1.69	0.56
1:A:673:A:O3'	7:G:86:ARG:NH2	2.39	0.56
1:A:1017:U:O2'	1:A:1018:G:O4'	2.23	0.56
5:E:107:PHE:HB3	5:E:145:ILE:HD11	1.87	0.56
1:A:1497:G:C8	1:A:1497:G:H5''	2.41	0.56
7:G:38:ARG:NH1	7:G:98:GLU:O	2.33	0.56
3:C:97:LEU:H	3:C:100:MET:HE3	1.68	0.56
4:D:110:GLU:HB2	4:D:144:LEU:HD12	1.88	0.56
1:A:691:G:O6	12:L:57:LYS:NZ	2.39	0.56
1:A:769:G:H4'	1:A:1513:A:H4'	1.87	0.56
1:A:819:A:O5'	1:A:819:A:H8	1.89	0.56
1:A:1297:G:H21	8:H:114:LYS:HB3	1.71	0.56
1:A:814:A:O2'	1:A:1510:C:O2'	2.24	0.55
1:A:1427:C:H2'	1:A:1428:A:H8	1.71	0.55
10:J:118:LEU:HD22	10:J:124:ARG:HG2	1.87	0.55
13:M:33:VAL:HG22	13:M:79:VAL:HG12	1.87	0.55
13:M:34:CYS:SG	13:M:37:VAL:HG23	2.47	0.55
3:C:97:LEU:HB2	3:C:100:MET:HG3	1.89	0.55
8:H:18:PHE:HB3	8:H:59:LEU:HD11	1.87	0.55
12:L:88:GLY:O	12:L:93:ARG:HD2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:G:H2'	1:A:822:U:C6	2.42	0.55
4:D:132:ARG:NH2	23:W:57:C:OP2	2.40	0.55
24:X:11:U:H4'	24:X:12:A:O5'	2.06	0.55
9:I:112:THR:HG23	9:I:115:ALA:H	1.72	0.55
1:A:23:C:H6	1:A:23:C:O5'	1.89	0.55
1:A:1318:A:OP2	1:A:1318:A:H8	1.90	0.55
2:B:18:THR:O	2:B:18:THR:OG1	2.22	0.55
10:J:123:ARG:NH1	10:J:124:ARG:O	2.39	0.55
1:A:1299:A:O2'	1:A:1301:U:O4'	2.24	0.55
1:A:1323:G:H2'	1:A:1324:A:C8	2.42	0.55
1:A:1536:C:H2'	1:A:1537:U:C6	2.42	0.55
21:U:35:VAL:HG21	21:U:54:MET:HG2	1.87	0.55
1:A:1499:A:H5'	1:A:1519:MA6:H92	1.89	0.54
6:F:156:LYS:NZ	9:I:73:GLU:OE2	2.39	0.54
1:A:926:G:O5'	1:A:926:G:H8	1.88	0.54
1:A:718:A:C5'	12:L:119:ASN:HD21	2.20	0.54
11:K:59:LYS:HE2	11:K:62:ARG:HH21	1.72	0.54
1:A:1070:U:H2'	1:A:1071:C:C6	2.42	0.54
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.89	0.54
2:B:76:GLU:HG3	3:C:18:HIS:HA	1.90	0.54
6:F:157:ARG:NH2	9:I:43:GLU:OE1	2.41	0.54
1:A:49:U:O2	1:A:362:G:H1'	2.07	0.53
1:A:1034:G:H2'	1:A:1035:A:C8	2.43	0.53
12:L:18:ASP:HB2	12:L:37:ARG:HH21	1.72	0.53
13:M:55:VAL:HG11	13:M:80:ILE:HD11	1.89	0.53
19:S:9:LYS:HA	24:X:14:U:H5'	1.90	0.53
1:A:866:C:C4	1:A:867:G:H1'	2.43	0.53
23:W:70:C:H2'	23:W:71:G:H8	1.73	0.53
5:E:132:ILE:HG23	5:E:135:TYR:HB2	1.90	0.53
23:W:72:C:H2'	23:W:73:A:H5'	1.90	0.53
1:A:844:G:H21	1:A:845:A:H2	1.56	0.53
1:A:1317:C:H5''	15:O:24:ARG:HH21	1.71	0.53
8:H:68:ASN:ND2	8:H:130:ASN:OD1	2.41	0.53
14:N:90:ARG:HB2	14:N:97:VAL:HG23	1.90	0.53
1:A:451:A:H61	1:A:481:G:H5'	1.73	0.53
1:A:526:C:C4	1:A:527:G7M:H1'	2.44	0.53
3:C:9:MET:HE3	3:C:47:VAL:HG22	1.90	0.53
1:A:606:G:N2	1:A:632:U:OP1	2.32	0.53
1:A:1497:G:H5''	1:A:1497:G:H8	1.74	0.53
1:A:816:A:OP1	1:A:1526:G:O2'	2.24	0.53
23:W:33:OMC:HM23	23:W:38:A:H61	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:G:H2'	1:A:338:A:C8	2.43	0.53
1:A:544:G:OP1	5:E:56:ARG:NH1	2.41	0.53
1:A:845:A:C8	19:S:10:PHE:HB2	2.41	0.52
6:F:40:GLY:HA3	6:F:117:VAL:HG13	1.91	0.52
10:J:3:GLU:OE2	10:J:4:ASN:ND2	2.42	0.52
1:A:1320:C:O2	20:T:36:ARG:NH1	2.41	0.52
1:A:926:G:H2'	1:A:1505:G:N3	2.25	0.52
1:A:890:G:O2'	1:A:906:A:N6	2.42	0.52
1:A:946:A:H2'	1:A:947:G:C8	2.45	0.52
1:A:874:G:C8	1:A:874:G:C5'	2.89	0.52
1:A:1423:G:N2	1:A:1477:U:O2	2.35	0.52
1:A:1534:A:O2'	22:V:54:LYS:NZ	2.43	0.52
23:W:51:U:H3	23:W:65:G:H1	1.56	0.52
1:A:79:G:H2'	1:A:80:A:C8	2.44	0.52
1:A:1498:UR3:H1'	1:A:1499:A:N7	2.23	0.52
23:W:56:PSU:OP2	23:W:56:PSU:H6	1.93	0.52
23:W:31:G:H2'	23:W:32:G:H8	1.75	0.52
1:A:864:A:O5'	1:A:864:A:C8	2.63	0.52
3:C:117:LEU:HD22	3:C:141:LEU:HB2	1.92	0.52
5:E:45:LYS:NZ	23:W:19:G:O6	2.43	0.52
1:A:1016:A:HO2'	1:A:1217:C:HO2'	1.58	0.52
1:A:1516:2MG:HM21	1:A:1519:MA6:H2	1.91	0.52
11:K:37:ARG:HH11	11:K:37:ARG:HB3	1.75	0.52
13:M:74:LEU:HD11	13:M:104:CYS:SG	2.49	0.52
24:X:18:G:H2'	24:X:19:U:O4'	2.09	0.52
1:A:460:A:H2'	1:A:461:A:C8	2.45	0.51
1:A:713:G:H2'	1:A:714:G:C8	2.45	0.51
1:A:1136:C:H3'	1:A:1137:C:H6	1.76	0.51
20:T:50:ALA:HB1	20:T:57:HIS:HB3	1.91	0.51
1:A:572:A:O2'	1:A:916:U:O2'	2.23	0.51
5:E:15:GLU:OE2	5:E:56:ARG:NH2	2.42	0.51
11:K:54:SER:OG	11:K:57:VAL:O	2.26	0.51
1:A:1382:C:O2'	8:H:79:ARG:NH1	2.43	0.51
20:T:30:PRO:HA	20:T:48:THR:HG23	1.92	0.51
23:W:17:C:H5''	23:W:18:U:C6	2.46	0.51
1:A:1225:A:H2'	1:A:1226:C:C5	2.45	0.51
1:A:87:C:H2'	1:A:88:U:C6	2.46	0.51
1:A:252:U:O4	1:A:253:A:N6	2.44	0.51
1:A:1062:U:H2'	1:A:1063:C:C6	2.45	0.51
3:C:69:PHE:HB3	3:C:80:VAL:HG22	1.92	0.51
1:A:202:G:O2'	1:A:468:A:H8	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:4OC:H6	1:A:1402:4OC:O5'	2.11	0.50
11:K:50:THR:HG22	11:K:62:ARG:HD3	1.93	0.50
22:V:63:GLU:HA	22:V:66:ARG:HE	1.77	0.50
9:I:9:ASP:OD2	9:I:13:ARG:NH1	2.43	0.50
17:Q:68:SER:HB3	17:Q:71:VAL:HG22	1.93	0.50
23:W:54:G:H3'	23:W:55:5MU:H73	1.93	0.50
1:A:1356:G:H2'	1:A:1357:A:C8	2.46	0.50
1:A:1478:U:H2'	1:A:1479:C:C6	2.45	0.50
3:C:56:GLU:HG2	3:C:198:PHE:CZ	2.46	0.50
5:E:4:TYR:CE2	5:E:11:LEU:HD21	2.45	0.50
5:E:72:PHE:HE1	5:E:94:LEU:HD11	1.77	0.50
6:F:89:HIS:HD2	6:F:135:ASN:HD22	1.58	0.50
12:L:16:VAL:O	12:L:17:SER:OG	2.25	0.50
1:A:966:2MG:N3	1:A:966:2MG:H2'	2.26	0.50
13:M:66:TYR:HB2	13:M:93:VAL:HG11	1.93	0.50
1:A:572:A:HO2'	1:A:916:U:HO2'	1.58	0.50
23:W:32:G:H3'	23:W:33:OMC:C5	2.46	0.49
1:A:525:C:H2'	1:A:526:C:O4'	2.11	0.49
1:A:692:U:O2'	1:A:694:A:N7	2.31	0.49
1:A:384:G:H2'	1:A:385:C:C6	2.47	0.49
1:A:859:G:H2'	1:A:860:A:C8	2.47	0.49
1:A:1425:U:H2'	1:A:1426:G:H8	1.76	0.49
4:D:153:VAL:HG12	4:D:157:LEU:HD21	1.93	0.49
12:L:17:SER:HA	12:L:79:ILE:HA	1.94	0.49
1:A:999:C:H2'	1:A:1000:A:C8	2.48	0.49
1:A:1009:U:H3	1:A:1020:G:H1	1.61	0.49
5:E:140:ASN:N	5:E:182:PHE:O	2.45	0.49
11:K:25:ILE:HD11	11:K:92:LEU:HD11	1.94	0.49
1:A:492:C:H2'	1:A:493:A:C8	2.47	0.49
1:A:1010:U:H2'	1:A:1011:C:C6	2.48	0.49
1:A:1034:G:H2'	1:A:1035:A:H8	1.77	0.49
23:W:20:G:H4'	23:W:21:H2U:OP2	2.12	0.49
1:A:399:G:H2'	1:A:400:C:C6	2.48	0.49
1:A:1218:C:H2'	1:A:1219:A:C8	2.48	0.49
5:E:99:ASP:OD2	5:E:133:ALA:HB1	2.13	0.48
19:S:32:TYR:O	19:S:40:VAL:HG12	2.14	0.48
1:A:1486:G:H2'	1:A:1487:G:C8	2.49	0.48
7:G:29:ILE:HD13	7:G:64:VAL:HG11	1.95	0.48
19:S:72:ASP:OD1	19:S:72:ASP:N	2.47	0.48
1:A:1377:A:OP1	8:H:92:ARG:NH2	2.46	0.48
1:A:531:U:H4'	1:A:532:A:OP1	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:C:HO2'	1:A:1141:C:C5'	2.26	0.48
1:A:1497:G:H4'	1:A:1497:G:OP1	2.14	0.48
3:C:134:ALA:O	3:C:138:THR:OG1	2.23	0.48
1:A:254:G:OP1	18:R:70:THR:HG22	2.13	0.48
4:D:179:ARG:NE	4:D:206:GLU:OE2	2.45	0.48
5:E:85:ASN:HB3	5:E:88:GLU:HG2	1.94	0.48
1:A:475:C:H2'	1:A:476:U:C6	2.48	0.48
1:A:501:C:OP1	13:M:114:ARG:NH2	2.35	0.48
1:A:522:C:H41	13:M:50:ARG:NH2	2.12	0.48
1:A:810:C:H5''	1:A:810:C:C6	2.48	0.48
1:A:1391:U:H2'	1:A:1392:G:C8	2.49	0.48
4:D:20:SER:OG	4:D:22:TRP:NE1	2.47	0.48
5:E:156:LYS:HE3	5:E:178:MET:HE1	1.95	0.48
1:A:1216:A:H5''	15:O:5:SER:HB3	1.97	0.47
2:B:97:THR:HA	2:B:100:LYS:HZ2	1.77	0.47
5:E:141:ASP:OD1	5:E:142:VAL:N	2.47	0.47
5:E:198:HIS:CD2	5:E:198:HIS:H	2.30	0.47
1:A:801:U:H2'	1:A:802:A:C8	2.49	0.47
1:A:521:G:H4'	13:M:70:GLU:HG2	1.97	0.47
1:A:1347:G:H5''	10:J:109:ARG:HB3	1.95	0.47
1:A:81:A:H2'	1:A:82:G:C8	2.49	0.47
1:A:502:A:OP1	13:M:115:SER:HB3	2.15	0.47
11:K:50:THR:HG23	11:K:64:GLN:HG2	1.96	0.47
2:B:18:THR:O	3:C:36:ASN:ND2	2.48	0.47
3:C:18:HIS:H	3:C:189:THR:HG22	1.79	0.47
7:G:45:ARG:O	7:G:56:LYS:HA	2.15	0.47
12:L:87:LYS:HD3	12:L:115:PRO:HD3	1.96	0.47
1:A:275:G:H5'	18:R:16:LYS:HD3	1.95	0.47
1:A:335:C:H2'	1:A:336:A:C8	2.50	0.47
1:A:819:A:H8	1:A:819:A:C5'	2.28	0.47
1:A:1071:C:H2'	1:A:1072:G:C8	2.49	0.47
1:A:1287:A:H2'	1:A:1288:A:C8	2.49	0.47
1:A:1499:A:C8	1:A:1519:MA6:H8	2.50	0.47
2:B:95:TRP:HA	2:B:98:LEU:HD12	1.96	0.47
17:Q:48:GLU:OE2	17:Q:51:ARG:NH2	2.43	0.47
1:A:864:A:H3'	1:A:865:A:C8	2.49	0.47
1:A:1427:C:H2'	1:A:1428:A:C8	2.49	0.47
6:F:99:ALA:CB	6:F:103:THR:HG21	2.45	0.47
7:G:69:GLU:H	7:G:69:GLU:CD	2.21	0.47
10:J:41:ARG:HD3	10:J:43:THR:HB	1.97	0.47
24:X:10:G:H4'	24:X:12:A:C5	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:MET:HA	3:C:107:VAL:HG21	1.97	0.47
23:W:57:C:H5'	23:W:57:C:C6	2.43	0.47
1:A:51:A:N7	1:A:114:U:O2'	2.44	0.47
1:A:266:G:H3'	18:R:69:LYS:HB2	1.97	0.47
1:A:864:A:H8	1:A:864:A:C5'	2.27	0.47
1:A:1297:G:O2'	8:H:114:LYS:HE3	2.15	0.47
1:A:664:G:OP1	19:S:57:ARG:NH2	2.44	0.46
1:A:923:A:H2'	1:A:924:C:O4'	2.15	0.46
1:A:1328:C:H5''	14:N:28:THR:HG21	1.97	0.46
1:A:22:G:C8	1:A:22:G:H5''	2.51	0.46
1:A:207:C:H2'	1:A:208:U:O4'	2.16	0.46
1:A:1417:G:O2'	1:A:1483:A:N6	2.40	0.46
23:W:52:C:H2'	23:W:53:G:O4'	2.16	0.46
1:A:995:C:H2'	1:A:996:A:H5''	1.97	0.46
1:A:1405:G:H2'	1:A:1406:U:C6	2.50	0.46
5:E:177:LYS:HB3	5:E:179:GLU:HG2	1.97	0.46
16:P:78:TYR:OH	16:P:89:ARG:O	2.21	0.46
24:X:19:U:H2'	24:X:20:U:O4'	2.15	0.46
1:A:216:U:H2'	1:A:217:C:C6	2.50	0.46
1:A:999:C:H2'	1:A:1000:A:H8	1.80	0.46
2:B:8:LEU:HD12	3:C:10:LEU:HD13	1.96	0.46
12:L:97:ILE:HG22	22:V:12:PHE:CZ	2.48	0.46
15:O:35:ASN:H	15:O:35:ASN:ND2	2.13	0.46
10:J:29:VAL:HG13	10:J:64:TYR:HA	1.97	0.46
16:P:32:LEU:HD22	16:P:59:MET:HG2	1.98	0.46
8:H:4:ARG:HH11	8:H:4:ARG:CG	2.26	0.46
14:N:10:PRO:HG2	14:N:13:LYS:HE2	1.97	0.46
1:A:371:A:H2'	1:A:372:C:O4'	2.16	0.46
3:C:18:HIS:H	3:C:189:THR:CG2	2.29	0.46
5:E:170:TRP:CD2	5:E:186:PRO:HB3	2.51	0.46
7:G:42:TRP:CZ2	7:G:102:MET:HG3	2.51	0.46
3:C:111:ILE:HD12	3:C:152:LYS:HA	1.97	0.46
8:H:2:PRO:HG3	8:H:7:ILE:HG12	1.98	0.46
1:A:1071:C:H6	1:A:1071:C:O5'	1.99	0.46
7:G:104:LYS:HE3	7:G:104:LYS:HA	1.98	0.46
1:A:171:A:H2'	1:A:172:A:C8	2.51	0.46
1:A:616:G:O2'	17:Q:47:GLU:OE2	2.34	0.46
1:A:1038:C:H2'	1:A:1039:G:H8	1.80	0.46
1:A:1140:C:O2'	1:A:1141:C:O5'	2.33	0.46
1:A:1273:C:H2'	1:A:1274:A:O4'	2.16	0.46
2:B:289:ASP:H	7:G:56:LYS:HG3	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:THR:HG22	3:C:39:HIS:CE1	2.51	0.46
6:F:162:GLU:CD	6:F:162:GLU:H	2.24	0.46
8:H:9:GLN:OE1	8:H:10:ARG:N	2.49	0.46
24:X:10:G:H2'	24:X:11:U:C6	2.51	0.46
1:A:79:G:H2'	1:A:80:A:H8	1.81	0.45
1:A:299:G:H2'	1:A:300:A:C8	2.51	0.45
1:A:1479:C:H2'	1:A:1480:A:C8	2.51	0.45
11:K:36:VAL:HB	11:K:76:ILE:HD13	1.98	0.45
1:A:763:G:H2'	1:A:764:C:C6	2.52	0.45
1:A:1268:G:H2'	1:A:1269:A:C8	2.51	0.45
1:A:1396:A:H4'	1:A:1397:C:H5''	1.99	0.45
4:D:151:VAL:HG12	4:D:200:VAL:HG22	1.98	0.45
23:W:32:G:H3'	23:W:33:OMC:C6	2.51	0.45
1:A:768:A:H1'	1:A:1512:U:H1'	1.99	0.45
1:A:923:A:H61	1:A:1393:U:H3	1.64	0.45
12:L:52:PHE:O	12:L:53:ARG:HD2	2.15	0.45
12:L:81:ASN:OD1	12:L:106:ARG:HD3	2.17	0.45
1:A:181:A:O2'	1:A:194:C:N4	2.49	0.45
9:I:102:ALA:N	9:I:113:ASP:OD2	2.34	0.45
24:X:10:G:H4'	24:X:12:A:N7	2.32	0.45
1:A:227:G:O2'	17:Q:63:GLN:OE1	2.24	0.45
1:A:235:C:H2'	1:A:236:A:C8	2.51	0.45
1:A:1539:C:H2'	1:A:1540:U:H6	1.80	0.45
2:B:89:ALA:O	2:B:93:GLU:HG3	2.17	0.45
1:A:108:G:H5''	1:A:109:A:H5''	1.99	0.45
1:A:410:G:H2'	1:A:429:U:C4	2.51	0.45
1:A:863:U:O5'	1:A:863:U:H6	1.99	0.45
1:A:932:C:OP1	8:H:4:ARG:HG2	2.17	0.45
6:F:80:THR:HG23	6:F:122:ASN:O	2.17	0.45
10:J:36:GLU:HA	10:J:45:ARG:HD3	1.98	0.45
16:P:18:ASP:OD1	16:P:21:ASP:HB2	2.17	0.45
1:A:60:A:H4'	1:A:61:G:O5'	2.17	0.45
1:A:81:A:H2'	1:A:82:G:H8	1.82	0.45
1:A:662:U:H2'	1:A:663:A:C8	2.52	0.45
1:A:1010:U:H2'	1:A:1011:C:H6	1.82	0.45
7:G:47:LEU:HD12	7:G:54:LEU:O	2.17	0.45
12:L:16:VAL:HG23	12:L:79:ILE:HG12	1.99	0.45
24:X:11:U:H1'	24:X:12:A:OP2	2.16	0.45
1:A:135:C:N3	17:Q:1:MET:HB2	2.32	0.45
4:D:120:ILE:HA	4:D:123:GLN:HE21	1.82	0.45
10:J:46:MET:SD	10:J:50:GLN:NE2	2.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:116:VAL:HG13	11:K:62:ARG:HH11	1.82	0.45
15:O:19:LYS:HE3	15:O:20:TYR:CE2	2.52	0.45
1:A:1517:G:C3'	1:A:1518:MA6:H8	2.47	0.44
6:F:45:ARG:HE	6:F:71:MET:HE3	1.82	0.44
1:A:161:A:H2'	1:A:162:A:C8	2.52	0.44
1:A:464:U:O2'	1:A:466:A:N7	2.47	0.44
1:A:1451:U:H5''	1:A:1452:C:H5	1.82	0.44
6:F:80:THR:HG22	6:F:81:LEU:H	1.81	0.44
5:E:101:VAL:O	5:E:105:MET:HG2	2.18	0.44
1:A:184:G:H2'	1:A:185:U:C6	2.52	0.44
1:A:335:C:H2'	1:A:336:A:H8	1.83	0.44
2:B:69:ASP:O	2:B:86:ARG:NE	2.50	0.44
4:D:23:PHE:CD1	11:K:97:ASP:HB2	2.53	0.44
19:S:48:ARG:HE	19:S:48:ARG:HB3	1.60	0.44
1:A:540:G:H21	5:E:40:GLN:NE2	2.14	0.44
1:A:1538:C:H2'	1:A:1539:C:H6	1.83	0.44
3:C:54:LEU:HD12	3:C:54:LEU:HA	1.85	0.44
4:D:110:GLU:OE1	4:D:110:GLU:N	2.45	0.44
1:A:975:A:N1	1:A:1366:C:O2'	2.38	0.44
4:D:155:GLY:HA2	4:D:163:ALA:HB1	1.98	0.44
5:E:87:GLY:HA3	5:E:197:GLU:HG3	1.99	0.44
9:I:56:LYS:HB3	9:I:56:LYS:HE2	1.78	0.44
9:I:89:LYS:HE3	9:I:89:LYS:HB3	1.58	0.44
14:N:66:GLU:OE1	14:N:70:ARG:NH1	2.46	0.44
21:U:70:ASN:O	21:U:74:ARG:HG3	2.17	0.44
1:A:382:A:H2'	1:A:383:A:C8	2.52	0.44
1:A:1081:A:H8	1:A:1081:A:H5''	1.82	0.44
7:G:4:TYR:CD2	7:G:71:ILE:HG13	2.52	0.44
1:A:501:C:H2'	1:A:502:A:C8	2.53	0.44
1:A:951:G:OP2	14:N:101:ARG:NH2	2.51	0.44
2:B:72:LEU:HA	2:B:84:LEU:HD23	1.99	0.44
4:D:150:LYS:HE3	4:D:201:TRP:CE3	2.53	0.44
5:E:50:ASP:OD1	5:E:50:ASP:N	2.49	0.44
5:E:190:ASP:OD1	5:E:190:ASP:N	2.51	0.44
16:P:15:PHE:CE2	16:P:84:ARG:HD2	2.53	0.44
21:U:28:MET:SD	21:U:67:ILE:HD12	2.57	0.44
23:W:10:G:C2	23:W:27:G:H1'	2.53	0.44
1:A:204:U:H2'	1:A:205:A:O4'	2.18	0.44
1:A:801:U:H2'	1:A:802:A:H8	1.81	0.44
1:A:958:A:C4	20:T:55:ARG:HD3	2.53	0.44
1:A:1498:UR3:H5'	1:A:1519:MA6:H103	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ALA:O	2:B:97:THR:HG22	2.18	0.43
5:E:49:SER:O	5:E:53:VAL:HG13	2.18	0.43
7:G:12:PRO:HB3	7:G:56:LYS:O	2.18	0.43
1:A:559:A:H4'	1:A:560:A:H3'	1.99	0.43
10:J:21:ILE:HG12	10:J:63:LEU:HD22	2.00	0.43
12:L:16:VAL:HG22	12:L:77:TYR:HB3	1.99	0.43
1:A:361:G:H2'	1:A:362:G:O4'	2.18	0.43
1:A:869:G:H8	1:A:869:G:O5'	2.01	0.43
1:A:1008:U:H2'	1:A:1009:U:C6	2.53	0.43
14:N:95:LEU:HD22	14:N:102:THR:HG21	2.00	0.43
17:Q:71:VAL:O	17:Q:75:ILE:HG13	2.18	0.43
21:U:28:MET:HE2	21:U:28:MET:HB3	1.81	0.43
1:A:819:A:C5'	1:A:819:A:C8	3.01	0.43
1:A:1098:C:O2'	22:V:71:TYR:OXT	2.34	0.43
3:C:6:MET:HE3	3:C:6:MET:HB2	1.80	0.43
10:J:17:ALA:HB2	10:J:67:VAL:HG13	2.01	0.43
2:B:43:LYS:NZ	3:C:188:ASP:OD2	2.42	0.43
7:G:51:ILE:O	7:G:54:LEU:HB2	2.19	0.43
23:W:34:U:O2	23:W:36:A:H3'	2.19	0.43
1:A:564:C:C6	1:A:564:C:OP1	2.72	0.43
1:A:628:G:H2'	1:A:629:A:C8	2.53	0.43
1:A:1538:C:H2'	1:A:1539:C:C6	2.53	0.43
5:E:50:ASP:O	5:E:53:VAL:HG22	2.19	0.43
1:A:459:A:H2'	1:A:460:A:C8	2.53	0.43
2:B:39:ASP:OD2	3:C:208:ARG:NE	2.49	0.43
18:R:23:VAL:HG11	18:R:59:VAL:HG21	2.01	0.43
3:C:67:ILE:H	3:C:89:GLN:NE2	2.17	0.43
3:C:187:VAL:HG22	3:C:191:SER:HB2	1.99	0.43
11:K:11:LYS:NZ	11:K:71:LEU:HD21	2.34	0.43
1:A:532:A:H5''	1:A:532:A:C4	2.53	0.43
1:A:1226:C:P	14:N:90:ARG:HH22	2.42	0.43
4:D:134:MET:HB2	4:D:151:VAL:HG21	2.01	0.43
13:M:102:LEU:HD23	13:M:102:LEU:HA	1.82	0.43
1:A:1140:C:O2'	1:A:1141:C:H6	2.02	0.43
3:C:157:LEU:HD13	3:C:179:LEU:HD13	2.00	0.43
4:D:7:PRO:HD2	4:D:184:TYR:CD2	2.53	0.43
5:E:146:ARG:HD3	5:E:148:LYS:HE2	2.01	0.43
6:F:100:SER:O	6:F:103:THR:HG22	2.19	0.43
23:W:48:U:O2'	23:W:49:C:OP2	2.24	0.43
1:A:343:U:H2'	1:A:345:C:C5	2.54	0.42
1:A:810:C:H3'	1:A:811:C:C6	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:5MC:H2'	1:A:1408:A:C8	2.54	0.42
1:A:1418:A:N6	1:A:1482:G:O2'	2.52	0.42
9:I:25:VAL:HG13	9:I:63:LEU:HD11	2.01	0.42
12:L:112:ASP:HB3	22:V:2:PRO:HG2	2.01	0.42
24:X:7:G:H2'	24:X:8:A:C8	2.54	0.42
1:A:131:A:H2'	1:A:132:C:C6	2.54	0.42
1:A:1171:A:H2'	1:A:1172:C:C6	2.54	0.42
5:E:98:LEU:O	5:E:102:VAL:HG12	2.19	0.42
21:U:32:ILE:HG12	21:U:54:MET:HE2	2.00	0.42
23:W:14:A:H2'	23:W:15:G:O4'	2.20	0.42
1:A:13:U:O2	1:A:914:A:H3'	2.19	0.42
1:A:92:U:H2'	1:A:93:U:C6	2.54	0.42
1:A:381:C:H2'	1:A:382:A:O4'	2.19	0.42
1:A:766:A:H61	1:A:1511:G:H1'	1.84	0.42
5:E:125:VAL:HG12	5:E:143:VAL:HG22	2.01	0.42
7:G:19:PRO:O	7:G:23:GLU:HG2	2.19	0.42
8:H:74:GLU:O	8:H:88:PRO:HA	2.19	0.42
1:A:1537:U:H2'	1:A:1538:C:C6	2.54	0.42
4:D:105:GLU:HG2	4:D:107:ARG:HD2	2.02	0.42
9:I:102:ALA:HB3	9:I:113:ASP:HB3	2.00	0.42
10:J:27:LYS:HE2	10:J:27:LYS:HB3	1.86	0.42
20:T:42:PRO:O	20:T:45:ILE:HG12	2.19	0.42
21:U:57:ILE:O	21:U:61:GLN:HG2	2.19	0.42
23:W:44:A:H2'	23:W:45:A:C8	2.55	0.42
1:A:208:U:H3'	1:A:210:C:N4	2.35	0.42
1:A:901:A:C5	1:A:902:G:H1'	2.55	0.42
1:A:1393:U:O5'	1:A:1393:U:H6	2.03	0.42
6:F:60:ILE:HD13	23:W:20:G:C2	2.54	0.42
23:W:14:A:C2	23:W:15:G:H1'	2.55	0.42
1:A:21:G:H1'	1:A:915:A:N6	2.34	0.42
1:A:142:G:O2'	1:A:196:A:N1	2.38	0.42
1:A:1119:C:H2'	1:A:1120:C:H6	1.85	0.42
2:B:75:VAL:O	2:B:82:THR:HG22	2.20	0.42
4:D:72:ARG:HG2	4:D:75:ILE:HD12	2.02	0.42
4:D:147:LYS:HE3	4:D:147:LYS:HB3	1.87	0.42
7:G:1:MET:HE3	7:G:65:GLU:HG2	2.01	0.42
7:G:81:ASN:O	7:G:83:ALA:N	2.47	0.42
1:A:967:5MC:H2'	1:A:968:A:C8	2.55	0.42
2:B:3:GLU:H	2:B:3:GLU:CD	2.26	0.42
5:E:65:TYR:OH	5:E:95:GLU:OE1	2.28	0.42
23:W:31:G:H2'	23:W:32:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:U:O2	1:A:1086:U:O4'	2.34	0.42
1:A:1391:U:H2'	1:A:1392:G:H8	1.84	0.42
10:J:84:THR:HG23	10:J:98:LEU:HD13	2.00	0.42
10:J:88:MET:HE2	10:J:95:ARG:N	2.34	0.42
12:L:113:VAL:HA	19:S:73:ARG:HD3	2.02	0.42
11:K:52:LEU:HB2	15:O:81:ARG:HD2	2.02	0.42
14:N:104:THR:OG1	14:N:105:ASN:N	2.51	0.42
1:A:789:U:O2'	1:A:791:G:N7	2.44	0.42
1:A:986:U:H2'	1:A:987:G:O4'	2.19	0.42
11:K:47:GLU:O	11:K:66:GLU:HA	2.20	0.42
23:W:1:C:H2'	23:W:2:G:H8	1.85	0.42
23:W:44:A:H2'	23:W:45:A:H8	1.85	0.42
23:W:72:C:C2'	23:W:73:A:H5'	2.50	0.42
2:B:6:ALA:O	2:B:10:GLU:HG2	2.20	0.41
12:L:25:ALA:HB1	12:L:90:GLY:HA3	2.01	0.41
24:X:17:U:H2'	24:X:18:G:O4'	2.20	0.41
1:A:924:C:C5'	1:A:924:C:C6	3.03	0.41
1:A:1151:A:HO2'	1:A:1152:A:H8	1.62	0.41
1:A:1255:G:O2'	1:A:1258:G:N3	2.43	0.41
1:A:236:A:H2'	1:A:237:G:C8	2.55	0.41
1:A:651:C:H2'	1:A:652:U:C6	2.55	0.41
1:A:862:C:O5'	1:A:862:C:H6	2.03	0.41
1:A:1329:A:OP1	14:N:29:ARG:HB2	2.21	0.41
4:D:89:LYS:HB2	4:D:89:LYS:HE2	1.72	0.41
1:A:180:U:H2'	1:A:181:A:H5'	2.02	0.41
1:A:864:A:O5'	1:A:864:A:H8	2.02	0.41
1:A:1229:A:OP2	14:N:113:ARG:HD3	2.20	0.41
1:A:1539:C:H2'	1:A:1540:U:C6	2.55	0.41
5:E:48:LEU:HD12	5:E:48:LEU:HA	1.84	0.41
12:L:85:MET:HE2	12:L:85:MET:HB3	1.91	0.41
15:O:47:LYS:HB3	15:O:47:LYS:HE3	1.82	0.41
21:U:54:MET:O	21:U:58:VAL:HG23	2.21	0.41
1:A:270:A:H2'	1:A:271:C:C6	2.55	0.41
1:A:921:U:H2'	1:A:922:G:O4'	2.20	0.41
1:A:1008:U:H2'	1:A:1009:U:H6	1.86	0.41
1:A:1152:A:OP1	11:K:70:HIS:ND1	2.44	0.41
1:A:1479:C:H2'	1:A:1480:A:H8	1.86	0.41
1:A:1489:G:H2'	1:A:1490:U:C6	2.56	0.41
2:B:51:GLU:OE1	2:B:52:GLN:HG2	2.20	0.41
6:F:156:LYS:HB3	6:F:156:LYS:HE2	1.82	0.41
9:I:87:LYS:HG3	9:I:125:ILE:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:C:H2'	1:A:614:C:C6	2.55	0.41
2:B:39:ASP:CG	3:C:208:ARG:HE	2.29	0.41
1:A:7:A:H2	6:F:128:TYR:OH	2.04	0.41
1:A:468:A:H3'	1:A:469:C:H6	1.86	0.41
1:A:532:A:N7	4:D:193:TYR:HE1	2.19	0.41
1:A:642:A:H8	1:A:642:A:O5'	2.04	0.41
1:A:1149:C:H2'	1:A:1150:A:C8	2.56	0.41
1:A:1477:U:H2'	1:A:1478:U:H6	1.82	0.41
11:K:6:ILE:HG13	11:K:76:ILE:HB	2.02	0.41
19:S:50:LYS:HE2	19:S:50:LYS:HB3	1.80	0.41
1:A:481:G:O2'	1:A:483:C:N4	2.46	0.41
1:A:494:G:O2'	1:A:496:A:H1'	2.20	0.41
1:A:1435:G:H2'	1:A:1436:U:C6	2.55	0.41
4:D:131:ARG:O	4:D:135:LYS:HB2	2.19	0.41
9:I:96:MET:HE2	9:I:96:MET:HB3	1.88	0.41
13:M:107:VAL:HG12	13:M:117:TYR:HB3	2.02	0.41
17:Q:6:LEU:HB3	17:Q:17:TYR:HB3	2.01	0.41
1:A:673:A:H2'	1:A:674:G:C8	2.56	0.41
1:A:868:C:H2'	1:A:869:G:O4'	2.21	0.41
1:A:1038:C:H2'	1:A:1039:G:C8	2.56	0.41
1:A:1535:C:H2'	1:A:1536:C:C6	2.56	0.41
2:B:57:GLN:OE1	2:B:57:GLN:N	2.52	0.41
4:D:86:LYS:O	4:D:90:VAL:HG12	2.20	0.41
6:F:99:ALA:HB3	6:F:103:THR:HG21	2.02	0.41
13:M:79:VAL:O	13:M:103:ASP:HB2	2.21	0.41
1:A:407:U:H2'	1:A:408:A:C8	2.56	0.41
1:A:555:U:H2'	1:A:556:C:C6	2.56	0.41
2:B:66:ASP:OD1	2:B:66:ASP:N	2.54	0.41
7:G:75:GLU:O	7:G:79:ARG:HG2	2.20	0.41
12:L:16:VAL:HG23	12:L:17:SER:H	1.85	0.41
12:L:34:ILE:HG13	12:L:70:CYS:SG	2.61	0.41
12:L:89:PRO:HG3	22:V:32:VAL:HG11	2.02	0.41
13:M:37:VAL:HG11	13:M:72:HIS:HE1	1.86	0.41
18:R:19:LYS:NZ	18:R:50:ASN:H	2.19	0.41
1:A:1275:A:H2'	1:A:1276:G:O4'	2.21	0.40
1:A:540:G:H21	5:E:40:GLN:HE22	1.68	0.40
1:A:812:G:H4'	1:A:813:U:H5'	2.03	0.40
1:A:1236:A:H2'	1:A:1237:C:C6	2.56	0.40
2:B:49:PRO:O	2:B:52:GLN:HG3	2.21	0.40
3:C:70:VAL:O	3:C:163:VAL:HA	2.20	0.40
7:G:67:PRO:O	7:G:70:VAL:HG12	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:13:LEU:HD13	8:H:13:LEU:HA	1.90	0.40
13:M:44:LYS:H	13:M:45:PRO:CD	2.32	0.40
21:U:67:ILE:HG12	21:U:71:LYS:HD3	2.04	0.40
1:A:948:C:OP1	14:N:108:THR:HG22	2.22	0.40
5:E:3:ARG:HE	5:E:115:ARG:NH1	2.19	0.40
16:P:80:GLN:HE22	16:P:84:ARG:HE	1.68	0.40
19:S:75:GLN:HE21	19:S:75:GLN:HB3	1.67	0.40
1:A:864:A:C8	1:A:864:A:C5'	3.04	0.40
1:A:941:G:H2'	1:A:942:G:O4'	2.22	0.40
1:A:967:5MC:OP1	1:A:969:A:H5'	2.22	0.40
1:A:1029:U:HO2'	1:A:1032:G:H1	1.67	0.40
2:B:31:ILE:HG12	2:B:63:GLN:HA	2.04	0.40
8:H:5:ARG:O	8:H:6:VAL:C	2.64	0.40
14:N:107:ARG:NH2	14:N:113:ARG:HA	2.36	0.40
17:Q:69:ASP:OD1	17:Q:70:ARG:N	2.55	0.40
1:A:89:U:H2'	1:A:90:C:C6	2.56	0.40
1:A:180:U:C2'	1:A:181:A:H5'	2.51	0.40
1:A:685:G:O2'	1:A:686:U:H5'	2.21	0.40
1:A:864:A:H3'	1:A:865:A:H8	1.87	0.40
2:B:23:ILE:HD11	2:B:92:HIS:ND1	2.37	0.40
3:C:60:ILE:HG12	3:C:63:ARG:HH21	1.87	0.40
10:J:41:ARG:HD3	10:J:41:ARG:HH11	1.78	0.40
21:U:43:ASP:OD1	21:U:44:LYS:N	2.54	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	350/557 (63%)	312 (89%)	37 (11%)	1 (0%)	36 70
3	C	224/241 (93%)	219 (98%)	5 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	209/233 (90%)	204 (98%)	5 (2%)	0	100	100
5	E	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
6	F	154/165 (93%)	145 (94%)	9 (6%)	0	100	100
7	G	102/131 (78%)	99 (97%)	3 (3%)	0	100	100
8	H	150/156 (96%)	142 (95%)	7 (5%)	1 (1%)	18	53
9	I	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
10	J	126/130 (97%)	122 (97%)	3 (2%)	1 (1%)	16	50
11	K	99/103 (96%)	95 (96%)	3 (3%)	1 (1%)	12	45
12	L	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
13	M	119/124 (96%)	112 (94%)	6 (5%)	1 (1%)	16	50
14	N	113/118 (96%)	111 (98%)	1 (1%)	1 (1%)	14	48
15	O	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
16	P	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
17	Q	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
18	R	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
19	S	65/75 (87%)	62 (95%)	1 (2%)	2 (3%)	3	19
20	T	81/92 (88%)	80 (99%)	1 (1%)	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	2731/3104 (88%)	2615 (96%)	108 (4%)	8 (0%)	37	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	5	ARG
11	K	57	VAL
14	N	66	GLU
2	B	262	LEU
13	M	44	LYS
19	S	10	PHE
19	S	22	ASP
10	J	13	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	86/461 (19%)	62 (72%)	24 (28%)	0	2
3	C	187/199 (94%)	176 (94%)	11 (6%)	18	50
4	D	172/190 (90%)	163 (95%)	9 (5%)	21	55
5	E	172/173 (99%)	155 (90%)	17 (10%)	7	30
6	F	119/126 (94%)	111 (93%)	8 (7%)	15	46
7	G	91/112 (81%)	79 (87%)	12 (13%)	4	18
8	H	125/129 (97%)	113 (90%)	12 (10%)	8	31
9	I	104/105 (99%)	99 (95%)	5 (5%)	23	57
10	J	106/107 (99%)	95 (90%)	11 (10%)	7	28
11	K	88/90 (98%)	82 (93%)	6 (7%)	14	45
12	L	90/99 (91%)	88 (98%)	2 (2%)	45	74
13	M	102/103 (99%)	94 (92%)	8 (8%)	11	39
14	N	93/96 (97%)	87 (94%)	6 (6%)	15	47
15	O	83/84 (99%)	83 (100%)	0	100	100
16	P	76/77 (99%)	74 (97%)	2 (3%)	40	72
17	Q	65/65 (100%)	59 (91%)	6 (9%)	8	33
18	R	74/78 (95%)	72 (97%)	2 (3%)	39	71
19	S	58/65 (89%)	52 (90%)	6 (10%)	7	28
20	T	72/79 (91%)	69 (96%)	3 (4%)	26	61
21	U	65/66 (98%)	61 (94%)	4 (6%)	16	49
22	V	60/61 (98%)	54 (90%)	6 (10%)	7	29
All	All	2088/2565 (81%)	1928 (92%)	160 (8%)	14	40

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	3	GLU
2	B	7	GLN
2	B	8	LEU
2	B	13	LEU
2	B	14	LYS
2	B	16	ILE
2	B	17	GLU
2	B	18	THR
2	B	31	ILE
2	B	51	GLU
2	B	52	GLN
2	B	57	GLN
2	B	62	ILE
2	B	63	GLN
2	B	64	VAL
2	B	67	GLU
2	B	69	ASP
2	B	75	VAL
2	B	87	GLU
2	B	93	GLU
2	B	95	TRP
2	B	97	THR
2	B	99	GLU
3	C	19	GLN
3	C	45	LYS
3	C	54	LEU
3	C	80	VAL
3	C	112	LYS
3	C	117	LEU
3	C	129	LEU
3	C	132	LYS
3	C	163	VAL
3	C	183	VAL
3	C	223	GLU
4	D	28	GLU
4	D	52	VAL
4	D	72	ARG
4	D	111	LEU
4	D	135	LYS
4	D	162	ILE
4	D	165	THR
4	D	192	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	206	GLU
5	E	11	LEU
5	E	28	ILE
5	E	29	ASP
5	E	47	ARG
5	E	48	LEU
5	E	129	VAL
5	E	131	ASN
5	E	132	ILE
5	E	136	GLN
5	E	171	LEU
5	E	173	VAL
5	E	184	ARG
5	E	188	ARG
5	E	189	SER
5	E	190	ASP
5	E	194	ASP
5	E	198	HIS
6	F	13	GLU
6	F	52	LYS
6	F	76	LEU
6	F	93	ARG
6	F	94	VAL
6	F	105	ILE
6	F	117	VAL
6	F	153	VAL
7	G	9	MET
7	G	17	GLN
7	G	36	ILE
7	G	56	LYS
7	G	61	LEU
7	G	69	GLU
7	G	74	LEU
7	G	76	THR
7	G	97	THR
7	G	102	MET
7	G	103	VAL
7	G	104	LYS
8	H	4	ARG
8	H	6	VAL
8	H	7	ILE
8	H	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	12	ILE
8	H	58	GLU
8	H	72	THR
8	H	75	VAL
8	H	78	ARG
8	H	80	VAL
8	H	106	GLU
8	H	113	ASP
9	I	50	LYS
9	I	55	THR
9	I	72	VAL
9	I	104	VAL
9	I	110	VAL
10	J	22	LYS
10	J	29	VAL
10	J	58	VAL
10	J	59	GLU
10	J	67	VAL
10	J	88	MET
10	J	89	GLU
10	J	105	THR
10	J	111	VAL
10	J	119	ARG
10	J	130	ARG
11	K	6	ILE
11	K	20	GLN
11	K	36	VAL
11	K	37	ARG
11	K	46	LYS
11	K	102	LEU
12	L	108	THR
12	L	111	THR
13	M	4	VAL
13	M	21	VAL
13	M	24	LEU
13	M	43	LYS
13	M	44	LYS
13	M	107	VAL
13	M	112	GLN
13	M	115	SER
14	N	16	VAL
14	N	28	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	56	LEU
14	N	58	ASP
14	N	102	THR
14	N	104	THR
16	P	6	GLU
16	P	17	ARG
17	Q	3	THR
17	Q	18	GLN
17	Q	21	VAL
17	Q	42	ILE
17	Q	45	GLU
17	Q	77	GLU
18	R	22	VAL
18	R	55	ILE
19	S	10	PHE
19	S	38	LYS
19	S	45	THR
19	S	67	LEU
19	S	74	HIS
19	S	75	GLN
20	T	51	VAL
20	T	58	VAL
20	T	79	THR
21	U	3	ASN
21	U	5	LYS
21	U	6	SER
21	U	67	ILE
22	V	4	ILE
22	V	21	ARG
22	V	24	GLU
22	V	44	GLU
22	V	59	LYS
22	V	63	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	7	GLN
2	B	63	GLN
3	C	39	HIS
3	C	89	GLN
3	C	120	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	3	GLN
4	D	123	GLN
5	E	40	GLN
5	E	136	GLN
5	E	164	GLN
6	F	89	HIS
6	F	122	ASN
6	F	132	ASN
6	F	135	ASN
7	G	37	HIS
7	G	52	ASN
10	J	32	GLN
10	J	37	GLN
10	J	75	GLN
11	K	58	ASN
12	L	15	GLN
12	L	101	ASN
12	L	119	ASN
14	N	8	ASN
15	O	35	ASN
15	O	66	GLN
16	P	20	ASN
16	P	35	GLN
16	P	80	GLN
19	S	75	GLN
21	U	13	GLN
21	U	20	HIS
21	U	52	ASN
21	U	70	ASN
22	V	64	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1537/1541 (99%)	237 (15%)	9 (0%)
23	W	76/77 (98%)	23 (30%)	3 (3%)
24	X	16/53 (30%)	3 (18%)	1 (6%)
All	All	1629/1671 (97%)	263 (16%)	13 (0%)

All (263) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	A
1	A	4	U
1	A	6	G
1	A	9	G
1	A	11	G
1	A	39	G
1	A	44	A
1	A	47	C
1	A	48	C
1	A	51	A
1	A	52	C
1	A	54	C
1	A	70	U
1	A	71	A
1	A	75	G
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	92	U
1	A	95	C
1	A	108	G
1	A	121	U
1	A	130	A
1	A	131	A
1	A	141	G
1	A	149	A
1	A	166	U
1	A	168	G
1	A	173	U
1	A	177	G
1	A	181	A
1	A	189	A
1	A	197	A
1	A	204	U
1	A	212	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	306	A
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	351	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	397	A
1	A	398	U
1	A	406	G
1	A	413	G
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	457	G
1	A	458	U
1	A	463	U
1	A	464	U
1	A	467	U
1	A	468	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	495	A
1	A	496	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	532	A
1	A	533	A
1	A	547	A
1	A	562	U
1	A	563	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	564	C
1	A	566	G
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	588	G
1	A	596	A
1	A	633	G
1	A	642	A
1	A	653	U
1	A	665	A
1	A	682	G
1	A	703	G
1	A	718	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	755	G
1	A	773	G
1	A	775	G
1	A	793	U
1	A	794	A
1	A	809	G
1	A	810	C
1	A	812	G
1	A	813	U
1	A	815	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	U
1	A	832	G
1	A	841	C
1	A	842	U
1	A	843	U
1	A	844	G
1	A	846	G
1	A	859	G
1	A	861	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	862	C
1	A	864	A
1	A	870	U
1	A	871	U
1	A	874	G
1	A	875	U
1	A	876	C
1	A	882	C
1	A	914	A
1	A	916	U
1	A	922	G
1	A	924	C
1	A	925	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	942	G
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C
1	A	992	U
1	A	993	G
1	A	994	A
1	A	996	A
1	A	1004	A
1	A	1009	U
1	A	1018	G
1	A	1020	G
1	A	1025	U
1	A	1027	C
1	A	1028	C
1	A	1031	C
1	A	1033	G
1	A	1044	A
1	A	1065	U
1	A	1066	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1070	U
1	A	1079	G
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1103	C
1	A	1104	G
1	A	1132	C
1	A	1133	G
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	1146	A
1	A	1151	A
1	A	1152	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1260	G
1	A	1278	G
1	A	1279	G
1	A	1280	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	1317	C
1	A	1320	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1332	A
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1394	A
1	A	1398	A
1	A	1429	A
1	A	1432	G
1	A	1441	A
1	A	1442	G
1	A	1446	A
1	A	1451	U
1	A	1453	G
1	A	1489	G
1	A	1497	G
1	A	1498	UR3
1	A	1506	U
1	A	1517	G
1	A	1520	C
1	A	1529	G
1	A	1530	G
1	A	1534	A
1	A	1537	U
23	W	8	4SU
23	W	9	G
23	W	13	C
23	W	16	C
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	43	G
23	W	44	A
23	W	48	U
23	W	49	C
23	W	54	G
23	W	56	PSU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	W	57	C
23	W	58	A
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 (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	428	G
1	A	429	U
1	A	463	U
1	A	532	A
1	A	641	U
1	A	874	G
1	A	924	C
1	A	1065	U
1	A	1078	U
23	W	21	H2U
23	W	48	U
23	W	57	C
24	X	11	U

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

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	$\# Z > 2$
1	4OC	A	1402	1	20,23,24	0.80	0	25,32,35	1.46	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	A	1518	1	23,26,27	0.28	0	33,38,41	0.65	1 (3%)
1	PSU	A	516	1,25	18,21,22	1.11	3 (16%)	21,30,33	2.14	6 (28%)
13	D2T	M	89	13	8,9,10	1.98	1 (12%)	6,11,13	2.38	3 (50%)
23	5MU	W	55	23	19,22,23	1.44	5 (26%)	27,32,35	2.24	6 (22%)
1	2MG	A	1207	1	23,26,27	1.30	4 (17%)	33,38,41	2.31	8 (24%)
1	2MG	A	966	1	23,26,27	1.28	4 (17%)	33,38,41	2.25	7 (21%)
1	G7M	A	527	1	23,26,27	0.73	1 (4%)	34,39,42	0.59	0
1	UR3	A	1498	1	19,22,23	1.00	0	26,32,35	2.09	6 (23%)
23	4SU	W	8	23	18,21,22	1.80	5 (27%)	25,30,33	2.40	6 (24%)
23	H2U	W	21	23	18,21,22	1.33	3 (16%)	19,30,33	1.19	1 (5%)
23	OMC	W	33	23	19,22,23	0.81	0	25,31,34	0.94	1 (4%)
23	PSU	W	56	23	18,21,22	1.35	2 (11%)	21,30,33	2.29	5 (23%)
1	5MC	A	967	1	19,22,23	1.66	3 (15%)	26,32,35	1.25	3 (11%)
1	5MC	A	1407	1	19,22,23	1.78	3 (15%)	26,32,35	1.31	5 (19%)
1	MA6	A	1519	1	23,26,27	0.28	0	33,38,41	0.88	1 (3%)
1	2MG	A	1516	1	23,26,27	1.29	4 (17%)	33,38,41	2.26	7 (21%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	9/11/29/30	0/3/3/3
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	5MC	C5-C4	6.54	1.49	1.44
1	A	967	5MC	C5-C4	5.98	1.48	1.44
23	W	8	4SU	C4-S4	-4.93	1.60	1.68
13	M	89	D2T	CB-CA	-4.80	1.53	1.54
23	W	21	H2U	C2-N3	-3.16	1.32	1.38
1	A	1207	2MG	C5-C4	3.15	1.47	1.38
23	W	56	PSU	C6-C5	3.12	1.38	1.35
1	A	966	2MG	C5-C4	3.07	1.47	1.38
1	A	1516	2MG	C5-C4	3.07	1.47	1.38
23	W	55	5MU	C4-N3	-2.99	1.33	1.38
23	W	8	4SU	C4-N3	-2.98	1.34	1.37
23	W	21	H2U	C4-N3	-2.91	1.32	1.37
1	A	516	PSU	C6-C5	2.79	1.38	1.35
23	W	56	PSU	C4-N3	-2.74	1.33	1.38
1	A	1407	5MC	C6-C5	2.74	1.39	1.34
1	A	967	5MC	C6-C5	2.74	1.39	1.34
1	A	527	G7M	C8-N7	2.60	1.37	1.33
23	W	8	4SU	C5-C4	-2.57	1.39	1.42
23	W	55	5MU	C6-C5	2.54	1.38	1.34
1	A	1207	2MG	C6-N1	-2.50	1.34	1.38
23	W	21	H2U	C2-N1	-2.50	1.32	1.35
23	W	55	5MU	C2-N3	-2.47	1.33	1.38
1	A	1516	2MG	C6-N1	-2.45	1.34	1.38
1	A	1516	2MG	C2-N3	2.41	1.36	1.32
1	A	966	2MG	C6-N1	-2.37	1.34	1.38
23	W	55	5MU	C6-N1	-2.37	1.34	1.38
1	A	1207	2MG	C2-N3	2.31	1.36	1.32
1	A	1407	5MC	C6-N1	-2.25	1.34	1.38
1	A	967	5MC	C6-N1	-2.23	1.34	1.38
1	A	516	PSU	O4'-C1'	-2.19	1.40	1.43
23	W	8	4SU	C2-N1	2.18	1.41	1.38
1	A	966	2MG	C2-N3	2.16	1.36	1.32
1	A	516	PSU	C4-C5	-2.10	1.38	1.44
1	A	966	2MG	C5-N7	-2.09	1.34	1.39
23	W	8	4SU	C2-N3	-2.03	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	55	5MU	C4-C5	2.03	1.48	1.44
1	A	1207	2MG	C5-N7	-2.01	1.35	1.39
1	A	1516	2MG	C5-N7	-2.01	1.35	1.39

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	UR3	C4-N3-C2	-7.34	118.67	124.58
1	A	1207	2MG	C2-N3-C4	7.28	121.10	112.00
1	A	1516	2MG	C2-N3-C4	7.18	120.99	112.00
1	A	966	2MG	C2-N3-C4	7.08	120.86	112.00
23	W	8	4SU	C4-N3-C2	-6.97	120.64	127.31
23	W	56	PSU	N1-C2-N3	6.69	122.23	115.17
1	A	1207	2MG	C5-C4-N3	-6.25	118.44	128.39
1	A	1516	2MG	C5-C4-N3	-6.12	118.65	128.39
23	W	8	4SU	C5-C4-N3	5.89	120.23	114.75
1	A	966	2MG	C5-C4-N3	-5.89	119.02	128.39
1	A	1402	4OC	C2'-C1'-N1	-5.64	103.53	114.24
23	W	55	5MU	N3-C2-N1	5.58	122.15	114.89
23	W	55	5MU	C4-N3-C2	-5.44	120.20	127.34
1	A	516	PSU	C4-N3-C2	-5.42	118.91	126.37
1	A	516	PSU	N1-C2-N3	5.09	120.53	115.17
1	A	1516	2MG	N9-C4-N3	4.71	135.38	125.95
23	W	56	PSU	C4-N3-C2	-4.56	120.08	126.37
1	A	1207	2MG	N9-C4-N3	4.50	134.94	125.95
23	W	55	5MU	C5-C4-N3	4.48	119.22	115.32
23	W	8	4SU	C5-C4-S4	-4.39	119.29	124.31
1	A	966	2MG	N9-C4-N3	4.36	134.67	125.95
23	W	8	4SU	N3-C2-N1	4.04	120.15	114.89
13	M	89	D2T	CB1-SB-CB	3.91	109.39	102.36
23	W	56	PSU	O2-C2-N1	-3.85	118.81	122.79
23	W	55	5MU	O4-C4-C5	-3.85	120.52	124.92
23	W	55	5MU	C5-C6-N1	-3.73	119.27	123.31
1	A	1407	5MC	C5-C6-N1	-3.61	119.39	123.31
1	A	1516	2MG	C2'-C1'-N9	-3.52	103.45	113.25
1	A	1498	UR3	C5-C4-N3	3.51	119.66	115.04
1	A	1207	2MG	C6-C5-N7	3.45	136.57	130.29
1	A	966	2MG	C6-C5-N7	3.38	136.44	130.29
1	A	967	5MC	C5-C6-N1	-3.28	119.75	123.31
13	M	89	D2T	OD2-CG-CB	3.22	120.11	113.15
1	A	1516	2MG	C6-C5-N7	3.19	136.10	130.29
1	A	516	PSU	C6-C5-C4	3.06	120.24	118.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	56	PSU	C3'-C2'-C1'	3.04	105.28	101.69
23	W	21	H2U	C3'-C2'-C1'	2.88	106.91	101.46
1	A	1498	UR3	C2'-C1'-N1	-2.84	105.36	113.25
1	A	966	2MG	C2'-C1'-N9	-2.81	105.43	113.25
1	A	1207	2MG	C4-C5-N7	-2.77	106.27	110.67
1	A	1498	UR3	O4'-C1'-N1	2.77	114.63	108.36
1	A	1518	MA6	C2-N1-C6	2.72	118.48	111.83
23	W	33	OMC	C2'-C1'-N1	-2.71	109.10	114.24
23	W	55	5MU	O2-C2-N1	-2.70	119.28	122.80
1	A	967	5MC	C5-C4-N3	-2.65	119.04	121.75
1	A	1519	MA6	C2-N1-C6	2.59	118.16	111.83
1	A	966	2MG	C4-C5-N7	-2.57	106.60	110.67
23	W	56	PSU	C5-C6-N1	-2.53	118.64	122.14
1	A	1407	5MC	C5-C4-N3	-2.52	119.18	121.75
1	A	1516	2MG	C4-C5-N7	-2.46	106.78	110.67
1	A	1498	UR3	C3U-N3-C4	2.42	121.22	117.87
1	A	1407	5MC	C2'-C1'-N1	-2.42	106.53	113.25
1	A	516	PSU	O2-C2-N1	-2.39	120.32	122.79
1	A	1402	4OC	C6-C5-C4	2.38	119.87	117.00
23	W	8	4SU	C3'-C2'-C1'	2.28	105.78	101.46
1	A	516	PSU	C5-C6-N1	-2.26	119.01	122.14
23	W	8	4SU	C2'-C1'-N1	-2.22	107.06	113.25
1	A	1207	2MG	C2'-C1'-N9	-2.20	107.11	113.25
1	A	1516	2MG	O6-C6-C5	-2.16	120.84	126.53
1	A	1207	2MG	C2-N1-C6	-2.15	121.95	124.55
1	A	966	2MG	O6-C6-C5	-2.13	120.92	126.53
1	A	1498	UR3	C3'-C2'-C1'	2.12	105.47	101.46
1	A	967	5MC	O2-C2-N3	-2.12	118.99	122.33
1	A	1207	2MG	O6-C6-C5	-2.06	121.09	126.53
13	M	89	D2T	OD2-CG-OD1	-2.04	119.44	124.08
1	A	516	PSU	O4'-C1'-C2'	2.03	107.95	105.15
1	A	1407	5MC	O2-C2-N3	-2.01	119.17	122.33
1	A	1407	5MC	CM5-C5-C6	-2.00	120.14	122.85

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1518	MA6	C5-C6-N6-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	N1-C6-N6-C10
1	A	1519	MA6	O4'-C1'-N9-C4
1	A	1519	MA6	O4'-C1'-N9-C8
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C10
1	A	1519	MA6	N1-C6-N6-C9
13	M	89	D2T	O-C-CA-CB
23	W	21	H2U	O4'-C1'-N1-C2
23	W	21	H2U	O4'-C1'-N1-C6
1	A	966	2MG	C3'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C10
23	W	56	PSU	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
23	W	56	PSU	O4'-C4'-C5'-O5'
23	W	55	5MU	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
23	W	55	5MU	C3'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
13	M	89	D2T	CG-CB-SB-CB1
1	A	527	G7M	C4'-C5'-O5'-P
1	A	1519	MA6	C4'-C5'-O5'-P
23	W	56	PSU	C4'-C5'-O5'-P
23	W	8	4SU	C4'-C5'-O5'-P
1	A	1207	2MG	O4'-C4'-C5'-O5'
13	M	89	D2T	CA-CB-CG-OD2
1	A	966	2MG	C4'-C5'-O5'-P

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0
1	A	1518	MA6	2	0
23	W	55	5MU	1	0
1	A	1207	2MG	1	0
1	A	966	2MG	1	0
1	A	527	G7M	1	0
1	A	1498	UR3	2	0
23	W	21	H2U	2	0
23	W	33	OMC	5	0
23	W	56	PSU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	967	5MC	2	0
1	A	1407	5MC	1	0
1	A	1519	MA6	4	0
1	A	1516	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 86 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

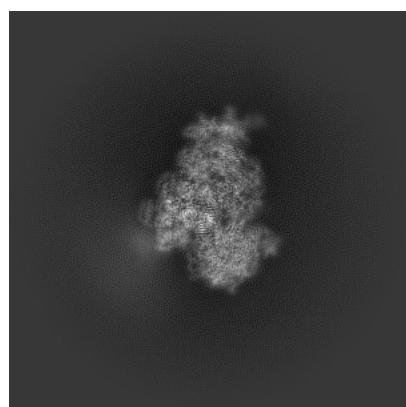
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51621. These allow visual inspection of the internal detail of the map and identification of artifacts.

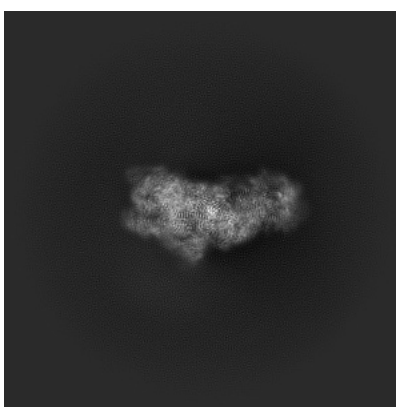
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

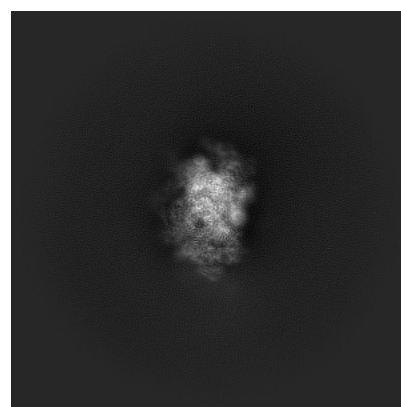
6.1.1 Primary map



X



Y

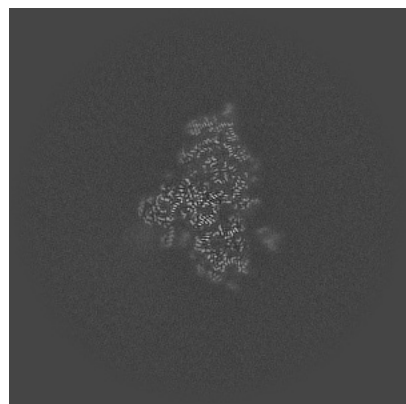


Z

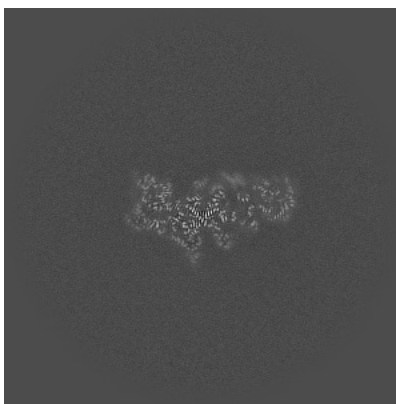
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

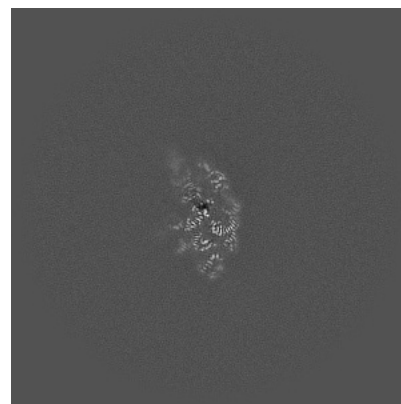
6.2.1 Primary map



X Index: 300



Y Index: 300

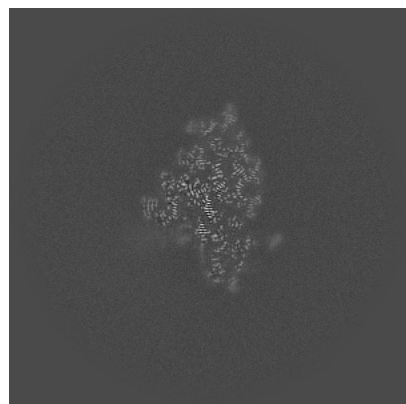


Z Index: 300

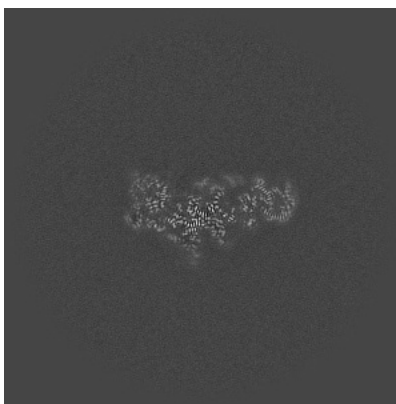
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

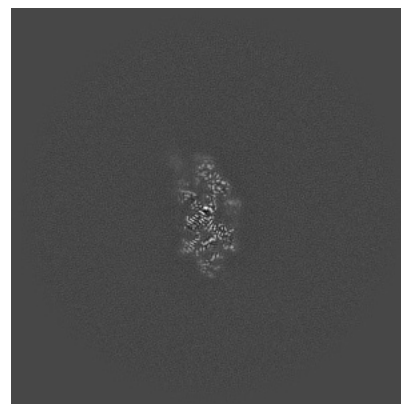
6.3.1 Primary map



X Index: 292



Y Index: 303

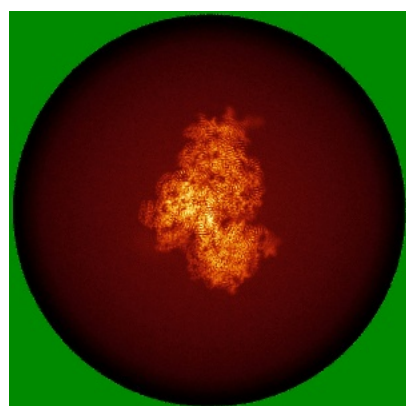


Z Index: 306

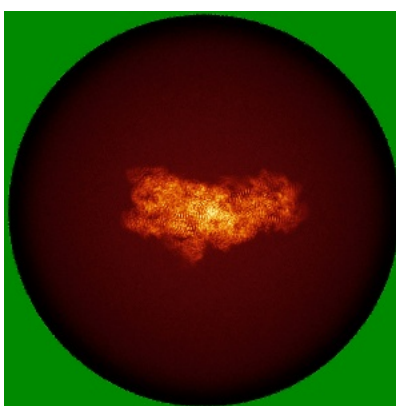
The images above show the largest variance slices of the map in three orthogonal directions.

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

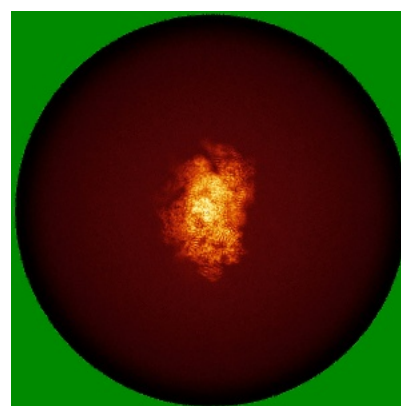
6.4.1 Primary map



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

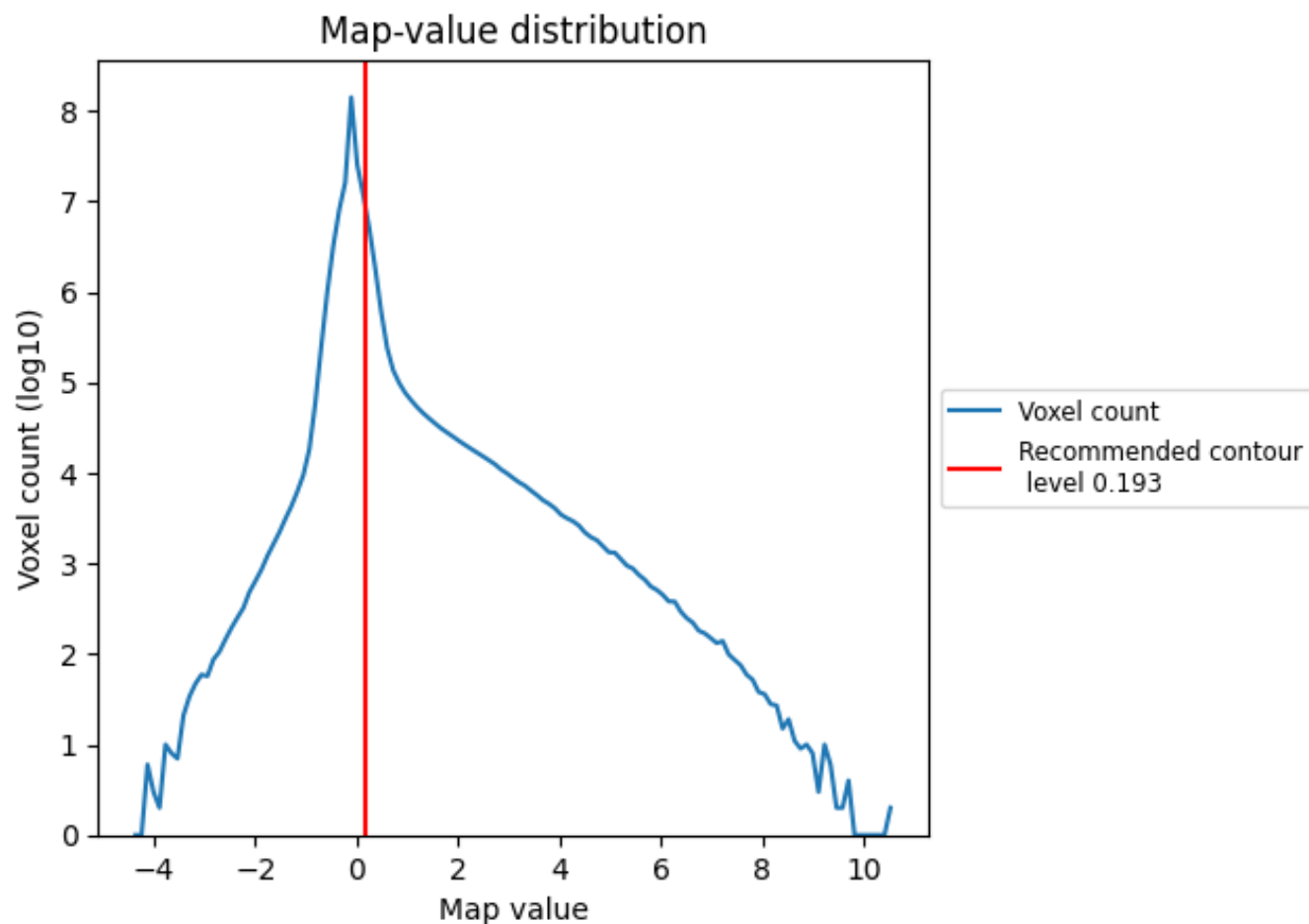
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

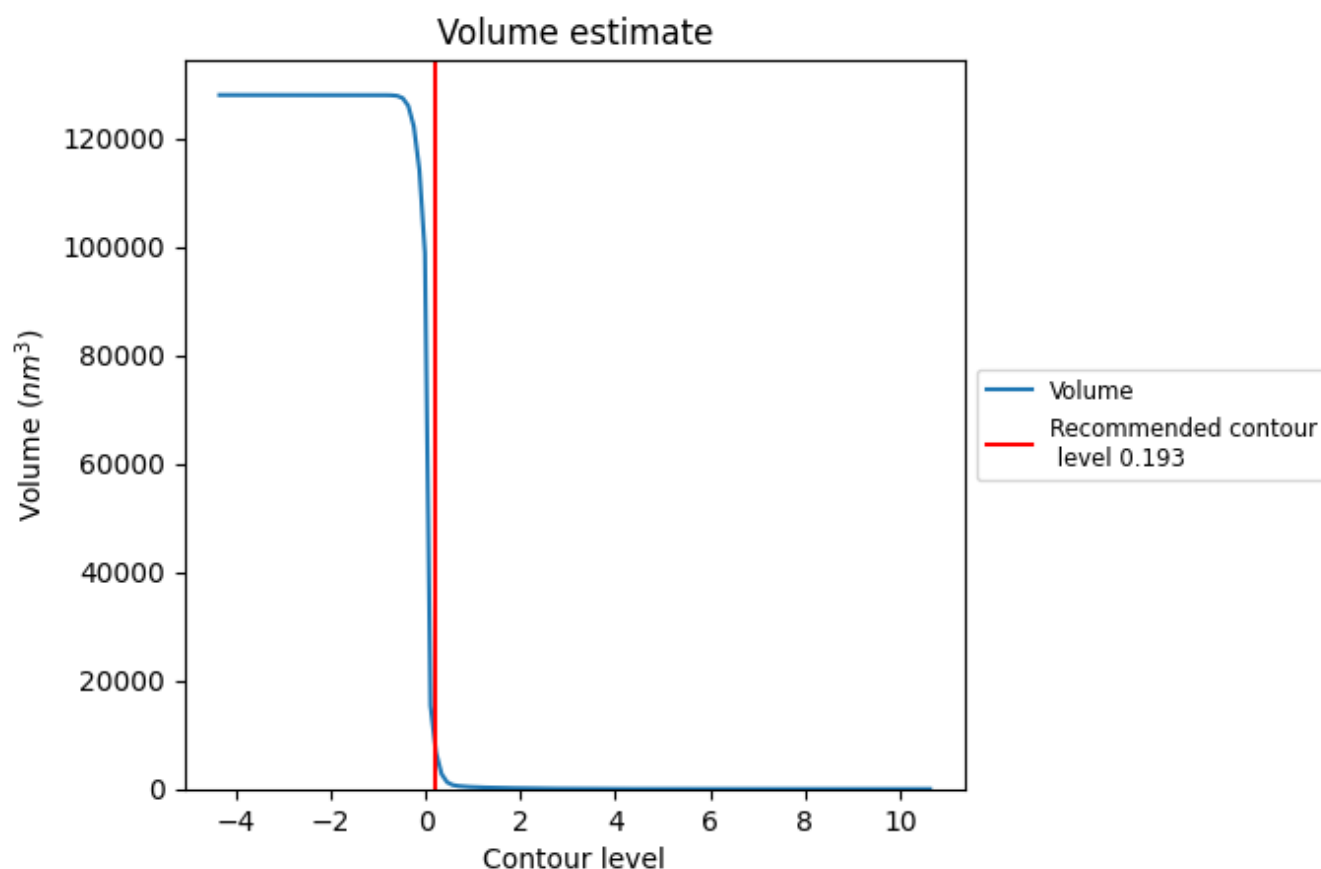
This section contains the results of statistical analysis of the map.

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.

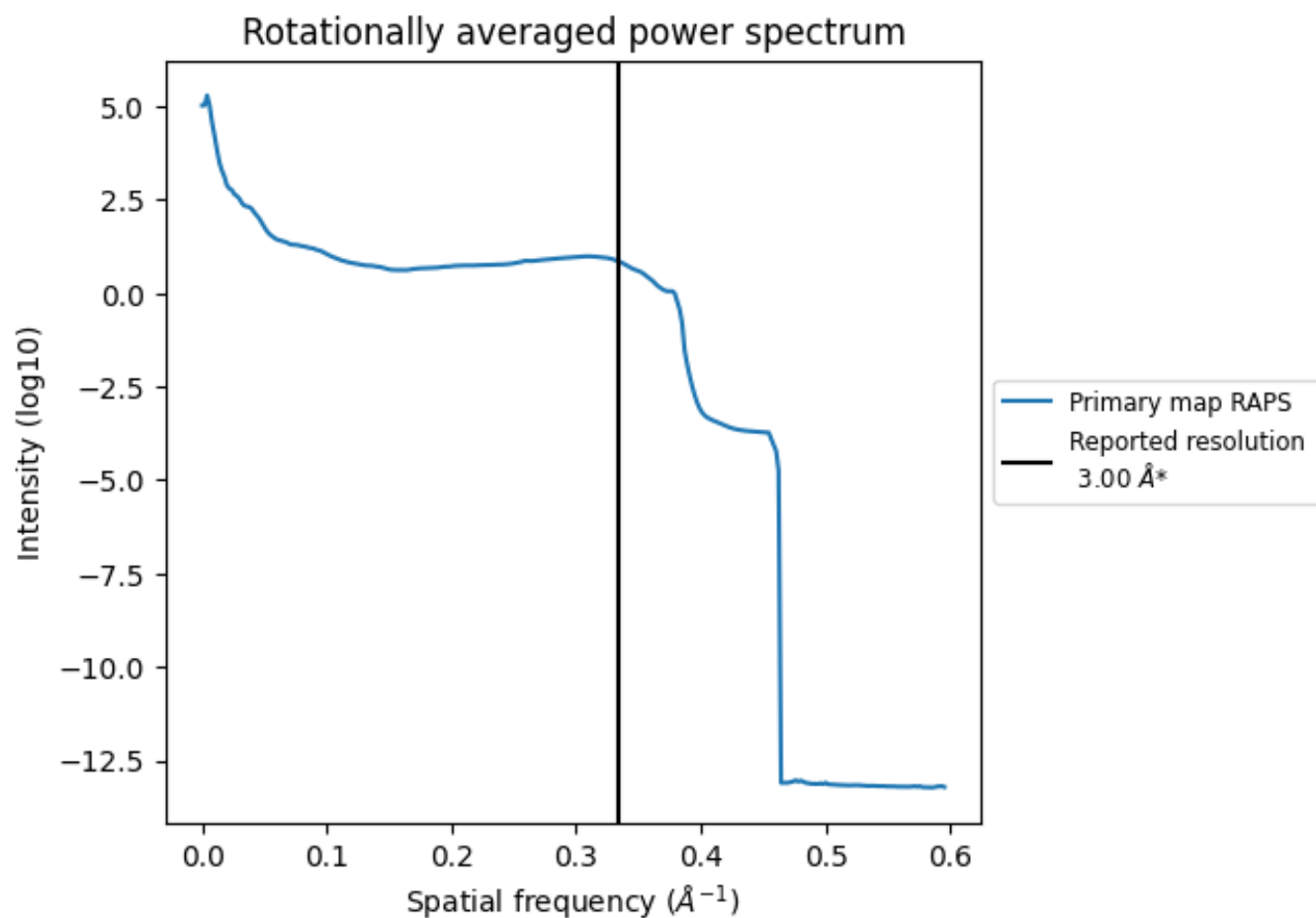
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8343 nm³; this corresponds to an approximate mass of 7537 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 0.333 Å⁻¹

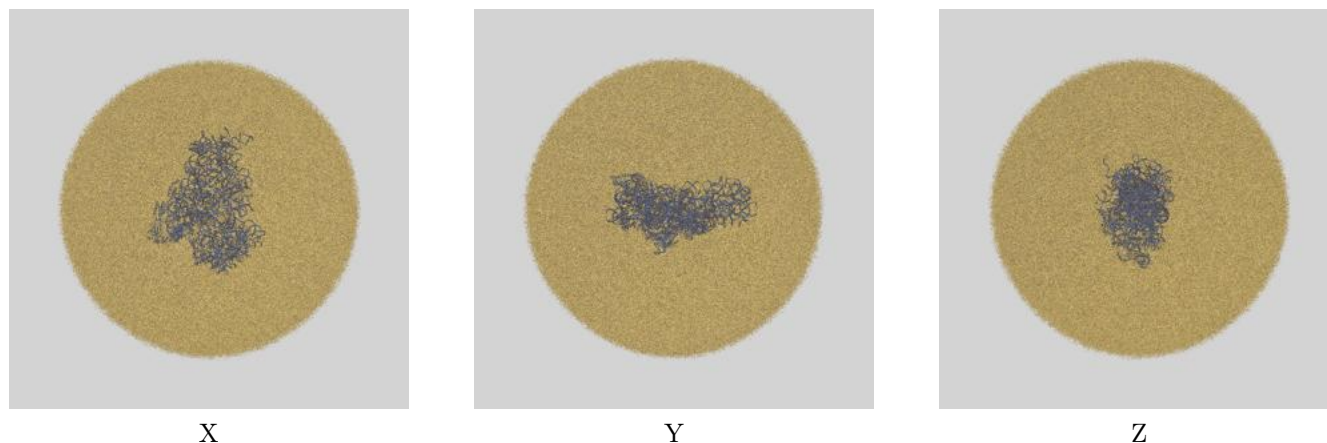
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

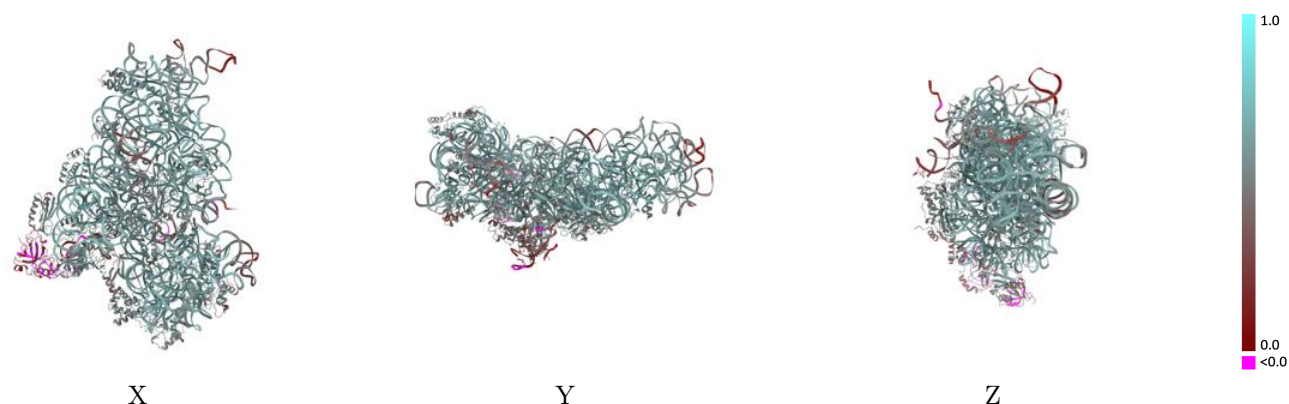
This section contains information regarding the fit between EMDB map EMD-51621 and PDB model 9GUV. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



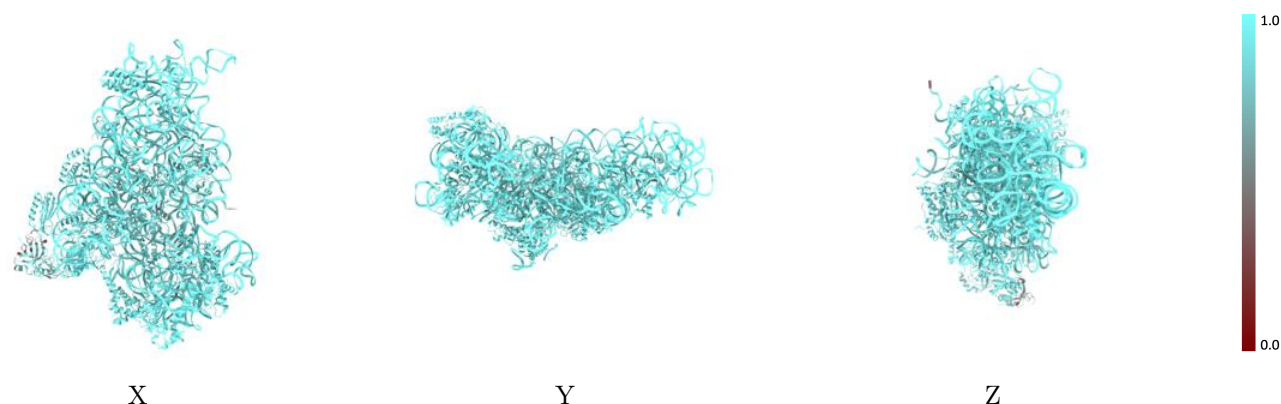
The images above show the 3D surface view of the map at the recommended contour level 0.193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



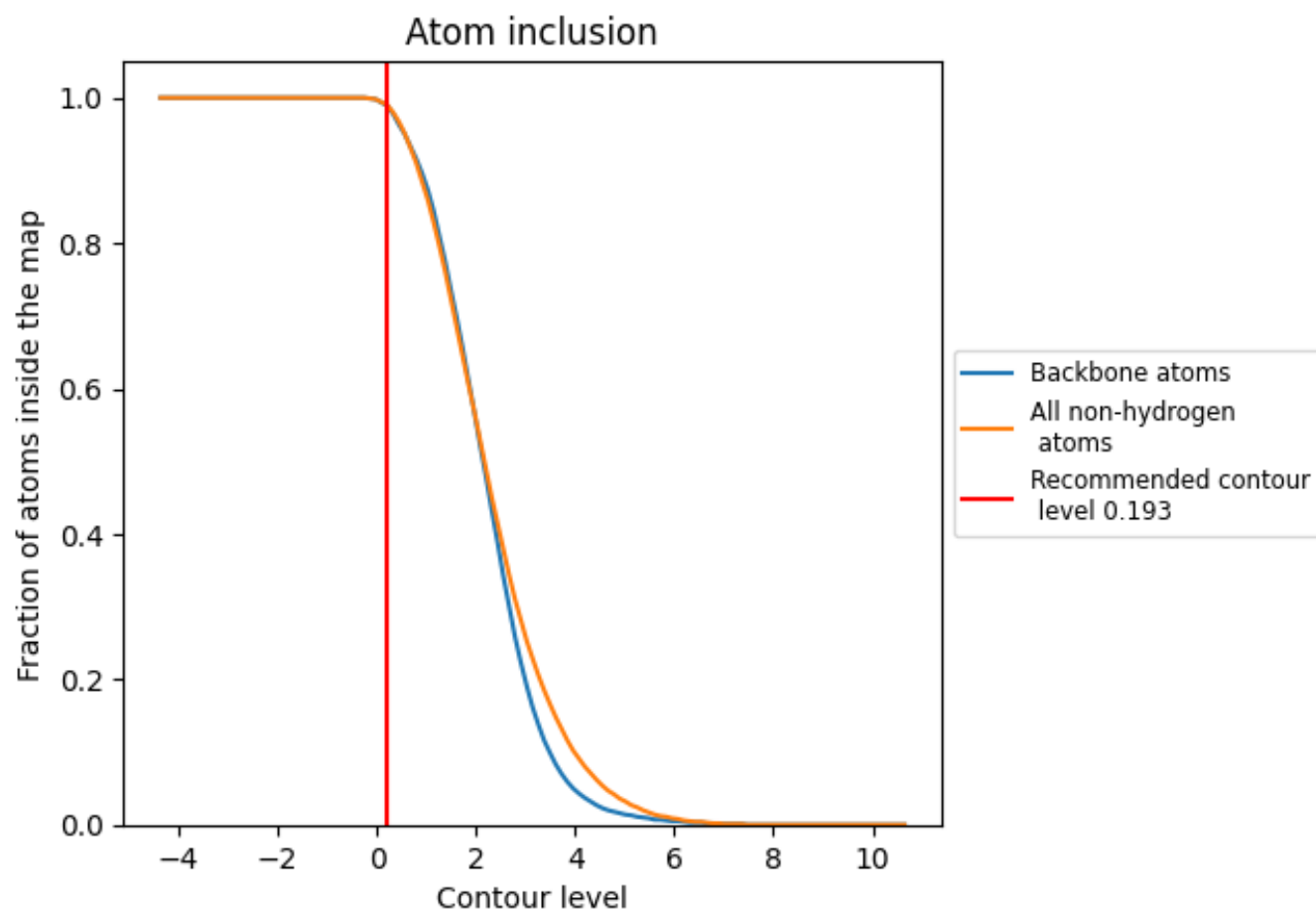
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.193).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9910	 0.5610
A	 1.0000	 0.6000
B	 0.8940	 0.2140
C	 0.9900	 0.5240
D	 0.9910	 0.5780
E	 0.9860	 0.5540
F	 0.9790	 0.5770
G	 0.9810	 0.5230
H	 0.9810	 0.4960
I	 0.9900	 0.5870
J	 0.9860	 0.5650
K	 0.9860	 0.5250
L	 0.9880	 0.5540
M	 0.9880	 0.5880
N	 0.9950	 0.5540
O	 0.9910	 0.5840
P	 0.9900	 0.5730
Q	 0.9860	 0.5910
R	 0.9890	 0.5540
S	 0.9930	 0.5790
T	 0.9910	 0.5770
U	 0.9940	 0.5740
V	 0.9890	 0.5000
W	 0.9630	 0.3020
X	 0.9810	 0.1610

