



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 11:45 AM EST

PDB ID : 6W7M
EMDB ID : EMD-21571
Title : 30S-Inactive-high-Mg2+ + carbon layer
Authors : Jahagirdar, D.; Jha, V.; Basu, B.; Gomez-Blanco, J.; Vargas, J.; Ortega, J.
Deposited on : 2020-03-19
Resolution : 3.80 Å(reported)
Based on initial model : 4V4Q

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

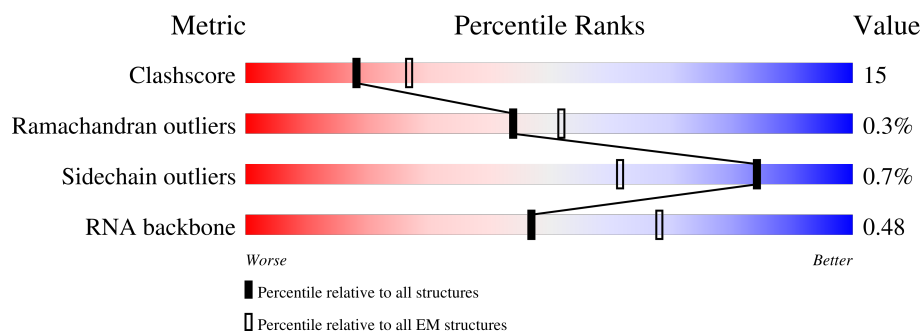
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1542	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 50694 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0
			32448	14471	5955	10510	1512		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	149	Total	C	N	O	S	0	0
			1163	724	222	213	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	122	Total	C	N	O	S	0	0
			949	587	195	163	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	87	Total	C	N	O	S	0	0
			708	436	143	128	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

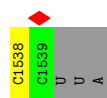
3 Residue-property plots

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 rRNA



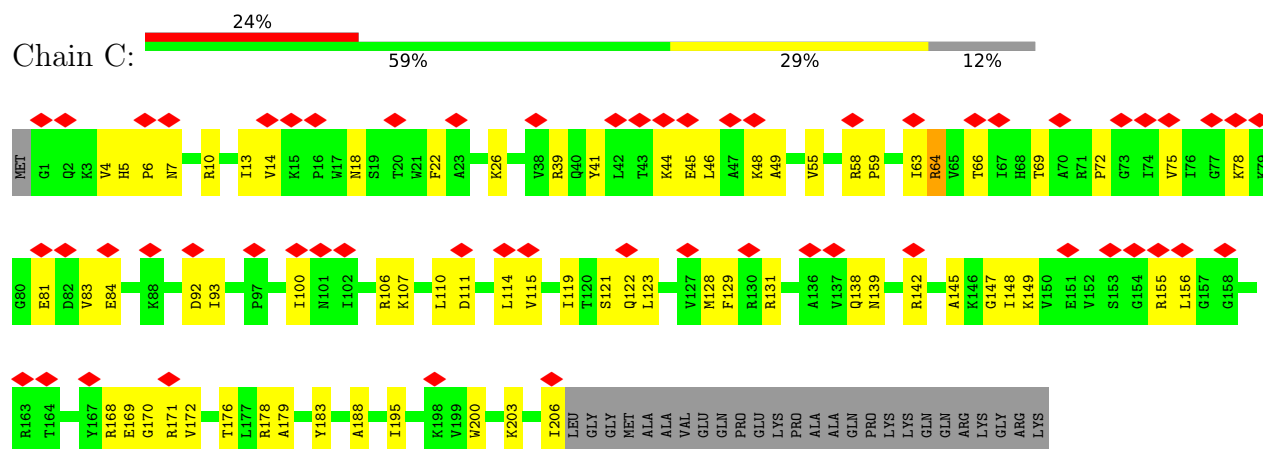




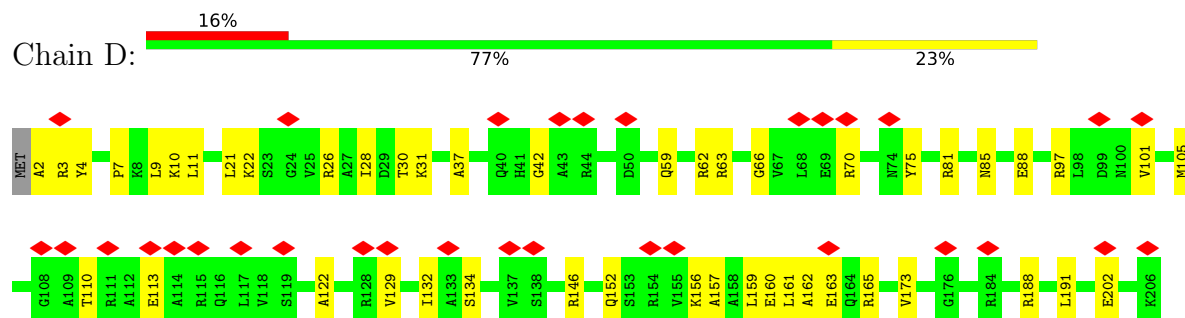
• Molecule 2: 30S ribosomal protein S2



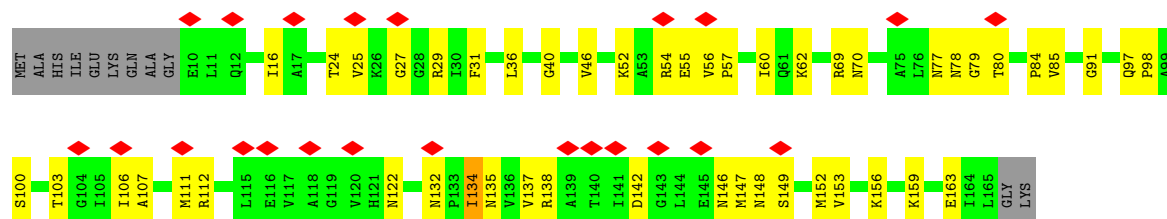
• Molecule 3: 30S ribosomal protein S3



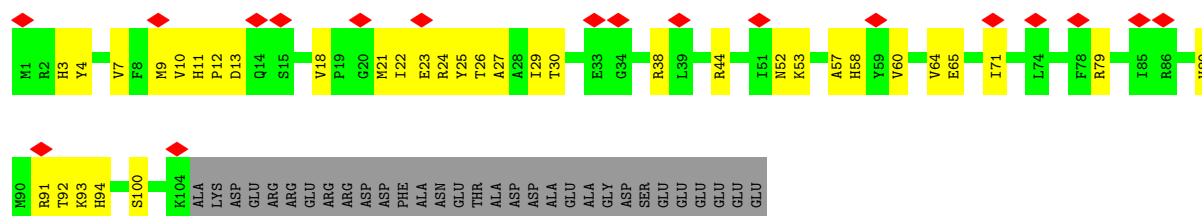
• Molecule 4: 30S ribosomal protein S4



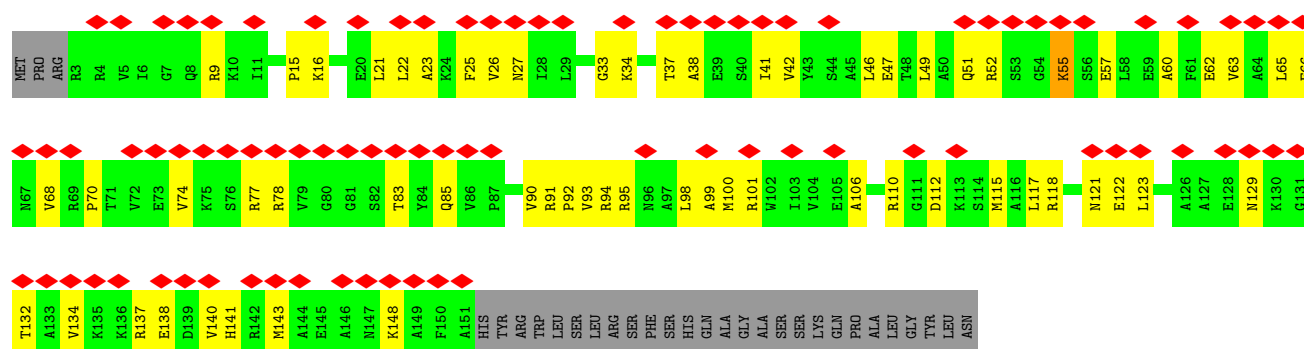
• Molecule 5: 30S ribosomal protein S5



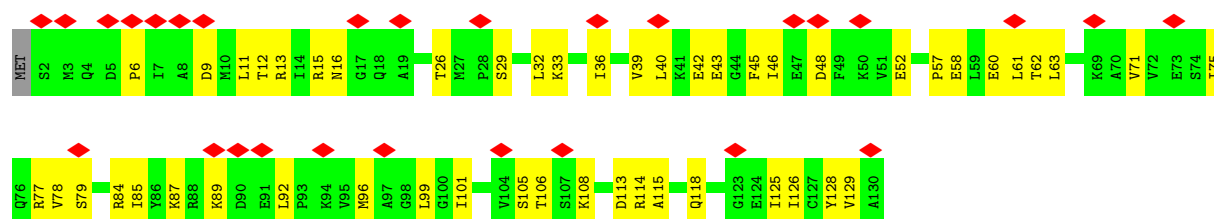
• Molecule 6: 30S ribosomal protein S6



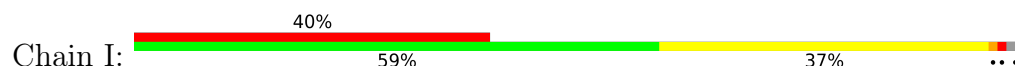
• Molecule 7: 30S ribosomal protein S7

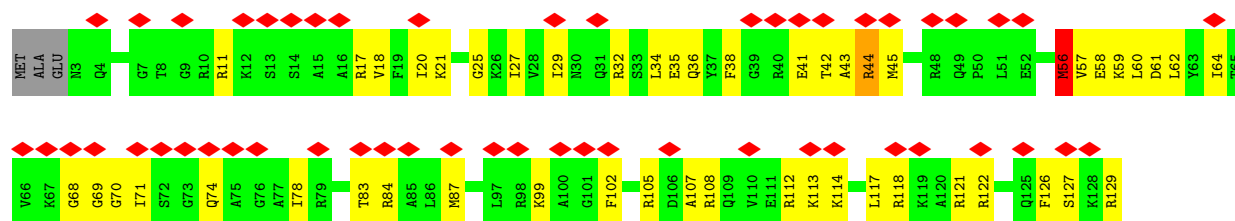


• Molecule 8: 30S ribosomal protein S8

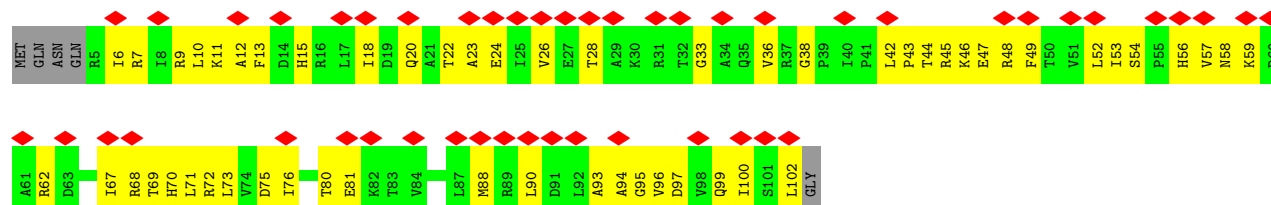


• Molecule 9: 30S ribosomal protein S9

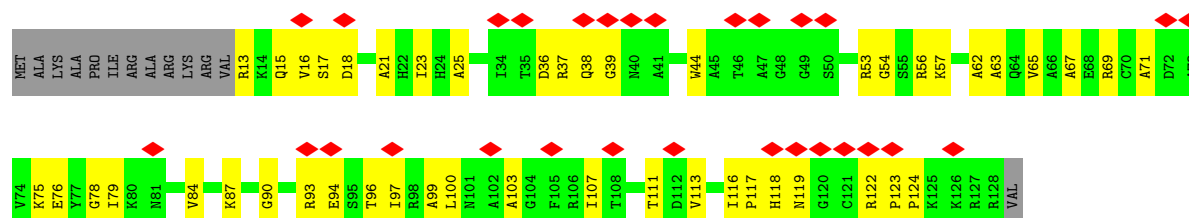




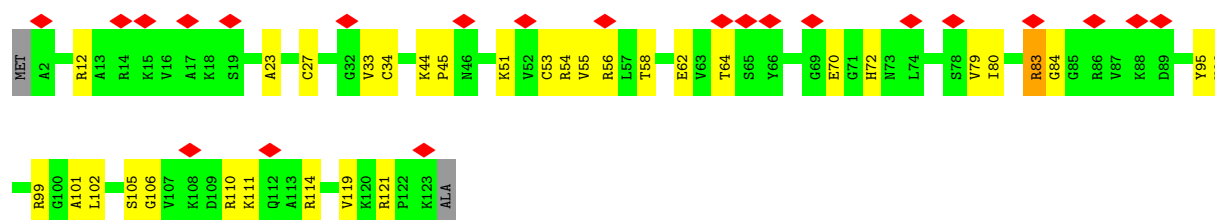
• Molecule 10: 30S ribosomal protein S10



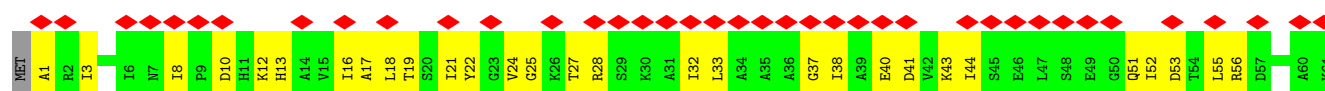
• Molecule 11: 30S ribosomal protein S11

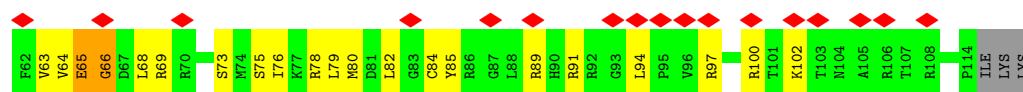


• Molecule 12: 30S ribosomal protein S12

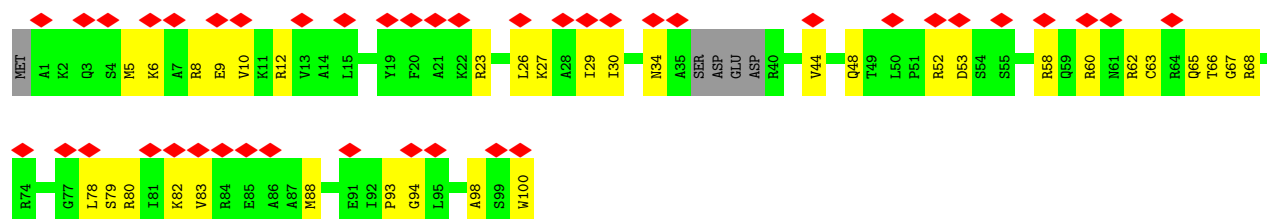
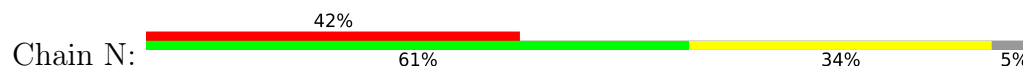


• Molecule 13: 30S ribosomal protein S13

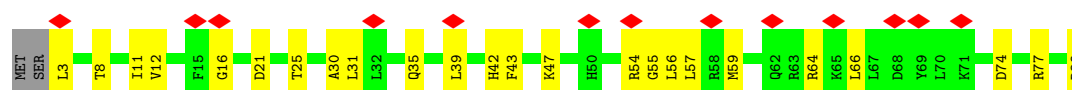




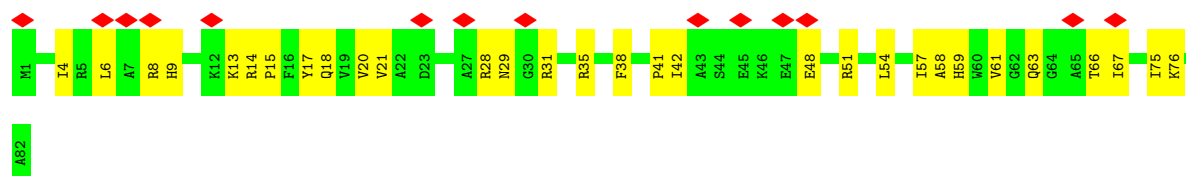
- Molecule 14: 30S ribosomal protein S14



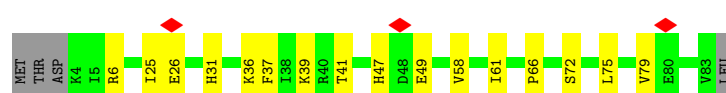
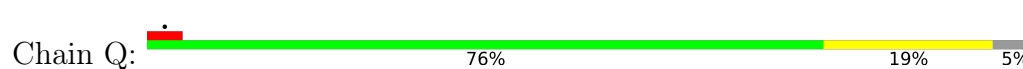
- Molecule 15: 30S ribosomal protein S15



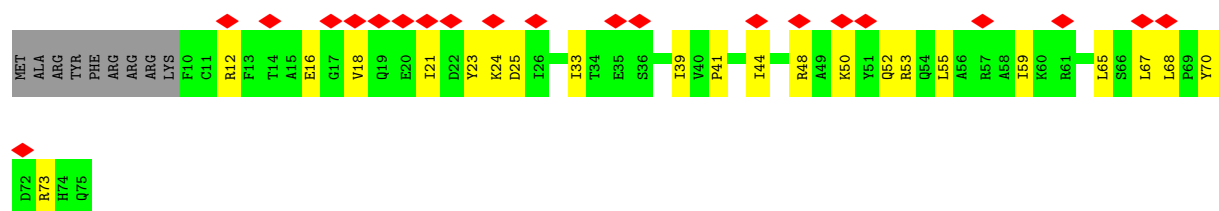
- Molecule 16: 30S ribosomal protein S16



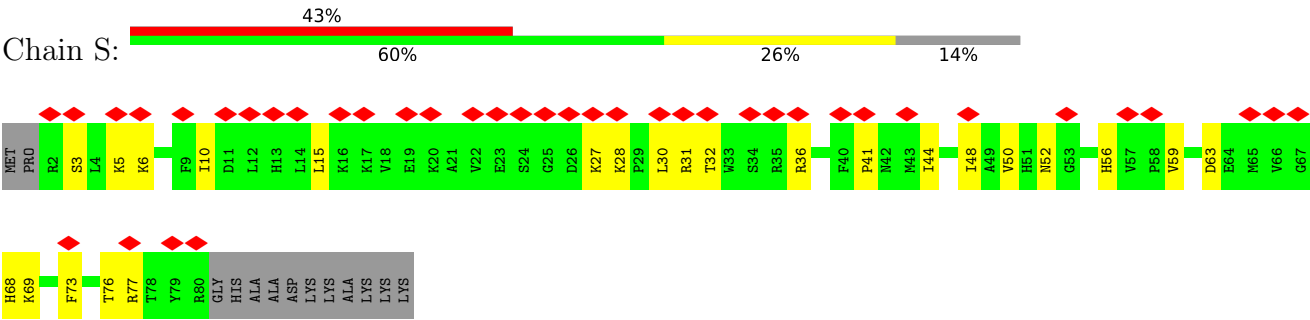
- Molecule 17: 30S ribosomal protein S17



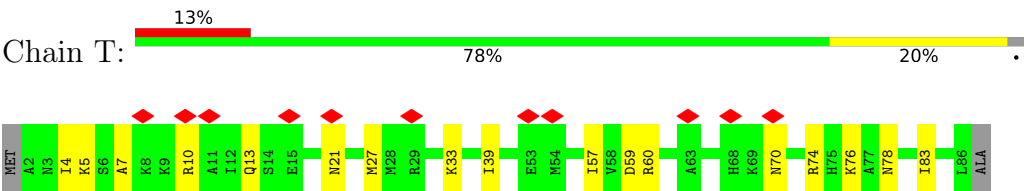
- Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	334903	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.824	Depositor
Minimum map value	-0.483	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.162	Depositor
Map size (Å)	326.192, 326.192, 326.192	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.073, 1.073, 1.073	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	1/36332 (0.0%)	0.84	36/56675 (0.1%)
2	B	0.27	0/1735	0.50	0/2338
3	C	0.24	0/1651	0.47	0/2225
4	D	0.24	0/1665	0.40	0/2227
5	E	0.25	0/1165	0.46	0/1568
6	F	0.25	0/867	0.44	0/1171
7	G	0.23	0/1176	0.42	0/1577
8	H	0.24	0/989	0.45	0/1326
9	I	0.23	0/1034	0.47	0/1375
10	J	0.23	0/796	0.49	0/1077
11	K	0.24	0/885	0.45	0/1195
12	L	0.23	0/963	0.46	0/1293
13	M	0.25	0/892	0.47	0/1193
14	N	0.24	0/785	0.46	0/1043
15	O	0.22	0/716	0.40	0/956
16	P	0.24	0/659	0.44	0/884
17	Q	0.24	0/657	0.46	0/881
18	R	0.23	0/553	0.43	0/743
19	S	0.24	0/652	0.45	0/877
20	T	0.24	0/670	0.37	0/888
All	All	0.23	1/54842 (0.0%)	0.74	36/81512 (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
2	B	0	2
9	I	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1158	C	C2-O2	-10.48	1.15	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1158	C	C6-N1-C2	-25.96	109.91	120.30
1	A	1181	G	N1-C6-O6	-17.23	109.56	119.90
1	A	1158	C	N1-C2-N3	16.54	130.78	119.20
1	A	1181	G	C5-C6-O6	14.81	137.49	128.60
1	A	1158	C	C5-C4-N4	11.74	128.42	120.20
1	A	1158	C	N3-C4-C5	-11.51	117.30	121.90
1	A	1158	C	N3-C2-O2	-11.49	113.86	121.90
1	A	1181	G	N1-C2-N2	-10.80	106.48	116.20
1	A	1158	C	O4'-C1'-N1	9.90	116.12	108.20
1	A	1181	G	N1-C2-N3	8.65	129.09	123.90
1	A	1181	G	N9-C4-C5	8.36	108.74	105.40
1	A	810	C	N1-C2-O2	8.01	123.71	118.90
1	A	754	C	N1-C2-O2	7.87	123.62	118.90
1	A	1181	G	C4-C5-N7	-7.83	107.67	110.80
1	A	754	C	C2-N1-C1'	7.83	127.41	118.80
1	A	810	C	N3-C2-O2	-7.67	116.53	121.90
1	A	1158	C	C4-C5-C6	7.41	121.11	117.40
1	A	1158	C	N1-C2-O2	-7.12	114.63	118.90
1	A	1181	G	C8-N9-C4	-7.11	103.56	106.40
1	A	1157	A	N9-C1'-C2'	6.41	122.34	114.00
1	A	754	C	N3-C2-O2	-6.27	117.51	121.90
1	A	1181	G	C6-N1-C2	-6.20	121.38	125.10
1	A	1432	G	O4'-C1'-N9	5.98	112.98	108.20
1	A	1158	C	C2-N1-C1'	5.91	125.30	118.80
1	A	739	C	N3-C2-O2	-5.58	118.00	121.90
1	A	1181	G	N3-C2-N2	5.57	123.80	119.90
1	A	1156	G	N9-C1'-C2'	-5.54	105.90	112.00
1	A	307	C	N1-C2-O2	5.49	122.19	118.90
1	A	754	C	C6-N1-C1'	-5.38	114.34	120.80
1	A	1047	G	N1-C6-O6	-5.35	116.69	119.90
1	A	1134	G	N1-C6-O6	-5.35	116.69	119.90
1	A	1158	C	N3-C4-N4	-5.33	114.27	118.00
1	A	1181	G	N3-C4-C5	-5.32	125.94	128.60
1	A	316	C	C2-N1-C1'	5.27	124.60	118.80
1	A	754	C	C6-N1-C2	-5.24	118.21	120.30
1	A	1047	G	C5-C6-O6	5.09	131.65	128.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	125	PHE	Peptide
2	B	127	LYS	Peptide
9	I	56	MET	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32448	0	16328	750	0
2	B	1704	0	1732	101	0
3	C	1624	0	1699	50	0
4	D	1643	0	1707	37	0
5	E	1152	0	1196	33	0
6	F	848	0	846	24	0
7	G	1163	0	1217	45	0
8	H	979	0	1031	34	0
9	I	1022	0	1070	41	0
10	J	786	0	828	47	0
11	K	869	0	878	35	0
12	L	949	0	1011	21	0
13	M	883	0	944	39	0
14	N	774	0	827	30	0
15	O	708	0	729	15	0
16	P	649	0	666	21	0
17	Q	648	0	691	11	0
18	R	544	0	560	20	0
19	S	637	0	665	19	0
20	T	664	0	714	15	0
All	All	50694	0	35339	1223	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 15.

All (1223) 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:1157:A:H61	1:A:1178:G:N2	1.20	1.39
1:A:1157:A:N6	1:A:1178:G:H21	1.21	1.33
1:A:1304:G:N2	1:A:1333:A:H62	1.41	1.16
1:A:1304:G:H21	1:A:1333:A:N6	1.44	1.13
1:A:888:G:N2	1:A:909:A:H62	1.53	1.07
1:A:888:G:H21	1:A:909:A:N6	1.55	1.04
1:A:1157:A:H1'	2:B:129:THR:HB	1.39	1.04
1:A:886:G:H1	1:A:911:U:H3	1.06	1.03
1:A:942:G:H1	1:A:1341:U:H3	1.06	0.97
1:A:1159:U:H4'	2:B:131:LYS:HB3	1.47	0.96
1:A:1157:A:H4'	2:B:128:LEU:HA	1.48	0.93
1:A:447:G:H21	1:A:487:A:H62	1.16	0.92
1:A:1445:U:H3	1:A:1457:G:H1	1.14	0.92
1:A:672:U:H3	1:A:734:G:H1	1.04	0.92
1:A:437:U:H3	1:A:495:A:H62	0.91	0.90
1:A:437:U:H3	1:A:495:A:N6	1.69	0.90
1:A:1160:G:C8	1:A:1182:G:N2	2.44	0.85
1:A:1159:U:H3'	2:B:135:MET:HB2	1.60	0.83
1:A:1160:G:N7	1:A:1182:G:N1	2.25	0.83
13:M:63:VAL:HB	13:M:68:LEU:HD22	1.59	0.82
10:J:42:LEU:HD23	10:J:71:LEU:HB3	1.60	0.82
1:A:1181:G:N2	2:B:128:LEU:O	2.13	0.82
1:A:1242:G:H1	1:A:1295:U:H3	0.85	0.82
1:A:1158:C:O2	2:B:130:LYS:HA	1.80	0.81
1:A:1160:G:N7	1:A:1182:G:C2	2.48	0.80
1:A:696:A:HO2'	1:A:786:G:HO2'	1.25	0.80
1:A:310:G:H5''	16:P:31:ARG:HB3	1.63	0.79
1:A:667:G:H2'	1:A:668:G:H8	1.47	0.78
1:A:978:A:OP2	1:A:1362:A:N6	2.16	0.78
1:A:1158:C:H2'	2:B:132:GLU:HB2	1.65	0.78
1:A:1158:C:O4'	2:B:128:LEU:HB3	1.82	0.78
1:A:1487:G:O2'	1:A:1488:G:N7	2.17	0.77
1:A:936:C:H1'	1:A:1382:C:H42	1.49	0.77
1:A:358:U:H2'	1:A:359:G:H8	1.50	0.76
1:A:1160:G:C8	1:A:1182:G:C2	2.74	0.76
7:G:112:ASP:HB2	7:G:118:ARG:HB3	1.67	0.75
1:A:665:A:H62	1:A:724:G:H1	1.34	0.75
1:A:977:A:O2'	1:A:982:U:O4	2.04	0.75
1:A:673:A:H2'	1:A:674:G:H8	1.49	0.75
1:A:1236:A:H4'	1:A:1304:G:H4'	1.67	0.75
1:A:484:G:H4'	1:A:485:U:H5'	1.67	0.75
1:A:670:G:O2'	6:F:79:ARG:NH1	2.19	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:G:N2	1:A:365:U:OP2	2.20	0.74
1:A:1250:A:H4'	9:I:69:GLY:H	1.52	0.74
14:N:30:ILE:HD13	14:N:44:VAL:HG21	1.69	0.74
1:A:1242:G:O6	1:A:1295:U:O4	2.05	0.73
2:B:101:THR:HB	2:B:178:LEU:HD21	1.70	0.73
4:D:202:GLU:HG2	5:E:112:ARG:HH12	1.53	0.73
1:A:1479:C:H2'	1:A:1480:A:H8	1.54	0.73
16:P:20:VAL:HG12	16:P:35:ARG:HA	1.70	0.73
18:R:39:ILE:HD13	18:R:59:ILE:HD12	1.69	0.73
1:A:1101:A:N6	2:B:174:GLU:OE1	2.22	0.72
4:D:59:GLN:HB3	4:D:63:ARG:HE	1.54	0.72
10:J:52:LEU:HB3	14:N:80:ARG:HD2	1.70	0.72
1:A:181:A:H1'	1:A:194:C:H41	1.54	0.72
3:C:106:ARG:HD2	3:C:107:LYS:HG3	1.70	0.72
2:B:98:GLY:O	2:B:102:ASN:ND2	2.22	0.72
1:A:1158:C:C2'	2:B:132:GLU:HB2	2.20	0.71
13:M:33:LEU:HD12	13:M:40:GLU:HG2	1.71	0.71
1:A:338:A:H2'	1:A:339:C:C6	2.25	0.71
1:A:263:A:OP1	20:T:74:ARG:NH2	2.23	0.71
3:C:64:ARG:NH2	10:J:94:ALA:O	2.23	0.71
14:N:9:GLU:HG3	14:N:62:ARG:HG3	1.72	0.70
1:A:1140:C:N4	1:A:1141:C:N4	2.39	0.70
11:K:63:ALA:HB1	11:K:96:THR:HB	1.74	0.70
1:A:297:G:N2	1:A:300:A:OP2	2.25	0.70
1:A:672:U:O2	1:A:734:G:N2	2.22	0.70
1:A:1049:U:H5''	1:A:1201:A:H5'	1.72	0.70
1:A:922:G:H1'	5:E:24:THR:HB	1.73	0.69
2:B:143:LEU:O	2:B:147:LEU:N	2.25	0.69
7:G:68:VAL:HA	7:G:137:ARG:HD2	1.74	0.69
3:C:7:ASN:HA	3:C:10:ARG:HB2	1.74	0.69
1:A:1246:A:N6	1:A:1292:G:O6	2.26	0.69
9:I:29:ILE:HG22	9:I:64:ILE:HB	1.75	0.69
1:A:112:G:H1	1:A:315:A:H61	1.39	0.68
13:M:63:VAL:HG12	13:M:64:VAL:H	1.57	0.68
1:A:864:A:H2'	1:A:865:A:C8	2.28	0.68
1:A:667:G:H2'	1:A:668:G:C8	2.28	0.68
1:A:1374:A:O2'	7:G:27:ASN:O	2.11	0.68
1:A:1228:C:H2'	1:A:1229:A:H8	1.58	0.68
2:B:132:GLU:HG2	2:B:135:MET:HB3	1.76	0.68
16:P:4:ILE:HG12	16:P:21:VAL:HG12	1.75	0.68
1:A:447:G:N2	1:A:487:A:H62	1.90	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:G:H5''	12:L:121:ARG:HH12	1.57	0.68
1:A:739:C:O2'	15:O:42:HIS:ND1	2.23	0.68
3:C:49:ALA:HB1	3:C:75:VAL:HG12	1.76	0.68
1:A:1081:A:H2'	1:A:1082:A:H8	1.59	0.67
1:A:1137:C:O2'	1:A:1138:G:N2	2.27	0.67
7:G:68:VAL:HG23	7:G:99:ALA:HB1	1.76	0.67
17:Q:58:VAL:HB	17:Q:79:VAL:O	1.95	0.67
2:B:9:LEU:HD12	2:B:11:ALA:H	1.60	0.67
2:B:173:LYS:O	2:B:177:ASN:ND2	2.28	0.67
12:L:83:ARG:NH2	12:L:84:GLY:O	2.27	0.67
1:A:1009:U:H3	1:A:1020:G:H1	1.42	0.67
1:A:785:G:H2'	1:A:786:G:H8	1.58	0.67
1:A:924:C:H2'	1:A:925:G:C5	2.29	0.67
19:S:27:LYS:HG2	19:S:28:LYS:H	1.59	0.67
1:A:107:G:C2	1:A:108:G:H1'	2.29	0.67
1:A:1158:C:HO2'	2:B:132:GLU:HB2	1.60	0.67
6:F:38:ARG:NH1	6:F:100:SER:OG	2.28	0.67
1:A:159:G:N2	1:A:162:A:OP2	2.28	0.66
1:A:177:G:OP1	20:T:60:ARG:NH2	2.27	0.66
1:A:1522:U:H2'	1:A:1523:G:H8	1.60	0.66
14:N:5:MET:SD	14:N:8:ARG:NH2	2.69	0.66
13:M:52:ILE:O	13:M:56:ARG:NH1	2.28	0.66
1:A:663:A:O2'	18:R:53:ARG:NH1	2.29	0.66
19:S:52:ASN:HB2	19:S:76:THR:HG22	1.78	0.66
1:A:995:C:N3	1:A:1046:A:O2'	2.29	0.65
3:C:110:LEU:HD22	3:C:203:LYS:HG2	1.78	0.65
1:A:1159:U:C4'	2:B:131:LYS:HB3	2.24	0.65
1:A:1181:G:H21	2:B:129:THR:CA	2.10	0.65
1:A:1351:U:H3	1:A:1371:G:H1	1.44	0.65
20:T:39:ILE:HD13	20:T:83:ILE:HD13	1.78	0.65
1:A:390:U:H2'	1:A:391:G:H8	1.61	0.65
1:A:1181:G:H21	2:B:129:THR:HA	1.60	0.65
1:A:1289:A:N3	7:G:34:LYS:NZ	2.45	0.65
1:A:1430:A:N6	1:A:1471:U:O4	2.30	0.65
1:A:1179:A:H2'	1:A:1180:A:C8	2.32	0.65
8:H:105:SER:HB2	8:H:126:ILE:HD11	1.77	0.65
9:I:32:ARG:NH2	9:I:36:GLN:O	2.29	0.65
1:A:1266:G:N2	1:A:1269:A:OP2	2.27	0.65
3:C:13:ILE:HG22	3:C:14:VAL:H	1.62	0.65
4:D:11:LEU:HB3	4:D:63:ARG:HD3	1.79	0.65
4:D:132:ILE:HG22	4:D:134:SER:H	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:C:C2	2:B:130:LYS:HA	2.32	0.65
1:A:1342:C:H2'	1:A:1343:G:C8	2.31	0.65
7:G:110:ARG:HH12	7:G:121:ASN:HB3	1.61	0.65
1:A:149:A:H1'	1:A:1446:A:C2	2.31	0.64
1:A:451:A:H61	1:A:481:G:H5'	1.62	0.64
1:A:1382:C:H4'	7:G:78:ARG:HH21	1.63	0.64
8:H:77:ARG:NH2	8:H:79:SER:O	2.29	0.64
1:A:722:G:H1	1:A:733:G:H1	1.42	0.64
1:A:766:A:OP2	1:A:812:G:N2	2.28	0.64
1:A:405:U:O4	4:D:2:ALA:N	2.30	0.64
12:L:33:VAL:HG22	12:L:79:VAL:HG12	1.80	0.64
1:A:1071:C:H2'	1:A:1072:G:H8	1.62	0.64
1:A:1485:U:H2'	1:A:1486:G:C8	2.32	0.64
1:A:1323:G:O2'	1:A:1362:A:O4'	2.15	0.63
1:A:1181:G:C5	2:B:130:LYS:HB2	2.33	0.63
1:A:108:G:H5'	1:A:109:A:H5''	1.80	0.63
1:A:144:G:N1	1:A:179:A:N7	2.46	0.63
1:A:1181:G:C4	2:B:130:LYS:HB2	2.33	0.63
1:A:437:U:O4	1:A:495:A:N7	2.31	0.63
3:C:149:LYS:HB3	3:C:200:TRP:HB2	1.80	0.63
7:G:70:PRO:HG3	7:G:98:LEU:HD23	1.81	0.63
1:A:335:C:H2'	1:A:336:A:H8	1.63	0.63
10:J:12:ALA:HB2	10:J:96:VAL:HG22	1.81	0.63
10:J:15:HIS:HA	10:J:18:ILE:HG22	1.79	0.63
1:A:85:U:H4'	1:A:86:G:H5'	1.80	0.63
1:A:694:A:H5'	11:K:54:GLY:HA2	1.80	0.63
1:A:1158:C:C5	2:B:125:PHE:HB3	2.34	0.63
1:A:691:G:H21	1:A:696:A:H62	1.46	0.63
1:A:946:A:H2'	1:A:947:G:H8	1.63	0.63
11:K:18:ASP:O	11:K:37:ARG:NH2	2.32	0.63
1:A:715:A:OP1	1:A:805:C:O2'	2.15	0.62
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.80	0.62
1:A:888:G:H21	1:A:909:A:H62	0.75	0.62
1:A:975:A:H5'	1:A:1363:A:H62	1.64	0.62
1:A:1301:U:OP2	1:A:1303:C:N4	2.30	0.62
11:K:111:THR:HB	18:R:73:ARG:HH12	1.64	0.62
1:A:338:A:H2'	1:A:339:C:H6	1.65	0.62
1:A:1305:G:H22	1:A:1331:G:H1'	1.64	0.62
1:A:673:A:H2'	1:A:674:G:C8	2.33	0.62
1:A:710:G:H5''	6:F:53:LYS:HE2	1.81	0.62
1:A:632:U:H5'	1:A:633:G:H8	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:G:H5'	16:P:8:ARG:HH12	1.65	0.62
1:A:1218:C:H2'	1:A:1219:A:H8	1.65	0.62
1:A:704:A:H61	11:K:44:TRP:HH2	1.48	0.62
1:A:925:G:O2'	1:A:926:G:O4'	2.16	0.62
1:A:1064:G:O2'	1:A:1190:G:N2	2.32	0.62
1:A:615:G:O6	1:A:625:U:O2	2.18	0.61
10:J:36:VAL:HG22	10:J:38:GLY:H	1.63	0.61
14:N:27:LYS:HD2	14:N:48:GLN:HG2	1.82	0.61
1:A:160:A:N6	1:A:346:G:N7	2.48	0.61
2:B:55:GLU:HA	2:B:58:LYS:HD2	1.82	0.61
14:N:66:THR:HG23	14:N:68:ARG:H	1.65	0.61
1:A:475:C:H2'	1:A:476:U:C6	2.35	0.61
7:G:16:LYS:NZ	9:I:45:MET:SD	2.73	0.61
1:A:1440:U:H3	1:A:1461:G:H1	1.47	0.61
7:G:49:LEU:HD22	7:G:52:ARG:HH21	1.64	0.61
8:H:15:ARG:HH22	8:H:75:ILE:H	1.48	0.61
1:A:1158:C:O2	2:B:128:LEU:O	2.18	0.61
1:A:1253:G:H2'	1:A:1254:A:C8	2.36	0.61
1:A:1355:G:H2'	1:A:1356:G:C8	2.36	0.61
8:H:48:ASP:OD1	8:H:62:THR:OG1	2.13	0.61
1:A:112:G:H1	1:A:315:A:N6	1.98	0.61
1:A:1250:A:N3	1:A:1370:G:O2'	2.28	0.61
1:A:680:C:H2'	1:A:681:A:C8	2.36	0.61
4:D:7:PRO:HB2	4:D:10:LYS:HG2	1.83	0.61
5:E:31:PHE:O	5:E:54:ARG:NH1	2.34	0.61
1:A:41:G:H2'	1:A:42:G:H8	1.66	0.60
2:B:110:ILE:HG12	2:B:147:LEU:HD21	1.82	0.60
1:A:942:G:O6	1:A:1341:U:O4	2.20	0.60
1:A:634:C:H2'	1:A:635:A:H8	1.67	0.60
9:I:21:LYS:HB2	9:I:61:ASP:HB3	1.82	0.60
1:A:1140:C:N4	1:A:1141:C:H41	2.00	0.60
1:A:946:A:H2'	1:A:947:G:C8	2.36	0.60
9:I:20:ILE:HA	9:I:61:ASP:O	2.01	0.60
1:A:501:C:H2'	1:A:502:A:H8	1.65	0.60
1:A:999:C:H2'	1:A:1000:A:H8	1.66	0.59
1:A:1079:G:O2'	1:A:1080:A:O4'	2.14	0.59
1:A:945:G:N2	1:A:1334:G:O2'	2.35	0.59
1:A:1157:A:N1	1:A:1181:G:H4'	2.17	0.59
8:H:43:GLU:HG2	8:H:101:ILE:HG21	1.84	0.59
1:A:447:G:H21	1:A:487:A:N6	1.94	0.59
4:D:26:ARG:HH21	4:D:30:THR:HG22	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:GLU:HG3	5:E:57:PRO:HD2	1.83	0.59
5:E:149:SER:HB3	5:E:152:MET:HG3	1.84	0.59
1:A:401:C:OP2	4:D:70:ARG:NH1	2.35	0.59
3:C:46:LEU:HG	3:C:49:ALA:HB3	1.85	0.59
6:F:12:PRO:O	6:F:44:ARG:NH2	2.36	0.59
1:A:375:U:O2	16:P:28:ARG:NH2	2.35	0.59
1:A:1118:U:H1'	1:A:1179:A:C8	2.38	0.59
7:G:90:VAL:HG13	7:G:95:ARG:HE	1.67	0.59
1:A:834:U:O3'	18:R:53:ARG:NH2	2.36	0.59
1:A:1253:G:H2'	1:A:1254:A:H8	1.67	0.59
3:C:149:LYS:HB2	3:C:172:VAL:HG21	1.85	0.59
1:A:401:C:O2'	1:A:621:A:N3	2.33	0.58
1:A:1251:A:HO2'	1:A:1369:C:HO2'	1.50	0.58
20:T:74:ARG:O	20:T:78:ASN:ND2	2.32	0.58
2:B:69:VAL:HG11	2:B:168:GLU:HG2	1.84	0.58
1:A:113:G:H1'	1:A:354:G:H5'	1.85	0.58
1:A:1375:A:O2'	7:G:101:ARG:NH2	2.31	0.58
5:E:25:VAL:HG23	5:E:27:GLY:H	1.68	0.58
13:M:13:HIS:HA	13:M:43:LYS:HA	1.85	0.58
1:A:101:A:OP1	20:T:5:LYS:NZ	2.35	0.58
2:B:148:GLY:HA2	2:B:151:LYS:HE3	1.86	0.58
4:D:85:ASN:HB3	4:D:88:GLU:HB2	1.84	0.58
10:J:80:THR:HG22	10:J:81:GLU:H	1.67	0.58
11:K:15:GLN:NE2	11:K:78:GLY:O	2.35	0.58
18:R:18:VAL:HG13	18:R:21:ILE:HG22	1.86	0.58
1:A:181:A:O2'	1:A:193:C:N4	2.36	0.58
1:A:419:C:OP1	1:A:513:C:O2'	2.21	0.58
1:A:714:G:H2'	1:A:715:A:C8	2.37	0.58
1:A:898:G:N2	1:A:901:A:OP2	2.37	0.58
16:P:6:LEU:HD12	16:P:17:TYR:HB3	1.85	0.58
1:A:107:G:OP2	1:A:108:G:N2	2.36	0.58
2:B:113:LEU:HD13	2:B:147:LEU:HD23	1.86	0.58
1:A:380:G:N2	1:A:383:A:OP2	2.32	0.58
1:A:144:G:H2'	1:A:145:G:C8	2.39	0.58
1:A:1157:A:H4'	2:B:128:LEU:CA	2.28	0.58
16:P:35:ARG:HH22	16:P:38:PHE:HB3	1.69	0.58
1:A:625:U:H2'	1:A:626:G:C8	2.39	0.57
1:A:1433:A:N6	1:A:1468:A:C6	2.72	0.57
16:P:66:THR:HG22	16:P:67:ILE:H	1.69	0.57
1:A:774:G:H2'	1:A:775:G:C8	2.39	0.57
1:A:1415:G:O6	1:A:1485:U:O2	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:C:H2'	1:A:1000:A:C8	2.38	0.57
3:C:59:PRO:HD3	3:C:64:ARG:CZ	2.33	0.57
10:J:23:ALA:HA	10:J:26:VAL:HG22	1.85	0.57
1:A:552:U:H2'	1:A:553:A:H8	1.68	0.57
1:A:578:C:O2'	1:A:728:A:N3	2.35	0.57
1:A:924:C:H42	1:A:1532:U:H3	1.51	0.57
1:A:1151:A:H5'	10:J:43:PRO:HA	1.87	0.57
9:I:34:LEU:HG	9:I:35:GLU:HG2	1.85	0.57
1:A:41:G:H2'	1:A:42:G:C8	2.39	0.57
1:A:123:U:OP1	1:A:311:C:O2'	2.20	0.57
1:A:745:G:H5'	1:A:851:G:H21	1.70	0.57
1:A:976:G:OP2	1:A:1358:U:O2'	2.22	0.57
1:A:1356:G:H2'	1:A:1357:A:C8	2.39	0.57
10:J:6:ILE:HG22	10:J:102:LEU:HG	1.85	0.57
1:A:233:C:H2'	1:A:234:C:H6	1.70	0.57
1:A:545:C:OP1	4:D:62:ARG:NH1	2.37	0.57
8:H:52:GLU:O	8:H:58:GLU:HB2	2.05	0.57
1:A:1233:G:O2'	1:A:1365:G:OP1	2.22	0.57
1:A:716:A:O2'	11:K:119:ASN:OD1	2.19	0.57
2:B:19:THR:O	2:B:21:TYR:N	2.37	0.57
18:R:33:ILE:HG21	18:R:68:LEU:HD11	1.86	0.57
1:A:339:C:H2'	1:A:340:U:C6	2.40	0.56
1:A:1130:A:OP1	9:I:17:ARG:NH2	2.38	0.56
1:A:1317:C:H3'	1:A:1318:A:H8	1.69	0.56
13:M:13:HIS:HB2	13:M:16:ILE:HG22	1.87	0.56
16:P:13:LYS:O	16:P:14:ARG:NE	2.36	0.56
1:A:717:U:H2'	1:A:734:G:H8	1.70	0.56
1:A:1088:G:H2'	1:A:1089:G:C8	2.40	0.56
1:A:1125:U:H2'	1:A:1126:U:H2'	1.86	0.56
1:A:1341:U:O2'	9:I:127:SER:O	2.24	0.56
1:A:1445:U:O4	1:A:1457:G:O6	2.24	0.56
8:H:9:ASP:HB3	8:H:13:ARG:HH21	1.71	0.56
1:A:231:U:H2'	1:A:232:G:H8	1.69	0.56
1:A:908:A:H2'	1:A:909:A:H8	1.71	0.56
1:A:501:C:H2'	1:A:502:A:C8	2.40	0.56
1:A:1218:C:H2'	1:A:1219:A:C8	2.40	0.56
1:A:1478:U:O2'	1:A:1479:C:O4'	2.23	0.56
11:K:116:ILE:HD12	11:K:117:PRO:HD2	1.88	0.56
1:A:1006:G:O6	1:A:1023:U:O2	2.24	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.41	0.56
1:A:861:G:H21	1:A:874:G:H5'	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:A:H2'	1:A:1103:C:C6	2.41	0.56
1:A:680:C:H2'	1:A:681:A:H8	1.70	0.56
1:A:1235:U:H2'	1:A:1236:A:C8	2.41	0.56
9:I:114:LYS:HD3	9:I:117:LEU:HD22	1.87	0.56
1:A:591:U:H2'	1:A:592:G:C8	2.41	0.56
2:B:100:LEU:HD22	2:B:178:LEU:HG	1.88	0.56
3:C:148:ILE:HG22	3:C:169:GLU:HB2	1.88	0.56
19:S:41:PRO:O	19:S:44:ILE:HG12	2.06	0.56
1:A:1158:C:H2'	2:B:132:GLU:H	1.70	0.56
10:J:9:ARG:HB2	10:J:99:GLN:HB2	1.88	0.56
15:O:12:VAL:O	15:O:16:GLY:N	2.36	0.56
1:A:706:A:H2'	1:A:707:U:C6	2.42	0.55
1:A:1160:G:C5	1:A:1182:G:N1	2.74	0.55
1:A:1293:C:H2'	1:A:1294:G:H8	1.71	0.55
14:N:63:CYS:HB3	14:N:67:GLY:H	1.71	0.55
1:A:1158:C:OP1	2:B:128:LEU:HD13	2.06	0.55
1:A:1158:C:C6	2:B:125:PHE:HB3	2.42	0.55
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.88	0.55
10:J:44:THR:HG21	10:J:68:ARG:HH11	1.72	0.55
1:A:645:G:H2'	1:A:646:G:H8	1.72	0.55
1:A:200:G:H2'	1:A:201:G:C8	2.42	0.55
1:A:214:C:H2'	1:A:215:C:C6	2.41	0.55
1:A:1107:C:OP2	3:C:171:ARG:NH1	2.36	0.55
1:A:1182:G:O3'	2:B:131:LYS:NZ	2.39	0.55
10:J:9:ARG:HG2	10:J:73:LEU:HD21	1.88	0.55
13:M:1:ALA:HB3	13:M:8:ILE:HG13	1.88	0.55
13:M:51:GLN:O	13:M:55:LEU:HG	2.06	0.55
1:A:8:A:N6	4:D:202:GLU:O	2.40	0.55
1:A:636:U:H2'	1:A:637:C:C6	2.41	0.55
1:A:1157:A:N6	1:A:1178:G:N2	2.03	0.55
1:A:1431:A:H4'	1:A:1432:G:OP1	2.05	0.55
15:O:64:ARG:NH1	15:O:89:ARG:OXT	2.39	0.55
19:S:44:ILE:HD12	19:S:63:ASP:HA	1.87	0.55
1:A:335:C:H2'	1:A:336:A:C8	2.40	0.55
1:A:339:C:H2'	1:A:340:U:H6	1.70	0.55
12:L:114:ARG:HB3	12:L:119:VAL:HB	1.88	0.55
13:M:78:ARG:HD3	13:M:79:LEU:HD23	1.89	0.55
1:A:829:G:H2'	1:A:830:G:H8	1.72	0.55
1:A:1008:U:OP1	14:N:23:ARG:NH1	2.39	0.55
1:A:1140:C:C4	1:A:1141:C:N4	2.74	0.55
3:C:147:GLY:HA2	3:C:170:GLY:HA3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:LEU:HG	8:H:45:PHE:HB2	1.88	0.55
1:A:113:G:H2'	1:A:114:U:C6	2.42	0.55
1:A:419:C:H5''	1:A:513:C:H4'	1.89	0.55
1:A:924:C:H2'	1:A:925:G:C4	2.42	0.55
2:B:26:MET:HB3	2:B:192:PRO:HG3	1.88	0.55
4:D:62:ARG:O	4:D:66:GLY:N	2.34	0.55
2:B:59:ILE:HG13	2:B:64:GLY:HA3	1.89	0.54
13:M:53:ASP:HA	13:M:56:ARG:HH11	1.72	0.54
1:A:1177:G:O6	1:A:1181:G:H5''	2.07	0.54
1:A:1301:U:H2'	1:A:1303:C:C6	2.43	0.54
1:A:1315:U:O2'	1:A:1360:A:N3	2.31	0.54
7:G:140:VAL:HA	7:G:143:MET:HG2	1.89	0.54
1:A:1043:G:H2'	1:A:1044:A:C8	2.42	0.54
1:A:601:G:H2'	1:A:602:A:H8	1.73	0.54
1:A:681:A:H2'	1:A:682:G:H8	1.71	0.54
1:A:1013:G:H21	1:A:1015:G:H8	1.54	0.54
19:S:30:LEU:H	19:S:30:LEU:HD23	1.72	0.54
1:A:711:G:H2'	1:A:712:A:H8	1.72	0.54
11:K:96:THR:O	11:K:100:LEU:HG	2.08	0.54
1:A:6:G:O6	5:E:100:SER:N	2.38	0.54
1:A:83:C:O2'	1:A:85:U:OP2	2.26	0.54
1:A:390:U:H2'	1:A:391:G:C8	2.43	0.54
2:B:165:ALA:HA	2:B:172:ILE:HD12	1.89	0.54
5:E:52:LYS:O	5:E:62:LYS:NZ	2.34	0.54
9:I:59:LYS:HG2	9:I:60:LEU:HG	1.89	0.54
10:J:24:GLU:O	10:J:28:THR:OG1	2.21	0.54
13:M:22:TYR:HB2	13:M:65:GLU:HG3	1.88	0.54
1:A:21:G:H2'	1:A:22:G:C8	2.43	0.54
1:A:235:C:H2'	1:A:236:A:H8	1.73	0.54
1:A:1329:A:H5'	13:M:25:GLY:HA3	1.89	0.54
1:A:1433:A:C5	1:A:1468:A:N1	2.76	0.54
13:M:19:THR:HG23	13:M:25:GLY:HA2	1.90	0.54
1:A:549:C:H2'	1:A:550:G:C8	2.43	0.54
1:A:959:A:HO2'	1:A:984:C:HO2'	1.40	0.54
1:A:976:G:N2	1:A:1362:A:HO2'	2.06	0.54
1:A:1178:G:N1	1:A:1181:G:O5'	2.40	0.54
1:A:1217:C:OP1	14:N:8:ARG:NH1	2.40	0.54
1:A:177:G:OP2	1:A:177:G:N2	2.32	0.54
1:A:258:G:H1	1:A:268:U:H3	1.54	0.54
1:A:1161:C:H2'	1:A:1162:C:C6	2.43	0.54
14:N:65:GLN:HG3	14:N:78:LEU:HG	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:4:ILE:HG23	20:T:7:ALA:H	1.73	0.54
1:A:212:G:H2'	1:A:213:G:H8	1.72	0.53
1:A:227:G:H2'	1:A:228:A:C8	2.43	0.53
20:T:59:ASP:OD1	20:T:76:LYS:NZ	2.30	0.53
1:A:709:U:H2'	1:A:710:G:C8	2.44	0.53
1:A:950:U:H2'	1:A:951:G:C8	2.43	0.53
1:A:1254:A:H2'	1:A:1255:G:C8	2.43	0.53
3:C:155:ARG:HB2	3:C:195:ILE:HG12	1.88	0.53
1:A:410:G:H21	1:A:432:A:H62	1.57	0.53
1:A:713:G:N2	1:A:777:A:O2'	2.37	0.53
1:A:774:G:H2'	1:A:775:G:H8	1.74	0.53
1:A:1159:U:O4'	2:B:131:LYS:HE2	2.08	0.53
1:A:1161:C:H2'	1:A:1162:C:H6	1.74	0.53
1:A:1250:A:H2'	1:A:1251:A:C8	2.42	0.53
14:N:6:LYS:O	14:N:10:VAL:HG23	2.09	0.53
1:A:1159:U:C3'	2:B:135:MET:HB2	2.37	0.53
1:A:1476:A:H2'	1:A:1477:U:C6	2.43	0.53
3:C:138:GLN:OE1	3:C:142:ARG:NH1	2.42	0.53
11:K:25:ALA:HB1	11:K:90:GLY:HA3	1.90	0.53
1:A:1178:G:N2	1:A:1180:A:H3'	2.23	0.53
6:F:26:THR:O	6:F:30:THR:HG23	2.08	0.53
1:A:637:C:H2'	1:A:638:U:C6	2.43	0.53
1:A:648:A:H2'	1:A:649:A:C8	2.44	0.53
1:A:792:A:O2'	1:A:794:A:N7	2.35	0.53
1:A:1355:G:H2'	1:A:1356:G:H8	1.73	0.53
10:J:45:ARG:HH21	10:J:69:THR:HG21	1.74	0.53
1:A:159:G:H21	1:A:161:A:H3'	1.72	0.53
10:J:88:MET:SD	10:J:88:MET:N	2.82	0.53
15:O:25:THR:HG23	15:O:66:LEU:HD22	1.91	0.53
1:A:88:U:O2'	1:A:89:U:OP1	2.27	0.53
1:A:150:U:O2'	1:A:151:A:O4'	2.27	0.53
1:A:455:G:H2'	1:A:456:A:C8	2.43	0.53
1:A:1348:U:H2'	1:A:1349:A:C8	2.44	0.53
1:A:1454:G:H2'	1:A:1455:G:H8	1.74	0.53
2:B:165:ALA:HB3	2:B:190:SER:HB3	1.89	0.53
6:F:9:MET:HA	6:F:58:HIS:O	2.07	0.53
5:E:16:ILE:HD12	5:E:36:LEU:HG	1.90	0.53
10:J:10:LEU:HB2	10:J:72:ARG:HB2	1.89	0.53
16:P:38:PHE:HZ	16:P:48:GLU:HG2	1.74	0.53
1:A:684:U:H2'	1:A:685:G:C8	2.44	0.53
1:A:1130:A:H2'	1:A:1131:G:H8	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:22:ILE:O	6:F:25:TYR:HB2	2.09	0.53
10:J:11:LYS:HG3	10:J:71:LEU:HG	1.91	0.53
15:O:39:LEU:HD23	15:O:56:LEU:HD13	1.91	0.53
1:A:28:A:O2'	1:A:296:U:OP1	2.27	0.52
2:B:127:LYS:HB2	2:B:128:LEU:HD23	1.89	0.52
4:D:188:ARG:HA	4:D:191:LEU:HD12	1.90	0.52
8:H:26:THR:OG1	8:H:60:GLU:OE1	2.20	0.52
12:L:110:ARG:HB3	12:L:119:VAL:HG21	1.91	0.52
1:A:107:G:N7	20:T:10:ARG:NH2	2.56	0.52
1:A:785:G:H2'	1:A:786:G:C8	2.43	0.52
13:M:12:LYS:HB2	13:M:17:ALA:HB2	1.89	0.52
1:A:154:U:H2'	1:A:155:A:H8	1.74	0.52
1:A:363:A:N6	12:L:27:CYS:SG	2.83	0.52
1:A:1060:U:H2'	1:A:1061:G:H8	1.75	0.52
1:A:1118:U:H1'	1:A:1179:A:N7	2.25	0.52
1:A:1433:A:C6	1:A:1468:A:C2	2.97	0.52
3:C:188:ALA:N	3:C:195:ILE:O	2.43	0.52
1:A:131:A:HO2'	1:A:262:A:HO2'	1.56	0.52
1:A:294:U:OP1	1:A:610:U:O2'	2.16	0.52
1:A:1151:A:HO2'	1:A:1152:A:H8	1.57	0.52
1:A:1213:A:H2'	1:A:1215:G:C8	2.44	0.52
4:D:9:LEU:HG	4:D:22:LYS:HE2	1.91	0.52
13:M:12:LYS:HB3	13:M:16:ILE:HG23	1.91	0.52
1:A:1045:C:H2'	1:A:1046:A:O4'	2.10	0.52
1:A:1189:U:H5''	3:C:4:VAL:HG11	1.91	0.52
1:A:1245:C:N4	1:A:1246:A:H62	2.08	0.52
8:H:6:PRO:HB2	8:H:33:LYS:HE3	1.92	0.52
9:I:126:PHE:HB3	9:I:129:ARG:HE	1.74	0.52
13:M:13:HIS:NE2	13:M:41:ASP:O	2.43	0.52
15:O:55:GLY:O	15:O:59:MET:HG3	2.09	0.52
1:A:1123:U:H2'	1:A:1124:G:C8	2.44	0.52
1:A:1376:U:O3'	7:G:94:ARG:NH2	2.42	0.52
10:J:47:GLU:HG3	10:J:49:PHE:CE2	2.45	0.52
1:A:336:A:H2'	1:A:337:G:H8	1.75	0.52
1:A:1438:G:H2'	1:A:1439:G:H8	1.73	0.52
10:J:11:LYS:HB2	10:J:97:ASP:HB3	1.92	0.52
1:A:889:A:H62	1:A:908:A:H62	1.56	0.52
1:A:1013:G:N2	1:A:1016:A:OP2	2.35	0.52
11:K:84:VAL:HG12	11:K:107:ILE:HD11	1.92	0.52
13:M:100:ARG:HG2	13:M:102:LYS:HG2	1.91	0.52
1:A:776:G:H22	1:A:802:A:H5''	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:C:H3'	1:A:1318:A:C8	2.44	0.52
1:A:1524:C:OP1	11:K:122:ARG:NH2	2.43	0.52
2:B:147:LEU:O	2:B:151:LYS:N	2.38	0.52
13:M:66:GLY:HA2	13:M:69:ARG:HB2	1.91	0.52
1:A:493:A:H2'	1:A:494:G:C8	2.45	0.52
1:A:1247:U:O2	1:A:1290:G:O6	2.28	0.52
1:A:1348:U:H2'	1:A:1349:A:H8	1.76	0.52
1:A:600:A:N6	1:A:639:G:O6	2.42	0.51
1:A:601:G:H2'	1:A:602:A:C8	2.45	0.51
1:A:942:G:N2	9:I:127:SER:OG	2.43	0.51
1:A:1144:G:N2	1:A:1146:A:H62	2.08	0.51
6:F:11:HIS:CE1	6:F:13:ASP:HB2	2.45	0.51
1:A:154:U:H2'	1:A:155:A:C8	2.45	0.51
1:A:1354:U:H2'	1:A:1355:G:C8	2.45	0.51
1:A:814:A:HO2'	1:A:1510:C:HO2'	1.58	0.51
1:A:973:G:H3'	1:A:974:A:H5''	1.93	0.51
7:G:91:ARG:HG2	7:G:93:VAL:HG12	1.91	0.51
1:A:699:C:N4	1:A:700:G:N7	2.59	0.51
1:A:1004:A:H2'	1:A:1005:A:O4'	2.10	0.51
1:A:1078:U:O2'	5:E:134:ILE:HD12	2.11	0.51
5:E:148:ASN:OD1	5:E:153:VAL:HG13	2.10	0.51
1:A:323:U:OP1	20:T:21:ASN:ND2	2.43	0.51
1:A:638:U:H2'	1:A:639:G:H8	1.74	0.51
1:A:1091:U:O2'	1:A:1093:A:N7	2.35	0.51
1:A:1181:G:C6	2:B:130:LYS:HE2	2.46	0.51
1:A:1465:A:H2'	1:A:1466:C:C6	2.46	0.51
2:B:49:PHE:O	2:B:53:LEU:HG	2.10	0.51
10:J:59:LYS:HE3	10:J:62:ARG:HE	1.75	0.51
14:N:26:LEU:HA	14:N:29:ILE:HD12	1.92	0.51
1:A:927:G:H3'	1:A:928:G:H8	1.75	0.51
1:A:1159:U:OP2	2:B:131:LYS:HB2	2.11	0.51
1:A:1477:U:H2'	1:A:1478:U:O4'	2.09	0.51
4:D:161:LEU:O	4:D:165:ARG:N	2.43	0.51
5:E:103:THR:N	5:E:122:ASN:OD1	2.32	0.51
1:A:68:G:H1'	1:A:171:A:C2	2.45	0.51
1:A:434:U:H2'	1:A:435:A:C8	2.46	0.51
1:A:720:C:H2'	1:A:721:G:C8	2.46	0.51
1:A:1004:A:OP1	1:A:1024:G:N2	2.43	0.51
1:A:1219:A:H2'	1:A:1220:G:C8	2.46	0.51
9:I:25:GLY:HA2	9:I:60:LEU:O	2.11	0.51
19:S:48:ILE:O	19:S:59:VAL:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:C:H2'	1:A:313:A:C8	2.46	0.51
1:A:384:G:H2'	1:A:385:C:C6	2.46	0.51
1:A:981:U:OP1	14:N:12:ARG:NH2	2.44	0.51
4:D:152:GLN:O	4:D:156:LYS:NZ	2.44	0.51
7:G:60:ALA:HA	7:G:63:VAL:HG22	1.92	0.51
9:I:41:GLU:HG2	9:I:71:ILE:HG21	1.93	0.51
12:L:44:LYS:HG3	12:L:45:PRO:HA	1.93	0.51
1:A:10:A:H2'	1:A:11:G:H8	1.76	0.51
1:A:982:U:OP2	14:N:62:ARG:NH2	2.43	0.51
1:A:1201:A:H4'	1:A:1202:U:O5'	2.11	0.51
13:M:82:LEU:HB3	19:S:73:PHE:HE1	1.76	0.51
1:A:591:U:H2'	1:A:592:G:H8	1.75	0.50
5:E:142:ASP:O	5:E:146:ASN:ND2	2.44	0.50
8:H:15:ARG:NH2	8:H:75:ILE:H	2.09	0.50
18:R:48:ARG:O	18:R:52:GLN:N	2.40	0.50
1:A:94:G:N2	1:A:97:G:OP2	2.44	0.50
1:A:1219:A:H2'	1:A:1220:G:H8	1.76	0.50
8:H:89:LYS:HA	8:H:92:LEU:HG	1.93	0.50
18:R:33:ILE:HG22	18:R:39:ILE:HG23	1.93	0.50
1:A:203:G:N2	1:A:204:G:O6	2.44	0.50
1:A:217:C:H2'	1:A:218:U:C6	2.46	0.50
1:A:1244:G:H2'	1:A:1245:C:C6	2.46	0.50
1:A:538:G:H5''	12:L:111:LYS:HB2	1.93	0.50
11:K:53:ARG:HA	11:K:57:LYS:HD2	1.92	0.50
1:A:512:U:H2'	1:A:513:C:H6	1.77	0.50
1:A:580:C:H2'	1:A:581:G:O4'	2.11	0.50
6:F:92:THR:HG22	6:F:94:HIS:H	1.76	0.50
9:I:83:THR:HG21	9:I:102:PHE:HB3	1.92	0.50
12:L:99:ARG:NH2	12:L:105:SER:O	2.39	0.50
13:M:10:ASP:HA	13:M:44:ILE:HD11	1.92	0.50
13:M:65:GLU:O	13:M:68:LEU:N	2.45	0.50
16:P:18:GLN:HE21	16:P:35:ARG:HH21	1.58	0.50
17:Q:72:SER:O	17:Q:72:SER:OG	2.30	0.50
1:A:570:G:H2'	1:A:571:U:C6	2.46	0.50
1:A:549:C:H2'	1:A:550:G:H8	1.77	0.50
1:A:1209:C:O2'	1:A:1214:C:N4	2.45	0.50
1:A:1312:G:H2'	1:A:1313:U:C6	2.47	0.50
2:B:185:ILE:HG22	2:B:199:ILE:HB	1.93	0.50
1:A:131:A:H2'	1:A:132:C:H6	1.77	0.50
1:A:181:A:H1'	1:A:194:C:N4	2.25	0.50
1:A:932:C:N4	1:A:933:G:O6	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:C:H2'	1:A:1072:G:C8	2.44	0.50
1:A:1072:G:N2	2:B:105:THR:HG21	2.27	0.50
1:A:1181:G:N2	2:B:129:THR:HA	2.27	0.50
11:K:16:VAL:HG12	11:K:18:ASP:H	1.76	0.50
1:A:1105:A:H2'	1:A:1106:G:H8	1.77	0.49
1:A:1481:U:H2'	1:A:1482:G:O4'	2.12	0.49
3:C:72:PRO:HA	3:C:75:VAL:HG22	1.94	0.49
15:O:3:LEU:HD13	15:O:35:GLN:HE22	1.76	0.49
1:A:1152:A:H4'	10:J:15:HIS:CE1	2.47	0.49
1:A:1158:C:O2'	2:B:132:GLU:OE1	2.30	0.49
1:A:1348:U:H5''	9:I:121:ARG:HG3	1.94	0.49
2:B:18:GLN:O	2:B:188:THR:OG1	2.30	0.49
5:E:159:LYS:HB3	5:E:163:GLU:HB2	1.95	0.49
1:A:625:U:H2'	1:A:626:G:H8	1.76	0.49
1:A:1371:G:H2'	1:A:1372:U:C6	2.47	0.49
1:A:1438:G:H1	1:A:1463:U:H3	1.59	0.49
9:I:56:MET:O	9:I:58:GLU:N	2.44	0.49
1:A:34:C:H2'	1:A:35:G:H8	1.77	0.49
1:A:912:C:H2'	1:A:913:A:C8	2.48	0.49
1:A:987:G:H21	1:A:1015:G:N2	2.09	0.49
2:B:160:LEU:HD22	2:B:162:VAL:HG22	1.94	0.49
9:I:41:GLU:HG3	9:I:42:THR:H	1.76	0.49
1:A:335:C:O2'	1:A:1433:A:N3	2.35	0.49
1:A:600:A:H2'	1:A:601:G:H8	1.78	0.49
1:A:691:G:N2	1:A:696:A:H62	2.11	0.49
1:A:1122:U:H2'	1:A:1123:U:C6	2.48	0.49
1:A:1163:A:H2'	1:A:1164:G:O4'	2.13	0.49
5:E:148:ASN:OD1	5:E:152:MET:HB2	2.13	0.49
1:A:94:G:H4'	1:A:95:C:H5'	1.93	0.49
1:A:407:U:H2'	1:A:408:A:H8	1.77	0.49
1:A:1017:U:H2'	1:A:1018:G:C8	2.47	0.49
1:A:1157:A:N6	1:A:1180:A:C5	2.80	0.49
2:B:93:HIS:CE1	2:B:145:ASN:HD22	2.31	0.49
1:A:728:A:H2'	1:A:729:A:C8	2.47	0.49
1:A:1433:A:C6	1:A:1468:A:N1	2.80	0.49
4:D:157:ALA:O	4:D:160:GLU:HG2	2.13	0.49
6:F:10:VAL:HG21	6:F:18:VAL:HG11	1.94	0.49
19:S:48:ILE:HB	19:S:59:VAL:HB	1.94	0.49
1:A:715:A:H2'	1:A:716:A:C8	2.47	0.49
2:B:164:ASP:O	2:B:168:GLU:HB2	2.12	0.49
1:A:936:C:H2'	1:A:937:A:H8	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:A:O2'	19:S:77:ARG:NH2	2.46	0.49
2:B:205:ALA:O	2:B:208:ALA:N	2.38	0.49
10:J:24:GLU:OE1	10:J:90:LEU:HB3	2.12	0.49
1:A:406:G:N1	1:A:437:U:O4	2.46	0.49
1:A:1438:G:H2'	1:A:1439:G:C8	2.47	0.49
14:N:78:LEU:HD23	14:N:82:LYS:HB3	1.94	0.49
17:Q:47:HIS:NE2	17:Q:49:GLU:OE2	2.46	0.49
1:A:200:G:H2'	1:A:201:G:H8	1.78	0.48
1:A:425:G:H2'	1:A:426:U:O4'	2.13	0.48
1:A:562:U:H1'	12:L:12:ARG:HD2	1.95	0.48
1:A:634:C:H2'	1:A:635:A:C8	2.46	0.48
1:A:834:U:H2'	1:A:835:U:C6	2.47	0.48
1:A:1467:C:H2'	1:A:1468:A:C8	2.48	0.48
1:A:1524:C:H2'	1:A:1525:G:C8	2.48	0.48
1:A:69:G:O2'	1:A:70:U:O4'	2.30	0.48
1:A:850:U:H2'	1:A:851:G:H5''	1.94	0.48
1:A:1073:U:H2'	1:A:1074:G:O4'	2.14	0.48
1:A:1287:A:H2'	1:A:1288:A:C8	2.48	0.48
4:D:26:ARG:HB2	4:D:31:LYS:HE3	1.94	0.48
7:G:25:PHE:CD1	7:G:100:MET:HB3	2.49	0.48
17:Q:31:HIS:N	17:Q:36:LYS:O	2.34	0.48
1:A:718:A:C8	11:K:118:HIS:HD2	2.31	0.48
1:A:722:G:O2'	1:A:724:G:OP1	2.28	0.48
4:D:159:LEU:O	4:D:163:GLU:HG2	2.13	0.48
8:H:115:ALA:HA	8:H:118:GLN:HG2	1.95	0.48
13:M:18:LEU:HD12	13:M:21:ILE:HD12	1.95	0.48
1:A:521:G:H4'	12:L:70:GLU:HG2	1.96	0.48
1:A:685:G:H22	1:A:706:A:H2	1.61	0.48
1:A:1083:U:O2'	1:A:1102:A:OP1	2.30	0.48
1:A:1222:G:OP1	1:A:1321:U:O2'	2.32	0.48
2:B:84:LEU:HB2	2:B:90:PHE:CE1	2.48	0.48
12:L:34:CYS:SG	12:L:53:CYS:HB2	2.53	0.48
12:L:99:ARG:HB3	12:L:106:GLY:HA2	1.95	0.48
1:A:404:G:O6	4:D:2:ALA:N	2.45	0.48
1:A:664:G:H22	1:A:741:G:H1	1.61	0.48
1:A:1342:C:H5'	9:I:127:SER:HA	1.95	0.48
2:B:72:LYS:NZ	2:B:203:ASP:HB3	2.28	0.48
3:C:78:LYS:HE2	3:C:81:GLU:HG3	1.95	0.48
5:E:107:ALA:HB1	5:E:111:MET:HE3	1.96	0.48
6:F:23:GLU:O	6:F:26:THR:OG1	2.20	0.48
7:G:23:ALA:HA	7:G:26:VAL:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:ARG:NH1	8:H:75:ILE:O	2.30	0.48
16:P:15:PRO:HD2	16:P:42:ILE:HD11	1.95	0.48
1:A:687:A:N1	1:A:703:G:O2'	2.36	0.48
1:A:1060:U:H5'	10:J:53:ILE:HG13	1.96	0.48
1:A:1300:G:H4'	1:A:1301:U:O5'	2.12	0.48
2:B:110:ILE:HG22	2:B:114:LYS:HE2	1.95	0.48
3:C:83:VAL:HG13	3:C:100:ILE:HD11	1.94	0.48
1:A:131:A:H2'	1:A:132:C:C6	2.48	0.48
1:A:167:A:H2'	1:A:168:G:H8	1.79	0.48
1:A:374:A:N1	1:A:390:U:O2'	2.46	0.48
1:A:600:A:H2'	1:A:601:G:C8	2.49	0.48
1:A:1372:U:H2'	1:A:1373:G:O4'	2.13	0.48
7:G:70:PRO:HA	7:G:141:HIS:HE1	1.79	0.48
1:A:373:A:H61	1:A:391:G:H1'	1.79	0.48
1:A:606:G:N2	1:A:633:G:N7	2.62	0.48
1:A:707:U:H2'	1:A:708:C:C6	2.49	0.48
1:A:886:G:O6	1:A:911:U:O4	2.31	0.48
7:G:78:ARG:HA	7:G:83:THR:HA	1.95	0.48
1:A:1181:G:H21	2:B:128:LEU:C	2.17	0.48
1:A:1347:G:C8	9:I:108:ARG:HG2	2.48	0.48
5:E:56:VAL:O	5:E:60:ILE:HG23	2.13	0.48
1:A:380:G:C2	1:A:382:A:H5''	2.48	0.48
1:A:1129:C:H4'	9:I:17:ARG:HH22	1.79	0.48
2:B:112:ARG:HA	2:B:115:ASP:OD2	2.14	0.48
4:D:110:THR:HG23	4:D:113:GLU:H	1.78	0.48
1:A:15:G:N2	1:A:921:U:O2	2.47	0.47
1:A:1228:C:H2'	1:A:1229:A:C8	2.45	0.47
1:A:1409:C:H2'	1:A:1410:A:C8	2.50	0.47
2:B:185:ILE:HG13	2:B:185:ILE:O	2.14	0.47
7:G:65:LEU:HA	7:G:68:VAL:HG22	1.94	0.47
11:K:13:ARG:N	11:K:76:GLU:OE1	2.47	0.47
1:A:648:A:H2'	1:A:649:A:H8	1.79	0.47
1:A:765:G:H1	1:A:812:G:HO2'	1.62	0.47
6:F:4:TYR:CD2	6:F:71:ILE:HG13	2.50	0.47
9:I:113:LYS:NZ	9:I:117:LEU:O	2.46	0.47
3:C:121:SER:OG	3:C:122:GLN:NE2	2.47	0.47
13:M:80:MET:SD	13:M:91:ARG:NH2	2.87	0.47
1:A:640:A:H2'	1:A:641:U:C6	2.48	0.47
1:A:1014:A:C4	1:A:1015:G:N2	2.82	0.47
1:A:1178:G:H22	1:A:1180:A:H3'	1.78	0.47
2:B:132:GLU:HA	2:B:135:MET:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:HIS:CD2	14:N:88:MET:HB3	2.49	0.47
1:A:416:G:H2'	1:A:417:G:H8	1.79	0.47
1:A:473:U:C2	1:A:474:G:C8	3.03	0.47
1:A:908:A:H2'	1:A:909:A:C8	2.49	0.47
1:A:973:G:O2'	10:J:56:HIS:HA	2.15	0.47
1:A:1329:A:H2'	1:A:1330:U:O4'	2.14	0.47
2:B:65:LYS:HB2	2:B:157:PRO:HA	1.97	0.47
3:C:178:ARG:HH11	3:C:206:ILE:HB	1.79	0.47
15:O:74:ASP:OD2	15:O:77:ARG:NH1	2.48	0.47
1:A:148:G:O2'	1:A:1447:A:H5'	2.15	0.47
1:A:327:A:O2'	1:A:328:C:O4'	2.28	0.47
1:A:681:A:H2'	1:A:682:G:C8	2.49	0.47
1:A:751:U:H2'	1:A:752:G:C4	2.50	0.47
1:A:826:C:O2	8:H:16:ASN:ND2	2.48	0.47
1:A:1226:C:H5''	13:M:94:LEU:HD11	1.96	0.47
13:M:73:SER:HA	13:M:76:ILE:HD12	1.95	0.47
1:A:112:G:N2	1:A:315:A:N1	2.62	0.47
1:A:312:C:H2'	1:A:313:A:H8	1.80	0.47
1:A:374:A:H4'	1:A:452:A:H2	1.80	0.47
1:A:424:G:H2'	1:A:425:G:H8	1.78	0.47
1:A:689:C:HO2'	1:A:705:G:HO2'	1.63	0.47
1:A:922:G:C2	1:A:923:A:C5	3.03	0.47
1:A:974:A:OP2	14:N:68:ARG:NH1	2.39	0.47
1:A:1041:G:H2'	1:A:1042:A:C8	2.50	0.47
1:A:1077:G:N2	1:A:1080:A:OP2	2.47	0.47
1:A:1415:G:C6	1:A:1485:U:O2	2.68	0.47
2:B:83:ALA:HA	2:B:88:GLN:HB2	1.97	0.47
3:C:92:ASP:OD1	3:C:93:ILE:N	2.47	0.47
5:E:84:PRO:HD2	8:H:96:MET:HA	1.96	0.47
13:M:33:LEU:O	13:M:37:GLY:N	2.47	0.47
19:S:27:LYS:HG2	19:S:28:LYS:N	2.29	0.47
1:A:512:U:H2'	1:A:513:C:C6	2.50	0.47
1:A:925:G:H2'	1:A:926:G:C8	2.49	0.47
1:A:941:G:H21	9:I:122:ARG:HH22	1.63	0.47
17:Q:26:GLU:HG3	17:Q:41:THR:HG22	1.97	0.47
1:A:217:C:H2'	1:A:218:U:H6	1.80	0.47
1:A:463:U:H2'	1:A:464:U:O4'	2.15	0.47
1:A:550:G:H2'	1:A:551:U:C6	2.50	0.47
1:A:1209:C:N3	1:A:1210:C:N4	2.58	0.47
1:A:1261:A:C8	1:A:1275:A:C6	3.03	0.47
1:A:750:C:H1'	15:O:21:ASP:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:C:H5	2:B:125:PHE:HB3	1.79	0.47
1:A:1278:G:N3	1:A:1279:G:N2	2.63	0.47
1:A:1351:U:O2	1:A:1371:G:N2	2.42	0.47
1:A:714:G:H2'	1:A:715:A:H8	1.80	0.46
1:A:976:G:N2	1:A:1362:A:O2'	2.48	0.46
1:A:1356:G:H2'	1:A:1357:A:H8	1.80	0.46
5:E:156:LYS:HD2	8:H:71:VAL:HA	1.97	0.46
6:F:24:ARG:O	6:F:27:ALA:HB3	2.14	0.46
7:G:129:ASN:HA	7:G:134:VAL:HG21	1.97	0.46
16:P:38:PHE:CE1	16:P:51:ARG:HB2	2.50	0.46
1:A:113:G:H2'	1:A:114:U:H6	1.80	0.46
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.46
1:A:923:A:C6	1:A:924:C:C4	3.03	0.46
1:A:1328:C:OP1	13:M:27:THR:OG1	2.27	0.46
4:D:37:ALA:HB3	4:D:42:GLY:HA2	1.96	0.46
5:E:69:ARG:HG3	5:E:70:ASN:ND2	2.30	0.46
5:E:85:VAL:HG21	5:E:147:MET:HG2	1.97	0.46
6:F:18:VAL:O	6:F:21:MET:HB2	2.14	0.46
1:A:665:A:H1'	1:A:733:G:H5'	1.97	0.46
1:A:1106:G:O2'	3:C:168:ARG:NH1	2.48	0.46
1:A:1287:A:N3	1:A:1353:G:O2'	2.46	0.46
1:A:1300:G:H1'	1:A:1301:U:OP2	2.15	0.46
8:H:87:LYS:HG3	8:H:125:ILE:HD11	1.96	0.46
10:J:52:LEU:HD13	10:J:59:LYS:HD2	1.97	0.46
1:A:86:G:H1'	1:A:87:C:O4'	2.15	0.46
1:A:711:G:H2'	1:A:712:A:C8	2.49	0.46
1:A:985:C:H2'	1:A:986:U:C6	2.51	0.46
1:A:1111:A:N1	3:C:176:THR:HG22	2.31	0.46
1:A:1118:U:H2'	1:A:1119:C:C6	2.51	0.46
1:A:1246:A:H2'	1:A:1247:U:O4'	2.15	0.46
7:G:106:ALA:HB2	7:G:132:THR:HB	1.97	0.46
10:J:46:LYS:HG2	10:J:68:ARG:HG2	1.97	0.46
13:M:13:HIS:CD2	13:M:43:LYS:HD3	2.51	0.46
1:A:15:G:N1	1:A:921:U:N3	2.64	0.46
1:A:427:U:OP2	1:A:428:G:O2'	2.21	0.46
1:A:492:C:H2'	1:A:493:A:C5	2.51	0.46
1:A:828:U:H5	1:A:870:U:H5	1.64	0.46
1:A:1118:U:H2'	1:A:1119:C:H6	1.80	0.46
5:E:91:GLY:HA3	5:E:135:ASN:CG	2.35	0.46
7:G:134:VAL:O	7:G:138:GLU:HG2	2.15	0.46
1:A:10:A:H2'	1:A:11:G:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:G:H2'	1:A:192:A:H8	1.80	0.46
1:A:1158:C:P	2:B:129:THR:HG22	2.56	0.46
1:A:1309:G:C6	1:A:1329:A:C6	3.04	0.46
1:A:398:U:H2'	1:A:399:G:H8	1.81	0.46
1:A:434:U:H2'	1:A:435:A:H8	1.81	0.46
1:A:1152:A:OP1	10:J:70:HIS:ND1	2.49	0.46
1:A:1159:U:H5'	2:B:135:MET:HB2	1.98	0.46
1:A:1260:G:H4'	1:A:1283:U:O2'	2.15	0.46
1:A:1347:G:H5''	9:I:108:ARG:HG3	1.98	0.46
1:A:1433:A:N6	1:A:1468:A:C5	2.84	0.46
15:O:11:ILE:HD11	15:O:30:ALA:HB1	1.96	0.46
1:A:260:G:H2'	1:A:261:U:C6	2.51	0.46
1:A:883:C:H2'	1:A:884:U:C6	2.51	0.46
1:A:959:A:O2'	1:A:984:C:O2'	2.12	0.46
1:A:1347:G:H22	1:A:1374:A:P	2.37	0.46
1:A:1386:G:H2'	1:A:1387:G:H8	1.81	0.46
5:E:77:ASN:HB2	5:E:80:THR:O	2.16	0.46
14:N:98:ALA:HB1	14:N:100:TRP:HZ3	1.81	0.46
1:A:17:U:H2'	1:A:18:C:C6	2.51	0.46
1:A:718:A:H61	18:R:70:TYR:HB3	1.81	0.46
1:A:1181:G:C6	2:B:130:LYS:HB2	2.51	0.46
1:A:1213:A:N7	1:A:1215:G:C2	2.84	0.46
1:A:1303:C:H2'	1:A:1304:G:O4'	2.16	0.46
1:A:1415:G:N2	1:A:1486:G:OP1	2.44	0.46
1:A:1464:U:O4	1:A:1465:A:N6	2.48	0.46
2:B:174:GLU:HA	2:B:177:ASN:HD21	1.80	0.46
16:P:54:LEU:HD23	16:P:57:ILE:HD12	1.97	0.46
1:A:264:C:O2'	17:Q:66:PRO:O	2.34	0.46
1:A:362:G:H5''	12:L:58:THR:HG21	1.98	0.46
1:A:375:U:H2'	1:A:376:G:O4'	2.16	0.46
1:A:1042:A:H2'	1:A:1043:G:C8	2.51	0.46
3:C:147:GLY:HA2	3:C:171:ARG:H	1.81	0.46
10:J:100:ILE:O	10:J:100:ILE:HG13	2.16	0.46
13:M:85:TYR:CE2	13:M:89:ARG:HG3	2.51	0.46
1:A:1372:U:O2'	7:G:33:GLY:O	2.21	0.45
2:B:132:GLU:OE1	2:B:136:ARG:HD2	2.16	0.45
1:A:947:G:H2'	1:A:948:C:H6	1.81	0.45
7:G:92:PRO:HA	7:G:95:ARG:HB2	1.97	0.45
9:I:18:VAL:HG13	9:I:64:ILE:HG12	1.97	0.45
10:J:93:ALA:O	10:J:95:GLY:N	2.48	0.45
13:M:75:SER:O	13:M:79:LEU:HG	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:C:H2'	1:A:937:A:C8	2.51	0.45
1:A:967:C:H5''	1:A:968:A:OP2	2.16	0.45
1:A:1314:C:H5	19:S:5:LYS:HE2	1.81	0.45
3:C:115:VAL:O	3:C:119:ILE:HG12	2.17	0.45
4:D:122:ALA:HA	4:D:146:ARG:HH11	1.82	0.45
16:P:28:ARG:NE	16:P:29:ASN:OD1	2.40	0.45
18:R:33:ILE:HD13	18:R:68:LEU:HD11	1.99	0.45
1:A:34:C:H2'	1:A:35:G:C8	2.51	0.45
1:A:171:A:H2'	1:A:172:A:C4	2.52	0.45
1:A:890:G:O2'	1:A:906:A:N6	2.38	0.45
1:A:1258:G:H2'	1:A:1259:C:C6	2.51	0.45
5:E:100:SER:OG	5:E:103:THR:OG1	2.29	0.45
11:K:23:ILE:O	11:K:87:LYS:HB3	2.16	0.45
1:A:744:C:H2'	1:A:745:G:C8	2.50	0.45
1:A:1524:C:H2'	1:A:1525:G:H8	1.82	0.45
2:B:105:THR:HA	2:B:108:GLN:HG2	1.99	0.45
8:H:32:LEU:O	8:H:36:ILE:HG12	2.16	0.45
17:Q:61:ILE:HA	17:Q:75:LEU:HA	1.98	0.45
1:A:835:U:OP1	18:R:53:ARG:NH1	2.49	0.45
1:A:837:U:H2'	1:A:838:G:H8	1.80	0.45
1:A:1158:C:O2'	2:B:132:GLU:HB2	2.15	0.45
1:A:1254:A:H2'	1:A:1255:G:H8	1.82	0.45
7:G:38:ALA:O	7:G:42:VAL:HG22	2.17	0.45
9:I:68:GLY:O	9:I:74:GLN:HG2	2.16	0.45
9:I:70:GLY:O	9:I:74:GLN:HG3	2.16	0.45
11:K:25:ALA:HB1	11:K:93:ARG:HG3	1.97	0.45
15:O:43:PHE:O	15:O:47:LYS:NZ	2.39	0.45
1:A:539:A:H2'	1:A:540:G:H8	1.82	0.45
1:A:1155:A:H2'	1:A:1156:G:O4'	2.16	0.45
14:N:29:ILE:HG23	14:N:34:ASN:HD22	1.80	0.45
1:A:19:A:H2'	1:A:20:U:C6	2.52	0.45
1:A:127:G:O2'	17:Q:6:ARG:NH2	2.49	0.45
1:A:751:U:H3'	1:A:752:G:C8	2.52	0.45
1:A:832:G:C2	1:A:833:G:C8	3.05	0.45
1:A:1124:G:O2'	1:A:1127:G:O6	2.34	0.45
1:A:1366:C:O3'	10:J:62:ARG:NH1	2.50	0.45
2:B:56:LEU:HD11	2:B:161:PHE:HE2	1.81	0.45
4:D:129:VAL:HG22	4:D:146:ARG:HH22	1.82	0.45
7:G:110:ARG:HD3	7:G:122:GLU:HG3	1.97	0.45
11:K:99:ALA:O	11:K:103:ALA:N	2.50	0.45
1:A:26:A:H61	1:A:558:G:H1'	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:U:H2'	1:A:151:A:H8	1.81	0.45
1:A:924:C:N4	1:A:1532:U:H3	2.15	0.45
1:A:1174:G:H2'	1:A:1175:G:O4'	2.17	0.45
2:B:83:ALA:HB3	2:B:90:PHE:HB3	1.98	0.45
12:L:101:ALA:O	12:L:102:LEU:HG	2.17	0.45
1:A:706:A:O2'	1:A:707:U:O4'	2.21	0.45
1:A:1102:A:H2'	1:A:1103:C:H6	1.81	0.45
1:A:1376:U:O4	7:G:9:ARG:NH2	2.50	0.45
15:O:31:LEU:O	15:O:35:GLN:HG2	2.17	0.45
1:A:981:U:O2'	14:N:60:ARG:HG3	2.17	0.44
1:A:1200:C:H5''	1:A:1201:A:H3'	1.99	0.44
1:A:1318:A:H1'	19:S:36:ARG:HH12	1.82	0.44
2:B:206:ILE:HA	2:B:209:VAL:HG12	1.99	0.44
3:C:10:ARG:HH21	3:C:179:ALA:HB3	1.81	0.44
4:D:11:LEU:HB3	4:D:63:ARG:HH11	1.82	0.44
5:E:134:ILE:H	5:E:134:ILE:HG12	1.50	0.44
12:L:55:VAL:HG21	12:L:80:ILE:HD11	1.99	0.44
18:R:25:ASP:OD2	18:R:25:ASP:N	2.50	0.44
1:A:750:C:H2'	1:A:751:U:C6	2.52	0.44
1:A:1467:C:H2'	1:A:1468:A:H8	1.82	0.44
3:C:188:ALA:HB3	3:C:195:ILE:HB	1.99	0.44
7:G:15:PRO:HG2	7:G:16:LYS:HE2	1.99	0.44
13:M:3:ILE:HD12	13:M:3:ILE:H	1.81	0.44
1:A:105:G:OP2	20:T:13:GLN:NE2	2.50	0.44
1:A:1018:G:H2'	1:A:1019:A:H8	1.81	0.44
1:A:1079:G:H2'	1:A:1080:A:C8	2.51	0.44
1:A:1332:A:H2'	1:A:1333:A:C8	2.52	0.44
10:J:7:ARG:HG2	10:J:75:ASP:OD1	2.17	0.44
10:J:13:PHE:HD2	14:N:93:PRO:HB2	1.82	0.44
1:A:407:U:H2'	1:A:408:A:C8	2.51	0.44
1:A:987:G:H21	1:A:1015:G:H21	1.65	0.44
1:A:1214:C:H5'	1:A:1215:G:H8	1.81	0.44
1:A:1343:G:H2'	1:A:1344:C:O4'	2.18	0.44
1:A:1354:U:H2'	1:A:1355:G:H8	1.81	0.44
1:A:1512:U:H2'	1:A:1513:A:C8	2.53	0.44
3:C:111:ASP:HB3	3:C:114:LEU:HD12	1.98	0.44
5:E:16:ILE:HD13	5:E:137:VAL:HG11	1.98	0.44
7:G:70:PRO:HA	7:G:141:HIS:CE1	2.53	0.44
11:K:93:ARG:O	11:K:96:THR:HG22	2.16	0.44
19:S:6:LYS:HD3	19:S:6:LYS:HA	1.83	0.44
1:A:131:A:O2'	1:A:262:A:O2'	2.27	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:U:O4	1:A:752:G:O2'	2.22	0.44
1:A:1120:C:H2'	1:A:1121:U:H6	1.82	0.44
5:E:153:VAL:HG21	8:H:99:LEU:HD12	1.98	0.44
12:L:56:ARG:HB2	12:L:62:GLU:OE1	2.18	0.44
14:N:12:ARG:HG2	14:N:53:ASP:OD2	2.18	0.44
1:A:45:G:H2'	1:A:46:G:C8	2.52	0.44
1:A:333:U:H2'	1:A:334:C:C6	2.53	0.44
1:A:411:A:OP1	4:D:26:ARG:NH1	2.50	0.44
1:A:1078:U:H5''	5:E:138:ARG:NH1	2.32	0.44
1:A:1120:C:H2'	1:A:1121:U:C6	2.53	0.44
1:A:1213:A:C2	1:A:1215:G:H1'	2.53	0.44
1:A:5:U:O3'	1:A:6:G:N2	2.51	0.44
1:A:102:G:OP1	20:T:5:LYS:HD2	2.17	0.44
1:A:262:A:H5''	20:T:70:ASN:HB2	1.99	0.44
1:A:335:C:C2	1:A:336:A:C8	3.06	0.44
1:A:673:A:OP1	6:F:52:ASN:ND2	2.48	0.44
7:G:49:LEU:HD11	7:G:123:LEU:HG	1.99	0.44
11:K:62:ALA:HA	11:K:65:VAL:HG22	2.00	0.44
12:L:54:ARG:NH1	12:L:64:THR:OG1	2.51	0.44
1:A:806:C:H2'	1:A:807:A:H8	1.83	0.44
1:A:1122:U:H2'	1:A:1123:U:C5	2.53	0.44
1:A:1174:G:C5	1:A:1175:G:C8	3.05	0.44
3:C:110:LEU:HB3	3:C:203:LYS:HE3	2.00	0.44
9:I:105:ARG:NH1	9:I:107:ALA:HA	2.33	0.44
11:K:21:ALA:HB3	11:K:84:VAL:HG23	1.99	0.44
18:R:71:THR:HG22	18:R:73:ARG:H	1.82	0.44
1:A:6:G:HO2'	1:A:7:A:H8	1.66	0.44
1:A:259:G:H2'	1:A:260:G:H8	1.82	0.44
1:A:386:C:H2'	1:A:387:U:C6	2.53	0.44
1:A:1041:G:H2'	1:A:1042:A:H8	1.82	0.44
1:A:1178:G:N2	1:A:1181:G:O5'	2.51	0.44
2:B:91:VAL:HG22	2:B:150:ILE:HD11	1.99	0.44
6:F:9:MET:HB2	6:F:57:ALA:HB1	2.00	0.44
7:G:62:GLU:O	7:G:66:GLU:HG2	2.17	0.44
13:M:33:LEU:HD22	13:M:38:ILE:HB	2.00	0.44
18:R:41:PRO:HD2	18:R:44:ILE:HD13	2.00	0.44
1:A:236:A:H2'	1:A:237:G:C8	2.51	0.43
1:A:252:U:O2	1:A:275:G:N2	2.51	0.43
1:A:763:G:H2'	1:A:764:C:C6	2.53	0.43
1:A:1155:A:C2	1:A:1156:G:H1'	2.52	0.43
1:A:1162:C:C2	1:A:1163:A:N7	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:A:H2'	1:A:1177:G:C8	2.53	0.43
2:B:11:ALA:HB1	2:B:14:HIS:NE2	2.33	0.43
5:E:97:GLN:HG2	5:E:98:PRO:HD2	2.00	0.43
9:I:20:ILE:HG21	9:I:60:LEU:HD13	1.99	0.43
11:K:17:SER:HA	11:K:79:ILE:HA	1.99	0.43
13:M:97:ARG:HD2	13:M:97:ARG:HA	1.81	0.43
16:P:58:ALA:HA	16:P:61:VAL:HG12	2.00	0.43
1:A:261:U:P	20:T:74:ARG:HH11	2.42	0.43
1:A:594:U:H3'	1:A:595:A:H8	1.84	0.43
1:A:947:G:H2'	1:A:948:C:C6	2.52	0.43
1:A:1237:C:H5'	1:A:1238:A:H8	1.83	0.43
13:M:32:ILE:HG23	13:M:33:LEU:HD23	2.00	0.43
1:A:19:A:OP2	5:E:132:ASN:ND2	2.51	0.43
1:A:73:C:C2'	1:A:74:A:H5'	2.48	0.43
1:A:868:C:H2'	1:A:869:G:O4'	2.18	0.43
1:A:1091:U:H2'	1:A:1093:A:OP2	2.18	0.43
1:A:1107:C:C4	1:A:1108:G:C8	3.07	0.43
18:R:23:TYR:CE2	18:R:24:LYS:HE2	2.54	0.43
1:A:19:A:H2'	1:A:20:U:H6	1.82	0.43
1:A:27:G:H2'	1:A:28:A:C8	2.53	0.43
1:A:340:U:H2'	1:A:341:C:C6	2.53	0.43
1:A:982:U:H1'	1:A:983:A:C6	2.54	0.43
1:A:1369:C:OP2	9:I:112:ARG:HG3	2.19	0.43
1:A:1381:U:H2'	1:A:1382:C:O4'	2.18	0.43
10:J:22:THR:O	10:J:26:VAL:HG13	2.18	0.43
14:N:79:SER:O	14:N:83:VAL:HG23	2.17	0.43
1:A:53:A:H2'	1:A:54:C:O4'	2.17	0.43
1:A:334:C:H2'	1:A:335:C:H6	1.84	0.43
1:A:608:A:C2	1:A:609:A:H1'	2.52	0.43
1:A:707:U:H2'	1:A:708:C:H6	1.84	0.43
1:A:763:G:H2'	1:A:764:C:H6	1.84	0.43
1:A:825:A:H2	8:H:12:THR:HG21	1.82	0.43
3:C:41:TYR:O	3:C:45:GLU:HG2	2.19	0.43
8:H:46:ILE:HG22	8:H:63:LEU:HD13	2.01	0.43
11:K:36:ASP:O	11:K:38:GLN:N	2.52	0.43
11:K:94:GLU:O	11:K:97:ILE:HG12	2.19	0.43
11:K:123:PRO:HA	11:K:124:PRO:HD3	1.90	0.43
12:L:51:LYS:HG2	12:L:72:HIS:CD2	2.53	0.43
1:A:231:U:H2'	1:A:232:G:C8	2.51	0.43
1:A:235:C:H2'	1:A:236:A:C8	2.53	0.43
1:A:717:U:H4'	11:K:119:ASN:HD21	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:G:H2'	1:A:830:G:C8	2.52	0.43
1:A:854:U:H5''	1:A:871:U:N3	2.33	0.43
1:A:1035:A:H2'	1:A:1036:A:C8	2.53	0.43
1:A:1250:A:H4'	9:I:69:GLY:N	2.28	0.43
2:B:96:LEU:O	2:B:99:MET:HG2	2.19	0.43
4:D:101:VAL:O	4:D:105:MET:HG2	2.19	0.43
8:H:46:ILE:HG21	8:H:61:LEU:HD13	2.00	0.43
1:A:81:A:N6	1:A:87:C:N3	2.65	0.43
1:A:456:A:H2'	1:A:457:G:C8	2.54	0.43
1:A:1161:C:C2	1:A:1162:C:C5	3.06	0.43
2:B:191:ASP:HB2	2:B:193:ASP:OD1	2.19	0.43
10:J:33:GLY:O	10:J:80:THR:OG1	2.33	0.43
10:J:52:LEU:HD11	10:J:59:LYS:HA	2.01	0.43
1:A:45:G:H2'	1:A:46:G:H8	1.84	0.43
1:A:91:U:H2'	1:A:92:U:H6	1.84	0.43
1:A:162:A:N7	1:A:163:C:H1'	2.33	0.43
1:A:986:U:H2'	1:A:987:G:H8	1.83	0.43
1:A:1301:U:HO2'	1:A:1302:C:H6	1.66	0.43
2:B:83:ALA:CB	2:B:90:PHE:HB3	2.49	0.43
2:B:107:ARG:HA	2:B:110:ILE:HB	2.01	0.43
2:B:218:ALA:HA	2:B:221:ARG:HD2	2.01	0.43
7:G:37:THR:O	7:G:41:ILE:HG12	2.19	0.43
1:A:73:C:H2'	1:A:74:A:H5'	2.00	0.43
1:A:1039:G:H2'	1:A:1040:U:C6	2.53	0.43
1:A:1070:U:H2'	1:A:1071:C:C6	2.54	0.43
1:A:1087:G:N3	1:A:1087:G:H2'	2.33	0.43
1:A:1098:C:H5'	1:A:1167:A:H61	1.83	0.43
1:A:1491:G:H2'	1:A:1492:A:C8	2.54	0.43
7:G:21:LEU:HG	7:G:22:LEU:HD22	2.01	0.43
7:G:112:ASP:HB3	7:G:117:LEU:HD22	2.00	0.43
8:H:84:ARG:HB2	17:Q:37:PHE:HE2	1.84	0.43
11:K:65:VAL:HG23	11:K:69:ARG:HH12	1.84	0.43
15:O:8:THR:O	15:O:12:VAL:HG23	2.18	0.43
1:A:320:A:H2'	1:A:321:A:C8	2.54	0.43
1:A:399:G:H2'	1:A:400:C:C6	2.54	0.43
1:A:836:G:OP2	18:R:50:LYS:HD3	2.19	0.43
1:A:898:G:H2'	1:A:900:A:OP2	2.19	0.43
1:A:941:G:H21	9:I:122:ARG:HH12	1.66	0.43
1:A:1057:G:H2'	1:A:1058:G:C8	2.53	0.43
1:A:1479:C:H2'	1:A:1480:A:C8	2.43	0.43
2:B:102:ASN:O	2:B:105:THR:HG22	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:91:ARG:HH12	6:F:93:LYS:HD3	1.83	0.43
7:G:62:GLU:HA	7:G:65:LEU:HG	2.01	0.43
16:P:66:THR:HG22	16:P:67:ILE:N	2.34	0.43
18:R:65:LEU:HD23	18:R:67:LEU:HD11	2.01	0.43
1:A:25:C:H2'	1:A:26:A:H8	1.84	0.42
1:A:160:A:H1'	1:A:344:A:C5	2.53	0.42
1:A:269:C:H2'	1:A:270:A:H8	1.84	0.42
1:A:779:C:H2'	1:A:780:A:C8	2.54	0.42
1:A:902:G:H2'	1:A:903:G:H8	1.83	0.42
1:A:1018:G:H2'	1:A:1019:A:C8	2.54	0.42
1:A:1160:G:C6	1:A:1161:C:C4	3.07	0.42
1:A:1179:A:C6	1:A:1180:A:C6	3.06	0.42
1:A:1203:C:H2'	1:A:1204:A:H8	1.84	0.42
2:B:147:LEU:HD12	2:B:150:ILE:HB	2.01	0.42
3:C:69:THR:HG21	3:C:75:VAL:HG21	2.01	0.42
4:D:75:TYR:OH	4:D:97:ARG:NH1	2.52	0.42
1:A:398:U:H2'	1:A:399:G:C8	2.54	0.42
1:A:636:U:H2'	1:A:637:C:H6	1.83	0.42
1:A:865:A:O5'	1:A:865:A:H8	2.02	0.42
1:A:1012:A:H2'	1:A:1013:G:C8	2.54	0.42
1:A:1160:G:N3	2:B:130:LYS:HD2	2.34	0.42
6:F:29:ILE:HD12	6:F:64:VAL:HG11	2.00	0.42
9:I:38:PHE:HE2	9:I:78:ILE:HD12	1.83	0.42
9:I:64:ILE:HG21	9:I:78:ILE:HG12	2.01	0.42
16:P:59:HIS:O	16:P:63:GLN:HG2	2.19	0.42
19:S:31:ARG:HH21	19:S:56:HIS:CE1	2.37	0.42
1:A:240:G:H2'	1:A:241:G:H8	1.84	0.42
1:A:545:C:H2'	1:A:546:A:O4'	2.19	0.42
1:A:737:C:H5'	6:F:89:VAL:O	2.20	0.42
1:A:1040:U:H2'	1:A:1041:G:C8	2.54	0.42
1:A:1251:A:H2'	1:A:1252:A:C8	2.54	0.42
3:C:145:ALA:O	3:C:147:GLY:N	2.50	0.42
1:A:358:U:H2'	1:A:359:G:C8	2.40	0.42
1:A:773:G:N1	1:A:807:A:C6	2.87	0.42
1:A:986:U:H2'	1:A:987:G:C8	2.54	0.42
1:A:1048:G:O2'	1:A:1050:G:OP1	2.37	0.42
3:C:58:ARG:HB3	3:C:63:ILE:HA	2.00	0.42
7:G:74:VAL:HG13	7:G:85:GLN:HB3	2.01	0.42
10:J:11:LYS:HE2	10:J:97:ASP:HB3	2.01	0.42
1:A:600:A:C6	1:A:639:G:C6	3.08	0.42
1:A:1158:C:O2	2:B:129:THR:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:G:H1'	2:B:130:LYS:CG	2.49	0.42
1:A:1181:G:H21	2:B:129:THR:N	2.16	0.42
1:A:1329:A:H5'	13:M:25:GLY:CA	2.48	0.42
3:C:129:PHE:CG	3:C:156:LEU:HD22	2.54	0.42
1:A:27:G:H2'	1:A:28:A:H8	1.85	0.42
1:A:62:U:H1'	1:A:379:C:H1'	2.02	0.42
1:A:321:A:H2'	1:A:322:C:C6	2.54	0.42
1:A:377:G:H2'	1:A:378:G:H8	1.83	0.42
1:A:879:C:H2'	1:A:880:C:C6	2.55	0.42
1:A:1456:A:C2	1:A:1457:G:H1'	2.54	0.42
2:B:27:LYS:HD2	2:B:30:ILE:HD12	2.01	0.42
1:A:82:G:H21	1:A:83:C:H4'	1.84	0.42
1:A:593:U:H2'	1:A:594:U:H6	1.84	0.42
1:A:1213:A:C5	1:A:1215:G:N3	2.87	0.42
1:A:1240:U:OP1	7:G:115:MET:HB2	2.20	0.42
1:A:1460:C:C2	1:A:1461:G:C8	3.08	0.42
8:H:75:ILE:HG13	8:H:129:VAL:HG22	2.02	0.42
10:J:67:ILE:HG23	14:N:94:GLY:O	2.19	0.42
1:A:102:G:H2'	1:A:103:U:C6	2.54	0.42
1:A:518:C:H6	1:A:530:G:H5'	1.84	0.42
1:A:682:G:C4	1:A:683:G:C8	3.08	0.42
1:A:901:A:C8	1:A:902:G:H1'	2.55	0.42
1:A:1070:U:H2'	1:A:1071:C:H6	1.85	0.42
1:A:1072:G:H2'	1:A:1073:U:C6	2.55	0.42
1:A:1209:C:H2'	1:A:1210:C:C5	2.55	0.42
1:A:1510:C:N4	1:A:1511:G:O6	2.53	0.42
3:C:128:MET:HB2	3:C:131:ARG:HD3	2.01	0.42
4:D:202:GLU:OE2	5:E:106:ILE:HA	2.20	0.42
7:G:55:LYS:HE3	7:G:57:GLU:OE1	2.19	0.42
1:A:710:G:H2'	1:A:711:G:C8	2.54	0.42
1:A:1105:A:H2'	1:A:1106:G:C8	2.55	0.42
1:A:1181:G:C2	2:B:130:LYS:N	2.88	0.42
2:B:72:LYS:HZ1	2:B:164:ASP:HB2	1.85	0.42
3:C:18:ASN:HD21	3:C:39:ARG:NH1	2.18	0.42
3:C:18:ASN:O	3:C:55:VAL:HA	2.20	0.42
6:F:7:VAL:HG21	18:R:24:LYS:NZ	2.35	0.42
8:H:75:ILE:HA	8:H:128:TYR:O	2.20	0.42
10:J:48:ARG:HD3	14:N:100:TRP:CZ2	2.54	0.42
10:J:57:VAL:HG12	10:J:58:ASN:N	2.35	0.42
1:A:259:G:H2'	1:A:260:G:C8	2.55	0.42
1:A:496:A:N3	1:A:496:A:H2'	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:A:H61	1:A:742:G:H1	1.68	0.42
1:A:911:U:H2'	1:A:912:C:C6	2.55	0.42
1:A:982:U:O2	1:A:983:A:N6	2.52	0.42
1:A:1469:C:H2'	1:A:1470:U:O4'	2.20	0.42
4:D:28:ILE:H	4:D:28:ILE:HD12	1.84	0.42
11:K:67:ALA:HB1	11:K:100:LEU:HD23	2.02	0.42
14:N:44:VAL:O	14:N:48:GLN:HG3	2.20	0.42
1:A:167:A:H2'	1:A:168:G:C8	2.55	0.41
1:A:691:G:O6	11:K:57:LYS:NZ	2.53	0.41
1:A:922:G:H2'	1:A:923:A:C8	2.55	0.41
1:A:1106:G:O3'	3:C:171:ARG:HB2	2.20	0.41
1:A:1120:C:C2	1:A:1121:U:C5	3.07	0.41
6:F:7:VAL:HA	6:F:60:VAL:O	2.19	0.41
7:G:91:ARG:O	7:G:95:ARG:N	2.52	0.41
9:I:113:LYS:HE2	9:I:118:ARG:O	2.20	0.41
14:N:9:GLU:HG2	14:N:12:ARG:HH11	1.84	0.41
1:A:518:C:C6	1:A:530:G:H5'	2.56	0.41
1:A:825:A:H1'	8:H:9:ASP:OD1	2.21	0.41
1:A:1431:A:H2'	1:A:1432:G:C4	2.54	0.41
2:B:160:LEU:HD13	2:B:175:ALA:HB2	2.02	0.41
8:H:39:VAL:O	8:H:42:GLU:HG3	2.20	0.41
1:A:516:U:H3'	1:A:517:G:C8	2.56	0.41
1:A:806:C:H2'	1:A:807:A:C8	2.56	0.41
2:B:67:LEU:HB2	2:B:160:LEU:HG	2.02	0.41
3:C:18:ASN:HD21	3:C:39:ARG:HH12	1.67	0.41
9:I:44:ARG:NH1	9:I:45:MET:HG2	2.34	0.41
11:K:75:LYS:NZ	11:K:79:ILE:O	2.53	0.41
11:K:113:VAL:O	11:K:113:VAL:HG12	2.20	0.41
15:O:54:ARG:O	15:O:57:LEU:HG	2.21	0.41
1:A:302:G:H2'	1:A:303:A:C8	2.55	0.41
1:A:416:G:H2'	1:A:417:G:C8	2.55	0.41
1:A:710:G:H2'	1:A:711:G:H8	1.85	0.41
1:A:1181:G:C2	2:B:130:LYS:HB2	2.55	0.41
2:B:22:TRP:HA	2:B:189:ASN:OD1	2.19	0.41
2:B:212:TYR:O	2:B:216:VAL:HG23	2.20	0.41
3:C:139:ASN:ND2	3:C:142:ARG:HH21	2.17	0.41
4:D:75:TYR:OH	4:D:134:SER:OG	2.32	0.41
9:I:42:THR:OG1	9:I:43:ALA:N	2.54	0.41
9:I:84:ARG:O	9:I:87:MET:HG2	2.19	0.41
9:I:105:ARG:HH11	9:I:107:ALA:HA	1.84	0.41
13:M:24:VAL:HG23	13:M:28:ARG:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:17:TYR:HE2	16:P:41:PRO:HG3	1.85	0.41
18:R:12:ARG:O	18:R:16:GLU:HG3	2.20	0.41
1:A:590:U:H2'	1:A:591:U:H6	1.85	0.41
1:A:980:C:O2	14:N:58:ARG:HA	2.19	0.41
1:A:1101:A:H1'	1:A:1102:A:OP2	2.19	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.54	0.41
2:B:27:LYS:HD2	2:B:27:LYS:HA	1.77	0.41
3:C:55:VAL:HB	3:C:66:THR:HB	2.02	0.41
11:K:65:VAL:O	11:K:69:ARG:HG2	2.21	0.41
12:L:23:ALA:HB3	12:L:95:TYR:OH	2.21	0.41
12:L:83:ARG:NH2	12:L:96:HIS:HB2	2.35	0.41
1:A:80:A:H2'	1:A:81:A:O4'	2.21	0.41
1:A:148:G:N2	1:A:175:C:O2	2.53	0.41
1:A:1017:U:H2'	1:A:1018:G:H8	1.85	0.41
1:A:1272:G:H2'	1:A:1273:C:C6	2.55	0.41
1:A:1323:G:H2'	1:A:1324:A:H8	1.84	0.41
1:A:1454:G:H2'	1:A:1455:G:C8	2.53	0.41
3:C:123:LEU:HD21	3:C:195:ILE:HD12	2.02	0.41
4:D:11:LEU:HD23	4:D:63:ARG:NH1	2.36	0.41
7:G:47:GLU:HG3	7:G:51:GLN:NE2	2.36	0.41
13:M:84:CYS:HB2	19:S:73:PHE:HA	2.01	0.41
19:S:3:SER:HB2	19:S:5:LYS:HZ1	1.84	0.41
19:S:32:THR:O	19:S:50:VAL:HA	2.19	0.41
1:A:424:G:H2'	1:A:425:G:C8	2.55	0.41
1:A:779:C:H2'	1:A:780:A:H8	1.85	0.41
1:A:979:C:C4	1:A:980:C:C4	3.09	0.41
1:A:1504:G:O2'	1:A:1505:G:O4'	2.20	0.41
6:F:11:HIS:HE1	6:F:13:ASP:HB2	1.83	0.41
10:J:36:VAL:HB	10:J:76:ILE:HG22	2.02	0.41
11:K:71:ALA:O	11:K:75:LYS:HG2	2.21	0.41
1:A:355:C:H1'	1:A:388:G:N3	2.36	0.41
1:A:374:A:H61	1:A:390:U:C2'	2.34	0.41
1:A:446:G:C2	1:A:489:C:C2	3.08	0.41
1:A:755:G:H2'	1:A:756:C:C6	2.56	0.41
1:A:879:C:H2'	1:A:880:C:H6	1.84	0.41
1:A:1013:G:H2'	1:A:1015:G:OP2	2.19	0.41
1:A:1381:U:C2	7:G:77:ARG:HD2	2.56	0.41
1:A:1455:G:H2'	1:A:1456:A:C8	2.56	0.41
3:C:6:PRO:HG2	3:C:183:TYR:CG	2.55	0.41
5:E:78:ASN:OD1	5:E:79:GLY:N	2.49	0.41
20:T:27:MET:SD	20:T:57:ILE:HD11	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:A:H5'	1:A:110:C:C5	2.55	0.41
1:A:518:C:C5	1:A:529:G:H3'	2.56	0.41
1:A:1144:G:H21	1:A:1146:A:H62	1.68	0.41
1:A:1268:G:N3	1:A:1326:U:O2'	2.54	0.41
1:A:1415:G:O6	1:A:1485:U:C2	2.74	0.41
3:C:22:PHE:CD2	10:J:97:ASP:HB2	2.56	0.41
3:C:69:THR:HG21	3:C:75:VAL:HG11	2.03	0.41
3:C:81:GLU:O	3:C:84:GLU:HG3	2.21	0.41
4:D:162:ALA:HA	4:D:165:ARG:HB2	2.02	0.41
7:G:46:LEU:O	7:G:49:LEU:HB2	2.20	0.41
8:H:11:LEU:HD12	8:H:77:ARG:HD2	2.03	0.41
8:H:106:THR:HG23	8:H:108:LYS:H	1.85	0.41
8:H:113:ASP:OD1	8:H:114:ARG:N	2.54	0.41
9:I:27:ILE:HG12	9:I:62:LEU:HB2	2.03	0.41
10:J:54:SER:OG	10:J:57:VAL:O	2.23	0.41
14:N:52:ARG:O	14:N:58:ARG:NH1	2.54	0.41
16:P:8:ARG:O	16:P:9:HIS:ND1	2.54	0.41
17:Q:25:ILE:O	17:Q:41:THR:HA	2.21	0.41
19:S:68:HIS:CD2	19:S:69:LYS:H	2.38	0.41
1:A:4:U:H5	4:D:81:ARG:HG3	1.86	0.41
1:A:81:A:N3	1:A:81:A:H2'	2.36	0.41
1:A:213:G:C5	1:A:214:C:C5	3.09	0.41
1:A:384:G:H2'	1:A:385:C:H6	1.85	0.41
1:A:394:G:H2'	1:A:395:C:C6	2.56	0.41
1:A:745:G:H2'	1:A:746:A:C8	2.55	0.41
1:A:950:U:H2'	1:A:951:G:H8	1.83	0.41
1:A:1256:A:C6	3:C:26:LYS:HE3	2.56	0.41
6:F:3:HIS:HD2	6:F:65:GLU:HB2	1.86	0.41
15:O:21:ASP:N	15:O:21:ASP:OD1	2.53	0.41
1:A:123:U:H2'	1:A:124:C:C6	2.56	0.40
1:A:153:C:C2	1:A:154:U:C5	3.09	0.40
1:A:489:C:C2	1:A:490:C:C5	3.09	0.40
1:A:559:A:H4'	1:A:560:A:H3'	2.03	0.40
1:A:592:G:O6	1:A:648:A:N6	2.54	0.40
1:A:1158:C:H5''	2:B:129:THR:O	2.21	0.40
1:A:1267:C:H2'	1:A:1268:G:O4'	2.21	0.40
16:P:75:ILE:HG13	16:P:76:LYS:N	2.35	0.40
1:A:866:C:C4	1:A:867:G:H1'	2.56	0.40
4:D:21:LEU:HD23	4:D:21:LEU:O	2.22	0.40
13:M:28:ARG:HD2	13:M:28:ARG:HA	1.85	0.40
1:A:22:G:H2'	1:A:23:C:C6	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:U:H1'	1:A:509:A:N7	2.36	0.40
1:A:724:G:H2'	1:A:725:G:C8	2.55	0.40
1:A:1157:A:C4'	2:B:129:THR:H	2.34	0.40
1:A:1481:U:H3'	1:A:1482:G:H8	1.86	0.40
8:H:78:VAL:HG12	8:H:85:ILE:HD13	2.04	0.40
10:J:20:GLN:NE2	10:J:24:GLU:OE2	2.54	0.40
10:J:57:VAL:HG12	10:J:58:ASN:H	1.86	0.40
13:M:65:GLU:HB3	13:M:66:GLY:H	1.65	0.40
18:R:55:LEU:O	18:R:59:ILE:HG12	2.21	0.40
19:S:10:ILE:HD11	19:S:15:LEU:HD22	2.03	0.40
1:A:107:G:O2'	1:A:378:G:O2'	2.06	0.40
1:A:142:G:H21	1:A:196:A:H2	1.68	0.40
1:A:159:G:N2	1:A:161:A:H3'	2.37	0.40
1:A:529:G:O2'	1:A:533:A:N6	2.54	0.40
1:A:708:C:O4'	11:K:39:GLY:HA3	2.21	0.40
1:A:740:U:H2'	1:A:741:G:H8	1.86	0.40
1:A:1525:G:H2'	1:A:1526:G:C8	2.57	0.40
10:J:11:LYS:HB2	10:J:11:LYS:HE2	1.99	0.40
10:J:68:ARG:HH12	10:J:70:HIS:CE1	2.39	0.40
14:N:9:GLU:HA	14:N:12:ARG:HB2	2.03	0.40
20:T:33:LYS:HA	20:T:33:LYS:HD3	1.80	0.40
1:A:236:A:H2'	1:A:237:G:H8	1.86	0.40
1:A:1010:U:H2'	1:A:1011:C:C6	2.56	0.40
1:A:1127:G:H22	1:A:1147:C:H42	1.69	0.40
1:A:1240:U:H5'	1:A:1241:G:O4'	2.21	0.40
1:A:1333:A:H2'	1:A:1334:G:O4'	2.21	0.40
1:A:1346:A:N1	1:A:1374:A:H5''	2.36	0.40
4:D:3:ARG:HG2	4:D:4:TYR:H	1.85	0.40
4:D:105:MET:SD	4:D:173:VAL:HG22	2.62	0.40
5:E:40:GLY:HA3	5:E:46:VAL:HG12	2.02	0.40
6:F:11:HIS:CD2	6:F:12:PRO:HD2	2.56	0.40
7:G:148:LYS:O	7:G:148:LYS:HG3	2.22	0.40
17:Q:26:GLU:OE2	17:Q:39:LYS:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	216/241 (90%)	186 (86%)	27 (12%)	3 (1%)	11	46
3	C	204/233 (88%)	183 (90%)	21 (10%)	0	100	100
4	D	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
5	E	154/167 (92%)	145 (94%)	9 (6%)	0	100	100
6	F	102/135 (76%)	100 (98%)	2 (2%)	0	100	100
7	G	147/179 (82%)	139 (95%)	8 (5%)	0	100	100
8	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	I	125/130 (96%)	106 (85%)	17 (14%)	2 (2%)	9	44
10	J	96/103 (93%)	80 (83%)	16 (17%)	0	100	100
11	K	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	M	112/118 (95%)	98 (88%)	12 (11%)	2 (2%)	8	42
14	N	92/101 (91%)	83 (90%)	9 (10%)	0	100	100
15	O	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
16	P	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	Q	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	R	64/75 (85%)	57 (89%)	7 (11%)	0	100	100
19	S	77/92 (84%)	71 (92%)	6 (8%)	0	100	100
20	T	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
All	All	2279/2505 (91%)	2103 (92%)	169 (7%)	7 (0%)	44	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	ARG
13	M	65	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	66	GLY
2	B	19	THR
9	I	56	MET
9	I	57	VAL
2	B	206	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	180/199 (90%)	178 (99%)	2 (1%)	73	85
3	C	170/190 (90%)	167 (98%)	3 (2%)	59	77
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	117 (98%)	2 (2%)	60	78
6	F	91/116 (78%)	91 (100%)	0	100	100
7	G	122/147 (83%)	121 (99%)	1 (1%)	81	89
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	102 (97%)	3 (3%)	42	67
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/99 (90%)	88 (99%)	1 (1%)	73	85
12	L	103/104 (99%)	102 (99%)	1 (1%)	76	86
13	M	92/96 (96%)	92 (100%)	0	100	100
14	N	79/84 (94%)	79 (100%)	0	100	100
15	O	75/77 (97%)	75 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	74/78 (95%)	74 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	70/79 (89%)	70 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
All	All	1918/2066 (93%)	1905 (99%)	13 (1%)	84	91

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

Mol	Chain	Res	Type
2	B	128	LEU
2	B	191	ASP
3	C	44	LYS
3	C	48	LYS
3	C	64	ARG
5	E	29	ARG
5	E	134	ILE
7	G	55	LYS
9	I	11	ARG
9	I	44	ARG
9	I	99	LYS
11	K	56	ARG
12	L	83	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	17	HIS
2	B	18	GLN
2	B	38	HIS
2	B	119	GLN
2	B	145	ASN
2	B	176	ASN
2	B	177	ASN
3	C	5	HIS
3	C	122	GLN
3	C	139	ASN
4	D	74	ASN
4	D	100	ASN
4	D	120	HIS
4	D	126	ASN
4	D	152	GLN
5	E	70	ASN
5	E	135	ASN
5	E	146	ASN
6	F	3	HIS
7	G	67	ASN
9	I	3	ASN
9	I	4	GLN
10	J	58	ASN
11	K	15	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	29	ASN
11	K	40	ASN
11	K	118	HIS
14	N	59	GLN
15	O	28	GLN
15	O	46	HIS
16	P	18	GLN
16	P	63	GLN
16	P	79	ASN
19	S	51	HIS
19	S	55	GLN
19	S	56	HIS
20	T	21	ASN
20	T	68	HIS
20	T	75	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1542 (97%)	416 (27%)	17 (1%)

All (416) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	4	U
1	A	5	U
1	A	6	G
1	A	8	A
1	A	9	G
1	A	30	U
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	54	C
1	A	58	C
1	A	66	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	67	C
1	A	68	G
1	A	69	G
1	A	70	U
1	A	71	A
1	A	74	A
1	A	75	G
1	A	77	A
1	A	82	G
1	A	83	C
1	A	85	U
1	A	87	C
1	A	88	U
1	A	89	U
1	A	91	U
1	A	94	G
1	A	95	C
1	A	108	G
1	A	120	A
1	A	121	U
1	A	130	A
1	A	131	A
1	A	134	G
1	A	146	G
1	A	163	C
1	A	164	G
1	A	171	A
1	A	173	U
1	A	181	A
1	A	182	A
1	A	184	G
1	A	196	A
1	A	197	A
1	A	207	C
1	A	209	U
1	A	210	C
1	A	211	G
1	A	212	G
1	A	220	G
1	A	226	G
1	A	240	G
1	A	244	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	279	A
1	A	281	G
1	A	289	G
1	A	298	A
1	A	306	A
1	A	307	C
1	A	316	C
1	A	321	A
1	A	322	C
1	A	325	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	345	C
1	A	351	G
1	A	352	C
1	A	354	G
1	A	363	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	374	A
1	A	375	U
1	A	379	C
1	A	382	A
1	A	392	C
1	A	393	A
1	A	402	G
1	A	406	G
1	A	411	A
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	426	U
1	A	428	G
1	A	429	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	450	G
1	A	454	G
1	A	456	A
1	A	457	G
1	A	458	U
1	A	460	A
1	A	462	G
1	A	463	U
1	A	467	U
1	A	468	A
1	A	469	C
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	485	U
1	A	493	A
1	A	496	A
1	A	505	G
1	A	508	U
1	A	509	A
1	A	511	C
1	A	514	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	527	G
1	A	529	G
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	580	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	588	G
1	A	589	U
1	A	615	G
1	A	618	C
1	A	627	G
1	A	632	U
1	A	633	G
1	A	650	G
1	A	653	U
1	A	656	G
1	A	659	U
1	A	666	G
1	A	671	G
1	A	678	U
1	A	683	G
1	A	684	U
1	A	687	A
1	A	689	C
1	A	690	G
1	A	699	C
1	A	700	G
1	A	705	G
1	A	706	A
1	A	709	U
1	A	716	A
1	A	719	C
1	A	720	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	732	C
1	A	734	G
1	A	735	C
1	A	739	C
1	A	740	U
1	A	747	A
1	A	750	C
1	A	752	G
1	A	753	A
1	A	755	G
1	A	760	G
1	A	777	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	781	A
1	A	782	A
1	A	787	A
1	A	790	A
1	A	792	A
1	A	793	U
1	A	795	C
1	A	797	C
1	A	802	A
1	A	803	G
1	A	809	G
1	A	815	A
1	A	817	C
1	A	818	G
1	A	821	G
1	A	824	G
1	A	828	U
1	A	832	G
1	A	835	U
1	A	836	G
1	A	838	G
1	A	841	C
1	A	842	U
1	A	844	G
1	A	845	A
1	A	846	G
1	A	847	G
1	A	848	C
1	A	849	G
1	A	851	G
1	A	852	G
1	A	854	U
1	A	870	U
1	A	871	U
1	A	894	G
1	A	901	A
1	A	902	G
1	A	914	A
1	A	917	G
1	A	920	U
1	A	921	U
1	A	922	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	925	G
1	A	927	G
1	A	928	G
1	A	934	C
1	A	939	G
1	A	942	G
1	A	943	U
1	A	944	G
1	A	949	A
1	A	960	U
1	A	961	U
1	A	965	U
1	A	967	C
1	A	968	A
1	A	969	A
1	A	974	A
1	A	976	G
1	A	982	U
1	A	983	A
1	A	989	U
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1002	G
1	A	1004	A
1	A	1008	U
1	A	1009	U
1	A	1010	U
1	A	1017	U
1	A	1020	G
1	A	1022	A
1	A	1027	C
1	A	1029	U
1	A	1030	U
1	A	1033	G
1	A	1035	A
1	A	1038	C
1	A	1045	C
1	A	1048	G
1	A	1049	U
1	A	1050	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1051	C
1	A	1053	G
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1081	A
1	A	1086	U
1	A	1088	G
1	A	1089	G
1	A	1092	A
1	A	1093	A
1	A	1094	G
1	A	1095	U
1	A	1097	C
1	A	1098	C
1	A	1099	G
1	A	1101	A
1	A	1102	A
1	A	1107	C
1	A	1118	U
1	A	1130	A
1	A	1133	G
1	A	1136	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1141	C
1	A	1143	G
1	A	1144	G
1	A	1149	C
1	A	1154	G
1	A	1155	A
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1161	C
1	A	1168	U
1	A	1169	A
1	A	1170	A
1	A	1174	G
1	A	1175	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1181	G
1	A	1182	G
1	A	1196	A
1	A	1197	A
1	A	1201	A
1	A	1202	U
1	A	1210	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1224	U
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1233	G
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1248	A
1	A	1249	C
1	A	1253	G
1	A	1256	A
1	A	1258	G
1	A	1260	G
1	A	1269	A
1	A	1270	G
1	A	1276	G
1	A	1278	G
1	A	1279	G
1	A	1280	A
1	A	1281	C
1	A	1285	A
1	A	1286	U
1	A	1287	A
1	A	1290	G
1	A	1296	C
1	A	1298	U
1	A	1300	G
1	A	1301	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1302	C
1	A	1305	G
1	A	1312	G
1	A	1313	U
1	A	1316	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1321	U
1	A	1322	C
1	A	1323	G
1	A	1332	A
1	A	1336	C
1	A	1338	G
1	A	1339	A
1	A	1340	A
1	A	1341	U
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1364	U
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1414	U
1	A	1415	G
1	A	1417	G
1	A	1430	A
1	A	1431	A
1	A	1432	G
1	A	1441	A
1	A	1445	U
1	A	1446	A
1	A	1447	A
1	A	1449	C
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1455	G
1	A	1471	U
1	A	1473	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1474	U
1	A	1475	G
1	A	1479	C
1	A	1486	G
1	A	1487	G
1	A	1488	G
1	A	1489	G
1	A	1506	U
1	A	1507	A
1	A	1515	G
1	A	1516	G
1	A	1517	G
1	A	1519	A
1	A	1529	G
1	A	1530	G
1	A	1532	U
1	A	1533	C
1	A	1535	C
1	A	1536	C
1	A	1537	U
1	A	1538	C

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	70	U
1	A	88	U
1	A	428	G
1	A	827	U
1	A	1065	U
1	A	1092	A
1	A	1101	A
1	A	1157	A
1	A	1159	U
1	A	1181	G
1	A	1201	A
1	A	1300	G
1	A	1320	C
1	A	1431	A
1	A	1505	G
1	A	1518	A
1	A	1531	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

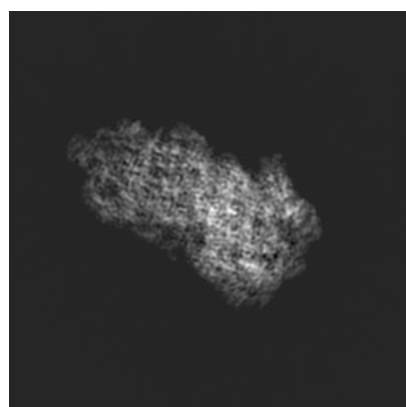
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21571. These allow visual inspection of the internal detail of the map and identification of artifacts.

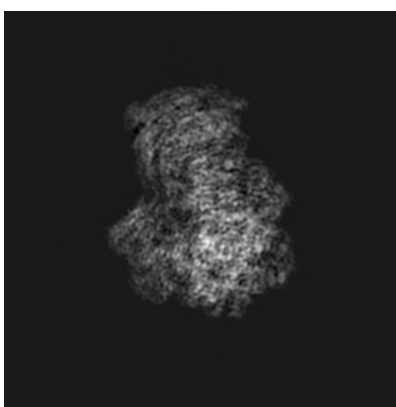
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

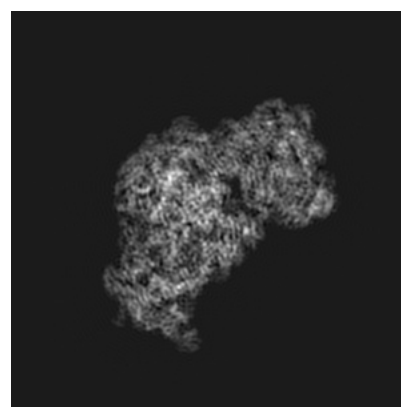
6.1.1 Primary map



X



Y

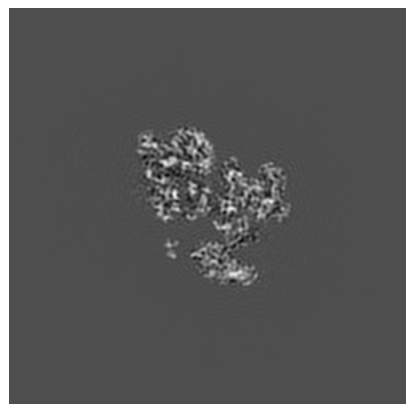


Z

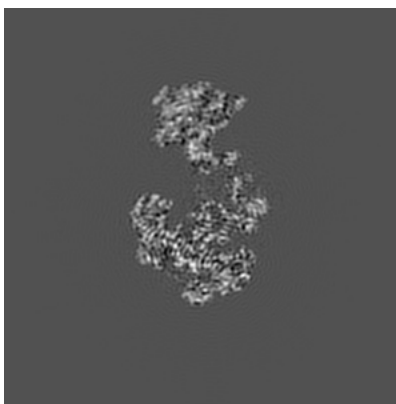
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

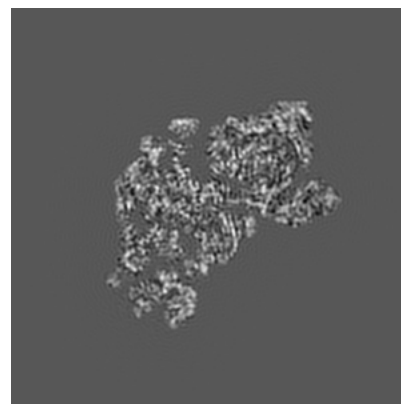
6.2.1 Primary map



X Index: 152



Y Index: 152

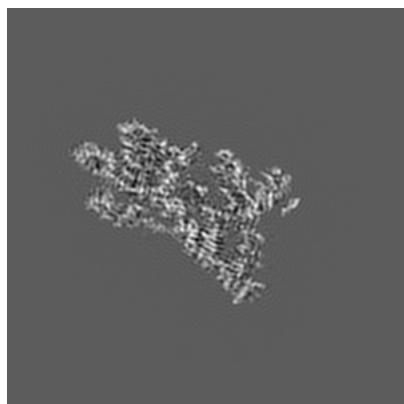


Z Index: 152

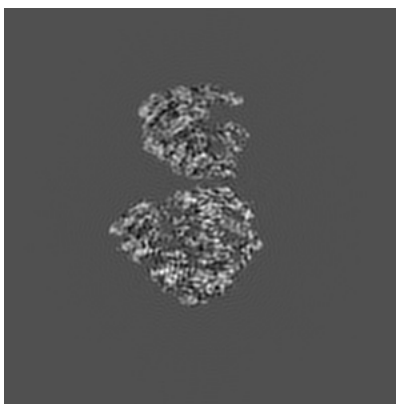
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

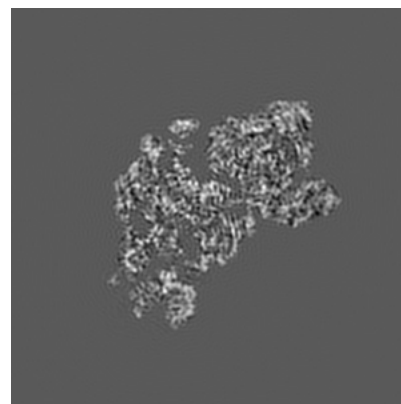
6.3.1 Primary map



X Index: 124



Y Index: 167



Z Index: 151

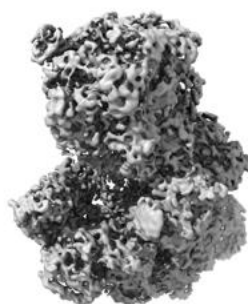
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.162. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

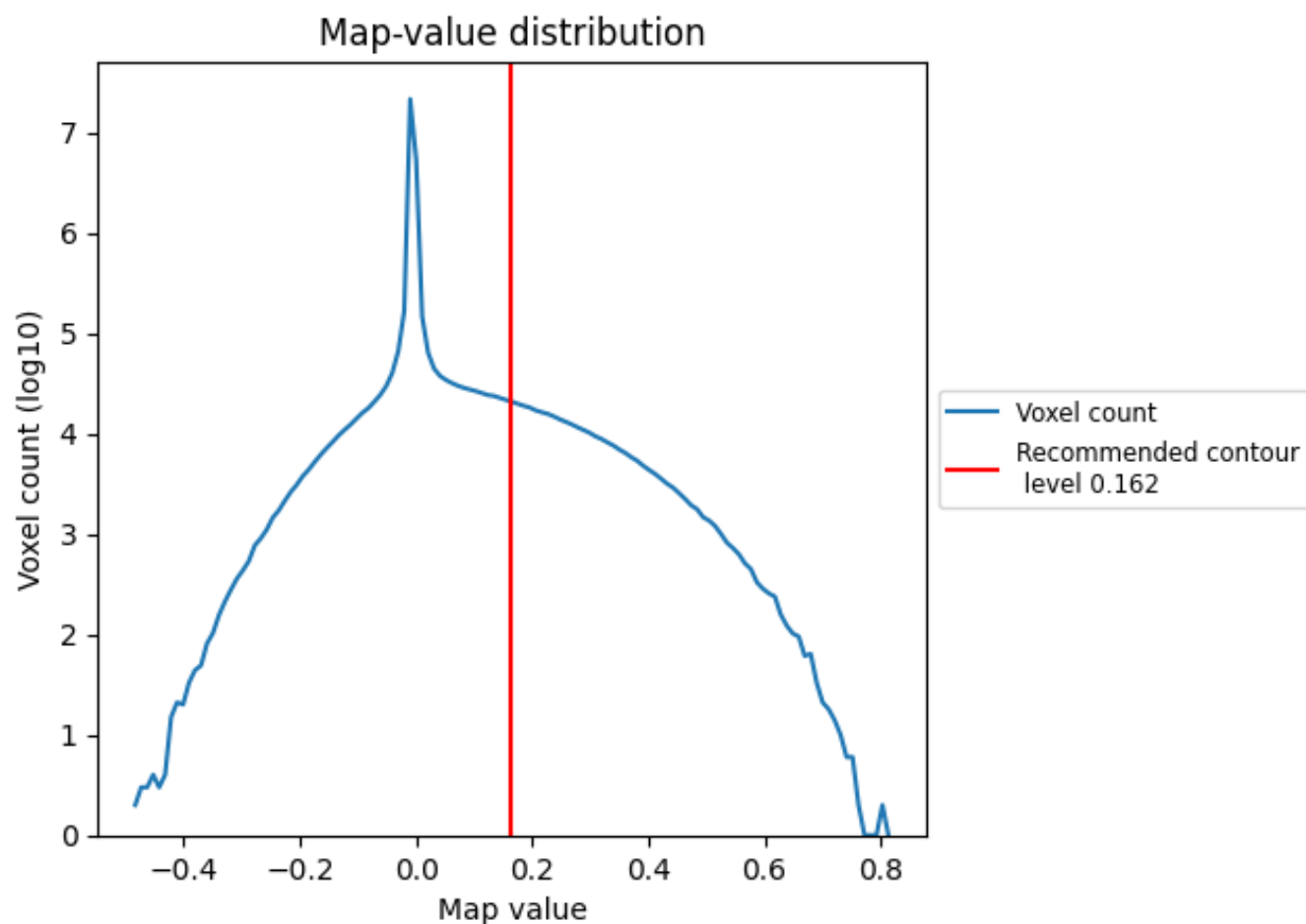
6.5 Mask visualisation

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

7 Map analysis [i](#)

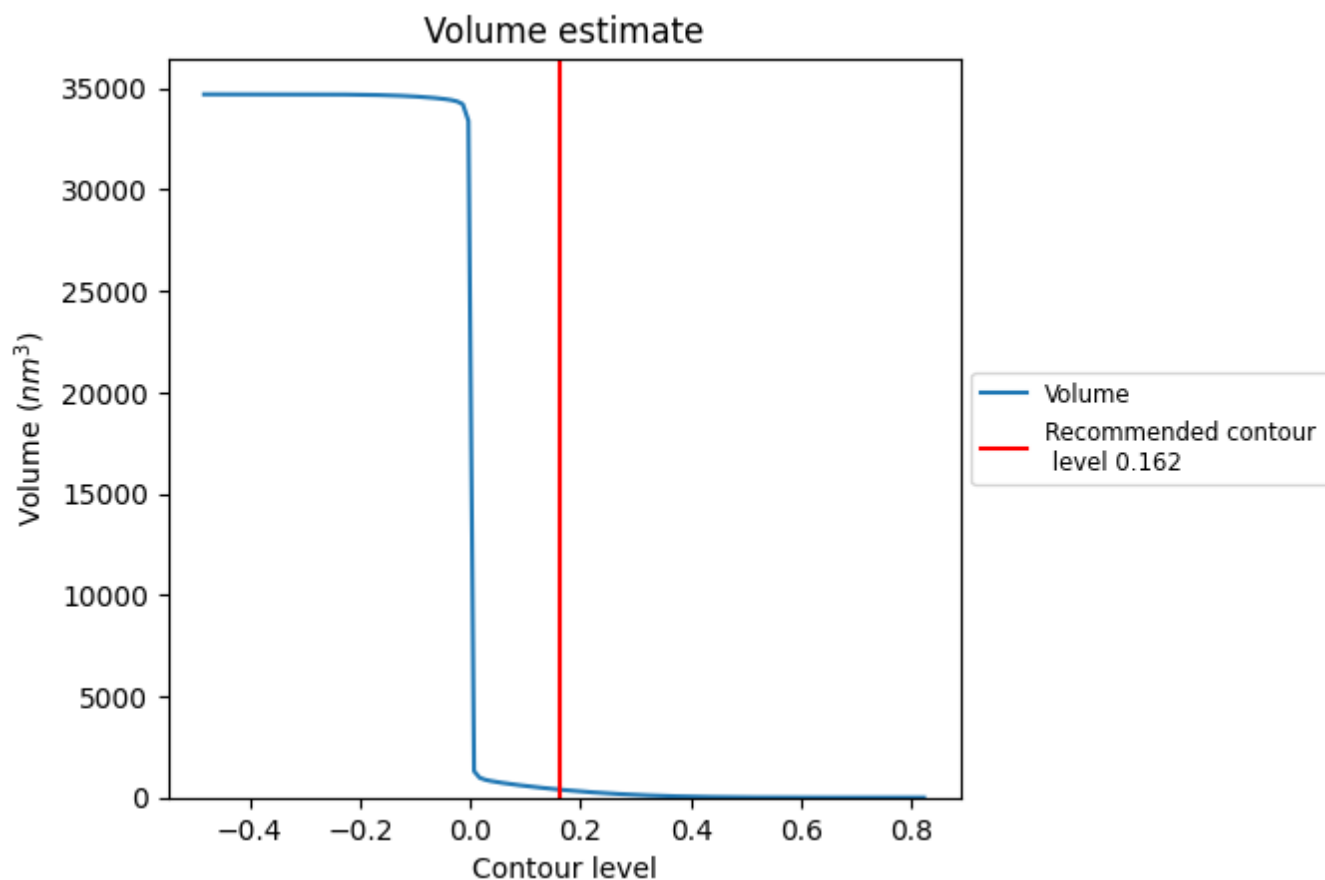
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

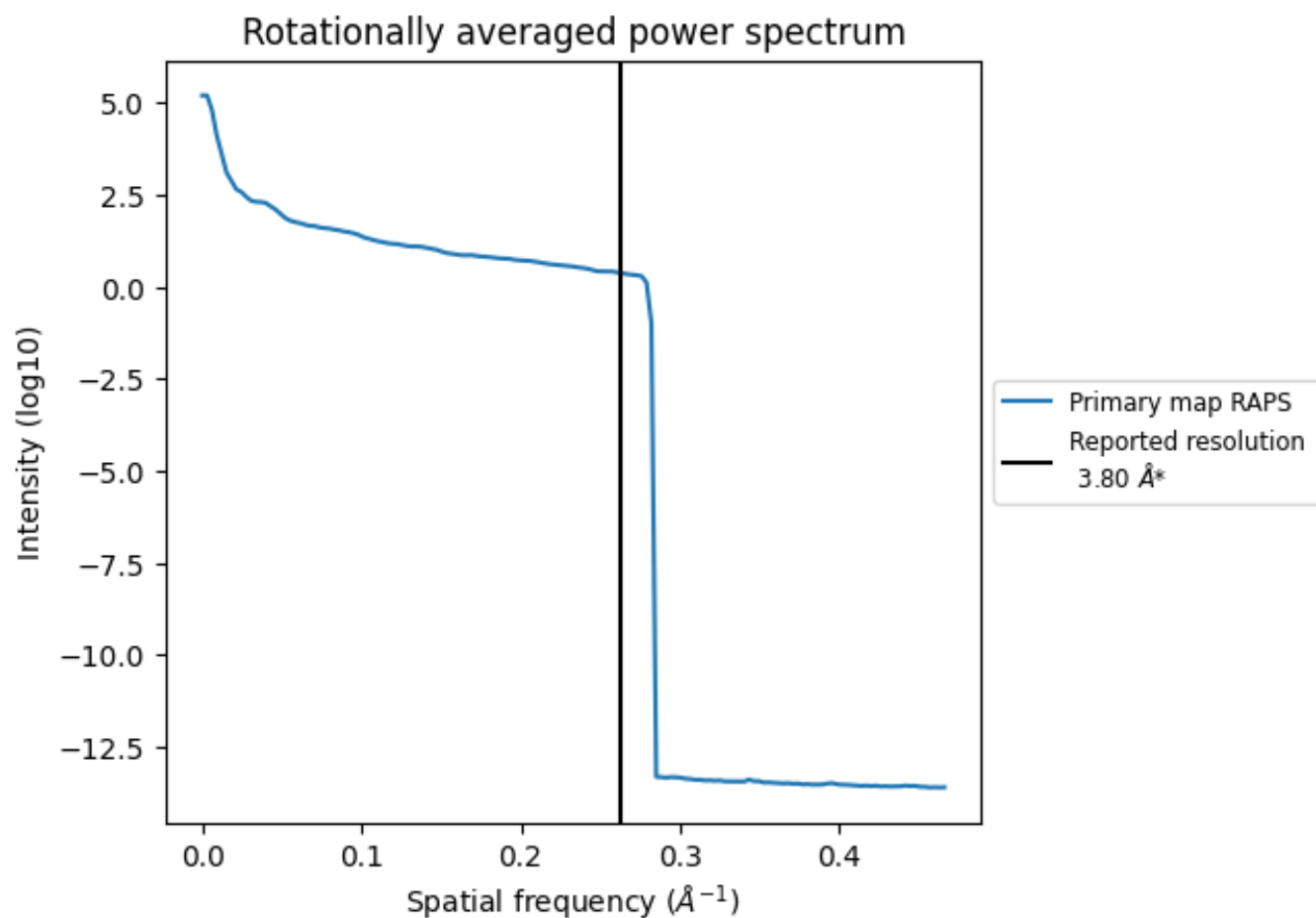
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 394 nm³; this corresponds to an approximate mass of 356 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 ⓘ

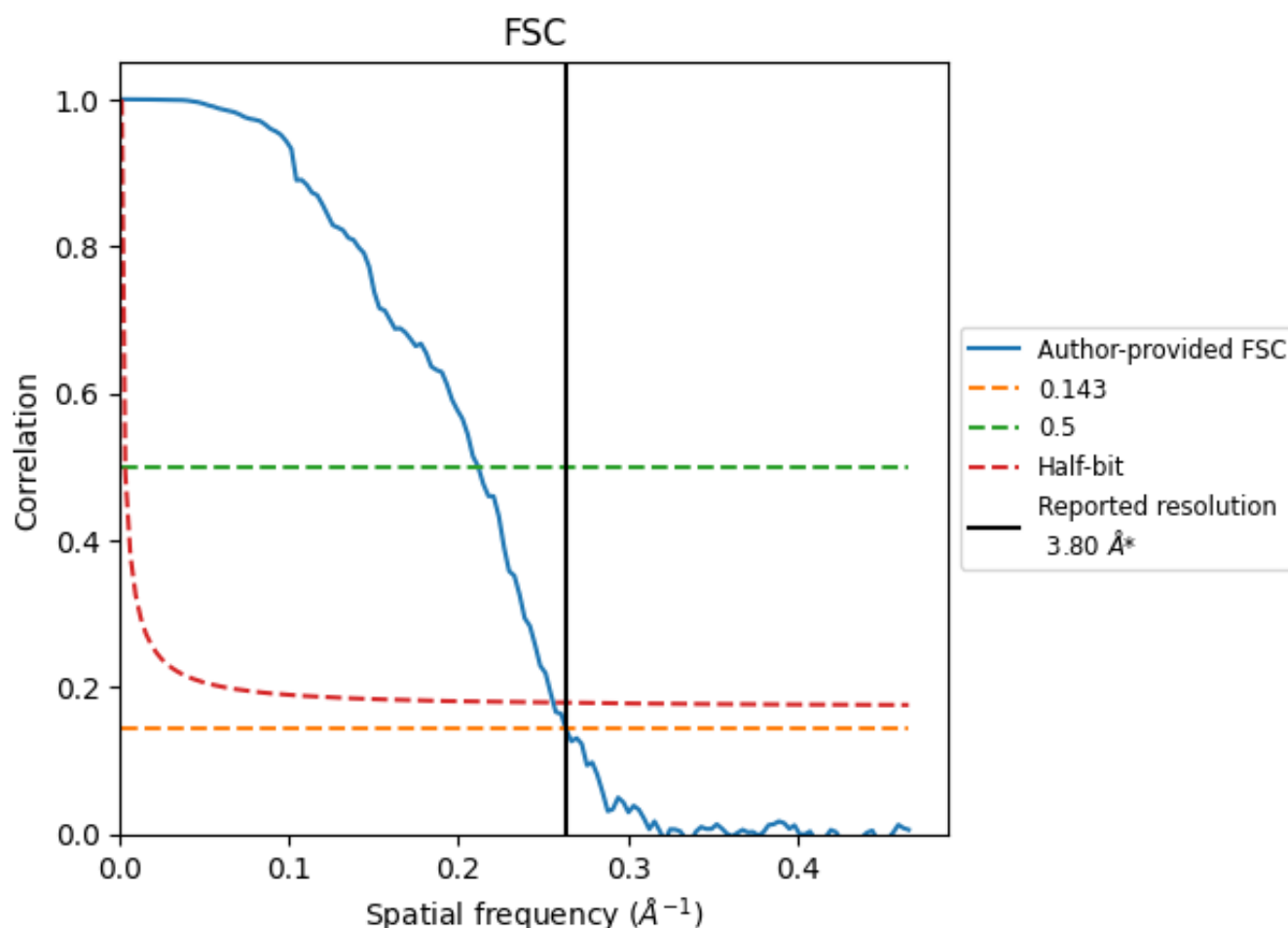


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

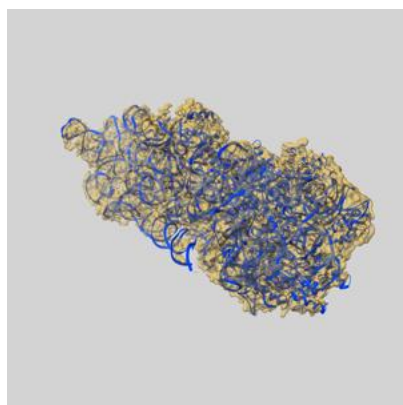
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.73	3.91
Unmasked-calculated*	-	-	-

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

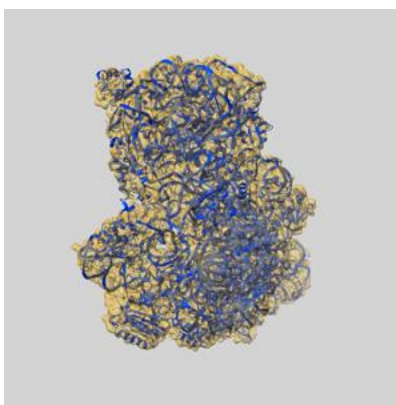
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21571 and PDB model 6W7M. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

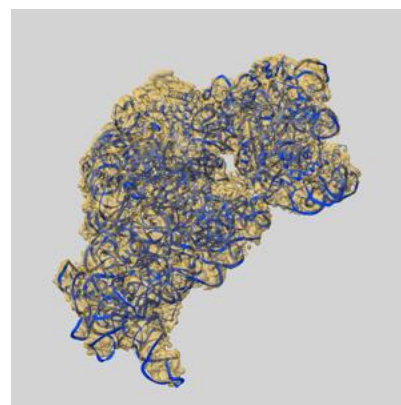
9.1 Map-model overlay [i](#)



X



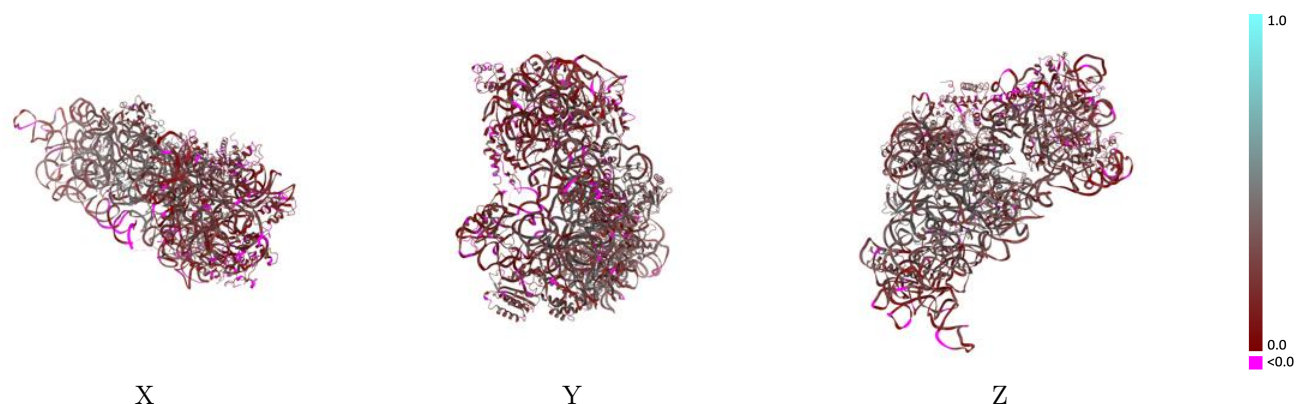
Y



Z

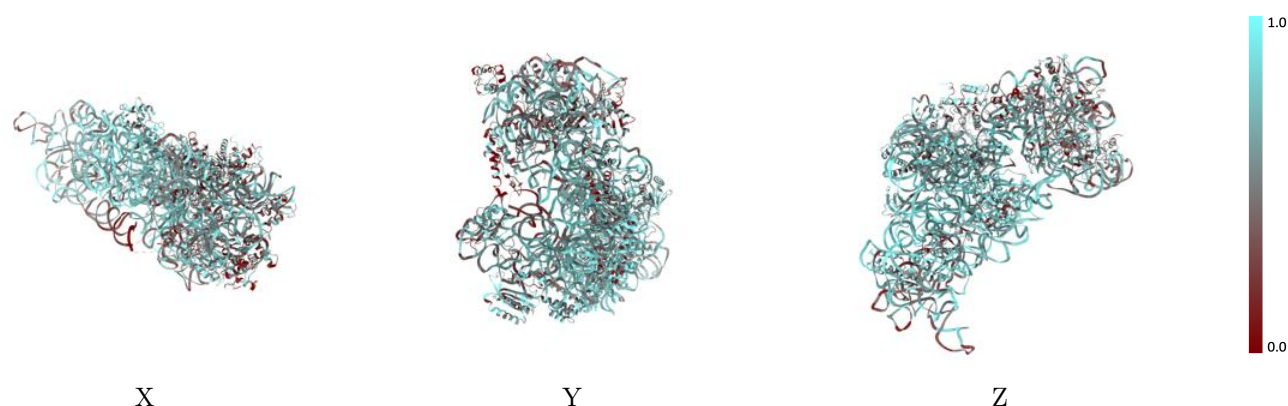
The images above show the 3D surface view of the map at the recommended contour level 0.162 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



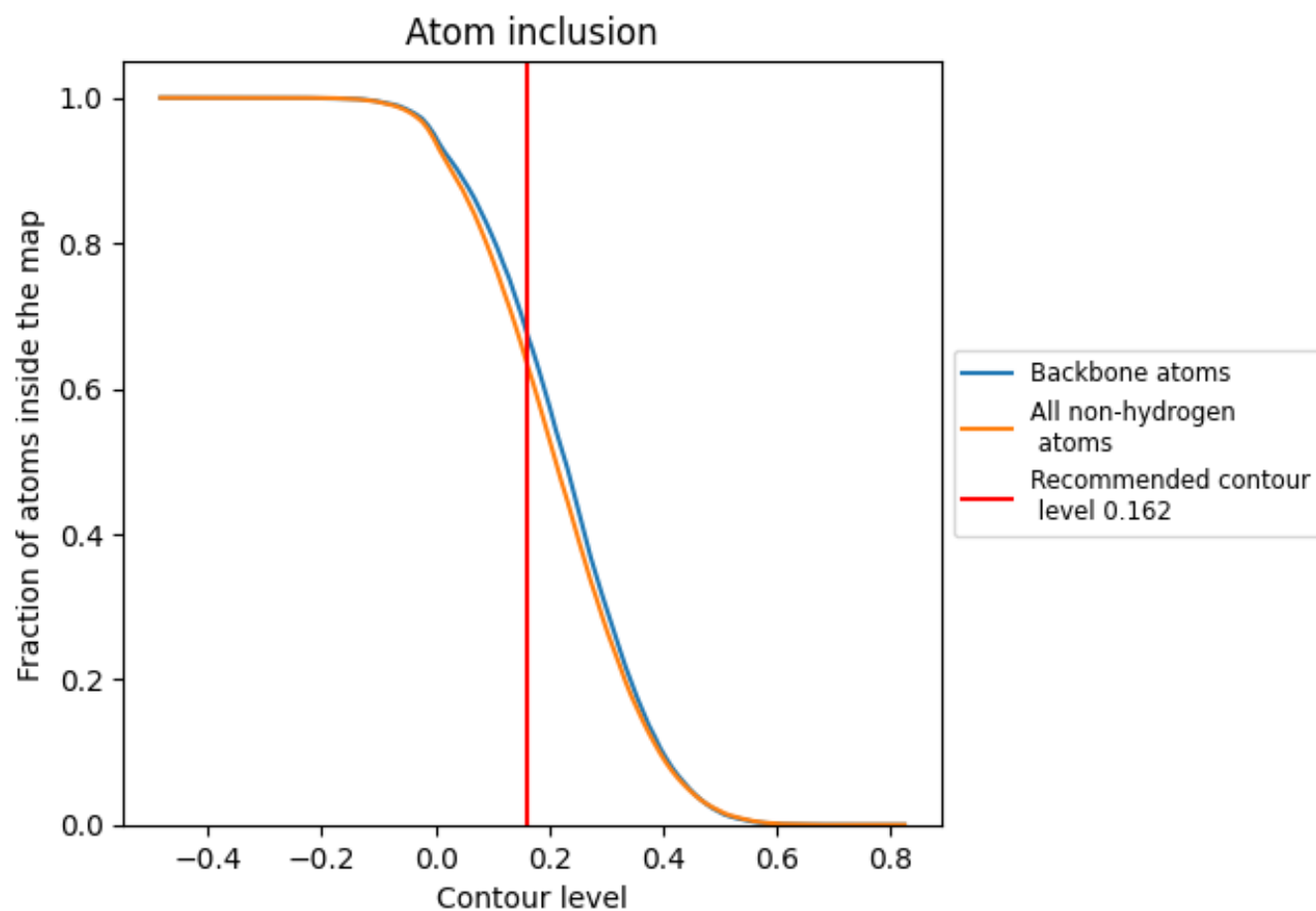
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.162).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 63% 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 (0.162) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6303	 0.2630
A	 0.6705	 0.2620
B	 0.4890	 0.1650
C	 0.5615	 0.2480
D	 0.6786	 0.3530
E	 0.6637	 0.3190
F	 0.6505	 0.2640
G	 0.3697	 0.1350
H	 0.5969	 0.3130
I	 0.4515	 0.1980
J	 0.4244	 0.2090
K	 0.5929	 0.2280
L	 0.6404	 0.3590
M	 0.4266	 0.1990
N	 0.4697	 0.2480
O	 0.6418	 0.3400
P	 0.6396	 0.3850
Q	 0.7009	 0.4140
R	 0.5067	 0.2620
S	 0.4332	 0.1950
T	 0.6425	 0.3210

