



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 09:07 PM UTC

PDB ID : 9H3S / pdb_00009h3s
EMDB ID : EMD-51836
Title : 50S subunit precursor C-CP_YjgA_L22
Authors : Lauer, S.; Nikolay, R.; Spahn, C.M.T.
Deposited on : 2024-10-17
Resolution : 4.16 Å(reported)
Based on initial model : 8RPY

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

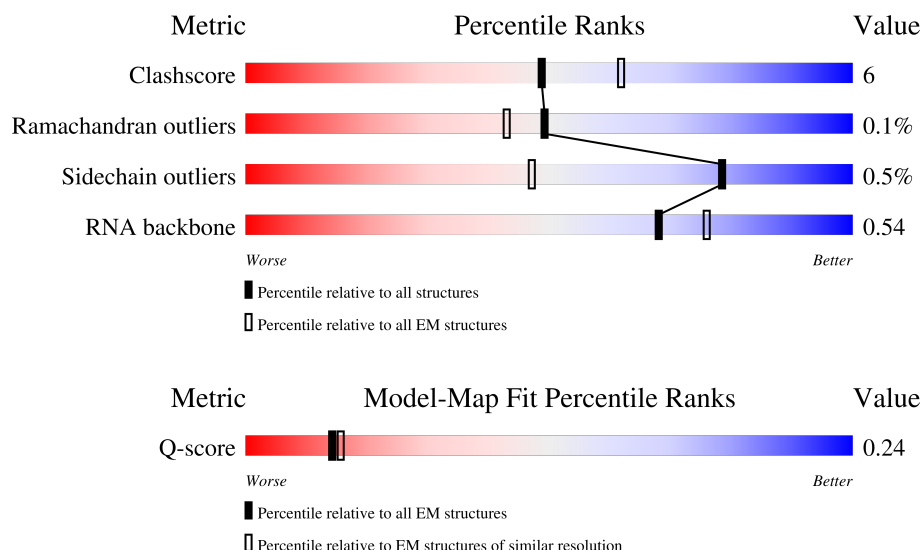
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.16 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.



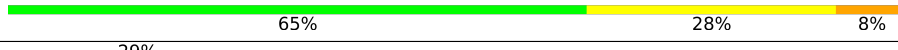
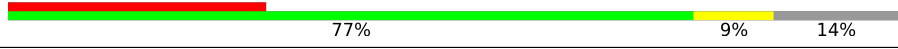
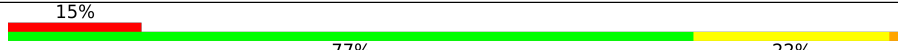
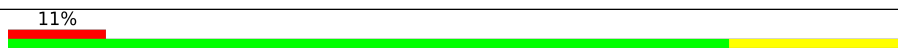
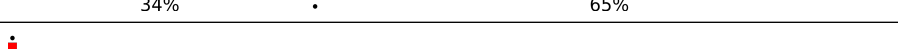
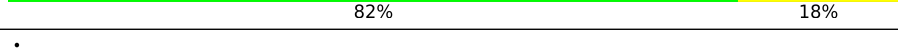
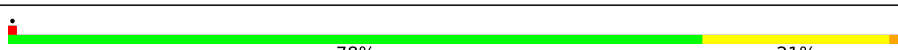
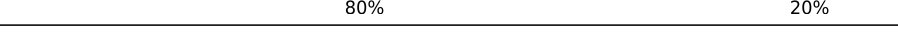
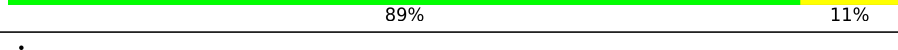
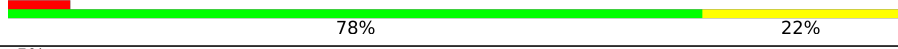
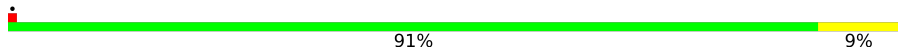
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5480 (3.66 - 4.66)

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	0	56	16% 77% 23%
2	2	46	78% 22%
3	4	38	16% 82% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	A	2903	
5	B	120	
6	C	183	
7	D	209	
8	E	201	
9	F	177	
10	G	176	
11	H	149	
12	J	142	
13	K	122	
14	L	143	
15	N	120	
16	O	116	
17	P	114	
18	Q	117	
19	R	103	
20	S	110	
21	T	93	
22	U	102	
23	V	94	
24	W	75	
25	X	77	
26	Y	63	
27	Z	58	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 82487 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 protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2715	Total	C	N	O	P	0	0
			58304	26009	10744	18836	2715		

- Molecule 5 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

- Molecule 6 is a protein called UPF0307 protein YjgA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	158	Total	C	N	O	S	0	0
			1298	805	253	238	2		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 8 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 11 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	52	Total	C	N	O	S	0	0
			400	256	73	70	1		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 15 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 16 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 17 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 19 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	110	Total	C	N	O	S	1	0
			868	538	170	157	3		

- Molecule 21 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 23 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 25 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

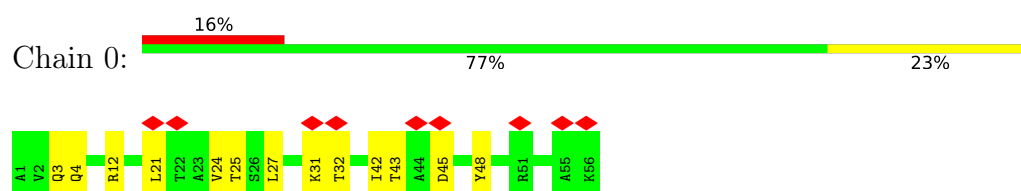
- Molecule 27 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

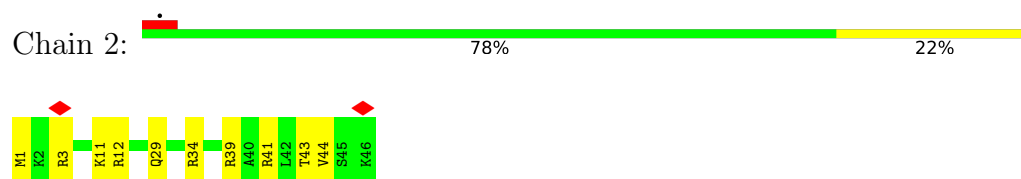
3 Residue-property plots

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.

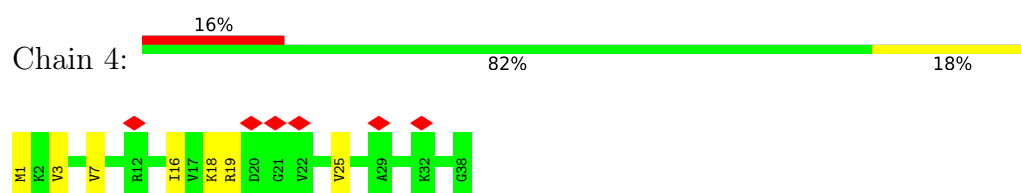
- Molecule 1: Large ribosomal subunit protein bL32



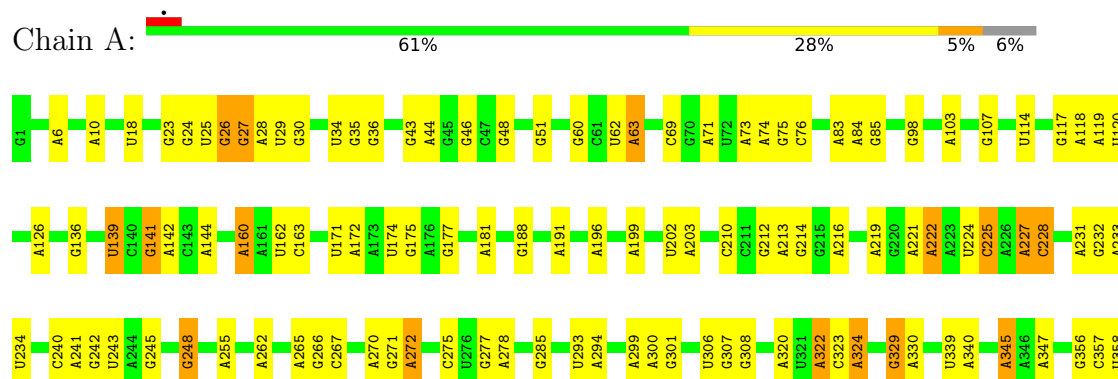
- Molecule 2: Large ribosomal subunit protein bL34

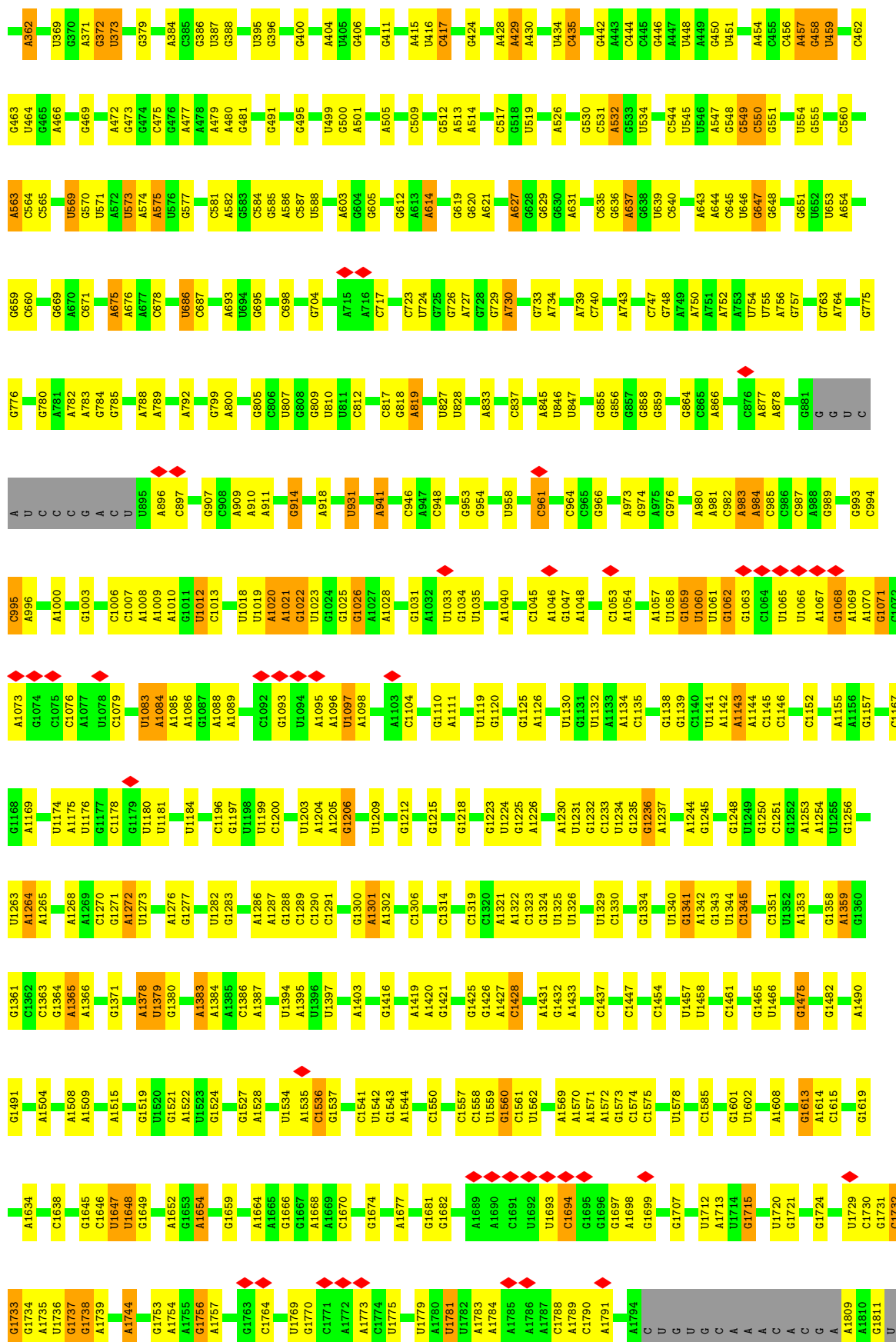


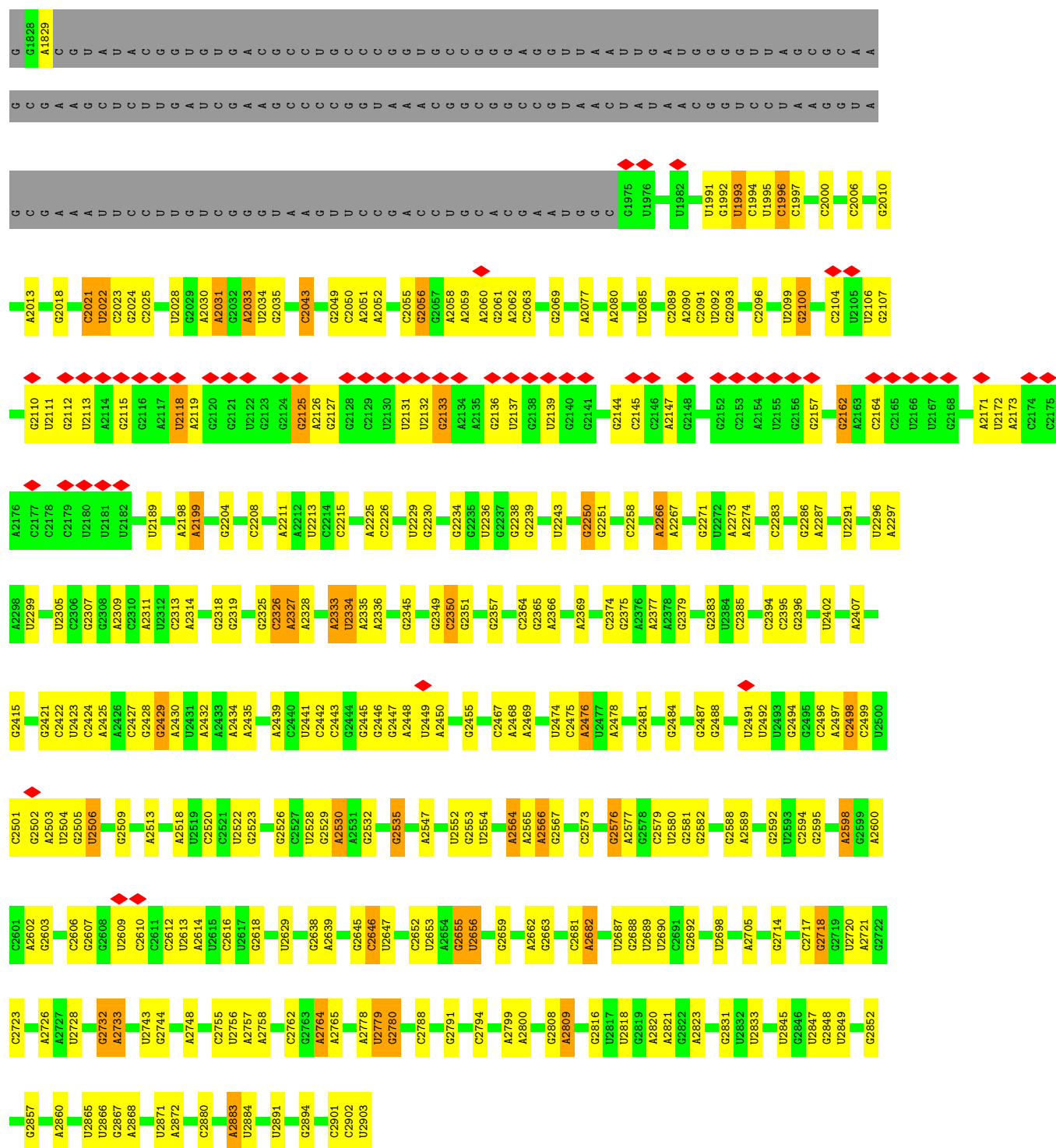
- Molecule 3: Large ribosomal subunit protein bL36A



- Molecule 4: 23S ribosomal RNA

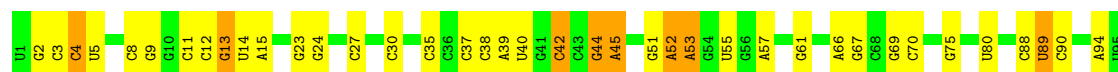






• Molecule 5: 5S ribosomal RNA

Chain B: 65% 28% 8%



Chain G:

11% 81% 19%

S1 K5 V9 D15 N29 G30 E31 K37 D38 A39 V40 A45 D46 M47 T48 R54 Y57 A58 D59 Q63 L70 G77 K85 L86 Q87 A95 K98 G99 N100 M103 D113 H114 Q115 L116 P117 A118 G119 T120 T128 E129 L132 K137 I140 G141 Q142 V143 D146 L147 E154 P155 Y156 D165 E166 V167 V168 R169 E172 A173 K174 K175 K176

[illegible]

Chain J: 82% 18%

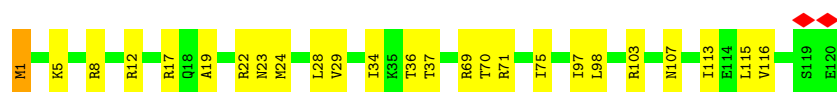
 M1 R2 T3 F4 T30 E31 L32 B37 A41 A42 E43 Y44 T50 G51 D52 V53 I54 K63 I84 T83 E91 P97 V100 I101 V105 M108 G115 M118 F119 R120 K121 L122 A123 V124 Q135 D141 I142

Chain K:

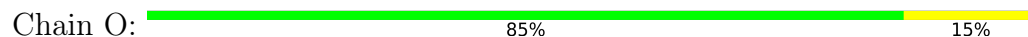
Chain L: 80% 19%

Amino Acid	Frequency	Color	Marked
R2	1	Green	No
L6	1	Green	No
L27	1	Green	No
G26	1	Green	No
K29	1	Green	No
T30	1	Green	No
R33	1	Green	No
R41	1	Green	No
S42	1	Green	Yes
G43	1	Green	Yes
E51	1	Green	No
M55	1	Green	No
A71	1	Green	No
T74	1	Green	No
A75	1	Green	No
T76	1	Green	No
T77	1	Green	No
R78	1	Green	No
G87	1	Green	Yes
G88	1	Green	Yes
D91	1	Green	No
L92	1	Green	No
N93	1	Green	No
T94	1	Green	No
L95	1	Green	No
I100	1	Green	No
I101	1	Green	No
G102	1	Green	No
I103	1	Green	No
Q104	1	Green	No
I111	1	Green	No
V127	1	Green	No
T128	1	Green	No
E136	1	Green	No
A137	1	Green	Yes
I142	1	Green	No
E143	1	Green	No
F144	1	Green	Yes

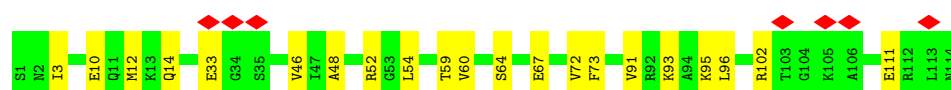
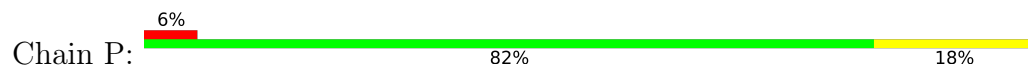
Chain N: 79% 20%



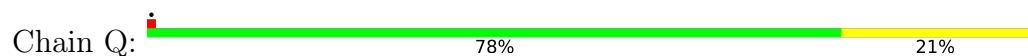
- Molecule 16: Large ribosomal subunit protein uL18



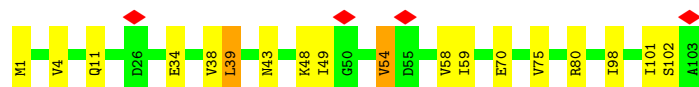
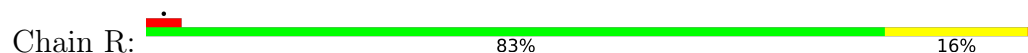
- Molecule 17: Large ribosomal subunit protein bL19



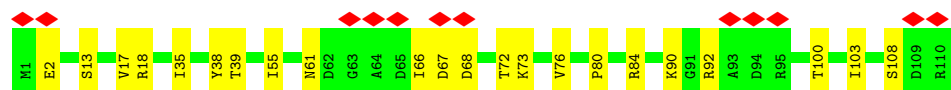
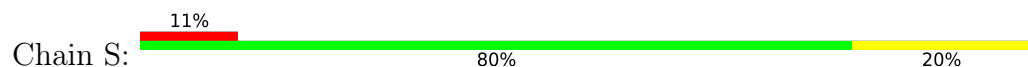
- Molecule 18: Large ribosomal subunit protein bL20



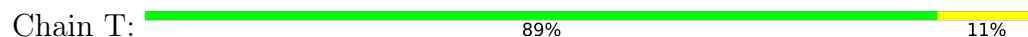
- Molecule 19: Large ribosomal subunit protein bL21



- Molecule 20: Large ribosomal subunit protein uL22

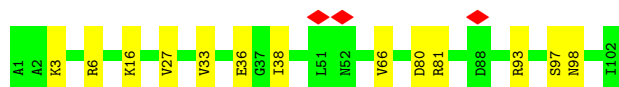


- Molecule 21: Large ribosomal subunit protein uL23



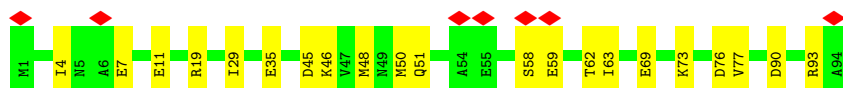
- Molecule 22: Large ribosomal subunit protein uL24

Chain U:  87% 13%



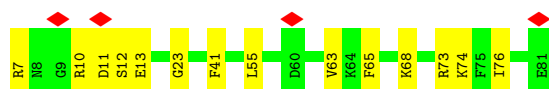
- Molecule 23: Large ribosomal subunit protein bL25

Chain V:  78% 22% 7%



- Molecule 24: Large ribosomal subunit protein bL27

Chain W:  81% 19% 5%

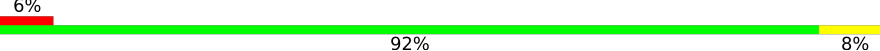


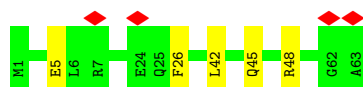
- Molecule 25: Large ribosomal subunit protein bL28

Chain X:  91% 9%



- Molecule 26: Large ribosomal subunit protein uL29

Chain Y:  92% 8% 6%



- Molecule 27: Large ribosomal subunit protein uL30

Chain Z:  76% 24% 1%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10197	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.659	Depositor
Minimum map value	-0.397	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.292	Depositor
Map size (Å)	424.0, 424.0, 424.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4133333, 1.4133333, 1.4133333	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	0	0.10	0/450	0.21	0/599
2	2	0.11	0/380	0.18	0/498
3	4	0.12	0/303	0.21	0/397
4	A	0.07	0/65303	0.22	6/101870 (0.0%)
5	B	0.06	0/2876	0.19	0/4483
6	C	0.09	0/1311	0.21	0/1753
7	D	0.09	0/1586	0.22	0/2134
8	E	0.09	0/1571	0.22	0/2113
9	F	0.10	0/1434	0.27	0/1926
10	G	0.09	0/1343	0.23	0/1816
11	H	0.12	0/405	0.24	0/544
12	J	0.09	0/1152	0.22	0/1551
13	K	0.09	0/947	0.22	0/1268
14	L	0.09	0/1054	0.26	0/1403
15	N	0.11	0/973	0.26	0/1301
16	O	0.07	0/902	0.22	0/1209
17	P	0.09	0/929	0.21	0/1242
18	Q	0.10	0/960	0.20	0/1278
19	R	0.11	0/829	0.26	0/1107
20	S	0.10	0/875	0.26	0/1170
21	T	0.10	0/744	0.21	0/994
22	U	0.10	0/787	0.23	0/1051
23	V	0.11	0/766	0.23	0/1025
24	W	0.07	0/582	0.21	0/769
25	X	0.10	0/635	0.21	0/848
26	Y	0.10	0/510	0.20	0/677
27	Z	0.11	0/453	0.23	0/605
All	All	0.08	0/90060	0.22	6/135631 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1770	G	OP1-P-OP2	-13.45	79.26	119.60
4	A	1769	U	OP2-P-O3'	-12.15	71.54	108.00
4	A	1770	G	O5'-P-OP1	-9.94	78.18	108.00
4	A	1769	U	OP1-P-O3'	9.17	135.51	108.00
4	A	1770	G	O5'-P-OP2	7.73	131.19	108.00
4	A	1769	U	O3'-P-O5'	-5.02	96.46	104.00

There are no chirality outliers.

There are no planarity outliers.

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	0	444	0	461	9	0
2	2	377	0	418	10	0
3	4	302	0	343	6	0
4	A	58304	0	29321	465	0
5	B	2572	0	1302	30	0
6	C	1298	0	1352	14	0
7	D	1565	0	1616	28	0
8	E	1552	0	1619	33	0
9	F	1410	0	1447	33	0
10	G	1323	0	1374	19	0
11	H	400	0	423	2	0
12	J	1129	0	1162	24	0
13	K	938	0	1012	17	0
14	L	1045	0	1117	24	0
15	N	960	0	1000	22	0
16	O	892	0	923	15	0
17	P	917	0	965	18	0
18	Q	947	0	1022	27	0
19	R	816	0	839	17	0
20	S	868	0	934	16	0
21	T	738	0	807	8	0
22	U	779	0	834	11	0
23	V	753	0	780	16	0
24	W	575	0	592	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	X	625	0	655	6	0
26	Y	509	0	543	4	0
27	Z	449	0	491	12	0
All	All	82487	0	53352	760	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (760) 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)
4:A:1351:C:O2'	4:A:1571:A:O2'	1.87	0.90
4:A:177:G:OP2	4:A:177:G:N2	2.05	0.88
4:A:275:C:O2	4:A:362:A:N6	2.08	0.87
5:B:5:U:OP1	5:B:61:G:O2'	1.92	0.86
4:A:1447:C:O2'	4:A:1544:A:N3	2.08	0.86
4:A:2646:C:OP2	4:A:2732:G:O2'	1.94	0.85
4:A:227:A:O2'	4:A:228:C:O5'	1.95	0.84
4:A:1007:C:OP2	4:A:1008:A:O2'	1.96	0.83
4:A:994:C:OP1	18:Q:52:ARG:NH2	2.11	0.83
4:A:2576:G:O2'	4:A:2579:C:OP2	1.97	0.83
4:A:248:G:O2'	4:A:2432:A:OP1	1.97	0.83
4:A:909:A:O2'	4:A:911:A:OP2	1.96	0.82
4:A:571:U:O2'	4:A:573:U:OP2	1.97	0.82
4:A:989:G:OP2	27:Z:11:SER:OG	1.98	0.82
3:4:1:MET:SD	4:A:2526:G:O2'	2.38	0.81
4:A:1681:G:OP2	4:A:1757:A:N6	2.12	0.81
4:A:2326:C:O2'	4:A:2327:A:OP1	1.97	0.81
4:A:605:G:OP1	8:E:99:LYS:NZ	2.14	0.81
4:A:2522:U:O2'	4:A:2647:U:OP1	1.97	0.81
4:A:2258:C:O2'	4:A:2427:C:OP2	1.99	0.80
4:A:1341:G:OP2	4:A:1394:U:O2'	1.99	0.79
4:A:2816:G:N3	4:A:2883:A:O2'	2.16	0.79
13:K:71:ARG:NH2	13:K:106:GLU:OE2	2.16	0.79
4:A:612:G:N2	4:A:614:A:O2'	2.16	0.79
4:A:534:U:O2'	18:Q:48:ASP:OD2	1.99	0.78
4:A:2581:G:N2	4:A:2581:G:OP2	2.17	0.78
10:G:37:ASN:ND2	10:G:63:GLN:OE1	2.16	0.78
4:A:1018:U:O2'	4:A:1120:G:N2	2.16	0.78
4:A:160:A:N3	4:A:2208:C:O2'	2.16	0.78
4:A:2377:A:O2'	16:O:117:PHE:O	2.02	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2085:U:O2	4:A:2234:G:O6	2.02	0.78
4:A:1138:G:N3	12:J:108:MET:HE1	2.00	0.77
4:A:2115:G:N2	4:A:2118:U:OP2	2.18	0.76
25:X:6:VAL:HG21	25:X:58:ILE:HD11	1.67	0.76
12:J:122:LEU:HD21	12:J:124:VAL:HG23	1.67	0.76
4:A:1724:G:O6	4:A:1737:G:N2	2.18	0.76
4:A:1068:G:N2	4:A:1095:A:O2'	2.20	0.75
16:O:31:THR:OG1	16:O:33:ARG:O	2.05	0.75
4:A:948:C:O2	4:A:984:A:O2'	2.04	0.74
4:A:2857:G:N2	4:A:2860:A:OP2	2.16	0.74
4:A:1060:U:O2'	4:A:1071:G:OP1	2.06	0.74
4:A:2865:U:OP2	4:A:2866:U:O2'	2.03	0.74
7:D:97:SER:OG	7:D:99:GLU:OE1	2.04	0.74
4:A:1125:G:OP2	4:A:1126:A:O2'	2.06	0.74
4:A:1697:G:OP2	4:A:1698:A:O2'	2.03	0.74
4:A:2125:G:N2	4:A:2171:A:OP1	2.21	0.74
21:T:6:ARG:O	21:T:10:VAL:HG13	1.87	0.73
23:V:58:SER:O	23:V:73:LYS:NZ	2.20	0.73
4:A:2564:A:O2'	4:A:2565:A:O4'	2.05	0.73
4:A:2595:G:N2	4:A:2598:A:OP2	2.20	0.73
4:A:631:A:N3	4:A:2415:G:O2'	2.22	0.73
9:F:117:SER:O	9:F:127:TYR:OH	2.05	0.73
4:A:29:U:O2	4:A:1215:G:O2'	2.07	0.73
4:A:2291:U:O2'	4:A:2374:C:O2	2.07	0.73
5:B:8:C:O2'	16:O:25:ARG:NH2	2.21	0.72
4:A:2006:C:O2'	4:A:2823:A:N3	2.21	0.72
4:A:2723:C:OP1	7:D:114:LYS:NZ	2.21	0.72
4:A:1288:G:OP2	4:A:1288:G:N2	2.19	0.72
4:A:219:A:N3	4:A:234:U:O2'	2.21	0.71
4:A:1019:U:OP1	4:A:1035:U:O2'	2.06	0.71
4:A:976:G:O2'	4:A:1155:A:O2'	2.08	0.71
4:A:1779:U:OP2	4:A:1784:A:N6	2.23	0.71
15:N:1:MET:SD	15:N:1:MET:N	2.63	0.71
4:A:1277:G:O2'	15:N:24:MET:SD	2.49	0.71
27:Z:46:MET:O	27:Z:50:VAL:HG22	1.90	0.71
4:A:833:A:O2'	14:L:51:GLU:OE1	2.08	0.70
23:V:48:MET:SD	23:V:51:GLN:NE2	2.64	0.70
4:A:1209:U:O2'	4:A:1237:A:N1	2.24	0.70
21:T:91:GLN:N	21:T:91:GLN:OE1	2.25	0.70
4:A:372:G:H3'	25:X:57:VAL:HG12	1.72	0.70
4:A:1426:G:OP2	4:A:1427:A:O2'	2.10	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:730:A:OP1	4:A:1775:U:O2'	2.06	0.70
4:A:2469:A:N6	4:A:2481:G:O2'	2.24	0.70
18:Q:97:ILE:HD11	18:Q:104:ALA:HB3	1.72	0.70
4:A:693:A:O2'	4:A:1353:A:N3	2.23	0.70
4:A:1363:C:O2'	4:A:1809:A:N3	2.22	0.70
7:D:16:THR:OG1	7:D:18:ASP:OD1	2.06	0.70
10:G:98:LYS:NZ	10:G:103:ASN:OD1	2.26	0.69
4:A:2144:G:O2'	4:A:2147:A:N1	2.24	0.69
4:A:2530:A:OP2	4:A:2535:G:N2	2.25	0.69
4:A:495:G:O2'	20:S:61:ASN:OD1	2.08	0.69
4:A:743:A:O2'	4:A:1659:G:OP1	2.10	0.69
4:A:2645:G:OP2	4:A:2645:G:N2	2.20	0.69
4:A:1218:G:N1	4:A:1232:G:N7	2.41	0.69
18:Q:108:LEU:HD22	19:R:48:LYS:HZ3	1.57	0.69
15:N:34:ILE:HG23	15:N:113:ILE:HG23	1.75	0.69
4:A:569:U:O2'	4:A:983:A:N1	2.25	0.68
17:P:64:SER:OG	17:P:67:GLU:O	2.09	0.68
4:A:584:C:N4	4:A:585:G:O6	2.26	0.68
4:A:2031:A:N3	4:A:2455:G:O2'	2.24	0.68
4:A:2655:G:O2'	4:A:2656:U:O5'	2.12	0.68
5:B:27:C:OP1	16:O:34:HIS:NE2	2.26	0.68
2:2:12:ARG:NH1	4:A:464:U:O2'	2.26	0.68
4:A:2528:U:O2'	4:A:2530:A:OP1	2.09	0.67
23:V:45:ASP:OD1	23:V:46:LYS:N	2.27	0.67
4:A:532:A:N1	4:A:2035:G:N2	2.41	0.67
4:A:858:G:OP1	24:W:74:LYS:NZ	2.26	0.67
4:A:1638:C:O2	4:A:2698:U:O2'	2.13	0.67
24:W:13:GLU:N	24:W:13:GLU:OE1	2.27	0.67
4:A:1668:A:N3	4:A:1670:C:N4	2.41	0.67
4:A:1677:A:O2'	4:A:1993:U:OP1	2.08	0.67
14:L:93:ASN:O	14:L:94:THR:OG1	2.11	0.67
4:A:577:G:O2'	4:A:1254:A:OP1	2.12	0.67
4:A:987:C:O2'	4:A:1000:A:N3	2.26	0.67
4:A:570:G:O4'	4:A:983:A:N6	2.27	0.67
4:A:1062:G:O2'	4:A:1063:G:O4'	2.07	0.67
5:B:55:U:O2'	9:F:25:MET:HE1	1.95	0.67
4:A:2091:C:OP2	4:A:2092:U:O2'	2.08	0.66
4:A:675:A:N3	4:A:2443:C:O2'	2.27	0.66
4:A:1264:A:OP2	4:A:1265:A:O2'	2.08	0.66
18:Q:64:ILE:HD12	18:Q:94:LEU:HD13	1.77	0.66
4:A:727:A:OP2	4:A:1431:A:O2'	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1536:C:O2'	4:A:1537:G:N2	2.28	0.66
18:Q:88:GLU:O	19:R:11:GLN:NE2	2.29	0.66
4:A:340:A:O2'	8:E:162:ARG:NH2	2.29	0.65
4:A:345:A:N3	4:A:347:A:N6	2.44	0.65
5:B:13:G:H1	5:B:69:G:HO2'	1.44	0.65
1:O:4:GLN:OE1	4:A:2056:G:O2'	2.13	0.65
22:U:3:LYS:O	22:U:93:ARG:NH1	2.29	0.65
4:A:210:C:O2'	4:A:1366:A:O2'	2.13	0.65
4:A:750:A:OP1	4:A:1615:C:N4	2.30	0.65
4:A:961:C:O2	4:A:2031:A:N6	2.30	0.65
4:A:400:G:N7	25:X:56:ARG:NH2	2.45	0.65
12:J:88:THR:OG1	12:J:91:GLU:OE1	2.15	0.65
16:O:60:GLU:OE1	16:O:60:GLU:N	2.29	0.64
4:A:18:U:O2'	4:A:554:U:OP1	2.15	0.64
12:J:97:PRO:O	12:J:100:VAL:HG22	1.97	0.64
2:2:29:GLN:NE2	4:A:210:C:OP1	2.30	0.64
4:A:1021:A:H61	4:A:1142:A:H61	1.46	0.64
8:E:139:LYS:NZ	8:E:144:GLU:OE1	2.26	0.64
9:F:120:SER:OG	9:F:128:SER:O	2.11	0.64
14:L:143:GLU:N	14:L:143:GLU:OE1	2.30	0.64
12:J:91:GLU:OE1	12:J:91:GLU:N	2.31	0.64
4:A:966:G:H4'	4:A:2271:G:H22	1.62	0.64
24:W:63:VAL:CG2	24:W:76:ILE:HD11	2.28	0.64
4:A:810:U:O4	14:L:30:THR:HG22	1.97	0.64
4:A:271:G:O2'	4:A:272:A:OP2	2.14	0.63
1:O:43:THR:OG1	1:O:45:ASP:OD1	2.11	0.63
4:A:2439:A:O2'	4:A:2600:A:OP1	2.16	0.63
4:A:560:C:O2	18:Q:47:ARG:NH2	2.31	0.63
17:P:10:GLU:N	17:P:10:GLU:OE1	2.29	0.63
4:A:2314:A:O2'	9:F:126:ASN:OD1	2.17	0.63
20:S:18:ARG:NH1	20:S:76:VAL:O	2.32	0.63
8:E:48:THR:OG1	8:E:51:GLU:OE1	2.17	0.62
4:A:1022:G:O6	12:J:68:LYS:NZ	2.26	0.62
4:A:2659:G:N2	4:A:2662:A:OP2	2.32	0.62
4:A:2788:C:O2'	4:A:2809:A:N3	2.30	0.62
4:A:807:U:OP2	14:L:41:ARG:NH2	2.32	0.62
4:A:227:A:HO2'	4:A:228:C:P	2.23	0.62
4:A:519:U:O2'	20:S:73:LYS:NZ	2.33	0.62
5:B:51:G:OP1	16:O:63:LYS:NZ	2.26	0.62
7:D:150:GLN:N	7:D:150:GLN:OE1	2.32	0.62
4:A:548:G:O2'	4:A:549:G:O4'	2.18	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:548:G:O2'	4:A:549:G:O5'	2.17	0.62
24:W:63:VAL:HG22	24:W:76:ILE:HD11	1.81	0.62
19:R:1:MET:HE2	19:R:43:ASN:OD1	1.99	0.62
4:A:191:A:O2'	4:A:678:C:O2	2.18	0.61
8:E:29:HIS:HA	14:L:6:LEU:HD21	1.82	0.61
23:V:62:THR:OG1	23:V:69:GLU:OE2	2.18	0.61
9:F:161:SER:N	9:F:164:GLU:OE2	2.32	0.61
2:2:39:ARG:NH1	4:A:469:G:O6	2.34	0.61
5:B:11:C:OP1	24:W:68:LYS:NZ	2.32	0.61
18:Q:89:ILE:CD1	19:R:39:LEU:HD21	2.31	0.61
18:Q:108:LEU:HD22	19:R:48:LYS:NZ	2.15	0.61
21:T:28:ASN:ND2	21:T:88:LYS:O	2.34	0.61
5:B:8:C:O3'	16:O:25:ARG:NH2	2.34	0.61
5:B:75:G:H1'	23:V:29:ILE:HG21	1.83	0.61
4:A:1287:A:N6	4:A:1649:G:O2'	2.34	0.61
4:A:964:C:O2'	4:A:2273:A:N3	2.28	0.61
8:E:46:GLN:O	8:E:88:ARG:NH2	2.33	0.61
6:C:140:TRP:NE1	6:C:182:GLU:OE1	2.34	0.61
4:A:564:C:OP2	19:R:80:ARG:NH2	2.33	0.60
4:A:1223:G:N2	4:A:1226:A:OP2	2.33	0.60
4:A:1226:A:OP1	18:Q:15:LYS:NZ	2.31	0.60
12:J:105:VAL:HG21	12:J:122:LEU:HD13	1.83	0.60
27:Z:26:LEU:O	27:Z:37:ARG:NH1	2.34	0.60
4:A:1754:A:N6	4:A:2717:C:O4'	2.34	0.60
4:A:2090:A:N6	4:A:2230:G:O6	2.34	0.60
1:0:12:ARG:NH2	4:A:517:C:OP1	2.33	0.60
2:2:34:ARG:NH2	2:2:41:ARG:O	2.34	0.60
4:A:2077:A:N3	4:A:2434:A:O2'	2.28	0.60
9:F:62:GLN:OE1	9:F:62:GLN:N	2.35	0.60
4:A:76:C:OP1	26:Y:48:ARG:NH1	2.35	0.60
18:Q:78:PHE:CE2	18:Q:82:LEU:HD11	2.37	0.60
4:A:144:A:H4'	21:T:2:ILE:HD11	1.84	0.59
4:A:676:A:HO2'	4:A:2442:C:HO2'	1.49	0.59
4:A:2266:A:N6	4:A:2273:A:OP2	2.32	0.59
4:A:2705:A:O2'	4:A:2852:G:OP1	2.18	0.59
4:A:1012:U:OP2	18:Q:69:ARG:NH2	2.34	0.59
7:D:4:LEU:HD13	7:D:101:PHE:CZ	2.37	0.59
23:V:35:GLU:OE2	23:V:93:ARG:NH1	2.35	0.59
4:A:698:C:O2'	4:A:734:A:N6	2.31	0.59
4:A:1248:G:OP1	8:E:44:ARG:NH1	2.35	0.59
14:L:136:GLU:OE2	14:L:142:ILE:HD11	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:7:VAL:O	4:A:1031:G:O2'	2.19	0.59
4:A:457:A:N7	4:A:472:A:N6	2.51	0.59
9:F:50:ASP:OD1	9:F:51:ASN:N	2.36	0.59
21:T:54:GLU:OE1	21:T:54:GLU:N	2.36	0.59
4:A:517:C:O2'	20:S:18:ARG:NH2	2.36	0.59
4:A:582:A:O3'	18:Q:10:ARG:NH1	2.33	0.59
23:V:11:GLU:N	23:V:11:GLU:OE1	2.36	0.59
13:K:106:GLU:OE1	13:K:106:GLU:N	2.36	0.58
4:A:448:U:O4'	8:E:79:ARG:NE	2.35	0.58
4:A:2821:A:OP2	7:D:115:GLY:N	2.35	0.58
12:J:44:TYR:O	18:Q:63:ARG:NE	2.33	0.58
4:A:1215:G:O6	4:A:1235:G:N2	2.36	0.58
4:A:2250:G:O2'	4:A:2496:C:OP1	2.21	0.58
4:A:1754:A:O2'	17:P:102:ARG:NH2	2.35	0.58
18:Q:85:ALA:O	18:Q:86:SER:OG	2.18	0.58
4:A:324:A:N6	4:A:339:U:O4'	2.37	0.58
4:A:1021:A:N6	4:A:1142:A:H61	2.01	0.58
4:A:2024:G:O2'	7:D:154:LYS:NZ	2.37	0.58
4:A:2743:U:OP2	4:A:2755:C:N4	2.37	0.58
18:Q:89:ILE:HD12	19:R:39:LEU:HD21	1.86	0.58
4:A:27:G:O2'	4:A:512:G:N2	2.31	0.58
4:A:210:C:HO2'	4:A:1366:A:HO2'	1.49	0.58
4:A:2566:A:N1	13:K:28:SER:OG	2.28	0.58
9:F:25:MET:O	9:F:29:ARG:NH1	2.36	0.58
4:A:627:A:OP1	14:L:78:ARG:NH1	2.36	0.58
4:A:2229:U:O2	25:X:33:HIS:NE2	2.36	0.58
4:A:2313:C:O4'	9:F:36:ASN:ND2	2.37	0.58
4:A:1340:U:OP1	21:T:19:LYS:NZ	2.36	0.57
4:A:2468:A:P	4:A:2476:A:H61	2.27	0.57
18:Q:93:ILE:HG21	19:R:4:VAL:HG11	1.85	0.57
4:A:931:U:O2	4:A:1167:C:O2'	2.20	0.57
4:A:1351:C:HO2'	4:A:1571:A:HO2'	1.30	0.57
4:A:586:A:OP2	4:A:1251:C:N4	2.38	0.57
4:A:2692:G:N3	4:A:2847:U:O2'	2.37	0.57
9:F:134:GLN:NE2	9:F:149:ARG:O	2.36	0.57
4:A:1528:A:OP2	4:A:1543:G:N2	2.37	0.57
4:A:2333:A:OP1	24:W:73:ARG:NH1	2.37	0.57
20:S:2:GLU:OE1	20:S:2:GLU:N	2.38	0.57
20:S:13:SER:O	20:S:17:VAL:HG23	2.04	0.57
24:W:7:ARG:O	24:W:10:ARG:NH1	2.38	0.57
4:A:48:G:H22	4:A:177:G:P	2.28	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:24:G:C2	4:A:25:U:C5	2.92	0.57
11:H:12:LEU:H	11:H:12:LEU:HD23	1.70	0.57
4:A:647:G:N2	4:A:2350:C:O2'	2.38	0.57
8:E:125:SER:O	8:E:137:LYS:NZ	2.34	0.57
8:E:154:ASP:OD1	8:E:154:ASP:N	2.37	0.57
9:F:51:ASN:OD1	9:F:52:ALA:N	2.38	0.57
19:R:58:VAL:N	19:R:102:SER:OG	2.38	0.57
4:A:1007:C:OP1	12:J:37:ARG:NH2	2.38	0.56
8:E:1:MET:N	8:E:14:VAL:O	2.36	0.56
7:D:33:ARG:HG3	7:D:73:VAL:HG13	1.86	0.56
27:Z:57:GLU:N	27:Z:57:GLU:OE1	2.37	0.56
4:A:2349:G:O6	4:A:2369:A:N6	2.38	0.56
5:B:14:U:OP2	5:B:70:C:O2'	2.23	0.56
8:E:127:GLU:N	8:E:127:GLU:OE1	2.36	0.56
4:A:2395:C:N3	6:C:80:ARG:NH2	2.52	0.56
8:E:171:ASP:OD1	8:E:172:ALA:N	2.39	0.56
14:L:91:ASP:OD1	14:L:92:LEU:N	2.37	0.56
4:A:1721:G:O2'	4:A:1739:A:N6	2.39	0.56
4:A:2299:U:O4	4:A:2318:G:N2	2.38	0.56
15:N:97:ILE:C	15:N:98:LEU:HD22	2.30	0.56
8:E:117:ARG:NH2	8:E:183:PHE:O	2.38	0.56
4:A:475:C:O2	4:A:479:A:N6	2.39	0.56
23:V:4:ILE:HD11	23:V:50:MET:SD	2.45	0.56
4:A:83:A:O2'	4:A:103:A:N6	2.39	0.56
4:A:1361:G:HO2'	4:A:2215:C:HO2'	1.54	0.56
15:N:69:ARG:O	15:N:70:THR:OG1	2.19	0.56
4:A:322:A:OP1	8:E:162:ARG:NE	2.39	0.56
4:A:1067:A:N6	4:A:1068:G:O6	2.40	0.55
16:O:116:GLN:N	16:O:116:GLN:OE1	2.37	0.55
3:4:19:ARG:NE	4:A:2756:U:OP2	2.38	0.55
4:A:2468:A:O5'	4:A:2476:A:N6	2.40	0.55
4:A:754:U:O2'	4:A:1272:A:N1	2.37	0.55
4:A:1325:U:OP1	4:A:1647:U:O2'	2.20	0.55
12:J:135:GLN:N	12:J:135:GLN:OE1	2.40	0.55
27:Z:50:VAL:O	27:Z:54:VAL:HG22	2.07	0.55
4:A:532:A:N7	4:A:2021:C:O2'	2.36	0.55
4:A:1712:U:OP2	4:A:1713:A:O2'	2.13	0.55
15:N:28:LEU:HD12	15:N:28:LEU:O	2.06	0.55
4:A:526:A:O2'	4:A:2043:C:O2	2.23	0.55
4:A:648:G:O2'	4:A:2351:G:OP1	2.13	0.55
4:A:2421:G:H4'	6:C:84:LEU:HD22	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2532:G:N2	4:A:2663:G:O2'	2.39	0.55
1:O:21:LEU:HD23	1:O:21:LEU:H	1.71	0.55
4:A:2780:G:OP2	12:J:120:ARG:NE	2.40	0.55
17:P:3:ILE:HD12	17:P:3:ILE:H	1.71	0.55
4:A:308:G:O2'	4:A:329:G:N2	2.40	0.54
4:A:1276:A:N6	4:A:1645:G:O6	2.40	0.54
4:A:2334:U:O2'	16:O:13:ARG:NH2	2.40	0.54
4:A:2594:C:N4	4:A:2595:G:O6	2.39	0.54
27:Z:6:ILE:HG21	27:Z:26:LEU:HD21	1.87	0.54
4:A:2022:U:O2'	4:A:2616:C:O2'	2.13	0.54
10:G:128:THR:HG23	10:G:129:GLU:OE1	2.07	0.54
14:L:27:LEU:HD23	14:L:27:LEU:H	1.72	0.54
14:L:76:GLU:OE1	14:L:76:GLU:N	2.40	0.54
27:Z:23:LEU:HD21	27:Z:53:MET:SD	2.47	0.54
4:A:1130:U:N3	4:A:2025:C:OP1	2.39	0.54
4:A:262:A:N3	4:A:430:A:O2'	2.33	0.54
4:A:300:A:O5'	22:U:81:ARG:NH2	2.40	0.54
9:F:161:SER:OG	9:F:164:GLU:OE1	2.25	0.54
4:A:84:A:N1	4:A:98:G:O2'	2.31	0.54
4:A:2049:G:H21	7:D:161:MET:CE	2.20	0.54
9:F:93:GLU:OE1	9:F:93:GLU:N	2.41	0.54
13:K:76:VAL:HG22	17:P:72:VAL:HG12	1.90	0.54
4:A:117:G:OP2	4:A:119:A:O2'	2.13	0.54
10:G:29:ASN:ND2	10:G:77:GLY:O	2.41	0.54
8:E:51:GLU:OE1	8:E:51:GLU:N	2.41	0.54
4:A:245:G:O2'	4:A:384:A:N1	2.40	0.54
4:A:372:G:O2'	4:A:373:U:P	2.65	0.54
4:A:1550:C:OP1	4:A:1720:U:O2'	2.11	0.54
5:B:52:A:O2'	5:B:53:A:O5'	2.22	0.53
26:Y:42:LEU:HD13	26:Y:45:GLN:OE1	2.08	0.53
2:2:3:ARG:NE	4:A:1613:G:O2'	2.36	0.53
4:A:837:C:N3	4:A:941:A:N6	2.56	0.53
4:A:1287:A:H61	4:A:1649:G:H1'	1.73	0.53
7:D:88:GLU:N	7:D:88:GLU:OE1	2.41	0.53
4:A:918:A:N3	5:B:80:U:O2'	2.41	0.53
4:A:1521:G:OP2	4:A:1522:A:O2'	2.15	0.53
17:P:91:VAL:HG11	17:P:96:LEU:HD21	1.91	0.53
4:A:1693:U:O2'	4:A:1694:C:OP1	2.22	0.53
4:A:2577:A:O4'	4:A:2612:C:N4	2.42	0.53
13:K:42:THR:HG22	13:K:57:VAL:HG22	1.89	0.53
18:Q:88:GLU:N	18:Q:88:GLU:OE1	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:80:ASP:OD1	22:U:81:ARG:N	2.42	0.53
23:V:58:SER:OG	23:V:59:GLU:OE1	2.26	0.53
4:A:225:C:N3	4:A:231:A:N6	2.57	0.53
4:A:477:A:N6	4:A:501:A:OP1	2.42	0.53
4:A:780:G:O2'	4:A:783:A:N6	2.37	0.53
4:A:1205:A:O2'	4:A:1206:G:OP1	2.26	0.53
5:B:52:A:O2'	5:B:53:A:P	2.66	0.53
4:A:2199:A:OP1	25:X:36:ARG:NH2	2.43	0.52
4:A:1028:A:OP2	4:A:1126:A:N6	2.41	0.52
4:A:1203:U:OP2	4:A:1204:A:O2'	2.07	0.52
4:A:2063:C:N4	4:A:2501:C:O2	2.33	0.52
4:A:329:G:O6	22:U:16:LYS:N	2.42	0.52
4:A:442:G:N2	8:E:43:THR:O	2.39	0.52
4:A:565:C:OP2	19:R:80:ARG:NH1	2.42	0.52
4:A:799:G:OP2	4:A:800:A:O2'	2.23	0.52
4:A:1790:C:H2'	4:A:1791:A:C8	2.45	0.52
1:0:31:LYS:HG3	1:0:32:THR:HG23	1.91	0.52
4:A:2000:C:OP1	15:N:5:LYS:NZ	2.43	0.52
24:W:11:ASP:OD1	24:W:12:SER:N	2.41	0.52
1:0:42:ILE:HG22	1:0:48:TYR:HB2	1.91	0.52
4:A:729:G:O2'	4:A:763:G:O5'	2.27	0.52
13:K:58:LEU:HD11	13:K:86:LEU:HD21	1.92	0.52
4:A:635:C:O2'	4:A:639:U:OP1	2.28	0.52
4:A:1048:A:OP2	4:A:1110:G:N2	2.38	0.52
4:A:1738:G:HO2'	4:A:1739:A:C5'	2.23	0.52
4:A:2682:A:N1	4:A:2728:U:O2'	2.41	0.52
5:B:45:A:O4'	9:F:91:ARG:NH1	2.43	0.52
8:E:176:ASP:OD1	8:E:179:SER:OG	2.17	0.52
4:A:993:G:OP2	18:Q:50:ARG:NH2	2.43	0.51
9:F:30:VAL:HG22	9:F:157:THR:HG22	1.92	0.51
4:A:2720:U:OP1	17:P:52:ARG:NH2	2.44	0.51
23:V:76:ASP:OD1	23:V:77:VAL:N	2.43	0.51
4:A:1715:G:N2	4:A:1744:A:OP2	2.37	0.51
4:A:2099:U:O2'	4:A:2100:G:O5'	2.27	0.51
4:A:222:A:H61	4:A:232:G:H1'	1.74	0.51
4:A:446:G:OP1	18:Q:4:LYS:NZ	2.41	0.51
7:D:99:GLU:OE1	7:D:99:GLU:N	2.39	0.51
4:A:2506:U:OP2	4:A:2576:G:N2	2.42	0.51
5:B:3:C:H3'	5:B:4:C:H5''	1.92	0.51
17:P:14:GLN:OE1	17:P:14:GLN:N	2.42	0.51
4:A:1020:A:H1'	4:A:1021:A:OP2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1139:G:O2'	4:A:1143:A:N1	2.39	0.51
4:A:1359:A:OP2	4:A:1371:G:N1	2.43	0.51
4:A:1811:G:OP2	6:C:162:ASN:ND2	2.41	0.51
4:A:2467:C:N4	4:A:2484:G:O6	2.44	0.51
4:A:1664:A:N6	4:A:1996:C:C4	2.79	0.51
13:K:59:LYS:N	13:K:89:ASN:OD1	2.42	0.51
4:A:2552:U:O2'	4:A:2553:G:N7	2.44	0.51
13:K:81:GLY:N	17:P:67:GLU:OE2	2.44	0.51
4:A:1282:U:O4	4:A:1286:A:N7	2.44	0.51
10:G:85:LYS:C	10:G:86:LEU:HD12	2.36	0.51
2:2:1:MET:N	4:A:1619:G:O2'	2.44	0.50
4:A:1534:U:O2'	4:A:1537:G:O6	2.19	0.50
4:A:2106:U:N3	4:A:2107:G:N7	2.60	0.50
18:Q:97:ILE:HD11	18:Q:104:ALA:CB	2.38	0.50
4:A:549:G:O2'	4:A:550:C:P	2.70	0.50
4:A:1084:A:N6	4:A:1085:A:N1	2.60	0.50
9:F:7:TYR:HA	9:F:11:VAL:HG12	1.94	0.50
4:A:671:C:OP1	14:L:43:GLY:N	2.42	0.50
4:A:2618:G:H21	7:D:155:VAL:HG21	1.76	0.50
6:C:93:ASP:OD1	6:C:94:VAL:N	2.45	0.50
14:L:104:GLN:OE1	14:L:104:GLN:N	2.38	0.50
7:D:81:GLU:OE1	7:D:81:GLU:N	2.43	0.50
19:R:34:GLU:N	19:R:34:GLU:OE1	2.45	0.50
4:A:85:G:OP1	22:U:6:ARG:N	2.45	0.50
4:A:1093:G:H21	4:A:1098:A:H62	1.60	0.50
4:A:727:A:P	4:A:1431:A:HO2'	2.33	0.49
4:A:1322:A:O2'	20:S:84:ARG:NH2	2.45	0.49
4:A:2509:G:N1	4:A:2580:U:O4	2.45	0.49
4:A:2831:G:N2	4:A:2884:U:OP2	2.45	0.49
20:S:67:ASP:OD1	20:S:68:ASP:N	2.44	0.49
4:A:514:A:N3	4:A:581:C:O2'	2.41	0.49
4:A:981:A:OP2	4:A:982:C:N4	2.44	0.49
4:A:1244:A:N6	4:A:1245:G:O6	2.44	0.49
4:A:2506:U:OP2	4:A:2576:G:N1	2.37	0.49
4:A:2718:G:O3'	17:P:95:LYS:NZ	2.40	0.49
10:G:100:ASN:ND2	10:G:115:GLN:OE1	2.45	0.49
10:G:142:GLN:NE2	10:G:146:ASP:OD1	2.45	0.49
4:A:1342:A:O2'	4:A:1344:U:OP1	2.24	0.49
1:0:3:GLN:NE2	4:A:1263:U:O2'	2.44	0.49
13:K:9:ASN:ND2	13:K:82:ASN:O	2.46	0.49
4:A:1652:A:OP1	15:N:8:ARG:NH1	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1287:A:N6	4:A:1649:G:HO2'	2.10	0.49
4:A:1664:A:H61	4:A:1996:C:N4	2.10	0.49
19:R:49:ILE:HG22	19:R:54:VAL:HG12	1.94	0.49
13:K:76:VAL:HG22	17:P:72:VAL:CG1	2.43	0.49
4:A:1666:G:H4'	13:K:6:THR:HG23	1.95	0.49
4:A:1058:U:H2'	4:A:1059:G:C4	2.48	0.49
4:A:1383:A:O2'	4:A:1384:A:O4'	2.17	0.49
4:A:1574:C:C2	4:A:1575:C:C5	3.01	0.49
7:D:181:ASP:N	7:D:181:ASP:OD1	2.45	0.49
17:P:33:GLU:N	17:P:33:GLU:OE1	2.46	0.49
21:T:18:GLU:OE1	21:T:18:GLU:N	2.41	0.49
4:A:966:G:O4'	4:A:2267:A:N6	2.46	0.48
13:K:90:ASN:OD1	13:K:91:SER:N	2.46	0.48
4:A:2089:C:N4	4:A:2090:A:H62	2.11	0.48
4:A:2375:G:N1	4:A:2379:G:O6	2.46	0.48
4:A:2497:A:N3	4:A:2498:C:N4	2.61	0.48
1:O:27:LEU:HD11	20:S:38:TYR:CE2	2.49	0.48
4:A:1184:U:OP2	27:Z:30:ARG:NH2	2.47	0.48
4:A:1326:U:O2'	4:A:2010:G:O2'	2.23	0.48
4:A:1779:U:O2	4:A:1783:A:N6	2.46	0.48
8:E:48:THR:O	8:E:52:VAL:HG23	2.13	0.48
15:N:115:LEU:N	15:N:115:LEU:HD12	2.28	0.48
4:A:240:C:OP2	4:A:241:A:O2'	2.19	0.48
4:A:1233:C:C2	4:A:1234:U:C5	3.01	0.48
4:A:1290:C:C2	4:A:1291:C:C5	3.01	0.48
14:L:93:ASN:OD1	14:L:94:THR:N	2.47	0.48
4:A:48:G:N2	4:A:177:G:OP2	2.47	0.48
4:A:434:U:O2	4:A:435:C:N4	2.42	0.48
4:A:587:C:O2	14:L:33:ARG:NH2	2.47	0.48
4:A:1664:A:N6	4:A:1996:C:N4	2.62	0.48
5:B:30:C:H1'	5:B:57:A:H61	1.78	0.48
4:A:462:C:N4	4:A:463:G:O6	2.47	0.48
4:A:2733:A:N3	7:D:208:LYS:NZ	2.52	0.48
8:E:142:ALA:C	8:E:143:LEU:HD12	2.39	0.48
10:G:172:GLU:OE1	10:G:172:GLU:N	2.47	0.48
4:A:442:G:O4'	8:E:41:GLN:NE2	2.46	0.48
7:D:1:MET:HE1	7:D:100:LEU:HB3	1.96	0.48
9:F:3:LEU:HD22	9:F:100:GLU:HG2	1.94	0.48
6:C:133:ILE:HD11	6:C:152:ILE:HD12	1.96	0.48
4:A:2307:G:N1	9:F:38:GLY:O	2.47	0.47
6:C:121:LEU:HD23	6:C:124:ARG:HH12	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:133:GLU:OE1	9:F:133:GLU:N	2.46	0.47
4:A:212:G:H2'	4:A:213:A:C8	2.48	0.47
4:A:704:G:O2'	4:A:727:A:N6	2.42	0.47
20:S:90:LYS:O	20:S:92:ARG:NH1	2.48	0.47
4:A:139:U:N3	4:A:141:G:N7	2.61	0.47
4:A:2429:G:O6	14:L:55:MET:HE1	2.13	0.47
5:B:42:C:C5	9:F:65:LEU:HD13	2.48	0.47
15:N:34:ILE:HG23	15:N:113:ILE:CG2	2.43	0.47
6:C:162:ASN:ND2	6:C:162:ASN:O	2.47	0.47
7:D:14:ILE:HD12	7:D:24:VAL:HG11	1.96	0.47
24:W:41:PHE:O	24:W:55:LEU:HD21	2.14	0.47
4:A:548:G:C2'	4:A:549:G:O4'	2.63	0.47
4:A:549:G:O2'	4:A:550:C:OP1	2.31	0.47
6:C:125:LEU:HD22	6:C:152:ILE:HD11	1.95	0.47
4:A:499:U:H2'	4:A:500:G:O4'	2.15	0.47
4:A:1020:A:H4'	4:A:1021:A:O5'	2.15	0.47
8:E:132:LYS:NZ	8:E:136:GLN:OE1	2.48	0.47
8:E:191:ASP:OD1	8:E:192:ALA:N	2.47	0.47
10:G:47:ASN:O	10:G:48:THR:HG23	2.15	0.47
4:A:25:U:H2'	4:A:26:G:O5'	2.15	0.47
4:A:1145:C:C2	4:A:1146:C:C5	3.03	0.47
4:A:1289:C:C2	4:A:1290:C:C5	3.03	0.47
4:A:2523:G:O2'	4:A:2764:A:O2'	2.19	0.47
5:B:37:C:O2	16:O:100:HIS:NE2	2.46	0.47
4:A:25:U:C2'	4:A:26:G:O5'	2.63	0.47
2:2:11:LYS:NZ	4:A:686:U:O4'	2.47	0.47
4:A:306:U:H2'	4:A:307:G:O4'	2.15	0.47
4:A:855:G:N2	24:W:23:GLY:O	2.41	0.47
4:A:1542:U:H2'	4:A:1543:G:O4'	2.15	0.47
4:A:2688:G:N1	4:A:2720:U:OP2	2.42	0.47
7:D:131:ASP:O	7:D:136:ASN:ND2	2.44	0.47
19:R:38:VAL:O	19:R:54:VAL:HG13	2.15	0.47
5:B:23:G:O2'	5:B:24:G:O4'	2.32	0.46
15:N:19:ALA:O	15:N:23:ASN:ND2	2.44	0.46
18:Q:48:ASP:OD1	18:Q:49:ARG:N	2.48	0.46
2:2:12:ARG:NH2	2:2:44:VAL:HG11	2.29	0.46
4:A:549:G:HO2'	4:A:550:C:P	2.39	0.46
4:A:1428:C:N4	4:A:1570:A:OP2	2.43	0.46
4:A:1753:G:H22	4:A:1756:G:P	2.38	0.46
4:A:2050:C:H2'	4:A:2051:A:O4'	2.16	0.46
5:B:114:C:H1'	16:O:47:VAL:HG11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:723:C:C2	4:A:724:U:C5	3.03	0.46
4:A:1215:G:O6	4:A:1235:G:C2	2.68	0.46
7:D:33:ARG:NH2	7:D:53:GLY:O	2.40	0.46
9:F:135:ILE:HD13	9:F:142:TYR:HB2	1.96	0.46
10:G:137:LYS:HA	10:G:140:ILE:HG22	1.97	0.46
14:L:71:ALA:HA	14:L:74:THR:HG22	1.96	0.46
4:A:629:G:N3	4:A:639:U:O2'	2.49	0.46
4:A:1432:G:H2'	4:A:1433:A:C8	2.51	0.46
4:A:1733:G:C2	4:A:1734:G:N7	2.84	0.46
4:A:2474:U:O2	4:A:2474:U:H2'	2.15	0.46
3:4:16:ILE:HD13	3:4:25:VAL:HG22	1.97	0.46
4:A:1270:C:N4	4:A:1648:U:O4	2.49	0.46
4:A:1378:A:O2'	4:A:1380:G:OP2	2.33	0.46
17:P:12:MET:HE2	17:P:54:LEU:N	2.31	0.46
23:V:4:ILE:HB	23:V:63:ILE:HD13	1.96	0.46
4:A:379:G:C6	4:A:396:G:O6	2.69	0.46
4:A:819:A:O2'	4:A:837:C:O2'	2.32	0.46
4:A:2756:U:H4'	4:A:2757:A:OP1	2.16	0.46
9:F:139:GLU:OE1	9:F:139:GLU:N	2.46	0.46
22:U:27:VAL:HG12	22:U:33:VAL:HG12	1.97	0.46
4:A:1003:G:O2'	4:A:1010:A:N1	2.43	0.46
9:F:134:GLN:N	9:F:134:GLN:OE1	2.49	0.46
4:A:2564:A:C2	4:A:2647:U:H4'	2.51	0.46
19:R:59:ILE:HD12	19:R:101:ILE:HD12	1.98	0.46
27:Z:6:ILE:CD1	27:Z:56:VAL:HG23	2.46	0.46
4:A:1006:C:O4'	12:J:30:THR:HG23	2.16	0.46
4:A:2652:C:H2'	4:A:2653:U:O4'	2.16	0.46
5:B:15:A:N3	5:B:109:A:N6	2.63	0.46
18:Q:64:ILE:CD1	18:Q:94:LEU:HD13	2.45	0.46
19:R:98:ILE:CG2	19:R:101:ILE:HD11	2.46	0.46
8:E:7:ASP:OD1	8:E:8:ALA:N	2.46	0.45
10:G:132:LEU:H	10:G:132:LEU:HD23	1.81	0.45
4:A:458:G:HO2'	4:A:459:U:P	2.39	0.45
4:A:636:G:C8	14:L:128:THR:HG21	2.51	0.45
4:A:1152:C:H4'	18:Q:79:ILE:HG21	1.98	0.45
5:B:2:G:H2'	5:B:3:C:C6	2.51	0.45
19:R:49:ILE:HG22	19:R:54:VAL:HA	1.98	0.45
4:A:1475:G:O2'	4:A:1732:C:N4	2.50	0.45
4:A:1527:G:N1	4:A:1544:A:OP2	2.40	0.45
12:J:32:LEU:CD2	12:J:54:ILE:HG21	2.47	0.45
4:A:188:G:O2'	4:A:1365:A:N6	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:372:G:O2'	4:A:373:U:O5'	2.34	0.45
4:A:733:G:N2	4:A:734:A:N7	2.64	0.45
4:A:1344:U:H3'	4:A:1345:C:H5'	1.97	0.45
4:A:2467:C:H2'	4:A:2468:A:O4'	2.17	0.45
4:A:2720:U:C2	4:A:2721:A:C8	3.04	0.45
8:E:161:ALA:CB	8:E:169:VAL:HG23	2.47	0.45
9:F:133:GLU:CG	9:F:135:ILE:HG22	2.47	0.45
4:A:756:A:H2'	4:A:757:G:O4'	2.17	0.45
4:A:1654:A:O2'	7:D:118:PHE:O	2.29	0.45
4:A:2655:G:O2'	4:A:2656:U:P	2.74	0.45
5:B:42:C:C4	9:F:65:LEU:HD22	2.51	0.45
5:B:94:A:OP1	23:V:19:ARG:NE	2.48	0.45
17:P:48:ALA:HB3	17:P:59:THR:HG22	1.97	0.45
22:U:33:VAL:HG13	22:U:66:VAL:HG12	1.98	0.45
4:A:224:U:O4	4:A:232:G:N2	2.49	0.45
4:A:450:G:N1	4:A:454:A:OP2	2.49	0.45
4:A:1142:A:C4	4:A:1144:A:N7	2.85	0.45
4:A:2133:G:N2	4:A:2157:G:O6	2.49	0.45
14:L:95:LEU:HD11	14:L:100:ILE:HD11	1.99	0.45
15:N:103:ARG:O	15:N:107:ASN:N	2.48	0.45
15:N:116:VAL:HG23	15:N:116:VAL:O	2.16	0.45
4:A:357:C:C2	4:A:358:U:C5	3.04	0.45
4:A:639:U:C2	4:A:640:C:C5	3.05	0.45
4:A:1788:C:C2	4:A:1789:A:C8	3.05	0.45
10:G:154:GLU:OE1	10:G:156:TYR:N	2.47	0.45
22:U:36:GLU:O	22:U:38:ILE:HD12	2.16	0.45
22:U:98:ASN:O	22:U:98:ASN:CG	2.59	0.45
12:J:50:THR:O	12:J:50:THR:HG22	2.16	0.45
14:L:29:LYS:O	14:L:30:THR:OG1	2.21	0.45
3:4:18:LYS:NZ	4:A:1034:G:O4'	2.40	0.45
4:A:458:G:O2'	4:A:459:U:P	2.74	0.45
4:A:627:A:C5	14:L:111:ILE:HD11	2.52	0.45
4:A:1141:U:H4'	4:A:1142:A:O4'	2.17	0.45
4:A:2243:U:O2'	4:A:2434:A:N1	2.38	0.45
4:A:2351:G:O2'	4:A:2366:A:N6	2.44	0.45
11:H:5:LEU:HD12	11:H:5:LEU:N	2.32	0.45
12:J:108:MET:N	12:J:108:MET:HE2	2.32	0.45
13:K:70:ARG:HD2	13:K:76:VAL:HG12	1.98	0.45
20:S:55:ILE:HG23	20:S:66:ILE:HG21	1.99	0.45
4:A:570:G:C1'	4:A:983:A:N6	2.80	0.45
9:F:48:LEU:HD12	9:F:48:LEU:C	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1235:G:O3'	4:A:1236:G:O4'	2.34	0.44
4:A:1323:C:N4	4:A:1324:G:O6	2.50	0.44
4:A:2589:A:N1	4:A:2606:C:N4	2.66	0.44
10:G:37:ASN:OD1	10:G:40:VAL:HG12	2.17	0.44
15:N:29:VAL:HG13	15:N:75:ILE:HD12	1.99	0.44
16:O:43:ASN:OD1	16:O:44:GLY:N	2.50	0.44
4:A:299:A:N6	4:A:322:A:O2'	2.40	0.44
4:A:754:U:C2	4:A:755:U:C5	3.05	0.44
4:A:864:G:O2'	4:A:914:G:O6	2.26	0.44
9:F:140:ILE:N	9:F:140:ILE:HD12	2.32	0.44
4:A:645:C:H2'	4:A:647:G:C8	2.52	0.44
4:A:864:G:H21	4:A:866:A:H62	1.66	0.44
4:A:1670:C:O2	4:A:1993:U:O2'	2.30	0.44
4:A:2845:U:O3'	17:P:52:ARG:NH1	2.51	0.44
15:N:28:LEU:HD13	15:N:34:ILE:HG22	1.99	0.44
4:A:415:A:H2'	4:A:416:U:C6	2.52	0.44
4:A:1737:G:O3'	4:A:1738:G:O4'	2.35	0.44
8:E:58:LYS:NZ	8:E:70:SER:O	2.46	0.44
15:N:70:THR:O	15:N:71:ARG:C	2.60	0.44
16:O:87:ILE:N	16:O:87:ILE:HD12	2.32	0.44
4:A:1753:G:N2	4:A:1756:G:OP2	2.40	0.44
2:2:34:ARG:NH1	4:A:466:A:OP1	2.51	0.44
4:A:107:G:O3'	4:A:293:U:O2'	2.30	0.44
4:A:1378:A:C4'	4:A:1379:U:OP1	2.66	0.44
4:A:2638:G:HO2'	4:A:2639:A:H8	1.63	0.44
4:A:320:A:H2'	8:E:131:THR:HG21	1.99	0.44
4:A:1341:G:OP1	4:A:1602:U:O2'	2.22	0.44
4:A:2681:C:OP1	7:D:114:LYS:NZ	2.51	0.44
10:G:45:ALA:O	10:G:46:ASP:C	2.60	0.44
4:A:1994:C:H2'	4:A:1995:U:C6	2.53	0.44
27:Z:4:ILE:HD11	27:Z:56:VAL:CG2	2.47	0.44
4:A:62:U:O2'	4:A:63:A:N7	2.46	0.44
4:A:2758:A:C2	10:G:70:LEU:HD11	2.53	0.44
7:D:22:ILE:HD12	7:D:22:ILE:N	2.33	0.44
12:J:43:GLU:N	12:J:43:GLU:OE1	2.51	0.44
4:A:1364:G:OP2	25:X:49:ARG:NH1	2.51	0.43
4:A:2552:U:H3'	4:A:2552:U:O2	2.18	0.43
5:B:39:A:C2	5:B:44:G:C2	3.05	0.43
8:E:142:ALA:O	8:E:143:LEU:HD12	2.18	0.43
8:E:149:ILE:HG23	8:E:149:ILE:O	2.18	0.43
12:J:101:ILE:O	12:J:105:VAL:HG22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:35:GLU:N	23:V:35:GLU:OE1	2.51	0.43
4:A:1083:U:O2'	4:A:1085:A:N7	2.45	0.43
9:F:118:ALA:O	9:F:166:ARG:NH1	2.44	0.43
14:L:136:GLU:CD	14:L:142:ILE:HD11	2.43	0.43
4:A:575:A:OP2	4:A:2499:C:O2'	2.36	0.43
4:A:2394:C:H42	6:C:80:ARG:NH2	2.16	0.43
8:E:176:ASP:OD1	8:E:176:ASP:N	2.50	0.43
4:A:1141:U:O2	4:A:1142:A:N6	2.52	0.43
4:A:1995:U:O2'	13:K:31:ARG:NH1	2.51	0.43
5:B:39:A:H2'	5:B:40:U:C6	2.54	0.43
15:N:28:LEU:HB2	15:N:34:ILE:HG21	1.99	0.43
3:4:3:VAL:O	3:4:3:VAL:HG22	2.18	0.43
4:A:6:A:N3	12:J:135:GLN:NE2	2.66	0.43
7:D:98:VAL:HG23	7:D:187:LEU:HD21	2.00	0.43
4:A:574:A:N6	4:A:2034:U:OP1	2.51	0.43
5:B:38:C:N4	5:B:39:A:N6	2.66	0.43
7:D:24:VAL:HG12	7:D:178:VAL:HG21	2.01	0.43
10:G:38:ASP:O	10:G:54:ARG:NH1	2.52	0.43
13:K:58:LEU:N	13:K:58:LEU:HD23	2.34	0.43
4:A:1083:U:N3	4:A:1086:A:OP2	2.51	0.43
4:A:1425:G:H2'	4:A:1426:G:O4'	2.19	0.43
4:A:2296:U:OP2	16:O:9:ARG:NH2	2.52	0.43
27:Z:19:HIS:O	27:Z:23:LEU:HD23	2.18	0.43
4:A:1541:C:H2'	4:A:1542:U:O4'	2.19	0.42
4:A:1736:U:H2'	4:A:1737:G:O4'	2.18	0.42
4:A:2506:U:O2	4:A:2506:U:O4'	2.37	0.42
20:S:35:ILE:O	20:S:39:THR:HG23	2.18	0.42
22:U:97:SER:O	22:U:98:ASN:OD1	2.37	0.42
4:A:36:G:N3	4:A:450:G:O2'	2.51	0.42
4:A:1426:G:O2'	4:A:1572:A:N6	2.53	0.42
7:D:3:GLY:C	7:D:4:LEU:HD12	2.44	0.42
7:D:98:VAL:HG22	7:D:98:VAL:O	2.19	0.42
8:E:154:ASP:OD2	8:E:157:LEU:HD12	2.19	0.42
4:A:1268:A:H1'	4:A:2013:A:H61	1.84	0.42
9:F:109:ARG:NH2	9:F:136:ILE:O	2.52	0.42
12:J:84:ILE:HG23	12:J:84:ILE:O	2.20	0.42
17:P:96:LEU:HD12	17:P:96:LEU:N	2.35	0.42
4:A:1319:C:N4	4:A:1334:G:O6	2.52	0.42
4:A:2779:U:O2'	12:J:120:ARG:NH2	2.53	0.42
13:K:37:ASP:OD1	13:K:38:ILE:N	2.53	0.42
23:V:7:GLU:N	23:V:7:GLU:OE1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:428:A:C2'	4:A:429:A:O5'	2.67	0.42
4:A:1264:A:O5'	4:A:1265:A:H2'	2.20	0.42
4:A:2446:G:N2	4:A:2449:U:O2	2.41	0.42
4:A:2450:A:N6	4:A:2501:C:O2	2.52	0.42
4:A:2645:G:H3'	4:A:2646:C:H5'	2.01	0.42
13:K:107:LEU:CD2	13:K:115:ILE:HG21	2.49	0.42
4:A:43:G:H2'	4:A:44:A:O4'	2.20	0.42
4:A:1068:G:H2'	4:A:1069:A:O4'	2.20	0.42
4:A:1558:C:O4'	4:A:1560:G:C8	2.73	0.42
4:A:1561:C:C2	4:A:1562:U:C5	3.08	0.42
4:A:1720:U:H2'	4:A:1721:G:O4'	2.20	0.42
6:C:146:GLN:OE1	6:C:146:GLN:N	2.43	0.42
15:N:36:THR:HG22	15:N:37:THR:N	2.35	0.42
18:Q:35:PHE:O	18:Q:38:VAL:HG22	2.20	0.42
4:A:563:A:C6	4:A:2018:G:C5	3.08	0.42
4:A:637:A:N1	4:A:651:G:O2'	2.42	0.42
4:A:2311:A:N3	9:F:78:ILE:HD13	2.35	0.42
4:A:2687:U:H2'	4:A:2688:G:O4'	2.20	0.42
6:C:110:GLN:O	6:C:114:LEU:HD23	2.20	0.42
23:V:29:ILE:HD11	23:V:90:ASP:OD2	2.20	0.42
4:A:550:C:H2'	4:A:551:G:H8	1.85	0.41
4:A:1289:C:O2'	4:A:1330:C:H4'	2.19	0.41
4:A:1386:C:H2'	4:A:1387:A:H8	1.84	0.41
8:E:188:MET:HE1	8:E:196:VAL:HG21	2.02	0.41
4:A:954:G:O2'	4:A:2274:A:N1	2.36	0.41
4:A:1026:G:OP2	4:A:1134:A:O2'	2.20	0.41
4:A:1199:U:H2'	4:A:1200:C:O4'	2.20	0.41
4:A:1601:G:H2'	4:A:1602:U:O4'	2.20	0.41
4:A:2580:U:H2'	4:A:2581:G:C4	2.55	0.41
4:A:2580:U:OP1	7:D:137:SER:OG	2.36	0.41
9:F:107:VAL:N	9:F:108:PRO:CD	2.83	0.41
4:A:1025:G:N2	4:A:1139:G:O6	2.50	0.41
4:A:1528:A:N6	4:A:1543:G:O2'	2.53	0.41
8:E:16:GLU:O	8:E:20:GLY:N	2.43	0.41
15:N:12:ARG:O	15:N:17:ARG:NH1	2.54	0.41
19:R:70:GLU:OE1	19:R:70:GLU:N	2.45	0.41
4:A:29:U:C2	4:A:30:G:C8	3.07	0.41
4:A:285:G:C6	4:A:356:G:C5	3.08	0.41
4:A:1096:A:H3'	4:A:1097:U:H5''	2.03	0.41
4:A:1465:G:H2'	4:A:1466:U:O4'	2.21	0.41
4:A:1557:C:OP2	4:A:1558:C:O2'	2.26	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:46:VAL:HG22	17:P:60:VAL:HG22	2.03	0.41
2:2:43:THR:OG1	2:2:44:VAL:N	2.53	0.41
4:A:1018:U:HO2'	4:A:1120:G:H21	1.59	0.41
4:A:1301:A:H2'	4:A:1301:A:N3	2.35	0.41
4:A:1572:A:C2	4:A:1573:G:C8	3.08	0.41
5:B:75:G:H1'	23:V:29:ILE:HD13	2.01	0.41
4:A:416:U:H2'	4:A:417:C:O4'	2.19	0.41
24:W:65:PHE:CE2	24:W:76:ILE:HD13	2.56	0.41
20:S:80:PRO:O	20:S:100:THR:OG1	2.33	0.41
4:A:174:U:C2	4:A:175:G:C8	3.08	0.41
4:A:2236:U:O2'	6:C:116:HIS:NE2	2.39	0.41
4:A:2592:G:C6	4:A:2603:G:C6	3.09	0.41
18:Q:48:ASP:OD1	18:Q:48:ASP:C	2.62	0.41
1:0:24:VAL:HG23	1:0:25:THR:N	2.36	0.41
4:A:28:A:H1'	4:A:513:A:N1	2.36	0.41
4:A:171:U:C2	4:A:172:A:C8	3.09	0.41
4:A:213:A:H2'	4:A:214:G:C8	2.56	0.41
4:A:395:U:H2'	4:A:396:G:C8	2.56	0.41
4:A:644:A:H2'	4:A:645:C:O4'	2.21	0.41
4:A:739:A:OP1	4:A:1781:U:P	2.79	0.41
4:A:995:C:O2	12:J:3:THR:OG1	2.30	0.41
4:A:1196:C:C2	4:A:1197:G:C8	3.09	0.41
4:A:1341:G:OP1	4:A:1397:U:N3	2.45	0.41
4:A:1614:A:N6	20:S:92:ARG:O	2.39	0.41
4:A:2423:U:O2	6:C:32:ILE:HG21	2.21	0.41
4:A:2487:G:C2	4:A:2488:G:C5	3.09	0.41
4:A:2717:C:O2'	17:P:93:LYS:NZ	2.46	0.41
9:F:133:GLU:HG2	9:F:135:ILE:HG22	2.02	0.41
10:G:46:ASP:O	10:G:47:ASN:CG	2.63	0.41
12:J:115:GLY:O	12:J:118:MET:HG2	2.21	0.41
15:N:28:LEU:HD12	15:N:28:LEU:C	2.46	0.41
15:N:34:ILE:CG2	15:N:113:ILE:HG23	2.48	0.41
16:O:2:ASP:OD1	16:O:3:LYS:N	2.47	0.41
4:A:23:G:C2	4:A:24:G:C8	3.09	0.41
4:A:202:U:H2'	4:A:203:A:O4'	2.21	0.41
4:A:301:G:OP2	22:U:81:ARG:NH2	2.46	0.41
4:A:554:U:H2'	4:A:555:G:O4'	2.21	0.41
4:A:619:G:O5'	4:A:620:G:N2	2.54	0.41
4:A:918:A:O2'	5:B:96:G:N2	2.54	0.41
4:A:1230:A:H2'	4:A:1231:U:O4'	2.21	0.41
9:F:90:LEU:HD23	9:F:90:LEU:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:116:LEU:HD12	10:G:120:ILE:CG2	2.51	0.41
14:L:95:LEU:HD23	14:L:101:ILE:HD13	2.03	0.41
4:A:227:A:O2'	4:A:228:C:O4'	2.38	0.40
4:A:270:A:N1	4:A:369:U:O2'	2.41	0.40
4:A:958:U:O2	5:B:89:U:O2'	2.29	0.40
4:A:2364:C:H2'	4:A:2365:G:O4'	2.21	0.40
4:A:2588:G:O6	4:A:2607:G:N1	2.54	0.40
26:Y:5:GLU:OE1	26:Y:5:GLU:N	2.49	0.40
27:Z:6:ILE:HD13	27:Z:56:VAL:HG23	2.04	0.40
10:G:143:VAL:O	10:G:147:LEU:HD23	2.20	0.40
12:J:4:PHE:CD2	18:Q:99:VAL:HG21	2.55	0.40
20:S:103:ILE:N	20:S:103:ILE:HD12	2.36	0.40
4:A:219:A:N6	4:A:428:A:OP2	2.54	0.40
4:A:549:G:C2'	4:A:550:C:O5'	2.69	0.40
4:A:1682:G:OP2	4:A:1699:G:N2	2.48	0.40
12:J:41:LYS:NZ	12:J:52:ASP:OD1	2.41	0.40
20:S:72:THR:HG21	20:S:108:SER:HB3	2.03	0.40
21:T:11:LEU:HD11	26:Y:26:PHE:CE1	2.56	0.40
4:A:28:A:C5	4:A:29:U:C5	3.09	0.40
4:A:69:C:O2	4:A:73:A:O2'	2.33	0.40
4:A:442:G:C6	4:A:444:C:N4	2.90	0.40
4:A:464:U:O4	4:A:788:A:C8	2.74	0.40
4:A:586:A:N1	4:A:809:G:O2'	2.50	0.40
4:A:1282:U:H2'	4:A:1283:G:O4'	2.22	0.40
4:A:2028:U:O4	4:A:2033:A:N7	2.54	0.40
14:L:103:ILE:N	14:L:103:ILE:HD12	2.36	0.40
4:A:817:C:H2'	4:A:818:G:O4'	2.21	0.40
4:A:1125:G:O6	4:A:1126:A:N6	2.55	0.40
4:A:2126:A:H2'	4:A:2162:G:H21	1.85	0.40
4:A:2327:A:H2'	4:A:2328:A:C8	2.56	0.40
4:A:2884:U:O2	4:A:2884:U:O4'	2.40	0.40
7:D:47:ALA:O	7:D:48:ILE:HD13	2.22	0.40
15:N:22:ARG:HG3	15:N:70:THR:HA	2.03	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	
1	0	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
2	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
3	4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
6	C	156/183 (85%)	155 (99%)	1 (1%)	0	100	100
7	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
8	E	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	24	61
9	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
10	G	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
11	H	50/149 (34%)	45 (90%)	5 (10%)	0	100	100
12	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
13	K	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
14	L	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
15	N	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
16	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
17	P	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
18	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
19	R	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	12	46
20	S	109/110 (99%)	104 (95%)	5 (5%)	0	100	100
21	T	91/93 (98%)	88 (97%)	3 (3%)	0	100	100
22	U	100/102 (98%)	87 (87%)	13 (13%)	0	100	100
23	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	W	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
25	X	75/77 (97%)	75 (100%)	0	0	100	100
26	Y	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
27	Z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2713/2884 (94%)	2598 (96%)	113 (4%)	2 (0%)	49 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	R	54	VAL
8	E	83	VAL

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
1	0	47/47 (100%)	47 (100%)	0	100 100
2	2	38/38 (100%)	38 (100%)	0	100 100
3	4	34/34 (100%)	34 (100%)	0	100 100
6	C	137/161 (85%)	137 (100%)	0	100 100
7	D	164/164 (100%)	164 (100%)	0	100 100
8	E	165/165 (100%)	163 (99%)	2 (1%)	63 72
9	F	148/148 (100%)	147 (99%)	1 (1%)	76 78
10	G	137/137 (100%)	136 (99%)	1 (1%)	76 78
11	H	41/114 (36%)	41 (100%)	0	100 100
12	J	116/116 (100%)	116 (100%)	0	100 100
13	K	103/103 (100%)	103 (100%)	0	100 100
14	L	102/102 (100%)	100 (98%)	2 (2%)	48 65
15	N	100/100 (100%)	99 (99%)	1 (1%)	68 75
16	O	86/86 (100%)	86 (100%)	0	100 100
17	P	99/99 (100%)	97 (98%)	2 (2%)	48 65
18	Q	89/89 (100%)	88 (99%)	1 (1%)	65 73
19	R	84/84 (100%)	82 (98%)	2 (2%)	43 63
20	S	94/93 (101%)	94 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	T	80/80 (100%)	80 (100%)	0	100	100
22	U	83/83 (100%)	83 (100%)	0	100	100
23	V	78/78 (100%)	78 (100%)	0	100	100
24	W	57/57 (100%)	57 (100%)	0	100	100
25	X	67/67 (100%)	67 (100%)	0	100	100
26	Y	55/55 (100%)	55 (100%)	0	100	100
27	Z	48/48 (100%)	48 (100%)	0	100	100
All	All	2252/2348 (96%)	2240 (100%)	12 (0%)	78	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	E	154	ASP
8	E	163	ASN
9	F	11	VAL
10	G	87	GLN
14	L	127	VAL
14	L	142	ILE
15	N	1	MET
17	P	73	PHE
17	P	111	GLU
18	Q	108	LEU
19	R	39	LEU
19	R	75	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	3	GLN
1	0	18	HIS
2	2	26	ASN
6	C	111	GLN
7	D	126	ASN
8	E	29	HIS
8	E	30	GLN
8	E	92	HIS
9	F	36	ASN
10	G	21	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	H	18	GLN
14	L	38	GLN
14	L	54	GLN
16	O	29	HIS
16	O	38	GLN
18	Q	19	GLN
18	Q	51	GLN
18	Q	55	GLN
22	U	39	ASN
24	W	46	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	2710/2903 (93%)	434 (16%)	16 (0%)
5	B	119/120 (99%)	14 (11%)	2 (1%)
All	All	2829/3023 (93%)	448 (15%)	18 (0%)

All (448) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	10	A
4	A	26	G
4	A	27	G
4	A	34	U
4	A	35	G
4	A	46	G
4	A	51	G
4	A	60	G
4	A	63	A
4	A	71	A
4	A	74	A
4	A	75	G
4	A	114	U
4	A	118	A
4	A	120	U
4	A	126	A
4	A	136	G
4	A	139	U
4	A	141	G
4	A	142	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	160	A
4	A	162	U
4	A	163	C
4	A	181	A
4	A	196	A
4	A	199	A
4	A	216	A
4	A	221	A
4	A	222	A
4	A	225	C
4	A	228	C
4	A	233	A
4	A	242	G
4	A	243	U
4	A	248	G
4	A	255	A
4	A	265	A
4	A	266	G
4	A	267	C
4	A	272	A
4	A	277	G
4	A	278	A
4	A	294	A
4	A	322	A
4	A	323	C
4	A	324	A
4	A	329	G
4	A	330	A
4	A	345	A
4	A	362	A
4	A	371	A
4	A	372	G
4	A	373	U
4	A	386	G
4	A	387	U
4	A	388	G
4	A	404	A
4	A	406	G
4	A	411	G
4	A	417	C
4	A	424	G
4	A	429	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	435	C
4	A	451	U
4	A	456	C
4	A	457	A
4	A	458	G
4	A	459	U
4	A	473	G
4	A	480	A
4	A	481	G
4	A	491	G
4	A	505	A
4	A	509	C
4	A	530	G
4	A	531	C
4	A	532	A
4	A	544	C
4	A	545	U
4	A	547	A
4	A	550	C
4	A	563	A
4	A	569	U
4	A	573	U
4	A	575	A
4	A	588	U
4	A	603	A
4	A	614	A
4	A	621	A
4	A	627	A
4	A	637	A
4	A	643	A
4	A	646	U
4	A	647	G
4	A	653	U
4	A	654	A
4	A	659	G
4	A	660	C
4	A	669	G
4	A	675	A
4	A	686	U
4	A	687	C
4	A	695	G
4	A	717	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	726	G
4	A	730	A
4	A	740	C
4	A	747	C
4	A	748	G
4	A	752	A
4	A	764	A
4	A	775	G
4	A	776	G
4	A	782	A
4	A	784	G
4	A	785	G
4	A	789	A
4	A	792	A
4	A	805	G
4	A	812	C
4	A	819	A
4	A	827	U
4	A	828	U
4	A	845	A
4	A	846	U
4	A	847	U
4	A	856	G
4	A	859	G
4	A	877	A
4	A	878	A
4	A	896	A
4	A	897	C
4	A	907	G
4	A	910	A
4	A	914	G
4	A	931	U
4	A	941	A
4	A	946	C
4	A	953	G
4	A	961	C
4	A	973	A
4	A	974	G
4	A	980	A
4	A	983	A
4	A	984	A
4	A	985	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	995	C
4	A	996	A
4	A	1009	A
4	A	1012	U
4	A	1013	C
4	A	1021	A
4	A	1023	U
4	A	1026	G
4	A	1033	U
4	A	1040	A
4	A	1045	C
4	A	1046	A
4	A	1047	G
4	A	1053	C
4	A	1054	A
4	A	1057	A
4	A	1059	G
4	A	1060	U
4	A	1061	U
4	A	1062	G
4	A	1065	U
4	A	1066	U
4	A	1068	G
4	A	1070	A
4	A	1071	G
4	A	1073	A
4	A	1076	C
4	A	1079	C
4	A	1083	U
4	A	1084	A
4	A	1088	A
4	A	1089	A
4	A	1097	U
4	A	1104	C
4	A	1111	A
4	A	1119	U
4	A	1132	U
4	A	1135	C
4	A	1143	A
4	A	1157	G
4	A	1169	A
4	A	1174	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	1175	A
4	A	1176	U
4	A	1178	C
4	A	1180	U
4	A	1181	U
4	A	1206	G
4	A	1212	G
4	A	1225	G
4	A	1236	G
4	A	1250	G
4	A	1253	A
4	A	1256	G
4	A	1264	A
4	A	1271	G
4	A	1272	A
4	A	1273	U
4	A	1300	G
4	A	1301	A
4	A	1302	A
4	A	1306	C
4	A	1314	C
4	A	1321	A
4	A	1329	U
4	A	1341	G
4	A	1343	G
4	A	1345	C
4	A	1359	A
4	A	1365	A
4	A	1378	A
4	A	1379	U
4	A	1383	A
4	A	1395	A
4	A	1403	A
4	A	1416	G
4	A	1419	A
4	A	1420	A
4	A	1421	G
4	A	1428	C
4	A	1437	C
4	A	1454	C
4	A	1458	U
4	A	1461	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	1475	G
4	A	1482	G
4	A	1490	A
4	A	1491	G
4	A	1504	A
4	A	1508	A
4	A	1509	A
4	A	1515	A
4	A	1519	G
4	A	1524	G
4	A	1535	A
4	A	1536	C
4	A	1559	U
4	A	1560	G
4	A	1569	A
4	A	1578	U
4	A	1585	C
4	A	1608	A
4	A	1613	G
4	A	1634	A
4	A	1646	C
4	A	1647	U
4	A	1648	U
4	A	1654	A
4	A	1674	G
4	A	1694	C
4	A	1707	G
4	A	1715	G
4	A	1729	U
4	A	1730	C
4	A	1731	G
4	A	1732	C
4	A	1733	G
4	A	1735	A
4	A	1737	G
4	A	1738	G
4	A	1744	A
4	A	1756	G
4	A	1764	C
4	A	1773	A
4	A	1781	U
4	A	1829	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	1991	U
4	A	1992	G
4	A	1993	U
4	A	1996	C
4	A	1997	C
4	A	2021	C
4	A	2022	U
4	A	2023	C
4	A	2030	A
4	A	2031	A
4	A	2033	A
4	A	2043	C
4	A	2052	A
4	A	2055	C
4	A	2056	G
4	A	2059	A
4	A	2060	A
4	A	2061	G
4	A	2062	A
4	A	2069	G
4	A	2080	A
4	A	2093	G
4	A	2096	C
4	A	2100	G
4	A	2104	C
4	A	2110	G
4	A	2111	U
4	A	2112	G
4	A	2113	U
4	A	2118	U
4	A	2119	A
4	A	2125	G
4	A	2127	G
4	A	2131	U
4	A	2132	U
4	A	2133	G
4	A	2136	G
4	A	2137	U
4	A	2139	U
4	A	2145	C
4	A	2162	G
4	A	2164	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	2172	U
4	A	2173	A
4	A	2189	U
4	A	2198	A
4	A	2199	A
4	A	2204	G
4	A	2211	A
4	A	2213	U
4	A	2225	A
4	A	2226	C
4	A	2238	G
4	A	2239	G
4	A	2250	G
4	A	2251	G
4	A	2266	A
4	A	2283	C
4	A	2286	G
4	A	2287	A
4	A	2297	A
4	A	2305	U
4	A	2309	A
4	A	2319	G
4	A	2325	G
4	A	2327	A
4	A	2333	A
4	A	2334	U
4	A	2335	A
4	A	2336	A
4	A	2345	G
4	A	2350	C
4	A	2357	G
4	A	2383	G
4	A	2385	C
4	A	2396	G
4	A	2402	U
4	A	2407	A
4	A	2422	C
4	A	2424	C
4	A	2425	A
4	A	2428	G
4	A	2429	G
4	A	2430	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	2435	A
4	A	2441	U
4	A	2445	G
4	A	2447	G
4	A	2448	A
4	A	2475	C
4	A	2476	A
4	A	2478	A
4	A	2491	U
4	A	2492	U
4	A	2494	G
4	A	2498	C
4	A	2502	G
4	A	2503	A
4	A	2504	U
4	A	2505	G
4	A	2506	U
4	A	2513	A
4	A	2518	A
4	A	2520	C
4	A	2529	G
4	A	2530	A
4	A	2535	G
4	A	2547	A
4	A	2554	U
4	A	2564	A
4	A	2566	A
4	A	2567	G
4	A	2573	C
4	A	2576	G
4	A	2582	G
4	A	2598	A
4	A	2602	A
4	A	2609	U
4	A	2610	C
4	A	2613	U
4	A	2614	A
4	A	2629	U
4	A	2646	C
4	A	2655	G
4	A	2656	U
4	A	2682	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	2689	U
4	A	2690	U
4	A	2714	G
4	A	2718	G
4	A	2726	A
4	A	2732	G
4	A	2733	A
4	A	2744	G
4	A	2748	A
4	A	2762	C
4	A	2764	A
4	A	2765	A
4	A	2778	A
4	A	2779	U
4	A	2780	G
4	A	2791	G
4	A	2794	C
4	A	2799	A
4	A	2800	A
4	A	2809	A
4	A	2818	U
4	A	2820	A
4	A	2833	U
4	A	2848	G
4	A	2849	U
4	A	2867	G
4	A	2868	A
4	A	2871	U
4	A	2872	A
4	A	2880	C
4	A	2883	A
4	A	2891	U
4	A	2894	G
4	A	2901	C
4	A	2902	C
4	A	2903	U
5	B	4	C
5	B	9	G
5	B	12	C
5	B	13	G
5	B	35	C
5	B	42	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	44	G
5	B	45	A
5	B	53	A
5	B	67	G
5	B	88	C
5	B	89	U
5	B	90	C
5	B	109	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	227	A
4	A	242	G
4	A	372	G
4	A	458	G
4	A	549	G
4	A	784	G
4	A	1020	A
4	A	1022	G
4	A	1224	U
4	A	1358	G
4	A	1378	A
4	A	1457	U
4	A	2058	A
4	A	2326	C
4	A	2655	G
4	A	2808	G
5	B	52	A
5	B	66	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 oligosaccharides 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.

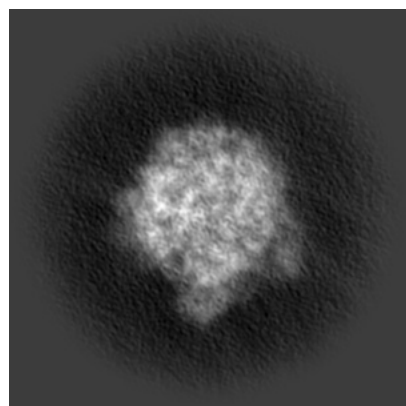
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51836. These allow visual inspection of the internal detail of the map and identification of artifacts.

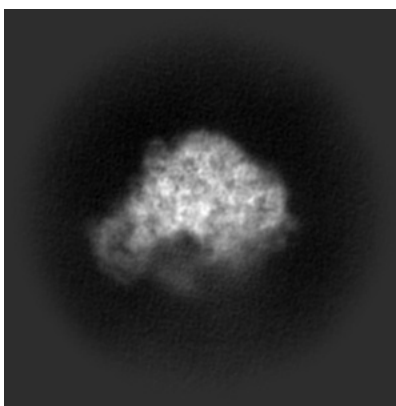
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

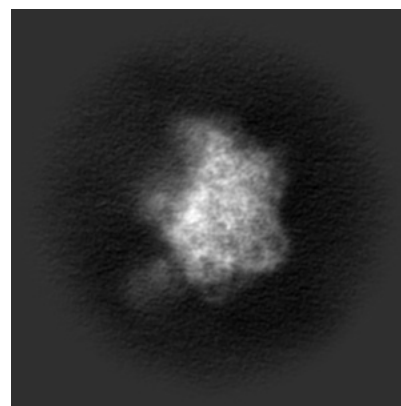
6.1.1 Primary map



X

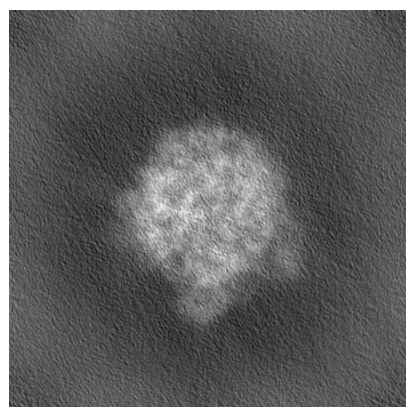


Y

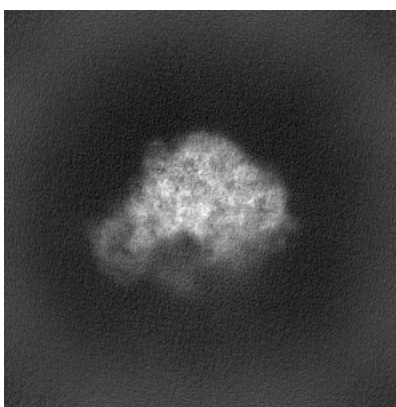


Z

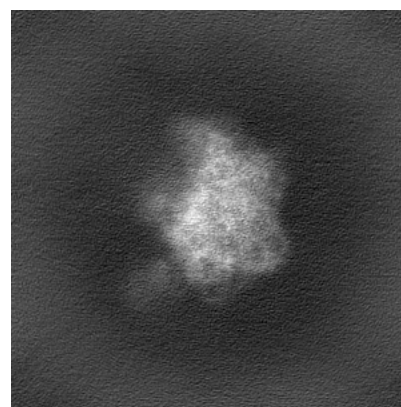
6.1.2 Raw map



X



Y

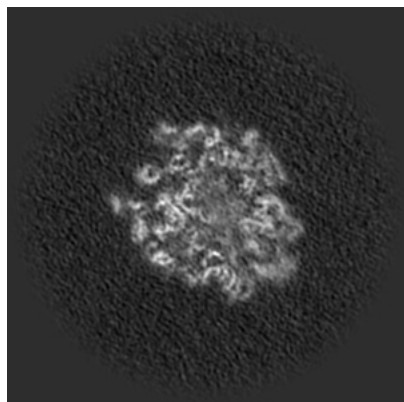


Z

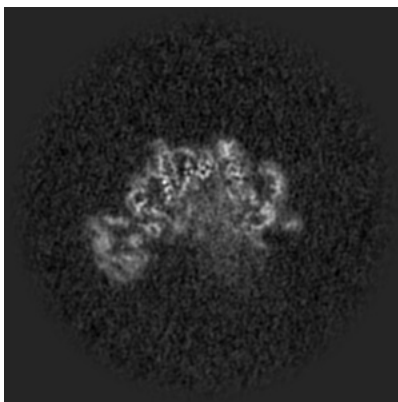
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

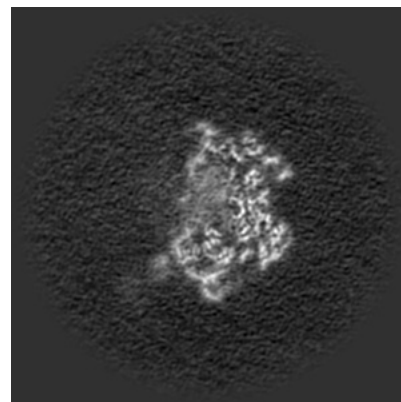
6.2.1 Primary map



X Index: 150

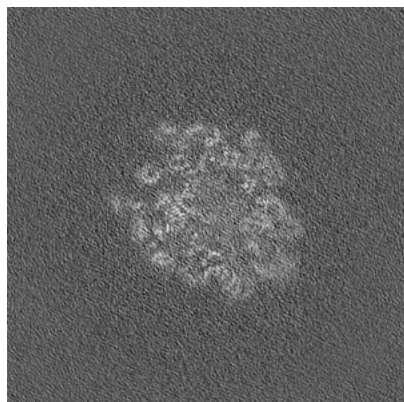


Y Index: 150

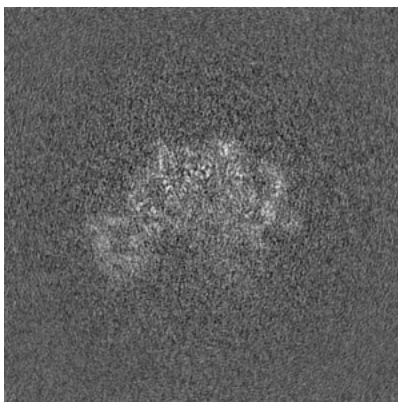


Z Index: 150

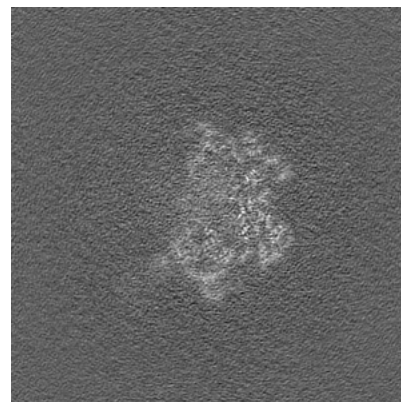
6.2.2 Raw map



X Index: 150



Y Index: 150

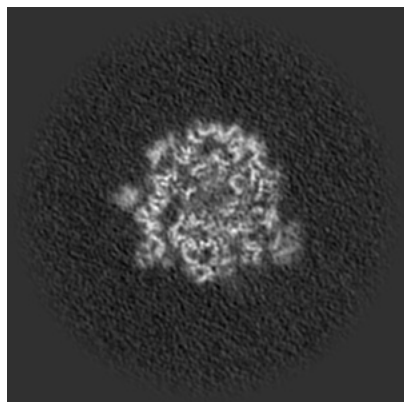


Z Index: 150

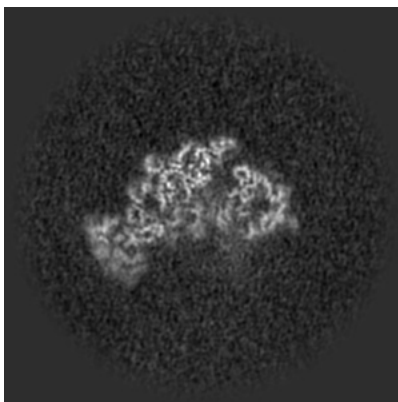
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

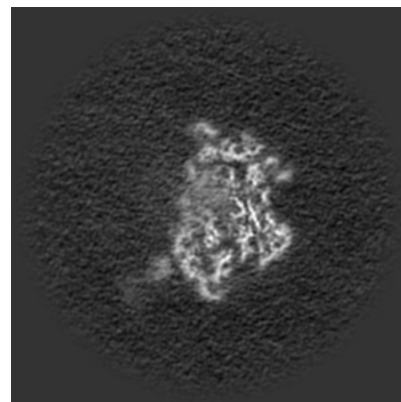
6.3.1 Primary map



X Index: 162

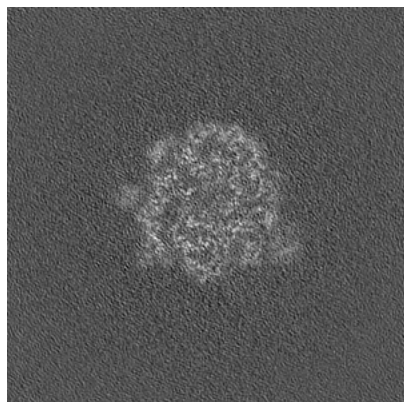


Y Index: 143

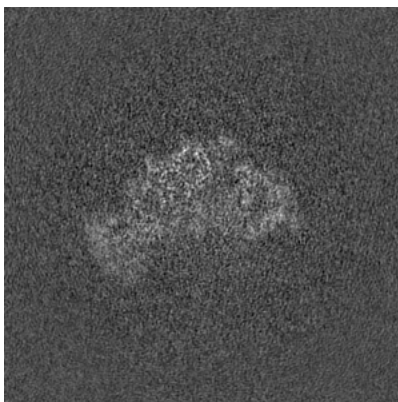


Z Index: 148

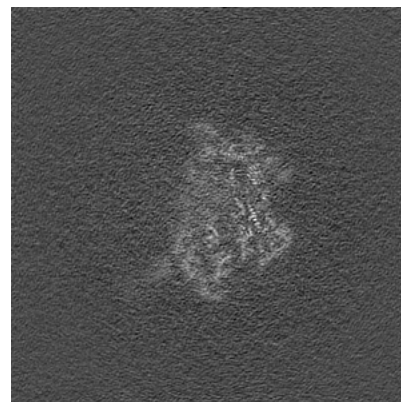
6.3.2 Raw map



X Index: 163



Y Index: 144

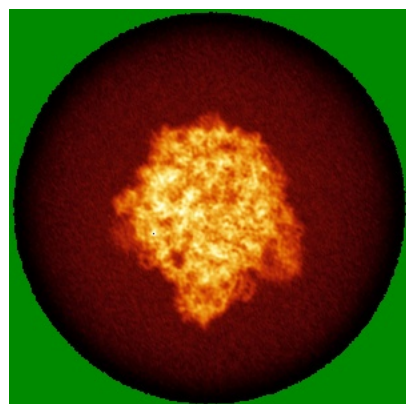


Z Index: 148

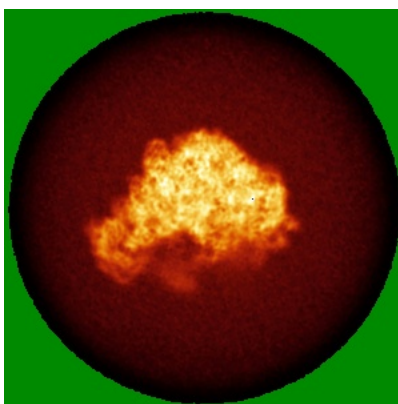
The images above show the largest variance slices of the map in three orthogonal directions.

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

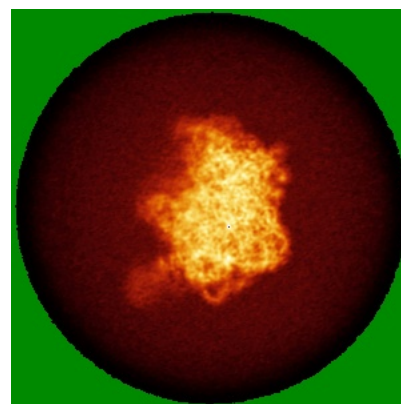
6.4.1 Primary map



X

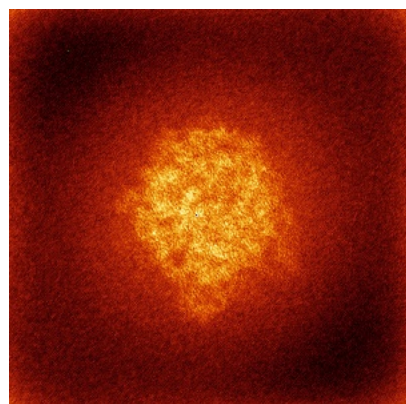


Y

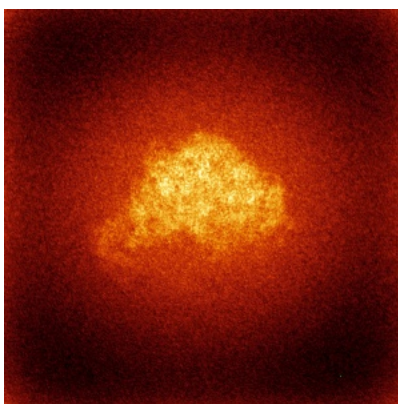


Z

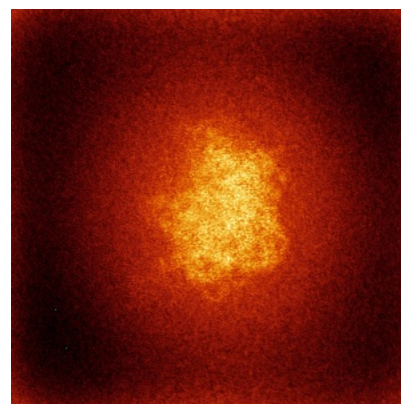
6.4.2 Raw map



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



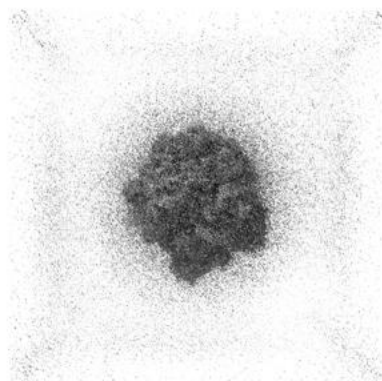
Y



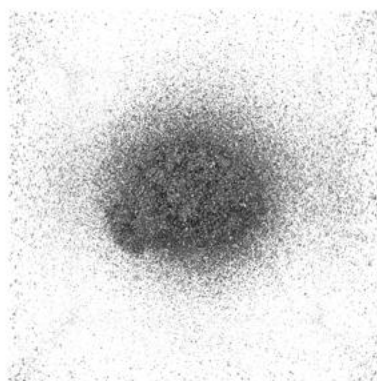
Z

The images above show the 3D surface view of the map at the recommended contour level 0.292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

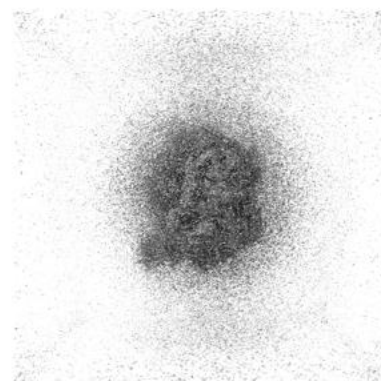
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

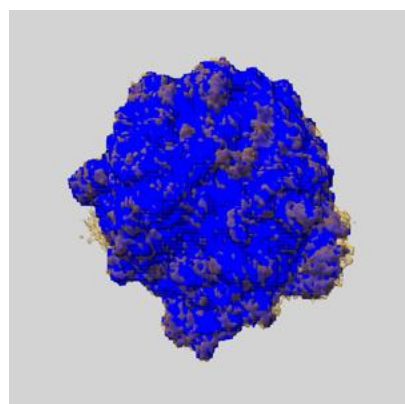
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

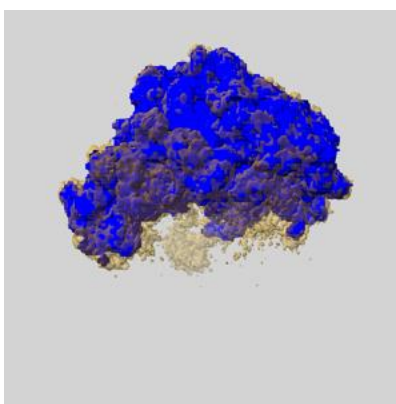
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

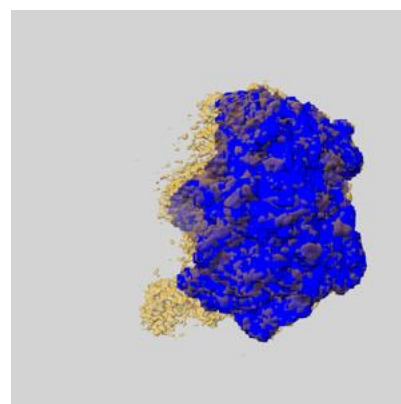
6.6.1 emd_51836_msk_1.map [i](#)



X



Y

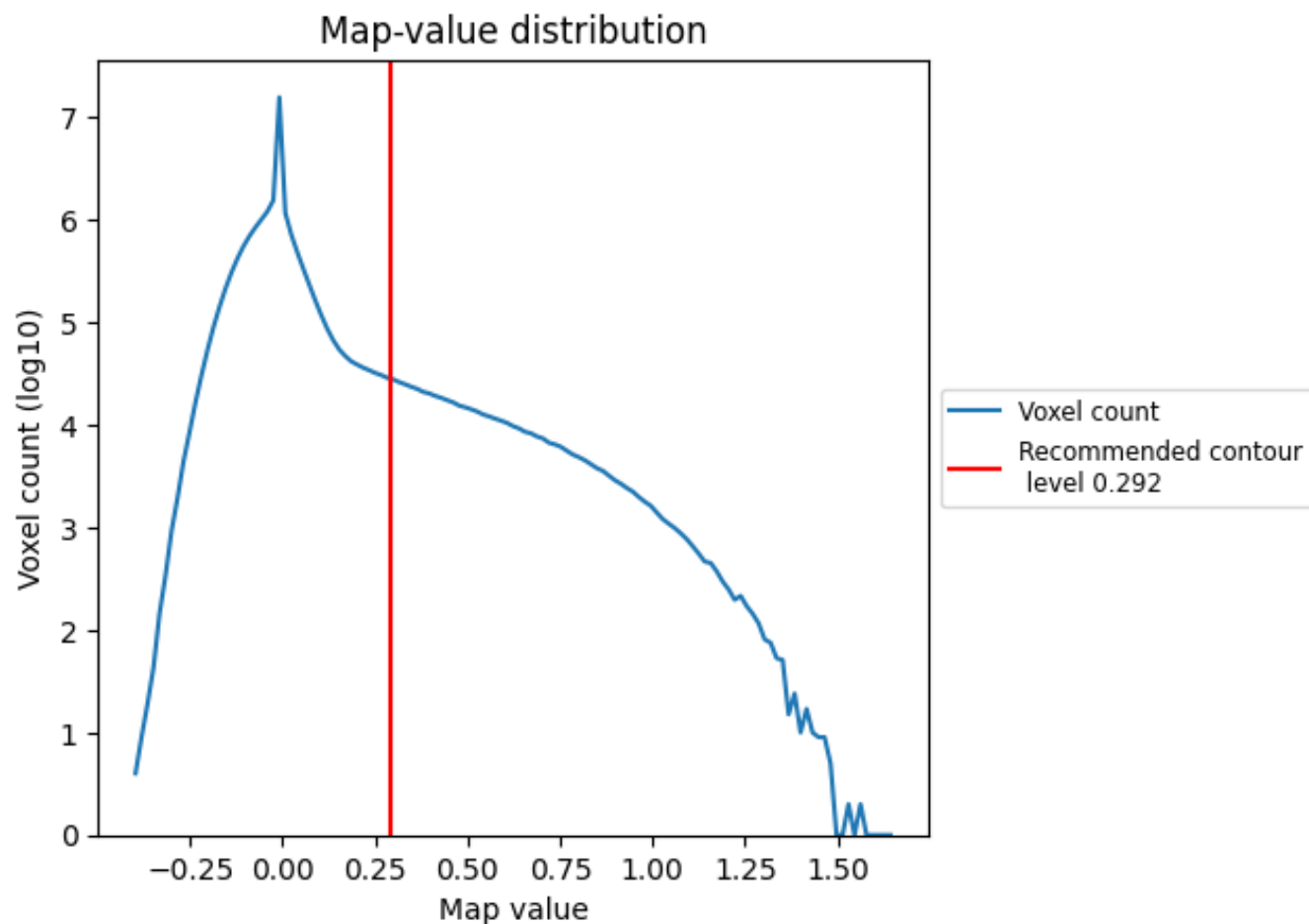


Z

7 Map analysis [i](#)

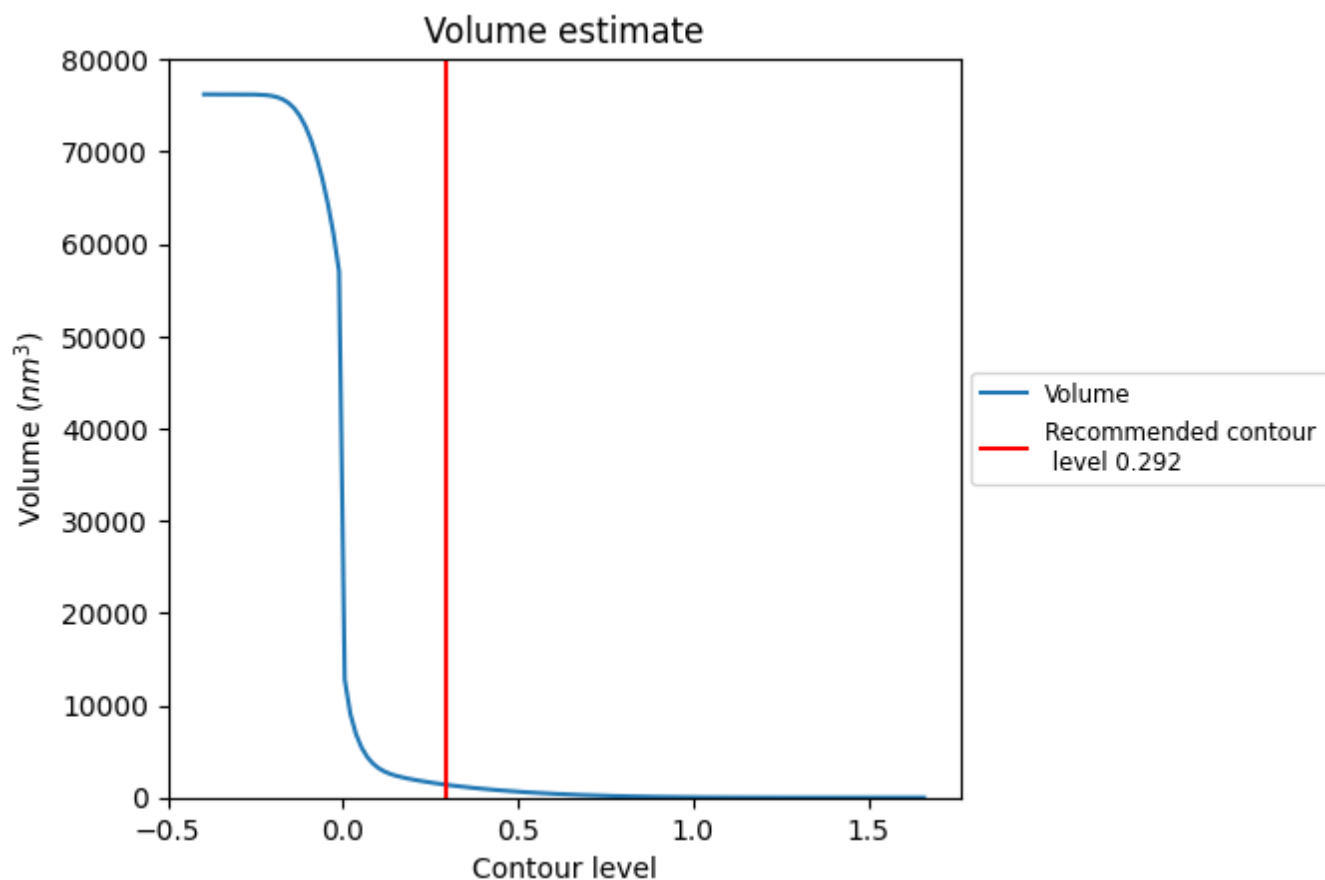
This section contains the results of statistical analysis of the map.

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.

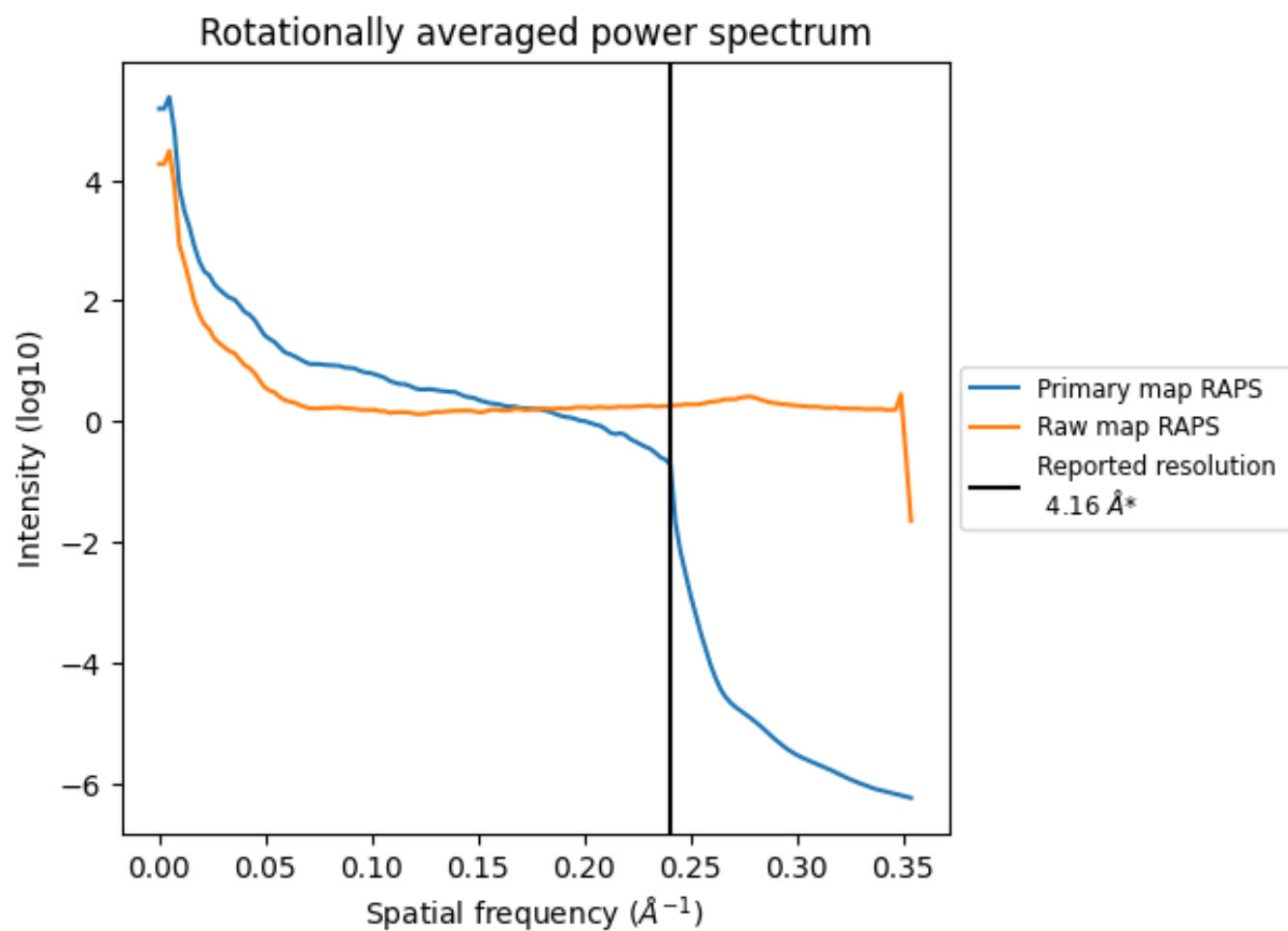
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1402 nm³; this corresponds to an approximate mass of 1267 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 ⓘ

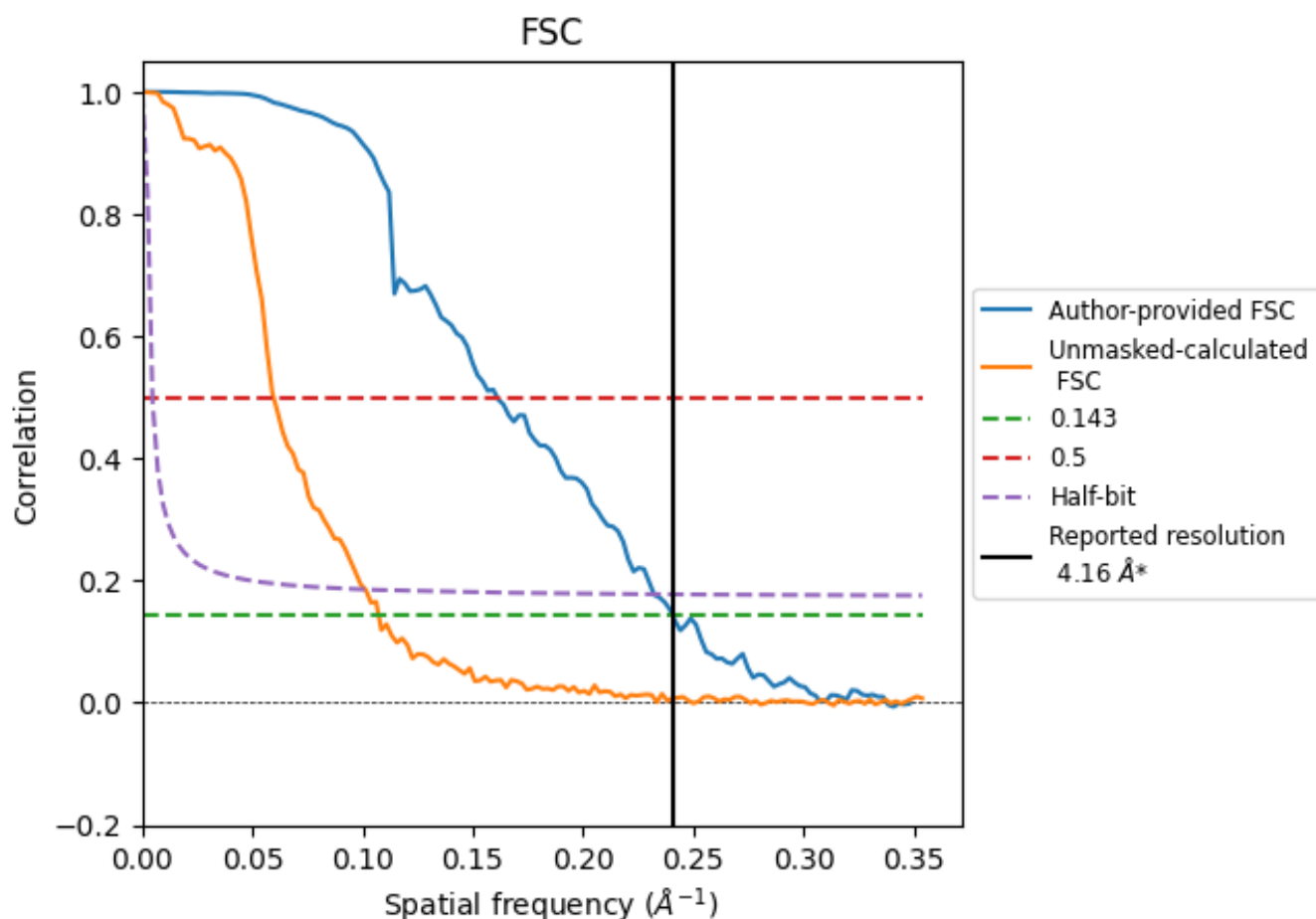


*Reported resolution corresponds to spatial frequency of 0.240 Å⁻¹

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 0.240 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

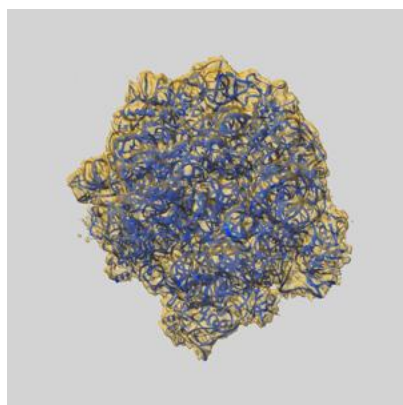
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.16	-	-
Author-provided FSC curve	4.16	6.21	4.31
Unmasked-calculated*	9.32	16.81	9.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.32 differs from the reported value 4.16 by more than 10 %

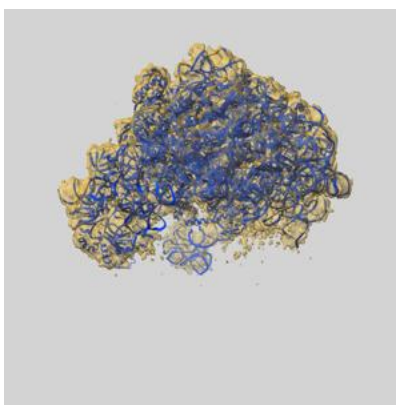
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51836 and PDB model 9H3S. Per-residue inclusion information can be found in section [3](#) on page [8](#).

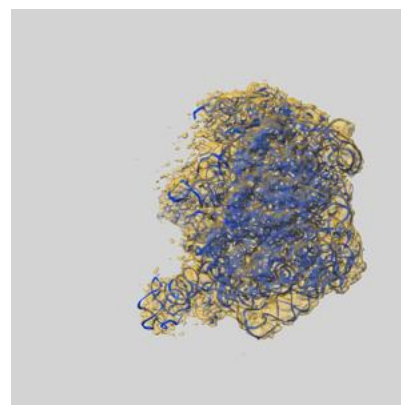
9.1 Map-model overlay [i](#)



X



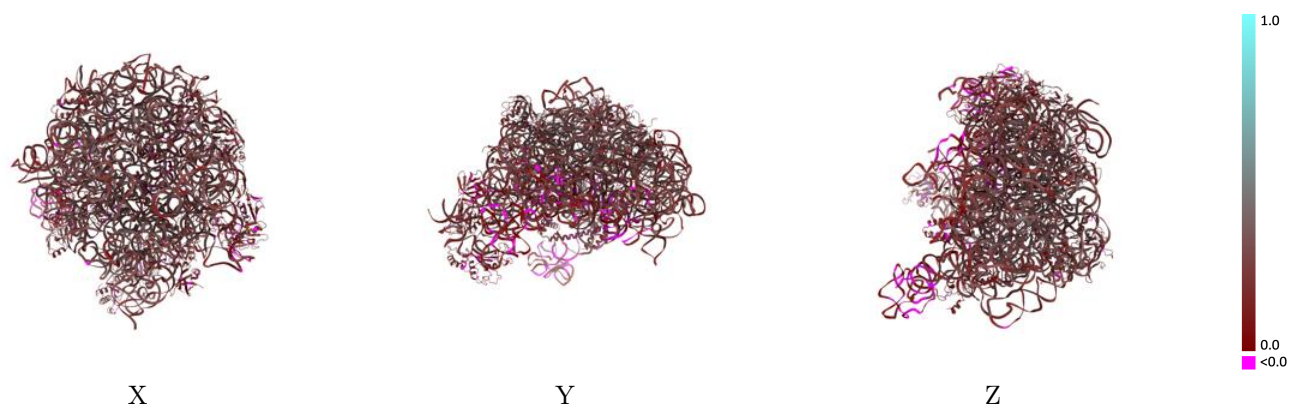
Y



Z

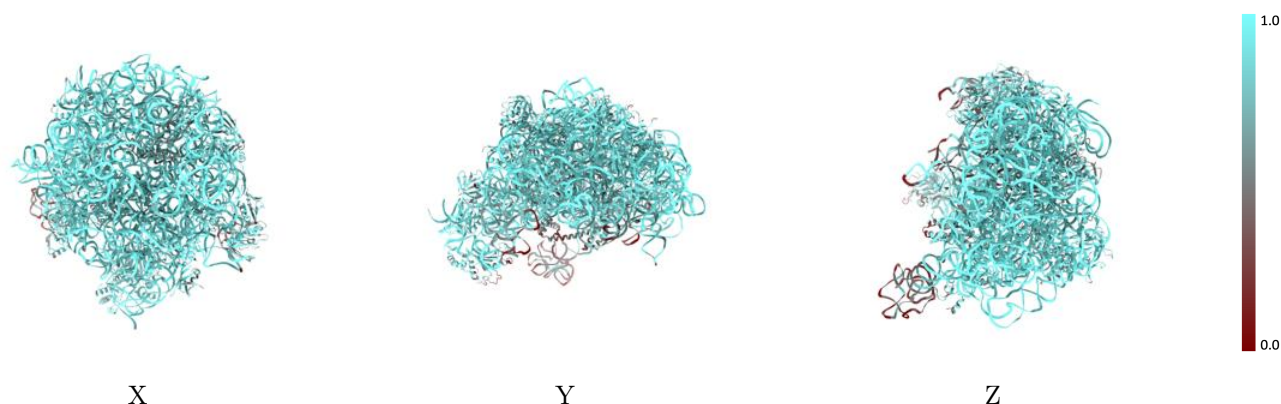
The images above show the 3D surface view of the map at the recommended contour level 0.292 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



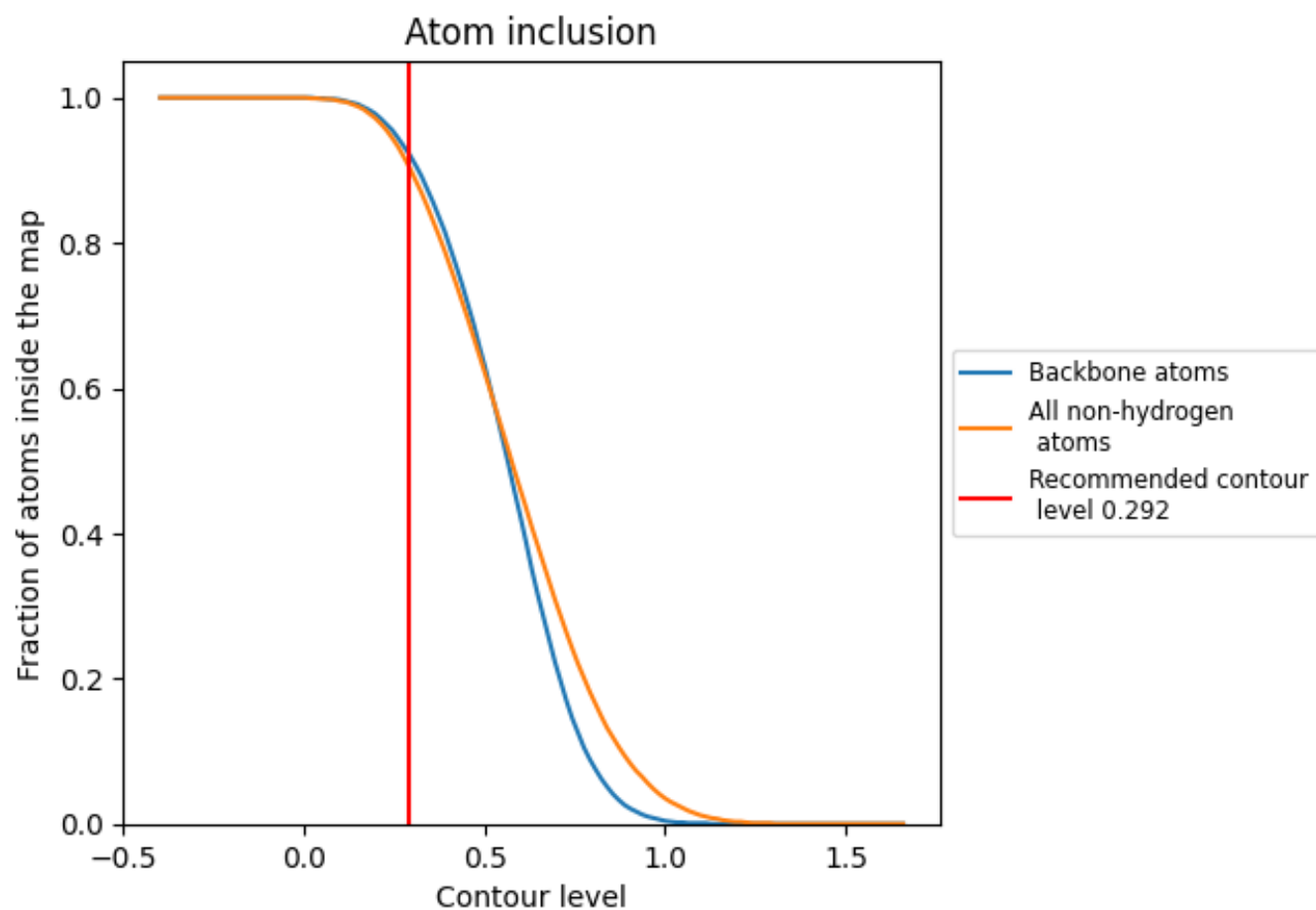
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.292).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.292) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.2400
0	 0.7430	 0.2360
2	 0.8900	 0.2660
4	 0.7060	 0.1910
A	 0.9290	 0.2480
B	 0.9790	 0.2240
C	 0.5650	 0.1310
D	 0.8560	 0.2520
E	 0.8380	 0.2270
F	 0.7390	 0.1400
G	 0.7460	 0.1750
H	 0.7020	 0.1440
J	 0.9080	 0.2790
K	 0.8340	 0.1840
L	 0.8410	 0.2310
N	 0.9140	 0.2520
O	 0.9290	 0.1860
P	 0.8200	 0.2310
Q	 0.9210	 0.2870
R	 0.8870	 0.2820
S	 0.7260	 0.2450
T	 0.8920	 0.2840
U	 0.9060	 0.2430
V	 0.8200	 0.1750
W	 0.8750	 0.2590
X	 0.9250	 0.2650
Y	 0.8550	 0.2370
Z	 0.9060	 0.2820

