



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:54 AM UTC

PDB ID : 9HA7 / pdb_00009ha7
EMDB ID : EMD-51979
Title : Pooled 50S subunit C-CP_(L22)- H61 precursor states supplemented with Api137
Authors : Lauer, S.; Nikolay, R.; Spahn, C.M.T.
Deposited on : 2024-11-01
Resolution : 4.37 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

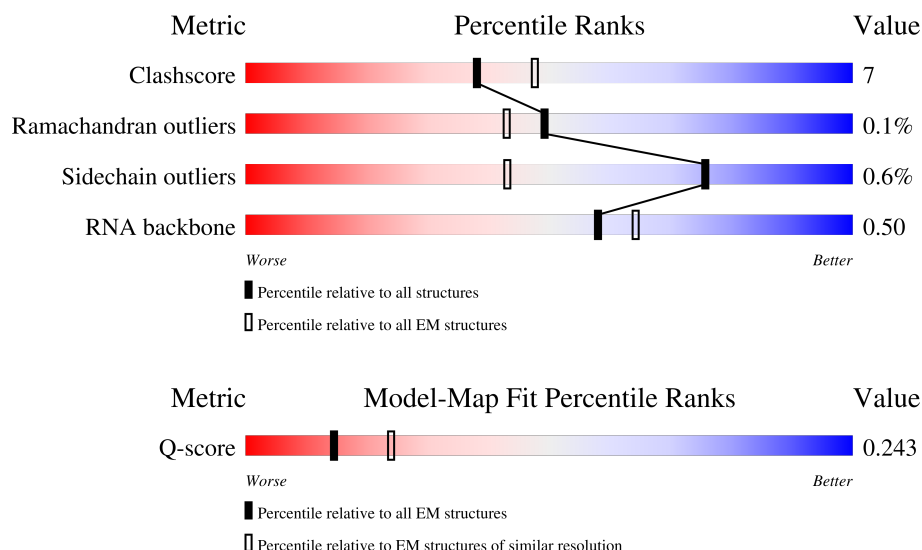
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.37 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.



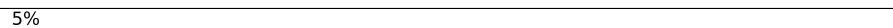
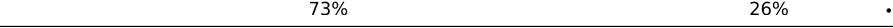
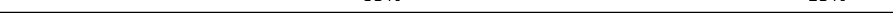
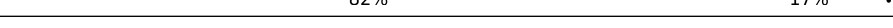
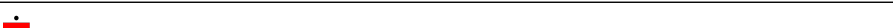
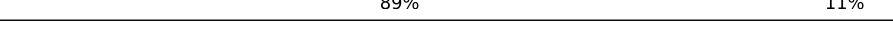
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3738 (3.87 - 4.87)

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	2	46	
2	B	120	
3	F	177	

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Mol	Chain	Length	Quality of chain
4	J	142	
5	L	143	
6	N	120	
7	O	116	
8	Q	117	
9	R	103	
10	T	93	
11	U	102	
12	V	94	
13	W	75	
14	Y	63	
15	Z	58	
16	A	2903	
17	D	209	
18	E	201	
19	y	17	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 59416 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 bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	38	Total	C	N	O	S	0	0
			309	185	77	46	1		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 3 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 4 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 6 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	120	Total	C	N	O	S	0	0
			957	592	196	164	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 8 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 9 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 12 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 13 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 16 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	1988	Total	C	N	O	P	0	0
			42736	19062	7924	13762	1988		

- Molecule 17 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	173	Total	C	N	O	S	0	0
			1284	805	231	244	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	176	Total	C	N	O	S	0	0
			1368	862	243	258	5		

- Molecule 19 is a protein called Apidaecins type 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	y	17	Total	C	N	O	0	0
			148	94	33	21		

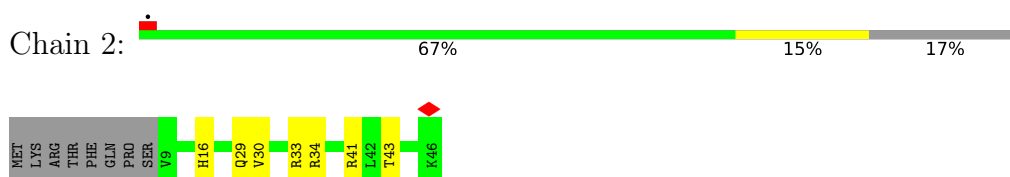
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	10	ARG	GLN	conflict	UNP P35581

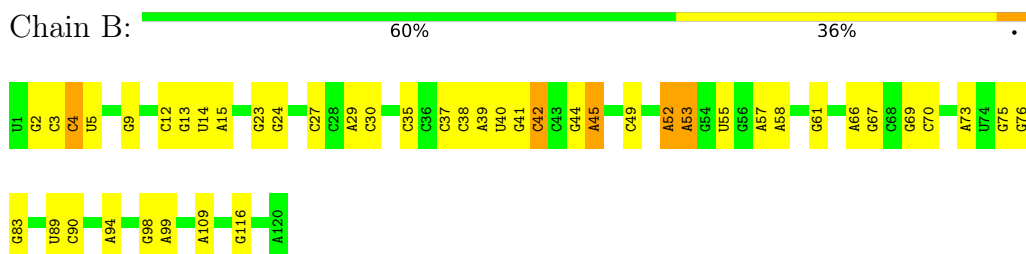
3 Residue-property plots

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.

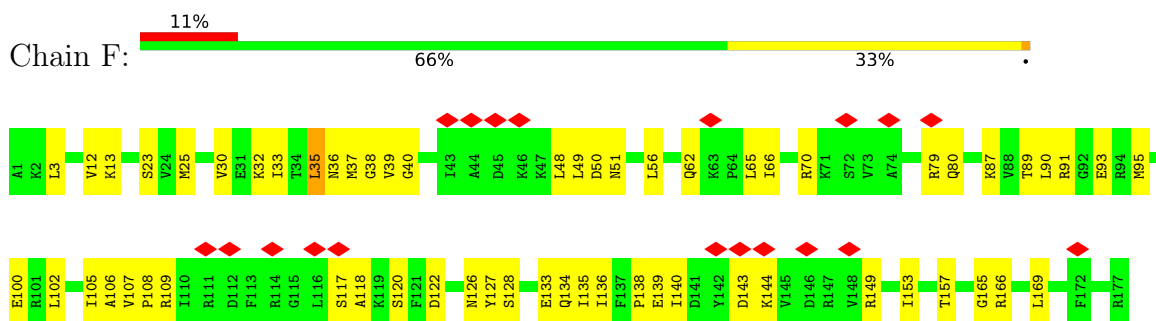
- Molecule 1: Large ribosomal subunit protein bL34



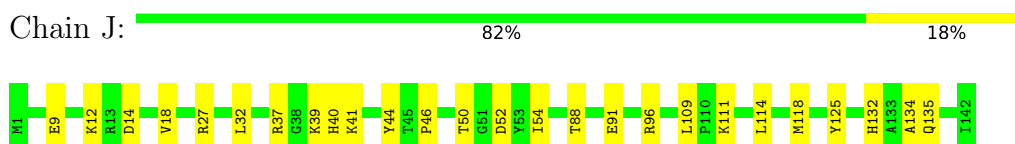
- Molecule 2: 5S ribosomal RNA



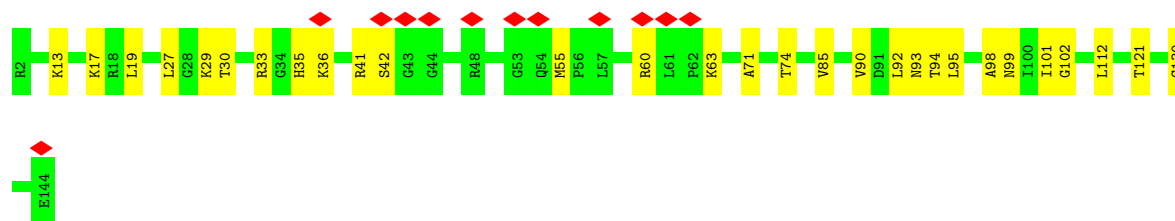
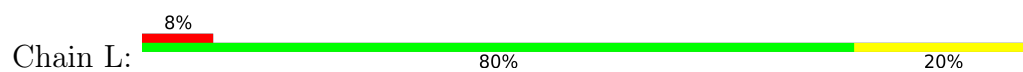
- Molecule 3: Large ribosomal subunit protein uL5



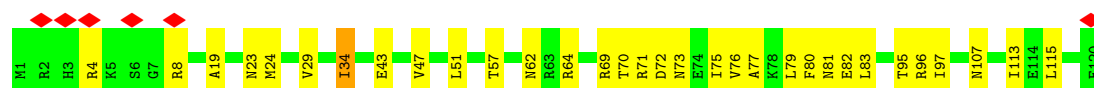
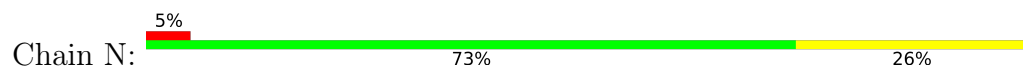
- Molecule 4: Large ribosomal subunit protein uL13



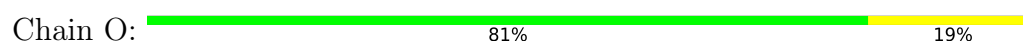
- Molecule 5: Large ribosomal subunit protein uL15



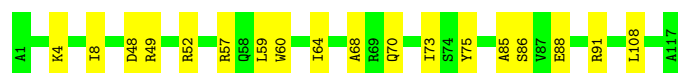
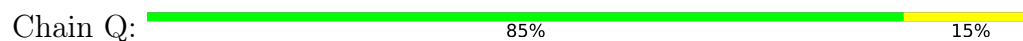
- Molecule 6: Large ribosomal subunit protein bL17



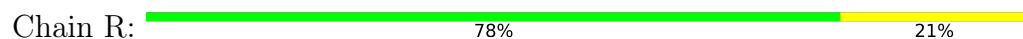
- Molecule 7: Large ribosomal subunit protein uL18



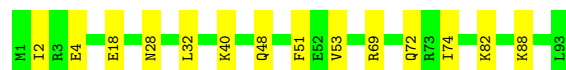
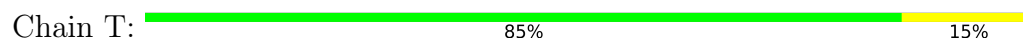
- Molecule 8: Large ribosomal subunit protein bL20



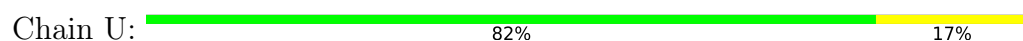
- Molecule 9: Large ribosomal subunit protein bL21



- Molecule 10: Large ribosomal subunit protein uL23

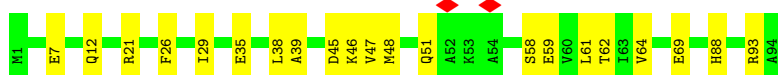
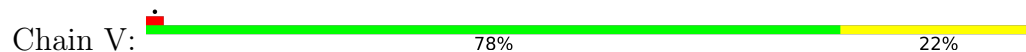


- Molecule 11: Large ribosomal subunit protein uL24

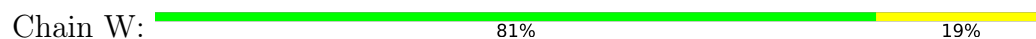




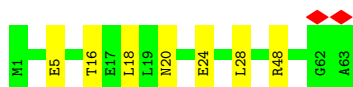
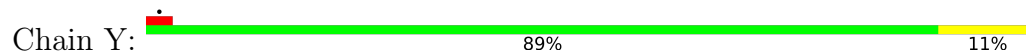
- Molecule 12: Large ribosomal subunit protein bL25



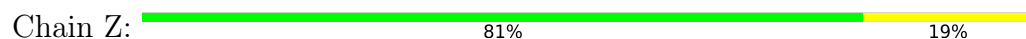
- Molecule 13: Large ribosomal subunit protein bL27



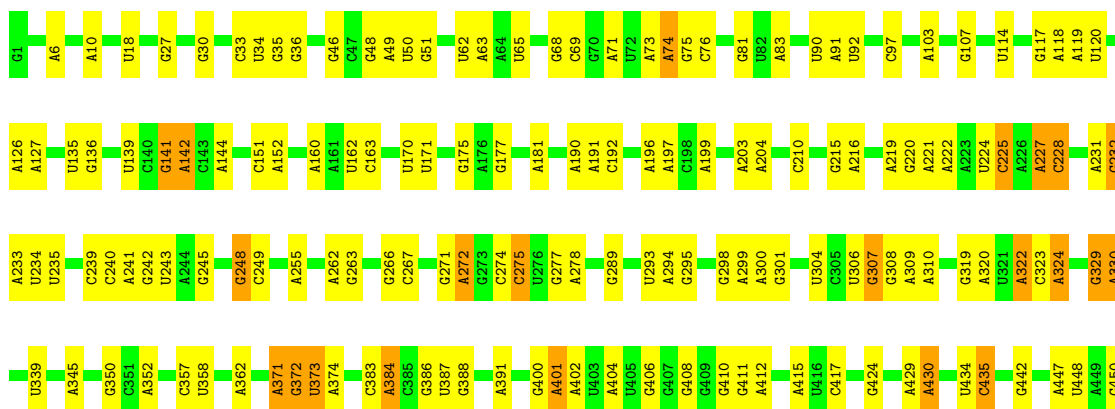
- Molecule 14: Large ribosomal subunit protein uL29



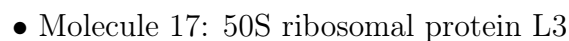
- Molecule 15: Large ribosomal subunit protein uL30



- Molecule 16: 23S ribosomal RNA



WORLDWIDE
PDB
PROTEIN DATA BANK





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28649	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 ($e^-/\text{\AA}^2$)	46.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.499	Depositor
Minimum map value	-0.761	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.255	Depositor
Map size ($\text{\AA}$)	399.6, 399.6, 399.6	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.998, 1.998, 1.998	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	2	0.06	0/310	0.16	0/405
2	B	0.06	0/2876	0.18	0/4483
3	F	0.11	0/1434	0.24	0/1926
4	J	0.09	0/1152	0.19	0/1551
5	L	0.09	0/1054	0.26	0/1403
6	N	0.10	0/970	0.23	0/1297
7	O	0.08	0/902	0.21	0/1209
8	Q	0.10	0/960	0.18	0/1278
9	R	0.12	0/829	0.27	0/1107
10	T	0.10	0/744	0.21	0/994
11	U	0.10	0/787	0.23	0/1051
12	V	0.11	0/766	0.22	0/1025
13	W	0.06	0/582	0.18	0/769
14	Y	0.11	0/510	0.24	0/677
15	Z	0.12	0/453	0.20	0/605
16	A	0.07	0/47875	0.20	0/74684
17	D	0.09	0/1296	0.20	0/1742
18	E	0.09	0/1382	0.17	0/1860
19	y	0.67	0/155	0.96	0/212
All	All	0.08	0/65037	0.20	0/98278

There are no bond length outliers.

There are no bond angle outliers.

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	2	309	0	344	5	0
2	B	2572	0	1302	34	0
3	F	1410	0	1447	49	0
4	J	1129	0	1162	22	0
5	L	1045	0	1117	25	0
6	N	957	0	998	22	0
7	O	892	0	923	17	0
8	Q	947	0	1022	17	0
9	R	816	0	839	16	0
10	T	738	0	807	11	0
11	U	779	0	834	14	0
12	V	753	0	780	17	0
13	W	575	0	592	9	0
14	Y	509	0	543	5	0
15	Z	449	0	491	11	0
16	A	42736	0	21494	422	0
17	D	1284	0	1339	25	0
18	E	1368	0	1421	33	0
19	y	148	0	151	45	0
All	All	59416	0	37606	678	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (678) 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)
16:A:1321:A:O2'	19:y:17:ARG:CZ	1.65	1.43
16:A:1321:A:C2'	19:y:15:HIS:O	1.80	1.27
16:A:1321:A:O2'	19:y:15:HIS:O	1.59	1.18
16:A:1321:A:O2'	19:y:17:ARG:NH2	1.80	1.13
16:A:507:A:H2'	19:y:10:ARG:HE	1.14	1.08
16:A:1321:A:C1'	19:y:15:HIS:O	2.08	1.00
16:A:239:C:HO2'	16:A:622:G:HO2'	1.07	0.95
16:A:62:U:H1'	19:y:3:ASN:OD1	1.65	0.94
16:A:1007:C:OP2	16:A:1008:A:O2'	1.90	0.88
16:A:1667:G:N2	16:A:1669:A:N6	2.24	0.86
4:J:134:ALA:O	16:A:2898:U:O2'	1.94	0.86
16:A:951:C:N4	16:A:952:G:O6	2.10	0.85
16:A:909:A:O2'	16:A:911:A:OP2	1.95	0.84
16:A:1321:A:O3'	19:y:17:ARG:NE	2.11	0.84
16:A:514:A:N3	16:A:581:C:O2'	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:2865:U:OP2	16:A:2866:U:O2'	1.95	0.84
16:A:542:C:N4	16:A:543:G:O6	2.11	0.83
16:A:1492:G:OP2	16:A:1493:C:O2'	1.96	0.83
16:A:507:A:H2'	19:y:10:ARG:NE	1.93	0.83
16:A:2642:G:N2	16:A:2772:C:O2	2.11	0.83
16:A:1321:A:H1'	19:y:15:HIS:O	1.69	0.83
16:A:1315:C:O2'	16:A:1392:A:N3	2.11	0.82
16:A:1378:A:O2'	16:A:1380:G:N7	2.12	0.82
16:A:83:A:O2'	16:A:103:A:N6	2.11	0.82
16:A:571:U:O2'	16:A:573:U:OP2	1.98	0.82
16:A:126:A:O2'	16:A:127:A:O4'	1.96	0.82
16:A:1287:A:N1	16:A:1648:U:O2'	2.11	0.82
16:A:508:A:O5'	19:y:13:PRO:HG3	1.81	0.81
16:A:1414:C:O2'	16:A:1415:U:O4'	1.98	0.81
18:E:46:GLN:O	18:E:88:ARG:NH2	2.13	0.81
2:B:39:A:O2'	2:B:40:U:O4'	1.99	0.81
3:F:109:ARG:NH2	3:F:136:ILE:O	2.14	0.81
16:A:675:A:N3	16:A:2443:C:O2'	2.13	0.81
16:A:177:G:OP2	16:A:177:G:N2	2.13	0.80
16:A:2049:G:N2	16:A:2619:C:O2	2.13	0.80
3:F:38:GLY:O	16:A:2306:C:N4	2.15	0.80
7:O:50:ALA:O	7:O:81:ARG:NH1	2.15	0.80
16:A:1667:G:H21	16:A:1669:A:N6	1.77	0.80
16:A:548:G:O2'	16:A:549:G:O4'	1.98	0.79
16:A:2743:U:OP2	16:A:2755:C:N4	2.15	0.79
2:B:14:U:OP2	2:B:70:C:O2'	2.01	0.79
16:A:1604:C:O2'	16:A:1610:A:N1	2.13	0.79
3:F:87:LYS:NZ	16:A:2314:A:OP1	2.16	0.79
2:B:5:U:OP1	2:B:61:G:O2'	2.00	0.79
16:A:1667:G:N2	16:A:1669:A:H62	1.80	0.78
12:V:58:SER:OG	12:V:59:GLU:OE1	2.01	0.78
16:A:2678:C:OP1	17:D:124:ARG:NH2	2.16	0.78
16:A:463:G:N2	16:A:466:A:OP2	2.16	0.78
3:F:70:ARG:NH1	16:A:2298:A:OP1	2.16	0.78
11:U:3:LYS:O	11:U:93:ARG:NH1	2.16	0.77
5:L:41:ARG:NH2	16:A:807:U:OP2	2.18	0.77
16:A:2050:C:O2	16:A:2618:G:N2	2.16	0.77
16:A:532:A:N1	16:A:2035:G:N2	2.33	0.77
16:A:966:G:O4'	16:A:2267:A:N6	2.18	0.77
16:A:2326:C:O2'	16:A:2327:A:OP1	2.02	0.77
16:A:234:U:O4	16:A:263:G:N2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:2645:G:OP2	16:A:2645:G:N2	2.17	0.76
16:A:2816:G:N3	16:A:2883:A:O2'	2.18	0.76
6:N:77:ALA:O	6:N:81:ASN:ND2	2.18	0.76
16:A:569:U:OP1	16:A:945:A:O2'	2.03	0.76
16:A:629:G:N3	16:A:639:U:O2'	2.19	0.76
16:A:2646:C:OP2	16:A:2732:G:O2'	2.02	0.76
3:F:133:GLU:OE1	3:F:133:GLU:N	2.19	0.76
16:A:1466:U:HO2'	16:A:1546:G:HO2'	1.00	0.76
16:A:227:A:O2'	16:A:228:C:O5'	2.02	0.76
3:F:120:SER:OG	3:F:128:SER:O	2.03	0.76
16:A:2788:C:O2'	16:A:2809:A:N3	2.17	0.75
16:A:117:G:OP2	16:A:119:A:O2'	2.03	0.75
16:A:805:G:N2	16:A:829:A:OP1	2.20	0.75
16:A:2009:A:O2'	16:A:2010:G:O4'	2.01	0.75
15:Z:18:LYS:NZ	16:A:850:U:OP1	2.19	0.74
16:A:1321:A:O2'	19:y:17:ARG:NH1	2.18	0.74
16:A:2258:C:O2'	16:A:2427:C:OP2	2.05	0.74
2:B:75:G:O2'	12:V:88:HIS:NE2	2.20	0.74
16:A:507:A:C4	19:y:10:ARG:CZ	2.70	0.74
16:A:1322:A:N1	16:A:1333:G:O2'	2.20	0.74
16:A:570:G:O2'	16:A:983:A:N1	2.20	0.74
17:D:16:THR:OG1	17:D:18:ASP:OD1	2.03	0.74
16:A:220:G:O2'	16:A:233:A:O2'	2.05	0.74
16:A:1321:A:N3	19:y:15:HIS:C	2.46	0.73
1:2:16:HIS:NE2	16:A:464:U:O2	2.21	0.72
16:A:192:C:O2'	16:A:802:A:N3	2.20	0.72
16:A:1321:A:H2'	19:y:15:HIS:O	1.88	0.72
16:A:1024:G:OP2	16:A:1025:G:O2'	2.03	0.72
16:A:1359:A:OP2	16:A:1371:G:N2	2.21	0.72
16:A:322:A:OP1	18:E:162:ARG:NE	2.21	0.72
16:A:239:C:O2'	16:A:622:G:O2'	1.96	0.71
16:A:1588:G:O2'	16:A:1589:U:O4'	2.05	0.71
6:N:95:THR:HB	6:N:113:ILE:HD11	1.72	0.71
16:A:18:U:O2'	16:A:554:U:OP1	2.07	0.71
5:L:55:MET:O	5:L:60:ARG:NH1	2.23	0.70
4:J:88:THR:OG1	4:J:91:GLU:OE1	2.09	0.70
16:A:931:U:O2	16:A:1167:C:O2'	2.09	0.70
16:A:1272:A:N6	16:A:1619:G:OP2	2.24	0.70
16:A:48:G:N2	16:A:177:G:OP1	2.22	0.70
18:E:122:GLU:N	18:E:122:GLU:OE1	2.25	0.70
9:R:80:ARG:NH1	16:A:572:A:OP2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:117:SER:O	3:F:127:TYR:OH	2.10	0.69
4:J:46:PRO:HD3	8:Q:59:LEU:HD11	1.73	0.69
14:Y:48:ARG:NH1	16:A:76:C:OP1	2.25	0.69
12:V:48:MET:SD	12:V:51:GLN:NE2	2.64	0.69
16:A:550:C:N4	16:A:551:G:O6	2.25	0.69
10:T:72:GLN:HB3	19:y:12:ARG:HH21	1.57	0.69
16:A:2043:C:OP1	16:A:2777:G:O2'	2.07	0.69
5:L:95:LEU:HD23	5:L:101:ILE:HD13	1.75	0.69
15:Z:4:ILE:HD11	15:Z:56:VAL:CG2	2.22	0.69
16:A:464:U:O4	16:A:684:G:O2'	2.11	0.69
8:Q:4:LYS:NZ	16:A:30:G:OP2	2.27	0.68
16:A:372:G:O2'	16:A:373:U:O5'	2.12	0.68
16:A:1026:G:OP2	16:A:1134:A:O2'	2.10	0.68
16:A:961:C:O2	16:A:2031:A:N6	2.26	0.68
16:A:1319:C:O2'	16:A:1320:C:OP1	2.12	0.68
16:A:1125:G:OP2	16:A:1126:A:O2'	2.08	0.68
1:2:29:GLN:NE2	16:A:210:C:OP1	2.26	0.68
12:V:64:VAL:HG22	12:V:69:GLU:OE1	1.93	0.68
12:V:45:ASP:OD1	12:V:46:LYS:N	2.28	0.67
7:O:60:GLU:OE1	7:O:60:GLU:N	2.26	0.67
16:A:612:G:N2	16:A:614:A:O2'	2.27	0.67
16:A:1209:U:O2'	16:A:1237:A:N1	2.25	0.67
16:A:475:C:O2	16:A:479:A:N6	2.27	0.67
16:A:224:U:OP2	16:A:408:G:N2	2.27	0.67
16:A:1341:G:OP1	16:A:1602:U:O2'	2.10	0.67
16:A:1638:C:OP1	16:A:2710:C:O2'	2.13	0.67
3:F:89:THR:OG1	3:F:91:ARG:NH2	2.27	0.67
10:T:48:GLN:NE2	10:T:53:VAL:O	2.27	0.67
10:T:40:LYS:NZ	16:A:1343:G:OP1	2.28	0.67
15:Z:30:ARG:NH2	16:A:1184:U:OP2	2.28	0.67
16:A:62:U:H1'	19:y:3:ASN:CG	2.20	0.67
16:A:248:G:O2'	16:A:2432:A:OP1	2.09	0.66
2:B:9:G:OP2	7:O:15:ARG:NH2	2.28	0.66
16:A:1651:G:O5'	16:A:2006:C:N4	2.29	0.66
16:A:659:G:O3'	18:E:94:GLN:NE2	2.27	0.66
16:A:1415:U:O2	16:A:1587:G:N2	2.28	0.66
2:B:42:C:H5	3:F:65:LEU:HD13	1.61	0.66
16:A:627:A:O4'	16:A:637:A:N6	2.29	0.66
16:A:453:A:N3	16:A:457:A:O2'	2.28	0.66
5:L:93:ASN:O	5:L:94:THR:OG1	2.09	0.66
16:A:227:A:HO2'	16:A:228:C:P	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:C:O2	7:O:100:HIS:NE2	2.28	0.65
7:O:2:ASP:OD1	7:O:3:LYS:N	2.29	0.65
16:A:605:G:OP1	18:E:99:LYS:NZ	2.29	0.65
9:R:23:GLU:OE2	9:R:91:GLN:NE2	2.29	0.65
16:A:631:A:N3	16:A:2415:G:O2'	2.27	0.65
3:F:37:MET:HE3	3:F:56:LEU:HD13	1.78	0.65
16:A:191:A:O2'	16:A:678:C:O2	2.13	0.65
16:A:62:U:C1'	19:y:3:ASN:CG	2.70	0.65
16:A:2751:G:N2	16:A:2751:G:OP1	2.26	0.65
16:A:1390:U:O2	16:A:1395:A:N7	2.30	0.65
16:A:1413:A:O2'	16:A:1414:C:O4'	2.14	0.65
5:L:13:LYS:NZ	16:A:1245:G:OP1	2.29	0.65
3:F:23:SER:OG	3:F:25:MET:SD	2.54	0.64
8:Q:52:ARG:NH2	16:A:994:C:OP1	2.30	0.64
16:A:62:U:O4'	19:y:3:ASN:CG	2.40	0.64
3:F:50:ASP:OD1	3:F:51:ASN:N	2.30	0.64
8:Q:88:GLU:N	8:Q:88:GLU:OE1	2.31	0.64
16:A:1650:A:O2'	16:A:1652:A:OP1	2.14	0.64
16:A:2822:G:OP1	17:D:164:GLN:NE2	2.30	0.64
6:N:64:ARG:NH1	16:A:2851:A:O2'	2.31	0.64
6:N:8:ARG:N	6:N:43:GLU:OE2	2.29	0.64
16:A:1024:G:O2'	16:A:1144:A:O2'	2.16	0.64
4:J:91:GLU:OE1	4:J:91:GLU:N	2.31	0.63
6:N:24:MET:SD	16:A:1277:G:O2'	2.56	0.63
16:A:2291:U:O2'	16:A:2374:C:O2	2.16	0.63
16:A:2659:G:N2	16:A:2662:A:OP2	2.31	0.63
16:A:91:A:O4'	19:y:7:TYR:CZ	2.52	0.63
4:J:109:LEU:HD13	4:J:118:MET:HG3	1.81	0.63
11:U:81:ARG:NH2	16:A:301:G:OP2	2.32	0.63
15:Z:4:ILE:HD11	15:Z:56:VAL:HG23	1.81	0.63
16:A:62:U:C1'	19:y:3:ASN:OD1	2.45	0.63
16:A:2633:G:N2	16:A:2786:U:O2	2.32	0.62
16:A:1422:G:O2'	16:A:1492:G:N2	2.32	0.62
16:A:569:U:O2'	16:A:971:G:N2	2.31	0.62
11:U:9:GLU:OE1	11:U:9:GLU:N	2.33	0.62
16:A:1270:C:O2	16:A:2010:G:N1	2.32	0.62
18:E:111:GLU:OE2	18:E:115:GLN:NE2	2.32	0.62
5:L:27:LEU:HD23	5:L:27:LEU:H	1.65	0.62
16:A:1651:G:N2	16:A:2006:C:OP2	2.31	0.62
16:A:448:U:O4'	18:E:79:ARG:NE	2.31	0.61
2:B:77:U:OP1	12:V:21:ARG:NH1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:844:A:N1	16:A:845:A:N6	2.48	0.61
3:F:33:ILE:CD1	3:F:95:MET:HE2	2.31	0.61
16:A:97:C:O2	16:A:103:A:O2'	2.17	0.61
17:D:26:VAL:CG1	17:D:186:LEU:HD12	2.30	0.61
4:J:39:LYS:NZ	16:A:1007:C:OP1	2.31	0.61
1:2:34:ARG:NH2	1:2:41:ARG:O	2.34	0.61
16:A:612:G:N2	16:A:614:A:HO2'	1.98	0.61
16:A:2446:G:N2	16:A:2449:U:O2	2.30	0.60
11:U:80:ASP:OD1	11:U:81:ARG:N	2.33	0.60
16:A:2692:G:N3	16:A:2847:U:O2'	2.34	0.60
17:D:33:ARG:HG3	17:D:73:VAL:HG13	1.83	0.60
3:F:35:LEU:HG	3:F:56:LEU:HD11	1.82	0.60
18:E:117:ARG:NH2	18:E:183:PHE:O	2.35	0.60
16:A:372:G:HO2'	16:A:373:U:P	2.24	0.60
2:B:27:C:OP1	7:O:34:HIS:NE2	2.34	0.60
6:N:107:ASN:ND2	16:A:1652:A:OP2	2.34	0.60
9:R:58:VAL:N	9:R:102:SER:OG	2.35	0.60
16:A:68:G:N2	16:A:74:A:O4'	2.35	0.60
16:A:1534:U:O2'	16:A:1535:A:OP1	2.20	0.60
16:A:442:G:N2	18:E:43:THR:O	2.33	0.60
17:D:3:GLY:C	17:D:4:LEU:HD12	2.27	0.60
17:D:25:THR:HG21	17:D:193:VAL:HG22	1.83	0.60
16:A:644:A:O2'	16:A:645:C:O5'	2.20	0.59
3:F:133:GLU:HG2	3:F:135:ILE:HG22	1.84	0.59
5:L:63:LYS:NZ	16:A:249:C:O2'	2.24	0.59
8:Q:57:ARG:NH2	16:A:998:C:OP2	2.36	0.59
16:A:2399:G:O6	16:A:2418:A:N6	2.35	0.59
16:A:152:A:N6	16:A:175:G:O6	2.36	0.59
16:A:2341:G:N2	16:A:2374:C:O3'	2.35	0.59
10:T:82:LYS:NZ	16:A:1339:G:OP1	2.36	0.59
3:F:93:GLU:OE1	3:F:93:GLU:N	2.35	0.59
4:J:135:GLN:N	4:J:135:GLN:OE1	2.36	0.59
16:A:1271:G:N2	16:A:1615:C:H42	2.01	0.58
18:E:46:GLN:N	18:E:46:GLN:OE1	2.36	0.58
5:L:33:ARG:NH2	16:A:587:C:O2	2.36	0.58
7:O:116:GLN:N	7:O:116:GLN:OE1	2.36	0.58
5:L:99:ASN:ND2	16:A:621:A:OP2	2.37	0.58
16:A:1651:G:H22	16:A:2006:C:P	2.26	0.58
6:N:96:ARG:O	6:N:113:ILE:HD12	2.04	0.58
3:F:134:GLN:N	3:F:134:GLN:OE1	2.36	0.58
16:A:2375:G:O2'	16:A:2377:A:N6	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:88:GLU:N	17:D:88:GLU:OE1	2.37	0.58
16:A:1451:C:O2'	16:A:1452:G:O4'	2.17	0.58
16:A:2017:U:O2'	16:A:2019:A:OP2	2.10	0.58
10:T:28:ASN:ND2	10:T:88:LYS:O	2.37	0.58
16:A:548:G:O2'	16:A:549:G:O5'	2.21	0.58
16:A:1321:A:N3	19:y:16:PRO:N	2.44	0.58
16:A:603:A:N6	16:A:655:A:O4'	2.37	0.57
16:A:1589:U:O4	16:A:1590:A:N6	2.37	0.57
16:A:2050:C:N3	16:A:2618:G:N1	2.45	0.57
6:N:82:GLU:HG2	6:N:83:LEU:HD22	1.86	0.57
16:A:224:U:O4	16:A:232:G:N2	2.36	0.57
16:A:324:A:N6	16:A:339:U:O4'	2.37	0.57
13:W:10:ARG:NH2	16:A:2279:G:N7	2.52	0.57
16:A:2007:U:O2'	16:A:2009:A:OP2	2.17	0.57
16:A:526:A:O2'	16:A:2043:C:O2	2.22	0.57
18:E:176:ASP:OD1	18:E:179:SER:OG	2.15	0.57
16:A:2049:G:N1	16:A:2619:C:N3	2.44	0.56
5:L:19:LEU:HD23	5:L:27:LEU:HD12	1.87	0.56
16:A:371:A:N6	16:A:402:A:OP2	2.38	0.56
2:B:80:U:O2'	16:A:918:A:N3	2.36	0.56
16:A:2723:C:OP1	17:D:114:LYS:NZ	2.28	0.56
19:y:4:ARG:N	19:y:5:PRO:HD2	2.20	0.56
2:B:75:G:HO2'	12:V:88:HIS:CD2	2.22	0.56
5:L:93:ASN:OD1	5:L:94:THR:N	2.38	0.56
16:A:1271:G:H22	16:A:1615:C:N4	2.04	0.56
16:A:987:C:O2'	16:A:1000:A:N3	2.34	0.56
16:A:2375:G:N2	16:A:2378:A:OP2	2.38	0.56
18:E:171:ASP:OD1	18:E:172:ALA:N	2.39	0.56
1:2:43:THR:OG1	16:A:126:A:N6	2.39	0.56
16:A:864:G:O2'	16:A:914:G:O6	2.23	0.56
16:A:63:A:C5	19:y:6:VAL:HG13	2.41	0.55
3:F:30:VAL:HG22	3:F:157:THR:HG22	1.88	0.55
2:B:38:C:O4'	7:O:100:HIS:NE2	2.39	0.55
16:A:1515:A:O2'	16:A:1556:C:O2	2.23	0.55
17:D:200:ASP:C	17:D:201:LEU:HD12	2.30	0.55
2:B:42:C:C5	3:F:65:LEU:HD13	2.41	0.55
7:O:31:THR:OG1	7:O:33:ARG:O	2.22	0.55
16:A:92:U:H1'	19:y:7:TYR:HE1	1.71	0.55
18:E:144:GLU:N	18:E:144:GLU:OE1	2.40	0.55
16:A:673:C:P	16:A:801:G:H21	2.29	0.55
16:A:2345:G:O2'	16:A:2381:A:N3	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:1:MET:SD	18:E:1:MET:N	2.79	0.55
3:F:62:GLN:OE1	3:F:62:GLN:N	2.40	0.55
16:A:644:A:O2'	16:A:645:C:O4'	2.23	0.54
16:A:2705:A:O2'	16:A:2852:G:OP1	2.25	0.54
3:F:134:GLN:NE2	3:F:149:ARG:O	2.40	0.54
8:Q:85:ALA:O	8:Q:86:SER:OG	2.25	0.54
2:B:76:G:OP2	12:V:12:GLN:NE2	2.39	0.54
2:B:55:U:O2'	3:F:25:MET:HE1	2.06	0.54
16:A:271:G:O2'	16:A:272:A:OP2	2.22	0.54
16:A:507:A:C5	19:y:10:ARG:CZ	2.91	0.54
16:A:1321:A:C3'	19:y:17:ARG:NE	2.70	0.54
4:J:37:ARG:NH1	4:J:44:TYR:OH	2.41	0.53
16:A:63:A:C6	19:y:6:VAL:HG13	2.43	0.53
16:A:1432:G:H2'	16:A:1433:A:C8	2.43	0.53
4:J:96:ARG:NH1	16:A:2640:G:OP1	2.42	0.53
16:A:549:G:HO2'	16:A:550:C:P	2.31	0.53
16:A:1414:C:HO2'	16:A:1415:U:C4'	2.20	0.53
3:F:32:LYS:C	3:F:33:ILE:HD12	2.33	0.53
8:Q:48:ASP:OD1	8:Q:49:ARG:N	2.42	0.53
16:A:549:G:O2'	16:A:550:C:OP1	2.26	0.53
18:E:189:THR:OG1	18:E:191:ASP:OD1	2.18	0.53
2:B:15:A:OP2	2:B:69:G:N2	2.37	0.53
5:L:30:THR:HG22	16:A:810:U:O4	2.08	0.53
16:A:69:C:O2	16:A:73:A:O2'	2.18	0.53
16:A:659:G:O2'	18:E:94:GLN:NE2	2.42	0.53
16:A:1319:C:HO2'	16:A:1320:C:P	2.30	0.53
8:Q:48:ASP:OD2	16:A:534:U:O2'	2.17	0.53
13:W:14:ALA:O	13:W:16:ARG:NH1	2.39	0.53
16:A:289:G:O6	16:A:352:A:N6	2.42	0.53
13:W:7:ARG:O	13:W:10:ARG:NH1	2.42	0.53
3:F:143:ASP:OD1	3:F:144:LYS:N	2.42	0.52
16:A:308:G:O2'	16:A:329:G:N2	2.43	0.52
16:A:1596:A:H2'	16:A:1597:A:H5'	1.92	0.52
16:A:2857:G:N2	16:A:2860:A:OP2	2.36	0.52
14:Y:16:THR:O	14:Y:20:ASN:ND2	2.41	0.52
16:A:2821:A:OP2	17:D:115:GLY:N	2.40	0.52
16:A:532:A:OP1	16:A:561:G:N2	2.33	0.52
9:R:15:SER:OG	9:R:18:GLN:NE2	2.43	0.52
16:A:1352:U:O2'	16:A:1570:A:N3	2.39	0.52
2:B:52:A:O2'	2:B:53:A:O5'	2.27	0.52
4:J:114:LEU:HD12	4:J:114:LEU:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:41:LYS:NZ	4:J:52:ASP:OD1	2.25	0.51
11:U:71:ILE:HD12	11:U:82:VAL:HG21	1.91	0.51
16:A:1244:A:N6	16:A:1245:G:O6	2.44	0.51
16:A:1656:C:N4	16:A:1657:U:O4	2.43	0.51
3:F:35:LEU:HD12	3:F:36:ASN:N	2.26	0.51
10:T:32:LEU:HD12	10:T:32:LEU:O	2.10	0.51
16:A:1021:A:N6	16:A:1142:A:H61	2.08	0.51
16:A:1271:G:H22	16:A:1615:C:H42	1.56	0.51
16:A:1358:G:O2'	16:A:1359:A:O5'	2.25	0.51
19:y:17:ARG:O	19:y:18:LEU:HB3	2.10	0.51
9:R:49:ILE:HG21	9:R:54:VAL:HG12	1.92	0.51
16:A:373:U:O4	16:A:401:A:N7	2.44	0.51
16:A:584:C:N4	16:A:585:G:O6	2.43	0.51
2:B:75:G:HO2'	12:V:88:HIS:CE1	2.27	0.51
9:R:38:VAL:O	9:R:54:VAL:HG13	2.11	0.51
16:A:274:C:H2'	16:A:275:C:C1'	2.39	0.51
16:A:673:C:OP1	16:A:801:G:N2	2.39	0.51
16:A:1402:U:O2'	16:A:1470:A:N1	2.29	0.51
16:A:2299:U:O4	16:A:2318:G:N2	2.44	0.51
16:A:2317:A:H2'	16:A:2318:G:O4'	2.11	0.51
4:J:40:HIS:O	8:Q:70:GLN:NE2	2.43	0.51
6:N:4:ARG:NH2	16:A:2874:C:OP1	2.43	0.51
16:A:1447:C:O2'	16:A:1544:A:N3	2.40	0.51
4:J:27:ARG:NH1	16:A:1012:U:O2	2.44	0.51
9:R:100:GLY:O	9:R:101:ILE:HD13	2.11	0.51
12:V:29:ILE:HD12	12:V:38:LEU:O	2.11	0.51
7:O:53:THR:HG23	7:O:74:VAL:CG2	2.40	0.51
12:V:26:PHE:HZ	12:V:47:VAL:HG11	1.76	0.51
16:A:1303:G:O6	16:A:1304:A:N6	2.44	0.51
18:E:140:ASP:OD1	18:E:141:MET:N	2.43	0.51
16:A:971:G:OP1	16:A:974:G:O2'	2.21	0.51
16:A:1329:U:OP2	16:A:1330:C:N4	2.42	0.51
2:B:52:A:O2'	2:B:53:A:P	2.68	0.50
9:R:58:VAL:H	9:R:102:SER:HG	1.57	0.50
16:A:68:G:N2	16:A:74:A:O5'	2.44	0.50
3:F:120:SER:OG	16:A:2303:G:O2'	2.29	0.50
6:N:73:ASN:OD1	16:A:1454:C:N4	2.43	0.50
6:N:69:ARG:O	6:N:70:THR:OG1	2.19	0.50
6:N:71:ARG:NH1	16:A:2707:U:O2	2.44	0.50
16:A:1016:G:O6	16:A:1147:A:N6	2.44	0.50
16:A:1321:A:N7	19:y:16:PRO:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:299:A:N3	16:A:319:G:O2'	2.25	0.50
16:A:1020:A:H4'	16:A:1021:A:O5'	2.12	0.50
10:T:51:PHE:O	10:T:53:VAL:HG13	2.11	0.50
4:J:135:GLN:NE2	16:A:6:A:N3	2.60	0.50
16:A:1205:A:O2'	16:A:1206:G:OP1	2.29	0.50
16:A:1413:A:H2'	16:A:1414:C:C6	2.47	0.50
16:A:1992:G:N1	16:A:1995:U:O4	2.45	0.50
16:A:591:U:O4	16:A:592:A:N6	2.43	0.50
16:A:640:C:N4	16:A:641:U:O4	2.45	0.50
18:E:25:GLU:OE1	18:E:25:GLU:N	2.40	0.50
6:N:57:THR:HG23	6:N:62:ASN:ND2	2.27	0.49
12:V:35:GLU:N	12:V:35:GLU:OE1	2.45	0.49
11:U:33:VAL:HG13	11:U:66:VAL:HG22	1.93	0.49
15:Z:57:GLU:N	15:Z:57:GLU:OE1	2.44	0.49
16:A:507:A:C5	19:y:10:ARG:NH2	2.80	0.49
18:E:148:ILE:HB	18:E:169:VAL:HG22	1.93	0.49
16:A:245:G:O2'	16:A:384:A:N1	2.42	0.49
10:T:18:GLU:OE1	10:T:18:GLU:N	2.41	0.49
16:A:434:U:O2	16:A:435:C:N4	2.41	0.49
2:B:49:C:OP2	7:O:30:ARG:NH1	2.46	0.49
10:T:2:ILE:HD11	16:A:144:A:H4'	1.93	0.49
16:A:554:U:H2'	16:A:555:G:O4'	2.13	0.49
16:A:107:G:O3'	16:A:293:U:O2'	2.26	0.49
16:A:231:A:H2'	16:A:232:G:O4'	2.12	0.49
16:A:508:A:C5'	19:y:13:PRO:HG3	2.42	0.49
17:D:40:LEU:HD13	17:D:44:GLY:O	2.12	0.49
18:E:3:LEU:HD13	18:E:120:VAL:HG21	1.94	0.49
16:A:307:G:N1	16:A:309:A:O5'	2.46	0.49
16:A:549:G:O2'	16:A:550:C:P	2.70	0.49
16:A:948:C:O2	16:A:984:A:O2'	2.07	0.49
16:A:1512:C:H2'	16:A:1513:U:N1	2.27	0.49
16:A:141:G:N2	16:A:142:A:N3	2.60	0.49
16:A:2326:C:HO2'	16:A:2327:A:P	2.33	0.49
16:A:2647:U:O2	16:A:2673:G:O6	2.31	0.49
2:B:42:C:C5	3:F:65:LEU:HD22	2.48	0.49
16:A:1028:A:OP2	16:A:1126:A:N6	2.44	0.49
3:F:3:LEU:HD22	3:F:100:GLU:HG2	1.93	0.49
9:R:63:VAL:HA	9:R:96:VAL:HG12	1.95	0.49
15:Z:4:ILE:HD12	15:Z:58:GLU:OE2	2.13	0.49
16:A:90:U:OP2	16:A:91:A:O2'	2.27	0.49
16:A:1321:A:O2'	19:y:17:ARG:NE	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:112:LEU:HD22	5:L:130:GLY:HA3	1.94	0.48
11:U:81:ARG:NH2	16:A:300:A:O5'	2.46	0.48
16:A:1170:C:N4	16:A:1171:G:O6	2.47	0.48
2:B:42:C:N3	3:F:89:THR:HG22	2.28	0.48
8:Q:57:ARG:NH1	16:A:997:G:OP2	2.45	0.48
12:V:62:THR:OG1	12:V:69:GLU:OE2	2.19	0.48
16:A:1386:C:H2'	16:A:1387:A:C8	2.47	0.48
2:B:3:C:H3'	2:B:4:C:H5''	1.94	0.48
6:N:97:ILE:CD1	6:N:113:ILE:HD13	2.43	0.48
16:A:1441:G:H2'	16:A:1442:U:C6	2.48	0.48
12:V:7:GLU:N	12:V:7:GLU:OE1	2.47	0.48
16:A:391:A:O2'	16:A:410:G:OP1	2.32	0.48
16:A:1266:G:N2	16:A:2012:G:O2'	2.47	0.48
16:A:1608:A:N7	16:A:1621:U:O2	2.46	0.48
16:A:330:A:N7	16:A:1210:G:O2'	2.42	0.48
2:B:78:A:H62	2:B:98:G:H21	1.61	0.48
16:A:956:G:O2'	16:A:960:A:N6	2.47	0.48
16:A:1448:G:H2'	16:A:1449:G:O4'	2.14	0.48
17:D:26:VAL:C	17:D:27:ILE:HD12	2.38	0.48
18:E:161:ALA:CB	18:E:169:VAL:HG23	2.43	0.48
18:E:191:ASP:OD1	18:E:192:ALA:N	2.46	0.48
16:A:1321:A:H5''	19:y:17:ARG:HB2	1.61	0.48
16:A:1324:G:O2'	16:A:1328:A:N6	2.46	0.48
16:A:1588:G:H2'	16:A:1589:U:C6	2.49	0.47
17:D:33:ARG:NH2	17:D:74:GLU:OE1	2.48	0.47
18:E:7:ASP:OD1	18:E:8:ALA:N	2.46	0.47
3:F:102:LEU:HD12	3:F:106:ALA:CB	2.45	0.47
6:N:19:ALA:O	6:N:23:ASN:ND2	2.42	0.47
16:A:415:A:N6	16:A:2409:G:O6	2.48	0.47
16:A:1383:A:O2'	16:A:1384:A:O4'	2.30	0.47
16:A:1434:A:H2'	16:A:1435:G:C8	2.49	0.47
16:A:1449:G:H3'	16:A:1450:G:O4'	2.15	0.47
7:O:43:ASN:OD1	7:O:44:GLY:N	2.47	0.47
15:Z:22:THR:HG22	16:A:850:U:O2'	2.14	0.47
16:A:1435:G:H2'	16:A:1436:G:C8	2.49	0.47
18:E:11:ALA:C	18:E:12:LEU:HD22	2.39	0.47
16:A:1466:U:O2'	16:A:1546:G:O2'	1.93	0.47
16:A:1386:C:H2'	16:A:1387:A:H8	1.79	0.47
2:B:39:A:H2'	2:B:40:U:C6	2.49	0.47
12:V:61:LEU:HD12	12:V:61:LEU:N	2.30	0.47
16:A:36:G:N3	16:A:450:G:O2'	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:573:U:O4	16:A:2029:G:O2'	2.20	0.47
16:A:508:A:OP2	19:y:13:PRO:HD3	2.15	0.47
18:E:31:VAL:HG21	18:E:104:ALA:HB2	1.96	0.47
5:L:85:VAL:HG13	5:L:98:ALA:HB2	1.97	0.47
17:D:26:VAL:HG12	17:D:186:LEU:HD12	1.97	0.47
9:R:11:GLN:N	9:R:11:GLN:OE1	2.48	0.47
15:Z:18:LYS:O	15:Z:22:THR:HG23	2.14	0.47
4:J:50:THR:O	4:J:50:THR:HG22	2.15	0.46
5:L:35:HIS:NE2	16:A:567:U:OP1	2.48	0.46
11:U:98:ASN:O	11:U:98:ASN:CG	2.58	0.46
12:V:38:LEU:HD23	12:V:39:ALA:N	2.30	0.46
16:A:357:C:C2	16:A:358:U:C5	3.03	0.46
16:A:2375:G:N1	16:A:2379:G:O6	2.48	0.46
6:N:72:ASP:O	6:N:76:VAL:HG23	2.14	0.46
10:T:4:GLU:CD	14:Y:18:LEU:HD13	2.41	0.46
16:A:203:A:OP2	16:A:204:A:O2'	2.14	0.46
16:A:1510:G:H2'	16:A:1511:G:C8	2.50	0.46
16:A:224:U:H2'	16:A:225:C:O4'	2.15	0.46
16:A:1551:A:H2'	16:A:1552:A:O4'	2.16	0.46
10:T:69:ARG:HG2	10:T:74:ILE:HG22	1.97	0.46
3:F:139:GLU:OE1	3:F:139:GLU:N	2.45	0.46
6:N:34:ILE:HD11	16:A:1278:C:O3'	2.16	0.46
16:A:974:G:OP1	16:A:1187:G:O2'	2.18	0.46
16:A:1524:G:H2'	16:A:1525:A:C8	2.51	0.46
13:W:32:ILE:N	13:W:32:ILE:HD12	2.30	0.46
16:A:451:U:C4	16:A:453:A:C8	3.03	0.46
16:A:1345:C:N4	16:A:1346:G:O6	2.48	0.46
3:F:35:LEU:HD13	3:F:153:ILE:HD13	1.97	0.46
13:W:79:GLU:OE1	13:W:79:GLU:N	2.49	0.46
15:Z:4:ILE:HD11	15:Z:56:VAL:HG21	1.95	0.46
16:A:932:U:O2'	16:A:934:U:O4	2.28	0.46
16:A:1000:A:OP2	16:A:1154:G:N1	2.43	0.46
16:A:1263:U:H2'	16:A:1264:A:N9	2.31	0.46
16:A:1360:G:C8	16:A:1361:G:C8	3.04	0.46
16:A:2047:C:O2'	16:A:2823:A:N1	2.46	0.46
2:B:116:G:H4'	7:O:54:VAL:HG12	1.97	0.45
15:Z:19:HIS:O	15:Z:23:LEU:HD23	2.15	0.45
16:A:549:G:C2'	16:A:550:C:O5'	2.64	0.45
16:A:1344:U:H3'	16:A:1345:C:H5'	1.98	0.45
4:J:125:TYR:HH	4:J:132:HIS:HE2	1.64	0.45
5:L:17:LYS:CE	5:L:27:LEU:HD13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1269:A:H2'	16:A:1270:C:O4'	2.16	0.45
17:D:183:GLU:OE1	17:D:183:GLU:N	2.43	0.45
2:B:29:A:O2'	2:B:58:A:N1	2.49	0.45
6:N:79:LEU:HD13	6:N:83:LEU:HB2	1.99	0.45
8:Q:75:TYR:OH	8:Q:91:ARG:NH1	2.48	0.45
13:W:60:ASP:OD1	13:W:61:GLY:N	2.49	0.45
16:A:81:G:O2'	16:A:295:G:O2'	2.33	0.45
17:D:27:ILE:HD12	17:D:27:ILE:N	2.31	0.45
16:A:543:G:O6	16:A:551:G:O6	2.34	0.45
18:E:79:ARG:O	18:E:80:SER:OG	2.32	0.45
16:A:299:A:N6	16:A:322:A:O2'	2.46	0.45
16:A:976:G:HO2'	16:A:1155:A:HO2'	1.62	0.45
16:A:1413:A:C2'	16:A:1414:C:O4'	2.65	0.45
16:A:219:A:N3	16:A:234:U:O2'	2.50	0.45
16:A:507:A:C2	19:y:10:ARG:HD2	2.52	0.45
3:F:33:ILE:O	3:F:90:LEU:HD23	2.17	0.45
4:J:114:LEU:HD11	16:A:557:C:O2'	2.17	0.45
16:A:500:G:O2'	16:A:505:A:N6	2.50	0.45
16:A:307:G:H22	16:A:309:A:H3'	1.82	0.45
16:A:1351:C:H2'	16:A:1352:U:O4'	2.16	0.45
16:A:1601:G:H2'	16:A:1602:U:O4'	2.17	0.45
16:A:2679:A:H5'	17:D:170:VAL:HG21	1.98	0.45
2:B:2:G:H2'	2:B:3:C:C6	2.52	0.44
16:A:1321:A:C4	19:y:16:PRO:CD	2.98	0.44
7:O:106:LEU:HD23	7:O:106:LEU:O	2.17	0.44
16:A:543:G:H2'	16:A:544:C:C6	2.52	0.44
16:A:1309:G:N2	16:A:1611:C:O4'	2.43	0.44
16:A:1484:U:H2'	16:A:1485:U:O4'	2.16	0.44
18:E:146:VAL:HG21	18:E:187:VAL:HG13	1.99	0.44
3:F:39:VAL:HG11	3:F:149:ARG:HH21	1.82	0.44
3:F:48:LEU:HD12	3:F:49:LEU:N	2.32	0.44
16:A:1542:U:H2'	16:A:1543:G:C8	2.53	0.44
16:A:320:A:H2'	18:E:131:THR:HG21	1.99	0.44
16:A:1443:U:C2	16:A:1444:G:C8	3.05	0.44
13:W:11:ASP:OD1	13:W:12:SER:N	2.51	0.44
16:A:548:G:C2'	16:A:549:G:O4'	2.65	0.44
16:A:820:A:OP2	16:A:973:A:N6	2.42	0.44
16:A:1307:A:H2'	16:A:1308:A:O4'	2.17	0.44
16:A:1342:A:O2'	16:A:1345:C:N4	2.50	0.44
16:A:1349:C:C2	16:A:1350:C:C5	3.05	0.44
16:A:1478:G:H2'	16:A:1479:G:C1'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:176:ASP:OD1	18:E:176:ASP:N	2.50	0.44
16:A:49:A:N1	16:A:177:G:N2	2.66	0.44
16:A:374:A:N6	16:A:400:G:O2'	2.51	0.44
16:A:151:C:N4	16:A:152:A:H62	2.16	0.44
16:A:471:A:OP1	18:E:79:ARG:NH1	2.47	0.44
19:y:17:ARG:HA	19:y:17:ARG:HH11	1.82	0.44
6:N:115:LEU:HD12	6:N:115:LEU:H	1.83	0.44
7:O:31:THR:O	7:O:102:ARG:NH2	2.49	0.44
9:R:40:MET:SD	9:R:41:ILE:N	2.91	0.44
16:A:383:C:N3	16:A:391:A:N6	2.64	0.44
3:F:118:ALA:O	3:F:166:ARG:NH1	2.48	0.44
4:J:32:LEU:HD23	4:J:54:ILE:HD13	2.00	0.44
5:L:90:VAL:N	5:L:121:THR:O	2.46	0.44
8:Q:68:ALA:HB1	8:Q:73:ILE:HG23	1.99	0.44
16:A:262:A:N3	16:A:430:A:O2'	2.41	0.44
16:A:966:G:H4'	16:A:2271:G:H22	1.83	0.44
9:R:74:ILE:N	9:R:74:ILE:HD12	2.31	0.43
16:A:630:G:N2	16:A:633:A:OP2	2.43	0.43
1:2:30:VAL:HG22	1:2:33:ARG:NH2	2.34	0.43
2:B:30:C:H1'	2:B:57:A:H61	1.83	0.43
11:U:27:VAL:HG12	11:U:33:VAL:HG12	2.00	0.43
16:A:1286:A:O2'	16:A:1288:G:OP2	2.27	0.43
17:D:188:LEU:HD12	17:D:188:LEU:N	2.33	0.43
2:B:77:U:O2	2:B:99:A:N7	2.51	0.43
16:A:240:C:OP2	16:A:241:A:O2'	2.20	0.43
16:A:507:A:C8	19:y:10:ARG:NH2	2.86	0.43
5:L:29:LYS:C	5:L:30:THR:HG23	2.43	0.43
5:L:42:SER:OG	16:A:672:C:OP2	2.32	0.43
9:R:98:ILE:HG21	9:R:101:ILE:HD11	2.00	0.43
16:A:298:G:O2'	16:A:322:A:N1	2.46	0.43
4:J:9:GLU:OE1	4:J:9:GLU:N	2.46	0.43
16:A:549:G:H2'	16:A:550:C:O4'	2.18	0.43
16:A:1346:G:H2'	16:A:1347:A:O4'	2.17	0.43
16:A:1348:C:C2	16:A:1349:C:C6	3.07	0.43
16:A:1425:G:H2'	16:A:1426:G:O4'	2.18	0.43
16:A:2321:U:O2	16:A:2321:U:H2'	2.19	0.43
17:D:40:LEU:HD13	17:D:44:GLY:C	2.44	0.43
17:D:97:SER:OG	17:D:98:VAL:N	2.52	0.43
18:E:118:LEU:HD23	18:E:119:ILE:N	2.33	0.43
3:F:66:ILE:N	3:F:66:ILE:HD12	2.33	0.43
6:N:29:VAL:HG11	6:N:75:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:48:ASP:OD1	8:Q:48:ASP:C	2.61	0.43
16:A:235:U:O4	16:A:263:G:N2	2.52	0.43
16:A:1205:A:HO2'	16:A:1206:G:P	2.42	0.43
16:A:1494:A:N3	16:A:1494:A:H2'	2.34	0.43
6:N:47:VAL:O	6:N:51:LEU:HD23	2.19	0.43
8:Q:8:ILE:HD12	8:Q:8:ILE:H	1.84	0.43
16:A:545:U:O4	16:A:548:G:O6	2.36	0.43
16:A:1566:A:H2'	16:A:1566:A:N3	2.34	0.43
16:A:2009:A:C2'	16:A:2010:G:O4'	2.66	0.43
11:U:97:SER:O	11:U:98:ASN:OD1	2.36	0.43
16:A:1414:C:O2'	16:A:1415:U:C4'	2.67	0.43
16:A:508:A:P	19:y:13:PRO:HG3	2.59	0.43
14:Y:5:GLU:OE1	14:Y:5:GLU:N	2.47	0.43
16:A:33:C:O2	16:A:447:A:N6	2.51	0.43
16:A:309:A:N3	16:A:329:G:O2'	2.51	0.43
16:A:2004:G:H2'	16:A:2005:A:O4'	2.18	0.43
17:D:101:PHE:HA	17:D:104:VAL:HG12	2.01	0.43
3:F:39:VAL:HG23	3:F:40:GLY:N	2.34	0.42
4:J:111:LYS:NZ	16:A:2039:U:OP1	2.37	0.42
16:A:465:G:H21	16:A:684:G:H1'	1.84	0.42
4:J:12:LYS:NZ	4:J:14:ASP:OD1	2.50	0.42
6:N:79:LEU:O	6:N:80:PHE:HB2	2.19	0.42
16:A:544:C:H2'	16:A:545:U:C2	2.53	0.42
16:A:2051:A:N3	16:A:2052:A:N6	2.67	0.42
5:L:29:LYS:O	5:L:30:THR:OG1	2.30	0.42
16:A:507:A:C4	19:y:10:ARG:NH2	2.87	0.42
16:A:1141:U:H4'	16:A:1142:A:O4'	2.20	0.42
16:A:1245:G:H2'	16:A:1246:A:C8	2.55	0.42
16:A:1319:C:O2'	16:A:1320:C:P	2.77	0.42
16:A:1364:G:O2'	16:A:1367:A:N6	2.53	0.42
16:A:1591:A:H2'	16:A:1592:C:O4'	2.18	0.42
5:L:92:LEU:O	5:L:92:LEU:HD23	2.20	0.42
16:A:170:U:C2	16:A:171:U:C5	3.07	0.42
16:A:832:U:O2	16:A:833:A:C8	2.73	0.42
16:A:1003:G:O2'	16:A:1010:A:N1	2.45	0.42
16:A:1576:U:H2'	16:A:1577:C:C6	2.55	0.42
16:A:2287:A:N6	16:A:2346:A:N7	2.68	0.42
3:F:165:GLY:O	3:F:169:LEU:HD13	2.19	0.42
16:A:92:U:H1'	19:y:7:TYR:CE1	2.53	0.42
16:A:2028:U:O4	16:A:2033:A:N7	2.52	0.42
5:L:71:ALA:HA	5:L:74:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:35:GLU:OE2	12:V:93:ARG:NH1	2.53	0.42
13:W:66:GLU:N	13:W:66:GLU:OE1	2.52	0.42
14:Y:24:GLU:O	14:Y:28:LEU:HD12	2.20	0.42
16:A:1370:C:H2'	16:A:1371:G:O4'	2.20	0.42
16:A:1430:G:C4	16:A:1431:A:C8	3.08	0.42
16:A:2399:G:C6	16:A:2418:A:C6	3.08	0.42
2:B:23:G:O2'	2:B:24:G:O4'	2.35	0.42
2:B:73:A:N3	2:B:73:A:H2'	2.35	0.42
9:R:75:VAL:HG22	9:R:86:GLN:OE1	2.19	0.42
16:A:507:A:C4	19:y:10:ARG:NE	2.88	0.42
16:A:1208:C:H2'	16:A:1209:U:O4'	2.19	0.42
16:A:1357:C:H2'	16:A:1358:G:O4'	2.20	0.42
17:D:33:ARG:CG	17:D:73:VAL:HG13	2.48	0.42
18:E:31:VAL:HG21	18:E:104:ALA:CB	2.48	0.42
16:A:1021:A:H61	16:A:1142:A:H61	1.68	0.42
16:A:1389:G:H2'	16:A:1390:U:O4'	2.20	0.42
16:A:1480:C:H2'	16:A:1481:U:O4'	2.19	0.42
16:A:1998:A:H2'	16:A:1999:C:C6	2.55	0.42
3:F:122:ASP:OD2	3:F:126:ASN:ND2	2.44	0.41
16:A:1504:A:N1	16:A:1505:A:N6	2.67	0.41
16:A:2831:G:N2	16:A:2884:U:OP2	2.53	0.41
8:Q:8:ILE:HD12	8:Q:8:ILE:N	2.35	0.41
3:F:48:LEU:O	3:F:51:ASN:ND2	2.53	0.41
7:O:108:ASP:OD1	7:O:109:ALA:N	2.54	0.41
8:Q:60:TRP:O	8:Q:64:ILE:HG12	2.20	0.41
13:W:64:LYS:N	13:W:77:SER:O	2.48	0.41
16:A:2345:G:O6	16:A:2371:G:O6	2.39	0.41
5:L:17:LYS:HE3	5:L:27:LEU:HD13	2.03	0.41
8:Q:91:ARG:NH1	16:A:1153:C:OP1	2.47	0.41
15:Z:46:MET:O	15:Z:50:VAL:HG22	2.20	0.41
16:A:1327:A:H2'	16:A:1328:A:O4'	2.21	0.41
16:A:1385:A:H1'	16:A:1386:C:C6	2.55	0.41
16:A:1561:C:H2'	16:A:1562:U:O4'	2.20	0.41
16:A:2720:U:C2	16:A:2721:A:C8	3.09	0.41
3:F:107:VAL:N	3:F:108:PRO:CD	2.84	0.41
16:A:65:U:O2'	16:A:456:C:O2	2.37	0.41
16:A:1595:C:H2'	16:A:1596:A:O4'	2.20	0.41
16:A:2848:G:O2'	16:A:2868:A:N6	2.46	0.41
9:R:23:GLU:OE1	9:R:24:LYS:N	2.50	0.41
16:A:62:U:O4'	19:y:3:ASN:ND2	2.53	0.41
16:A:1346:G:N1	16:A:1601:G:C6	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1353:A:N7	16:A:1377:G:N2	2.68	0.41
16:A:1414:C:C2'	16:A:1415:U:O4'	2.68	0.41
3:F:12:VAL:HG13	3:F:13:LYS:N	2.36	0.41
3:F:33:ILE:HD12	3:F:33:ILE:N	2.36	0.41
9:R:82:HIS:ND1	9:R:82:HIS:O	2.53	0.41
16:A:967:U:H2'	16:A:968:C:C6	2.56	0.41
16:A:1234:U:H2'	16:A:1235:G:O4'	2.21	0.41
16:A:1593:A:H2'	16:A:1594:U:O4'	2.21	0.41
3:F:65:LEU:HD23	3:F:65:LEU:H	1.86	0.41
11:U:85:ARG:NH2	11:U:101:THR:OG1	2.54	0.41
16:A:306:U:H2'	16:A:307:G:O4'	2.20	0.41
16:A:1358:G:N1	16:A:1372:U:OP2	2.45	0.41
16:A:1451:C:C2'	16:A:1452:G:OP2	2.69	0.41
16:A:1528:A:OP2	16:A:1543:G:N2	2.41	0.41
4:J:18:VAL:CG2	4:J:54:ILE:HD11	2.51	0.41
11:U:35:VAL:HG23	11:U:38:ILE:HB	2.02	0.41
16:A:1425:G:N2	16:A:1574:C:N4	2.69	0.41
16:A:1607:C:O4'	16:A:1621:U:N3	2.53	0.41
16:A:1630:A:H2'	16:A:1631:G:O4'	2.20	0.41
16:A:1665:A:C2'	16:A:1666:G:O5'	2.69	0.41
19:y:15:HIS:HB2	19:y:16:PRO:HD2	2.02	0.41
2:B:83:G:O6	2:B:94:A:N6	2.53	0.41
3:F:79:ARG:NH1	3:F:80:GLN:O	2.54	0.41
16:A:1351:C:H1'	16:A:1572:A:H1'	2.03	0.41
16:A:2368:C:O2	16:A:2369:A:C8	2.74	0.41
3:F:105:ILE:HD12	3:F:138:PRO:HG2	2.03	0.40
7:O:62:LEU:HD22	7:O:62:LEU:N	2.36	0.40
11:U:9:GLU:O	11:U:72:PHE:N	2.46	0.40
11:U:28:LEU:HD22	11:U:28:LEU:N	2.36	0.40
16:A:1354:A:H62	16:A:1377:G:H21	1.68	0.40
17:D:25:THR:HG21	17:D:193:VAL:CG2	2.50	0.40
16:A:1513:U:H2'	16:A:1514:G:O4'	2.22	0.40
16:A:2812:G:N2	16:A:2889:C:C2	2.89	0.40
2:B:45:A:O4'	3:F:91:ARG:NH1	2.55	0.40
5:L:35:HIS:O	5:L:36:LYS:C	2.64	0.40
18:E:154:ASP:OD1	18:E:154:ASP:N	2.48	0.40
3:F:140:ILE:N	3:F:140:ILE:HD12	2.36	0.40
16:A:635:C:O2'	16:A:639:U:OP1	2.40	0.40
16:A:928:A:H2'	16:A:929:U:C6	2.56	0.40
16:A:1347:A:C5	16:A:1348:C:C6	3.09	0.40
17:D:35:THR:HG22	17:D:73:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:101:ILE:HG13	5:L:102:GLY:N	2.37	0.40
16:A:458:G:C2'	16:A:459:U:OP2	2.70	0.40
16:A:499:U:H2'	16:A:500:G:O4'	2.22	0.40
16:A:1372:U:O4	16:A:1373:A:N6	2.55	0.40
16:A:1394:U:H2'	16:A:1395:A:O4'	2.22	0.40
16:A:1413:A:H2'	16:A:1414:C:O4'	2.22	0.40
16:A:1574:C:H2'	16:A:1575:C:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	36/46 (78%)	36 (100%)	0	0	100	100
3	F	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
4	J	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
5	L	141/143 (99%)	129 (92%)	12 (8%)	0	100	100
6	N	118/120 (98%)	107 (91%)	11 (9%)	0	100	100
7	O	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
8	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
9	R	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	12	47
10	T	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
11	U	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
12	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
13	W	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
14	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
15	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	D	169/209 (81%)	163 (96%)	6 (4%)	0	100	100
18	E	172/201 (86%)	168 (98%)	3 (2%)	1 (1%)	21	58
19	y	15/17 (88%)	11 (73%)	4 (27%)	0	100	100
All	All	1769/1876 (94%)	1692 (96%)	75 (4%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	R	54	VAL
18	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	2	30/38 (79%)	30 (100%)	0	100	100
3	F	148/148 (100%)	147 (99%)	1 (1%)	76	79
4	J	116/116 (100%)	116 (100%)	0	100	100
5	L	102/102 (100%)	102 (100%)	0	100	100
6	N	99/100 (99%)	98 (99%)	1 (1%)	68	76
7	O	86/86 (100%)	86 (100%)	0	100	100
8	Q	89/89 (100%)	88 (99%)	1 (1%)	65	74
9	R	84/84 (100%)	84 (100%)	0	100	100
10	T	80/80 (100%)	80 (100%)	0	100	100
11	U	83/83 (100%)	82 (99%)	1 (1%)	63	73
12	V	78/78 (100%)	78 (100%)	0	100	100
13	W	57/57 (100%)	56 (98%)	1 (2%)	51	66
14	Y	55/55 (100%)	55 (100%)	0	100	100
15	Z	48/48 (100%)	48 (100%)	0	100	100
17	D	134/164 (82%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	E	146/165 (88%)	144 (99%)	2 (1%)	59	71
19	y	17/17 (100%)	16 (94%)	1 (6%)	18	40
All	All	1452/1510 (96%)	1444 (99%)	8 (1%)	76	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	35	LEU
6	N	34	ILE
8	Q	108	LEU
11	U	98	ASN
13	W	65	PHE
18	E	19	PHE
18	E	163	ASN
19	y	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	J	47	HIS
4	J	80	HIS
7	O	98	GLN
9	R	18	GLN
11	U	52	ASN
17	D	36	GLN
18	E	94	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	A	1981/2903 (68%)	428 (21%)	17 (0%)
2	B	119/120 (99%)	14 (11%)	2 (1%)
All	All	2100/3023 (69%)	442 (21%)	19 (0%)

All (442) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	C
2	B	12	C

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Mol	Chain	Res	Type
2	B	13	G
2	B	35	C
2	B	41	G
2	B	42	C
2	B	44	G
2	B	45	A
2	B	53	A
2	B	66	A
2	B	67	G
2	B	89	U
2	B	90	C
2	B	109	A
16	A	10	A
16	A	27	G
16	A	34	U
16	A	35	G
16	A	46	G
16	A	50	U
16	A	51	G
16	A	71	A
16	A	74	A
16	A	75	G
16	A	114	U
16	A	118	A
16	A	120	U
16	A	135	U
16	A	136	G
16	A	139	U
16	A	141	G
16	A	142	A
16	A	160	A
16	A	162	U
16	A	163	C
16	A	181	A
16	A	190	A
16	A	196	A
16	A	197	A
16	A	199	A
16	A	215	G
16	A	216	A
16	A	221	A
16	A	222	A

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Mol	Chain	Res	Type
16	A	225	C
16	A	228	C
16	A	232	G
16	A	242	G
16	A	243	U
16	A	248	G
16	A	255	A
16	A	266	G
16	A	267	C
16	A	272	A
16	A	275	C
16	A	277	G
16	A	278	A
16	A	294	A
16	A	304	U
16	A	307	G
16	A	310	A
16	A	322	A
16	A	323	C
16	A	324	A
16	A	329	G
16	A	330	A
16	A	345	A
16	A	350	G
16	A	362	A
16	A	371	A
16	A	372	G
16	A	373	U
16	A	384	A
16	A	386	G
16	A	387	U
16	A	388	G
16	A	401	A
16	A	404	A
16	A	406	G
16	A	411	G
16	A	412	A
16	A	417	C
16	A	424	G
16	A	429	A
16	A	430	A
16	A	435	C

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Mol	Chain	Res	Type
16	A	456	C
16	A	457	A
16	A	458	G
16	A	459	U
16	A	465	G
16	A	466	A
16	A	473	G
16	A	480	A
16	A	481	G
16	A	491	G
16	A	505	A
16	A	509	C
16	A	510	C
16	A	529	A
16	A	530	G
16	A	531	C
16	A	532	A
16	A	543	G
16	A	544	C
16	A	545	U
16	A	547	A
16	A	549	G
16	A	550	C
16	A	563	A
16	A	568	U
16	A	572	A
16	A	573	U
16	A	575	A
16	A	588	U
16	A	603	A
16	A	614	A
16	A	621	A
16	A	627	A
16	A	637	A
16	A	645	C
16	A	646	U
16	A	647	G
16	A	654	A
16	A	668	A
16	A	669	G
16	A	670	A
16	A	671	C

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Mol	Chain	Res	Type
16	A	675	A
16	A	684	G
16	A	801	G
16	A	805	G
16	A	812	C
16	A	819	A
16	A	827	U
16	A	828	U
16	A	830	G
16	A	845	A
16	A	846	U
16	A	847	U
16	A	856	G
16	A	857	G
16	A	910	A
16	A	914	G
16	A	918	A
16	A	931	U
16	A	932	U
16	A	941	A
16	A	946	C
16	A	952	G
16	A	953	G
16	A	957	C
16	A	959	A
16	A	961	C
16	A	973	A
16	A	974	G
16	A	981	A
16	A	983	A
16	A	985	C
16	A	995	C
16	A	996	A
16	A	1009	A
16	A	1012	U
16	A	1013	C
16	A	1021	A
16	A	1022	G
16	A	1023	U
16	A	1026	G
16	A	1129	A
16	A	1132	U

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Mol	Chain	Res	Type
16	A	1135	C
16	A	1143	A
16	A	1151	A
16	A	1157	G
16	A	1169	A
16	A	1171	G
16	A	1174	U
16	A	1175	A
16	A	1176	U
16	A	1178	C
16	A	1180	U
16	A	1206	G
16	A	1212	G
16	A	1225	G
16	A	1236	G
16	A	1250	G
16	A	1253	A
16	A	1255	U
16	A	1256	G
16	A	1263	U
16	A	1265	A
16	A	1266	G
16	A	1267	U
16	A	1269	A
16	A	1271	G
16	A	1272	A
16	A	1273	U
16	A	1274	A
16	A	1275	A
16	A	1280	G
16	A	1284	A
16	A	1288	G
16	A	1289	C
16	A	1300	G
16	A	1301	A
16	A	1306	C
16	A	1307	A
16	A	1312	U
16	A	1315	C
16	A	1320	C
16	A	1321	A
16	A	1325	U

Continued on next page...

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Mol	Chain	Res	Type
16	A	1327	A
16	A	1329	U
16	A	1332	G
16	A	1333	G
16	A	1334	G
16	A	1340	U
16	A	1341	G
16	A	1343	G
16	A	1345	C
16	A	1352	U
16	A	1355	G
16	A	1356	G
16	A	1359	A
16	A	1361	G
16	A	1362	C
16	A	1365	A
16	A	1374	G
16	A	1379	U
16	A	1380	G
16	A	1383	A
16	A	1386	C
16	A	1391	U
16	A	1394	U
16	A	1395	A
16	A	1397	U
16	A	1400	U
16	A	1403	A
16	A	1404	C
16	A	1407	G
16	A	1413	A
16	A	1416	G
16	A	1419	A
16	A	1420	A
16	A	1421	G
16	A	1427	A
16	A	1428	C
16	A	1432	G
16	A	1434	A
16	A	1436	G
16	A	1445	G
16	A	1449	G
16	A	1450	G

Continued on next page...

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Mol	Chain	Res	Type
16	A	1452	G
16	A	1453	A
16	A	1454	C
16	A	1458	U
16	A	1459	G
16	A	1461	C
16	A	1467	U
16	A	1468	U
16	A	1469	A
16	A	1473	G
16	A	1474	U
16	A	1475	G
16	A	1478	G
16	A	1480	C
16	A	1482	G
16	A	1483	G
16	A	1484	U
16	A	1486	U
16	A	1493	C
16	A	1495	A
16	A	1497	U
16	A	1498	C
16	A	1501	G
16	A	1504	A
16	A	1508	A
16	A	1509	A
16	A	1515	A
16	A	1516	G
16	A	1519	G
16	A	1528	A
16	A	1529	G
16	A	1532	A
16	A	1535	A
16	A	1536	C
16	A	1537	G
16	A	1542	U
16	A	1546	G
16	A	1548	A
16	A	1553	A
16	A	1554	U
16	A	1555	G
16	A	1558	C

Continued on next page...

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Mol	Chain	Res	Type
16	A	1559	U
16	A	1560	G
16	A	1563	U
16	A	1566	A
16	A	1567	G
16	A	1569	A
16	A	1575	C
16	A	1576	U
16	A	1578	U
16	A	1579	A
16	A	1583	A
16	A	1584	U
16	A	1585	C
16	A	1592	C
16	A	1593	A
16	A	1596	A
16	A	1597	A
16	A	1598	A
16	A	1603	A
16	A	1607	C
16	A	1608	A
16	A	1613	G
16	A	1614	A
16	A	1615	C
16	A	1616	A
16	A	1618	A
16	A	1619	G
16	A	1620	G
16	A	1622	G
16	A	1627	G
16	A	1628	G
16	A	1634	A
16	A	1635	A
16	A	1636	U
16	A	1637	A
16	A	1644	C
16	A	1647	U
16	A	1648	U
16	A	1649	G
16	A	1650	A
16	A	1651	G
16	A	1652	A

Continued on next page...

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Mol	Chain	Res	Type
16	A	1653	G
16	A	1654	A
16	A	1656	C
16	A	1657	U
16	A	1660	G
16	A	1662	U
16	A	1663	G
16	A	1664	A
16	A	1666	G
16	A	1667	G
16	A	1992	G
16	A	1993	U
16	A	1997	C
16	A	1998	A
16	A	2003	A
16	A	2004	G
16	A	2006	C
16	A	2007	U
16	A	2008	C
16	A	2009	A
16	A	2011	U
16	A	2012	G
16	A	2013	A
16	A	2015	A
16	A	2022	U
16	A	2023	C
16	A	2030	A
16	A	2031	A
16	A	2043	C
16	A	2052	A
16	A	2250	G
16	A	2251	G
16	A	2266	A
16	A	2279	G
16	A	2283	C
16	A	2286	G
16	A	2287	A
16	A	2297	A
16	A	2305	U
16	A	2309	A
16	A	2319	G
16	A	2327	A

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Mol	Chain	Res	Type
16	A	2333	A
16	A	2334	U
16	A	2335	A
16	A	2336	A
16	A	2343	U
16	A	2350	C
16	A	2383	G
16	A	2385	C
16	A	2388	A
16	A	2402	U
16	A	2407	A
16	A	2422	C
16	A	2424	C
16	A	2425	A
16	A	2429	G
16	A	2430	A
16	A	2434	A
16	A	2435	A
16	A	2441	U
16	A	2448	A
16	A	2449	U
16	A	2615	U
16	A	2629	U
16	A	2630	G
16	A	2646	C
16	A	2647	U
16	A	2655	G
16	A	2656	U
16	A	2682	A
16	A	2689	U
16	A	2690	U
16	A	2714	G
16	A	2726	A
16	A	2732	G
16	A	2733	A
16	A	2744	G
16	A	2748	A
16	A	2764	A
16	A	2765	A
16	A	2778	A
16	A	2779	U
16	A	2780	G

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Mol	Chain	Res	Type
16	A	2791	G
16	A	2794	C
16	A	2799	A
16	A	2800	A
16	A	2809	A
16	A	2818	U
16	A	2820	A
16	A	2833	U
16	A	2835	A
16	A	2849	U
16	A	2867	G
16	A	2872	A
16	A	2873	A
16	A	2880	C
16	A	2883	A
16	A	2893	A
16	A	2894	G
16	A	2901	C
16	A	2902	C
16	A	2903	U

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	52	A
2	B	66	A
16	A	227	A
16	A	242	G
16	A	372	G
16	A	458	G
16	A	548	G
16	A	549	G
16	A	644	A
16	A	1020	A
16	A	1022	G
16	A	1319	C
16	A	1358	G
16	A	1427	A
16	A	1534	U
16	A	2010	G
16	A	2318	G
16	A	2326	C

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Mol	Chain	Res	Type
16	A	2655	G

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.

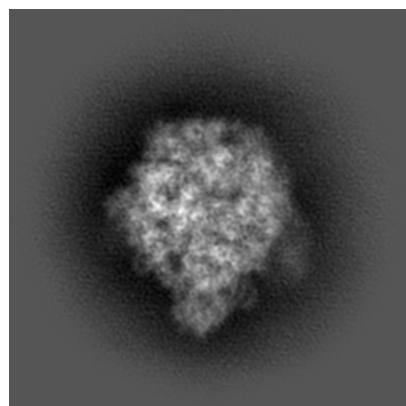
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51979. These allow visual inspection of the internal detail of the map and identification of artifacts.

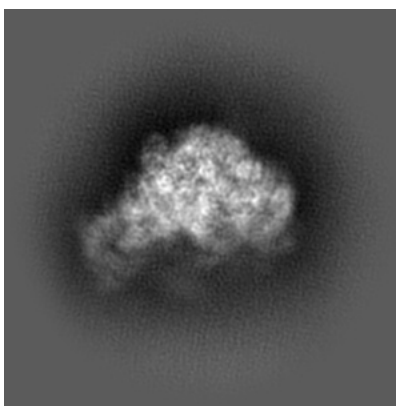
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

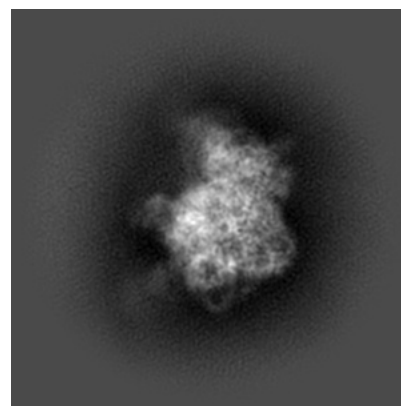
6.1.1 Primary map



X

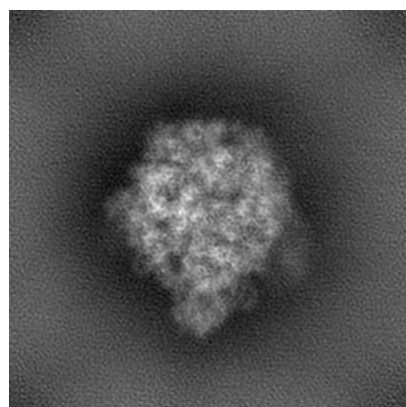


Y

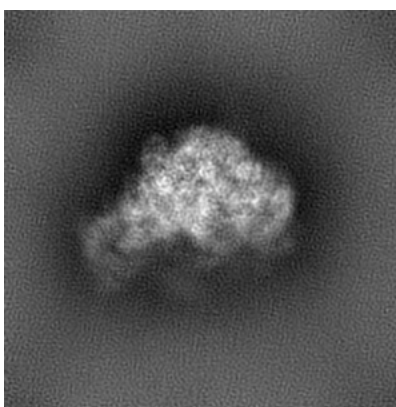


Z

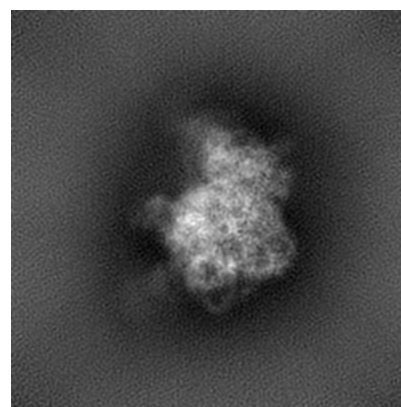
6.1.2 Raw map



X



Y

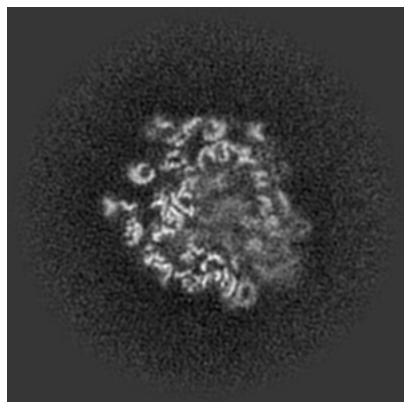


Z

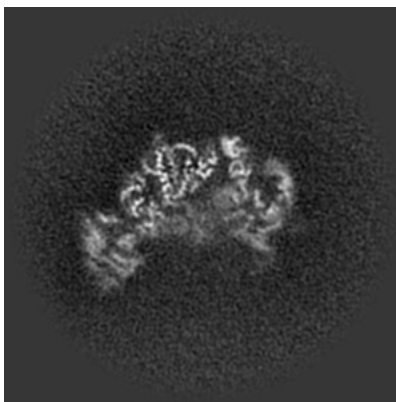
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

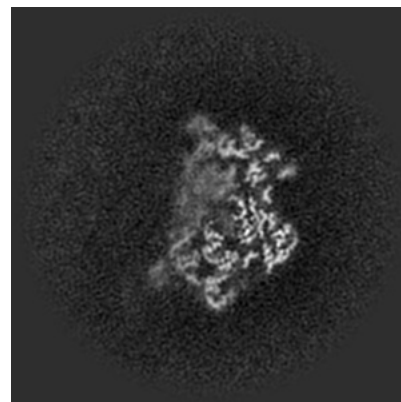
6.2.1 Primary map



X Index: 100

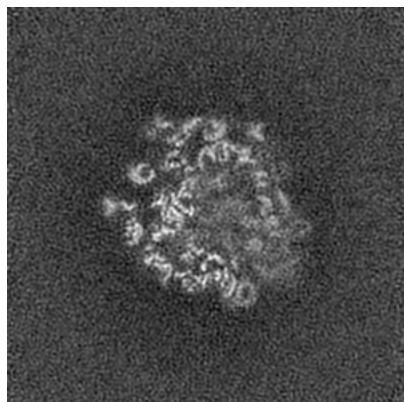


Y Index: 100

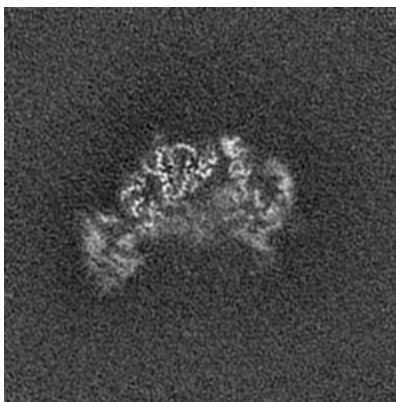


Z Index: 100

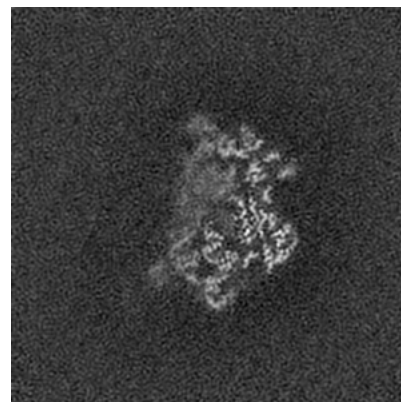
6.2.2 Raw map



X Index: 100



Y Index: 100

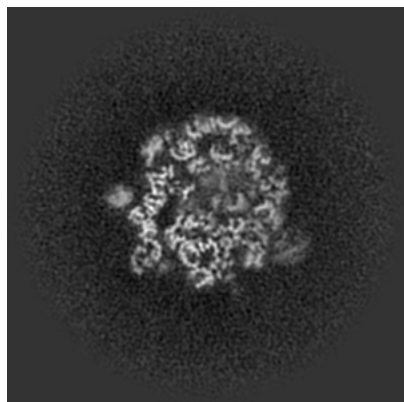


Z Index: 100

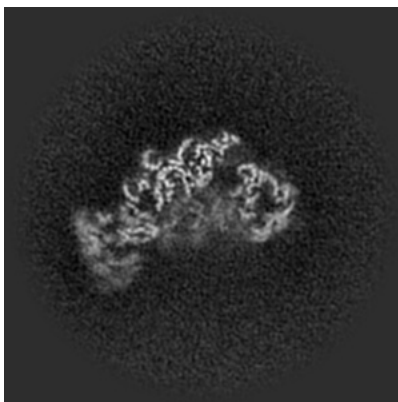
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

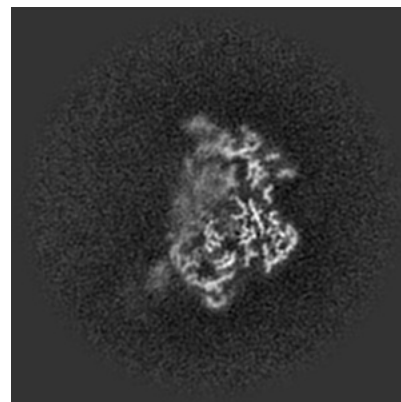
6.3.1 Primary map



X Index: 109

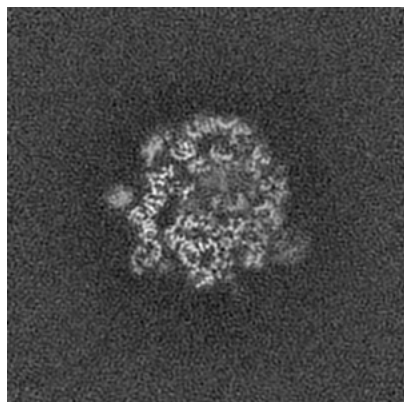


Y Index: 95

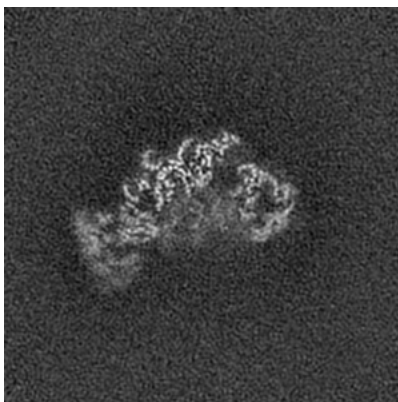


Z Index: 99

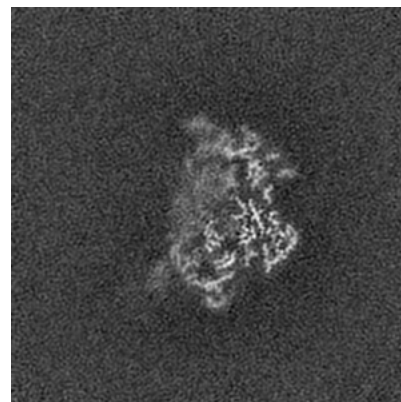
6.3.2 Raw map



X Index: 109



Y Index: 95

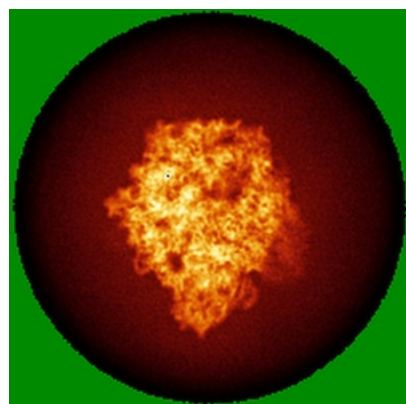


Z Index: 99

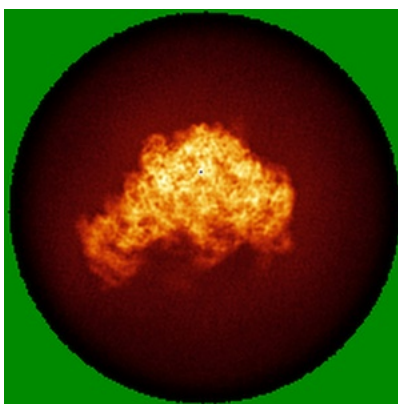
The images above show the largest variance slices of the map in three orthogonal directions.

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

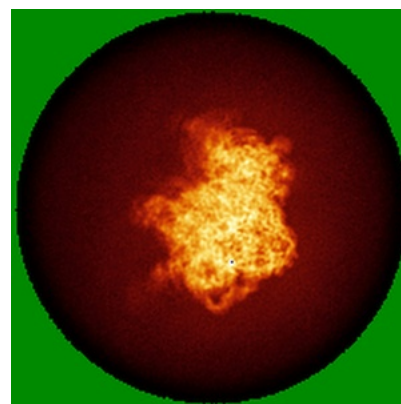
6.4.1 Primary map



X

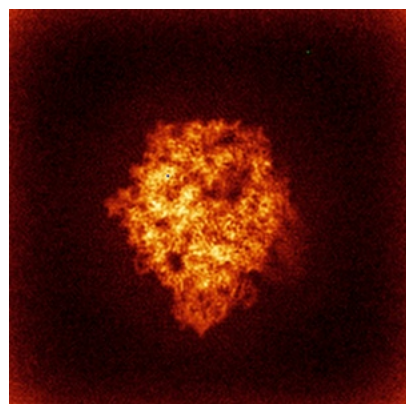


Y

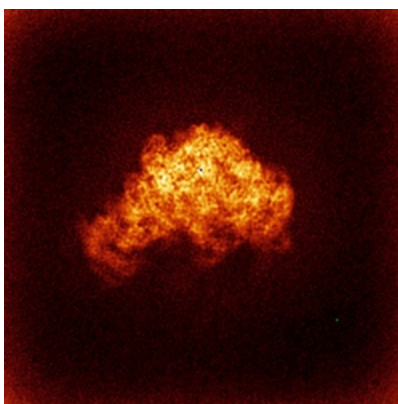


Z

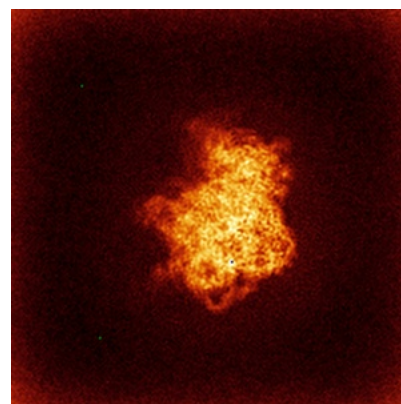
6.4.2 Raw map



X



Y

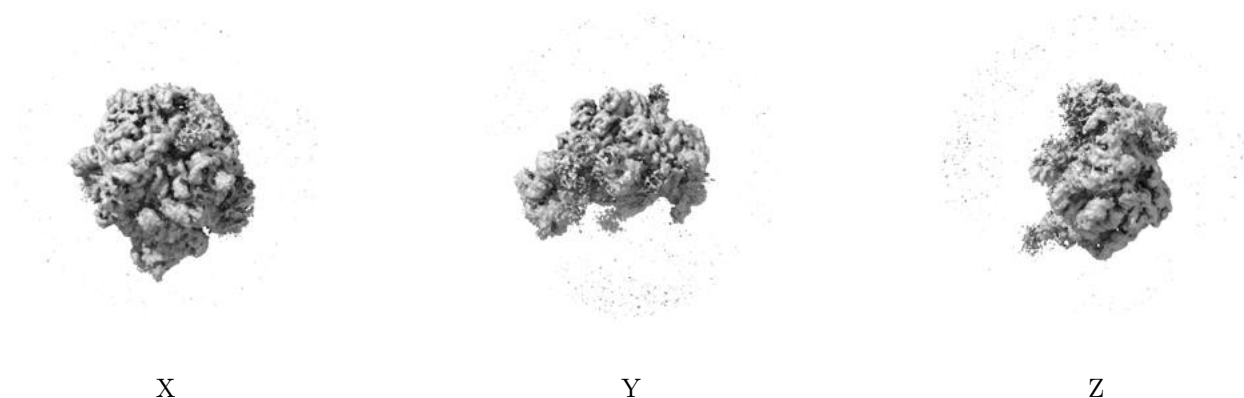


Z

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.

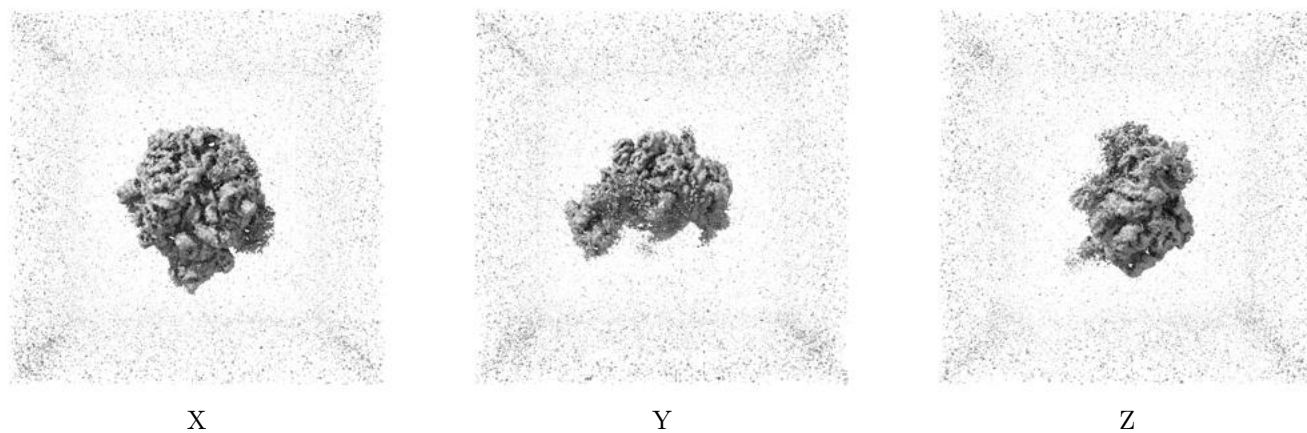
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.255. 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



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.

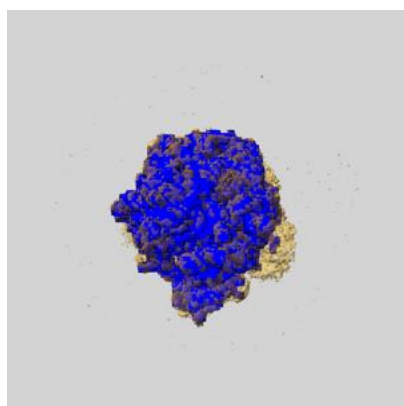
6.6 Mask visualisation [i](#)

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

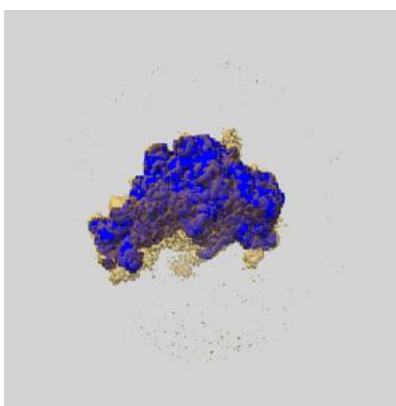
A mask typically either:

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

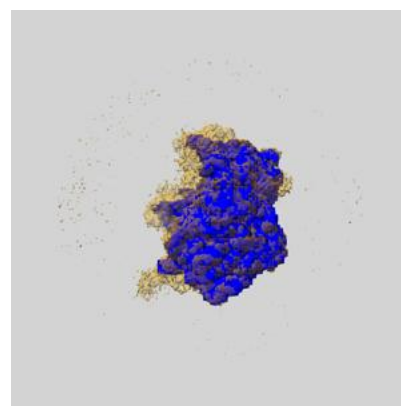
6.6.1 emd_51979_msk_1.map [i](#)



X



Y

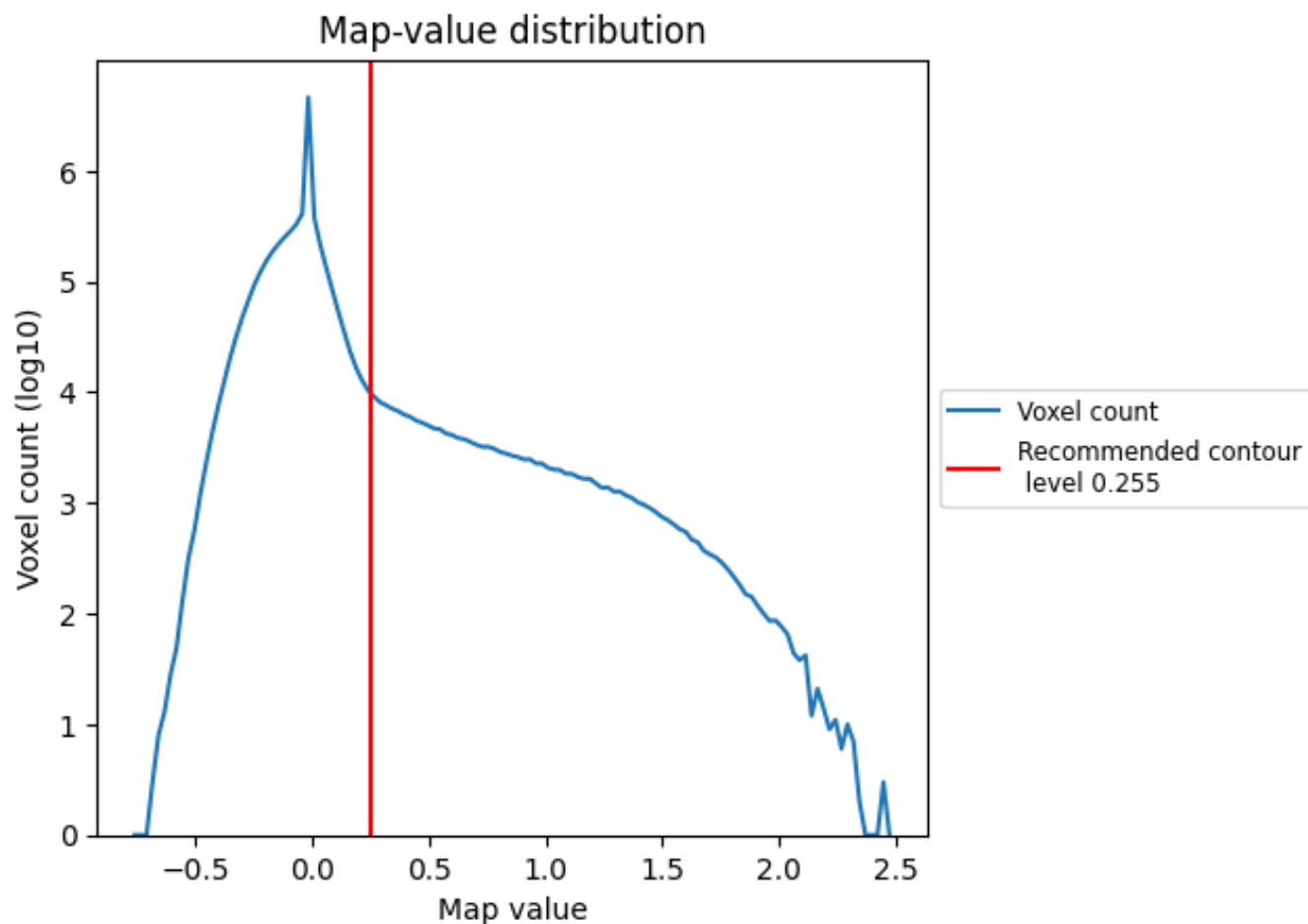


Z

7 Map analysis [i](#)

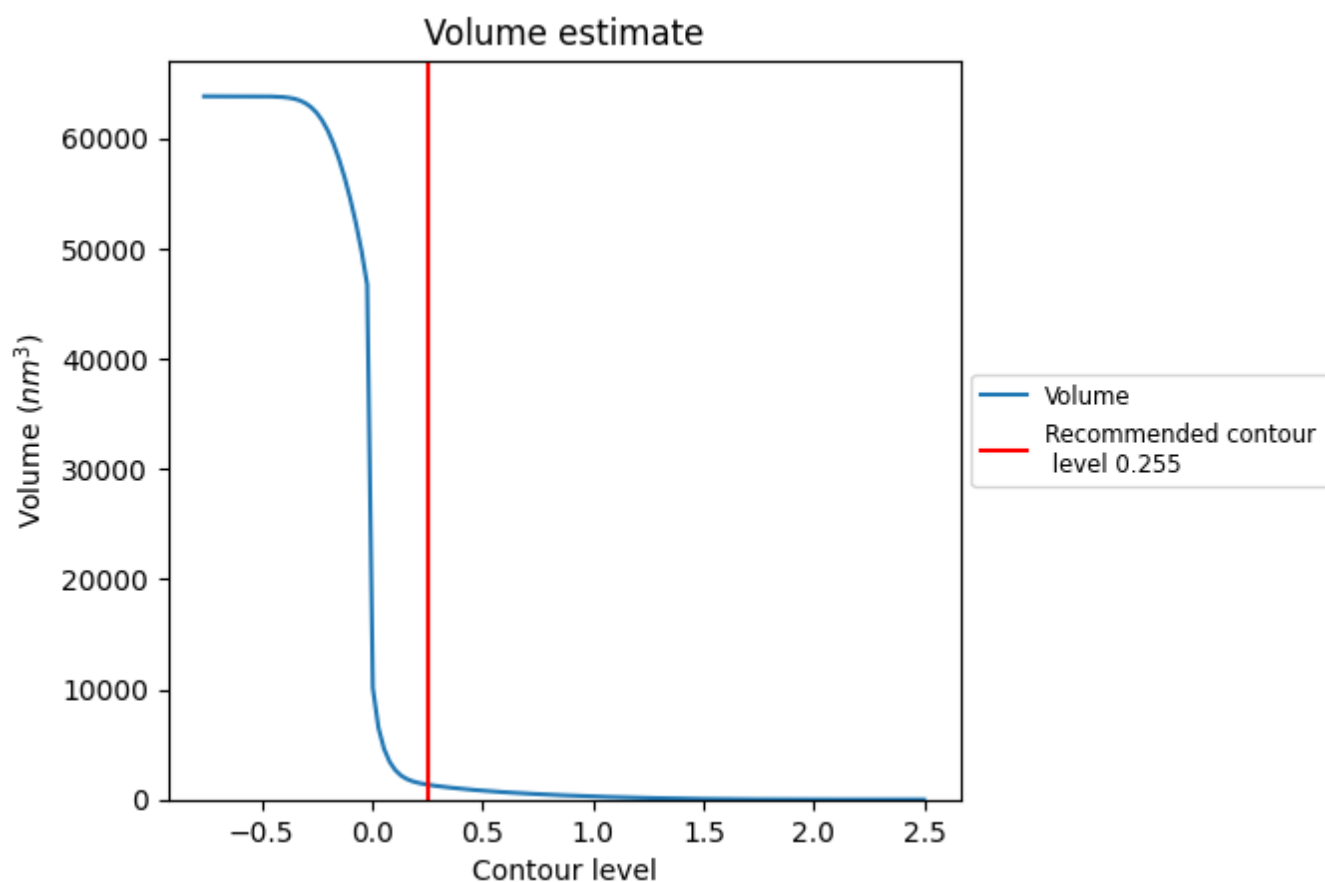
This section contains the results of statistical analysis of the map.

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.

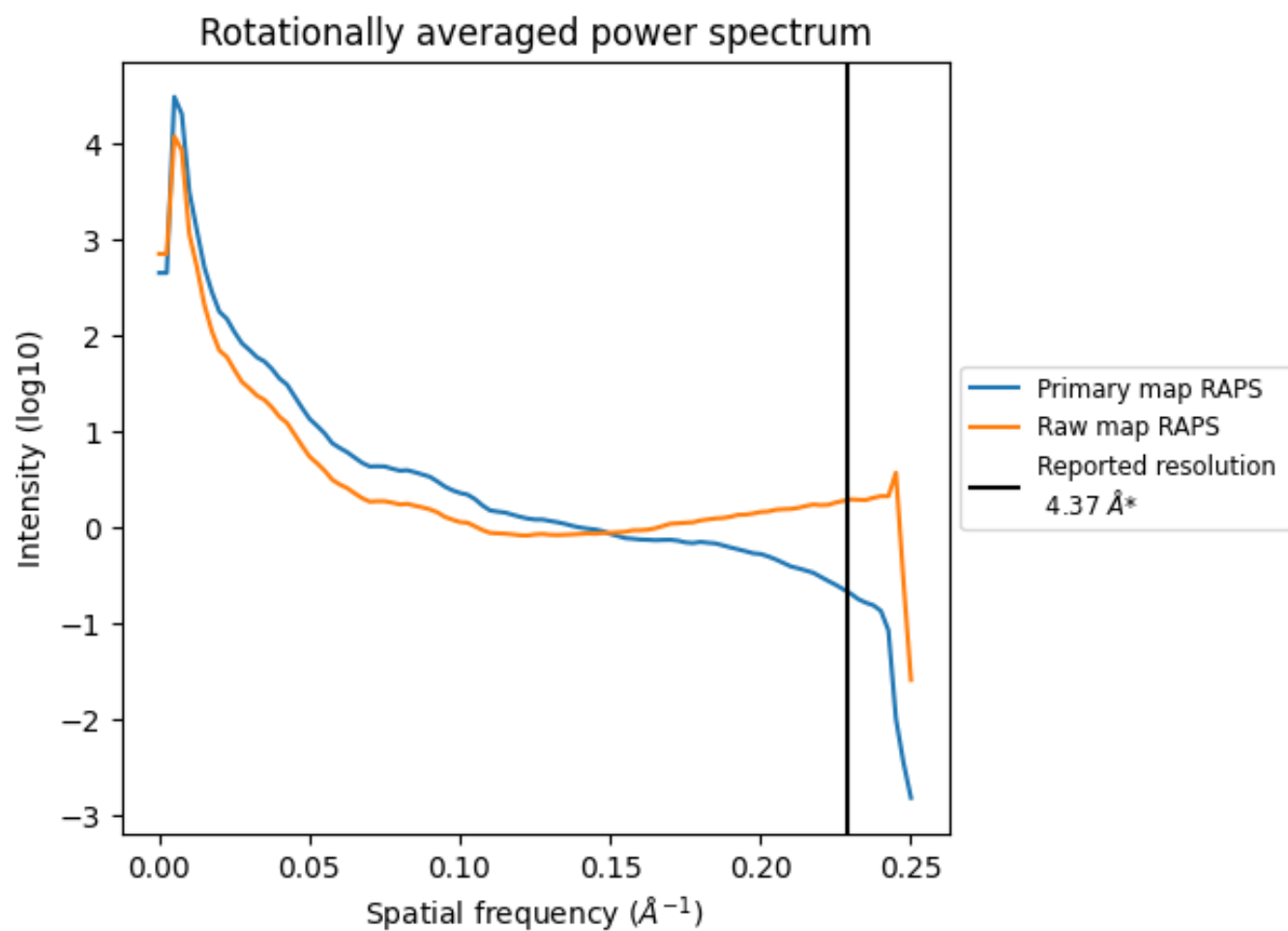
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1342 nm³; this corresponds to an approximate mass of 1212 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 ⓘ

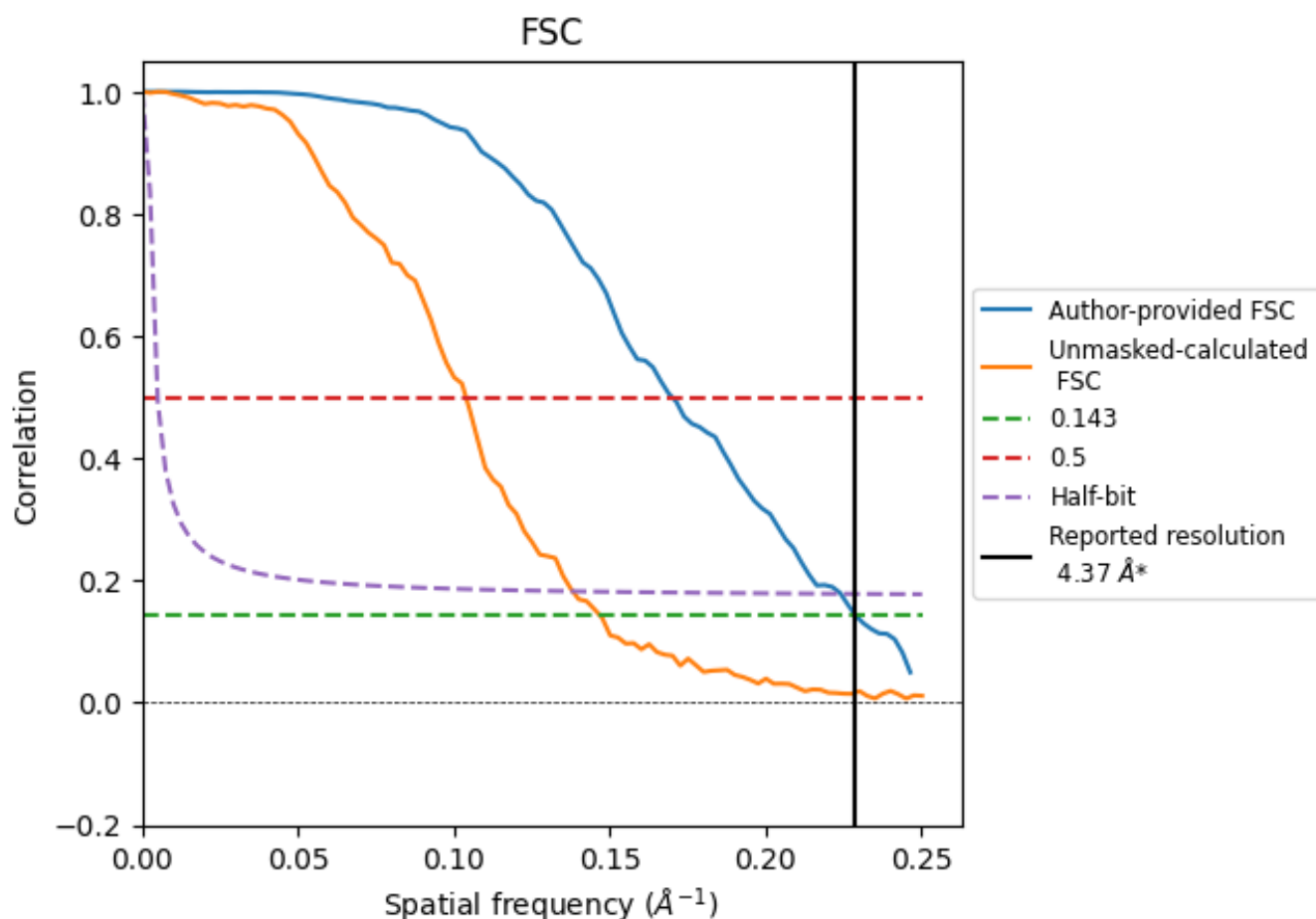


*Reported resolution corresponds to spatial frequency of 0.229 Å⁻¹

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 0.229 Å⁻¹

8.2 Resolution estimates [i](#)

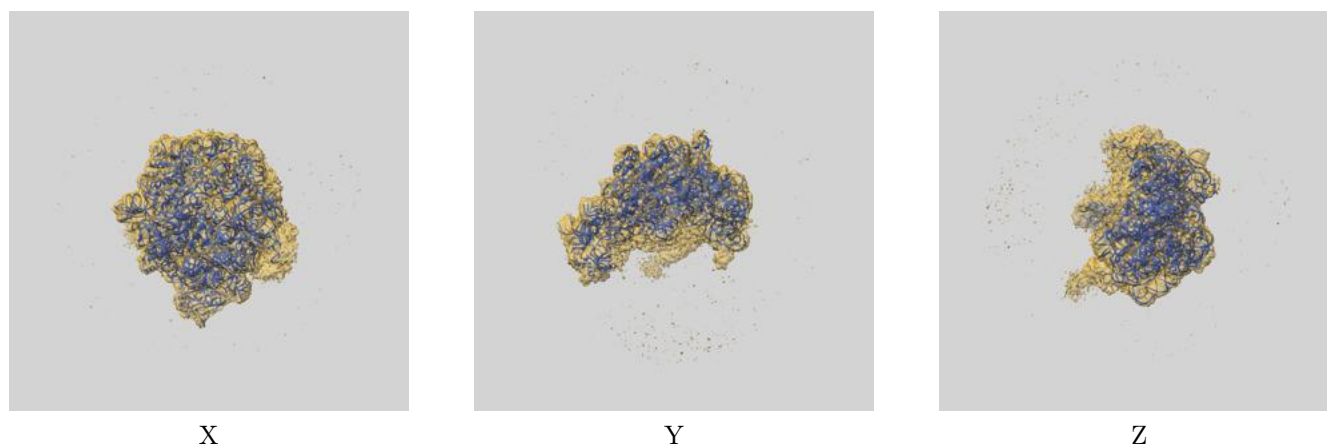
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.37	-	-
Author-provided FSC curve	4.37	5.88	4.46
Unmasked-calculated*	6.81	9.62	7.24

*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 6.81 differs from the reported value 4.37 by more than 10 %

9 Map-model fit [i](#)

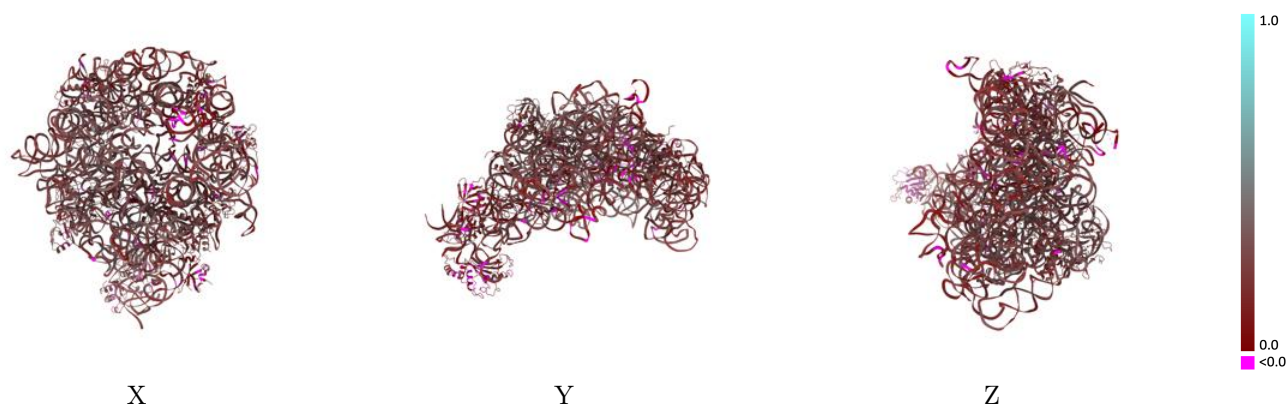
This section contains information regarding the fit between EMDB map EMD-51979 and PDB model 9HA7. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



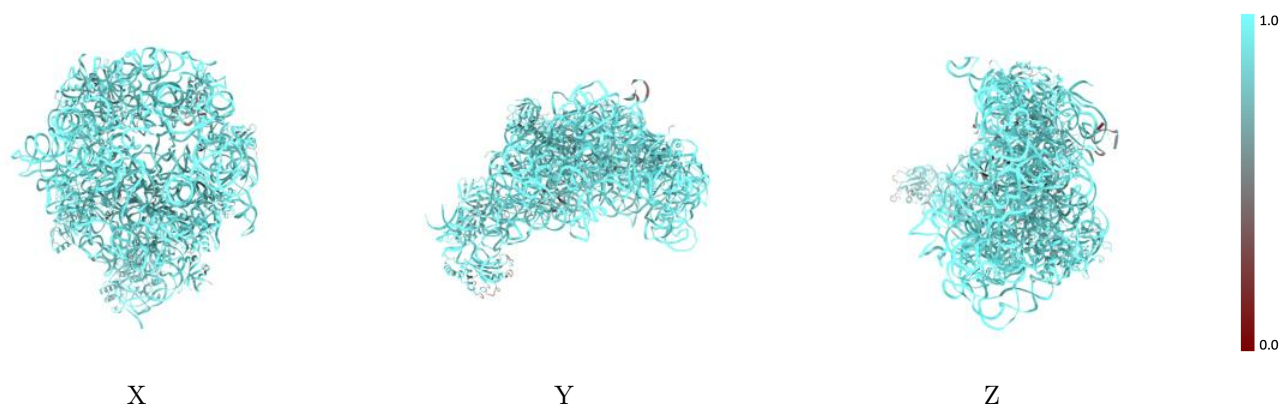
The images above show the 3D surface view of the map at the recommended contour level 0.255 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



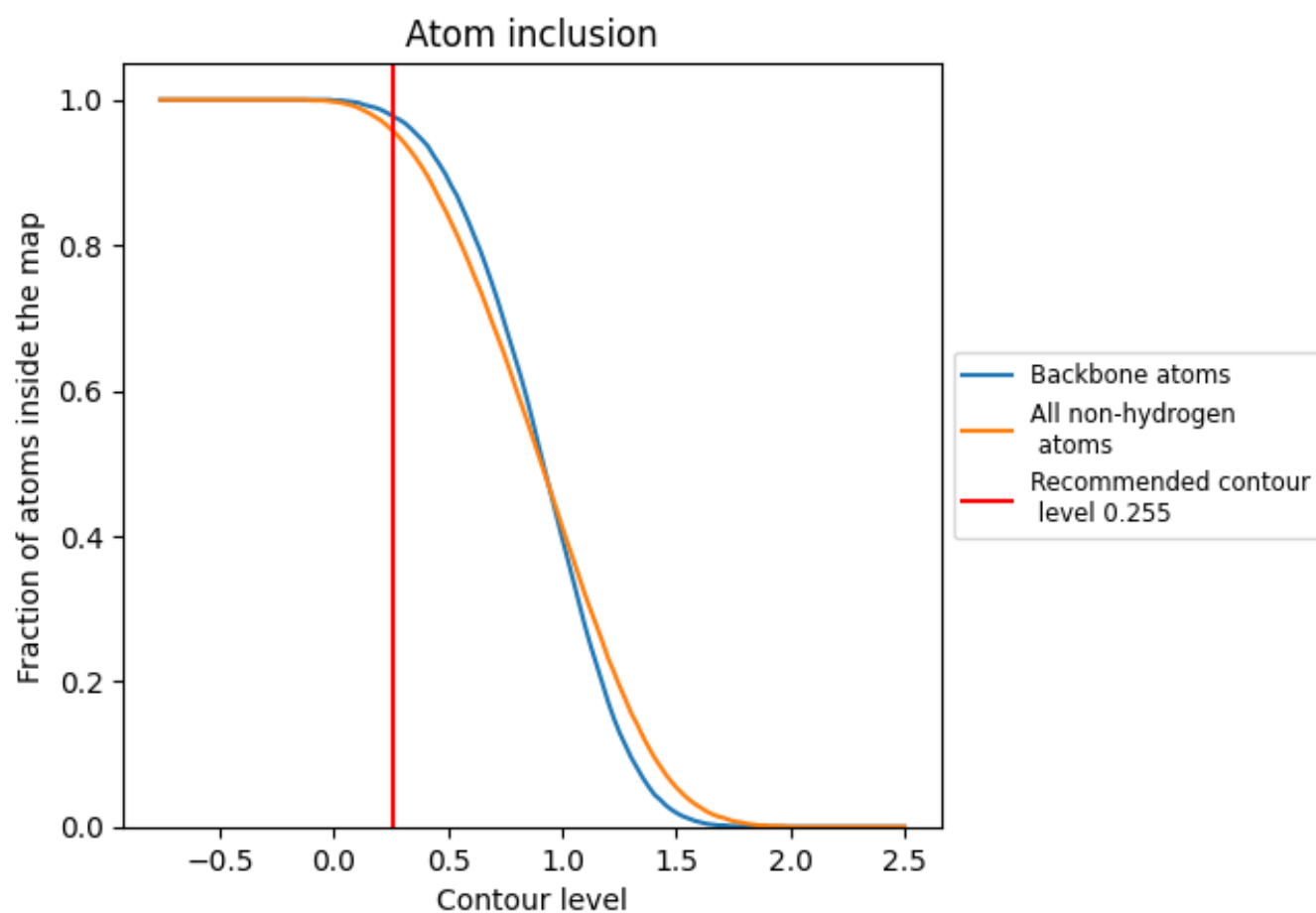
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.255).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.255) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.2430
2	 0.9030	 0.2520
A	 0.9810	 0.2550
B	 0.9760	 0.1940
D	 0.8870	 0.1710
E	 0.8960	 0.2690
F	 0.8030	 0.1160
J	 0.9370	 0.2770
L	 0.8130	 0.1800
N	 0.8760	 0.1920
O	 0.9300	 0.1730
Q	 0.9350	 0.2620
R	 0.9250	 0.3000
T	 0.8890	 0.2500
U	 0.9330	 0.2920
V	 0.8560	 0.1370
W	 0.9120	 0.2270
Y	 0.8790	 0.2260
Z	 0.9290	 0.2440
y	 0.4100	 0.0950

