



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:13 PM UTC

PDB ID : 6YTF / pdb_00006ytf
EMDB ID : EMD-10915
Title : Acinetobacter baumannii ribosome-tigecycline complex - 30S subunit head
Authors : Nicholson, D.; Edwards, T.A.; O'Neill, A.J.; Ranson, N.A.
Deposited on : 2020-04-24
Resolution : 3.00 Å(reported)
Based on initial models : 5AFI, 6YS5

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

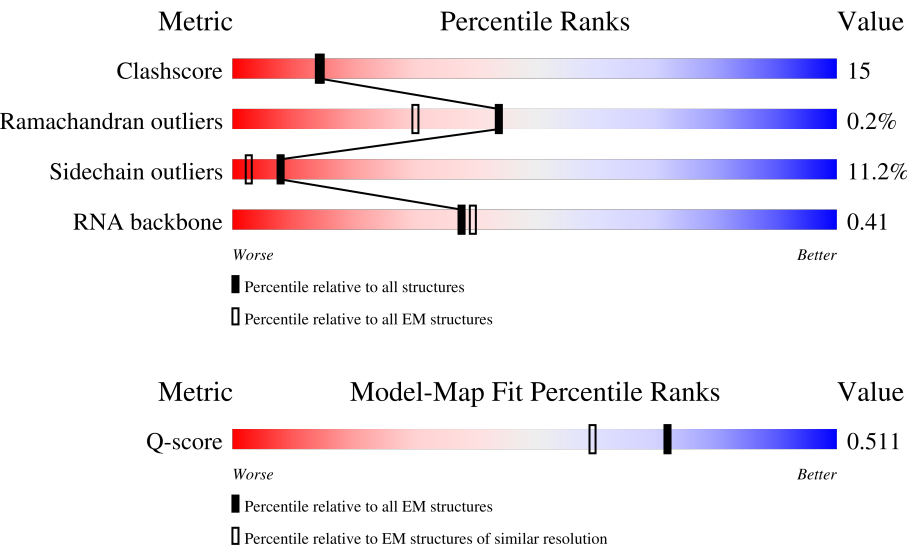
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	3	1544	 11% 15% . 71%
2	7	77	 19% 6% 17% . 74%
3	9	4	 100% 50% 50%

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Mol	Chain	Length	Quality of chain
4	d	250	
5	h	156	
6	j	128	
7	k	103	
8	n	118	
9	o	101	
10	t	91	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16906 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	453	Total	C	N	O	P	0	0
			9676	4320	1742	3161	453		

- Molecule 2 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	20	Total	C	N	O	P	0	0
			428	191	79	138	20		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	9	4	Total	C	N	O	P	0	0
			80	36	8	32	4		

- Molecule 4 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	210	Total	C	N	O	S	0	0
			1649	1040	310	292	7		

- Molecule 5 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	117	Total	C	N	O	S	0	0
			871	547	161	159	4		

- Molecule 6 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	127	Total	C	N	O	S	0	0
			995	621	198	175	1		

- Molecule 7 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	100	Total	C	N	O	S	0	0
			797	498	149	147	3		

- Molecule 8 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	n	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 9 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	o	100	Total	C	N	O	S	0	0
			791	493	158	136	4		

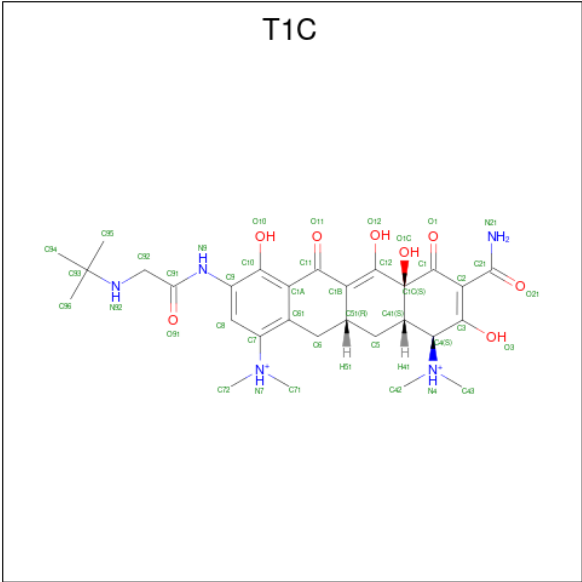
- Molecule 10 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	t	83	Total	C	N	O	S	0	0
			650	414	126	108	2		

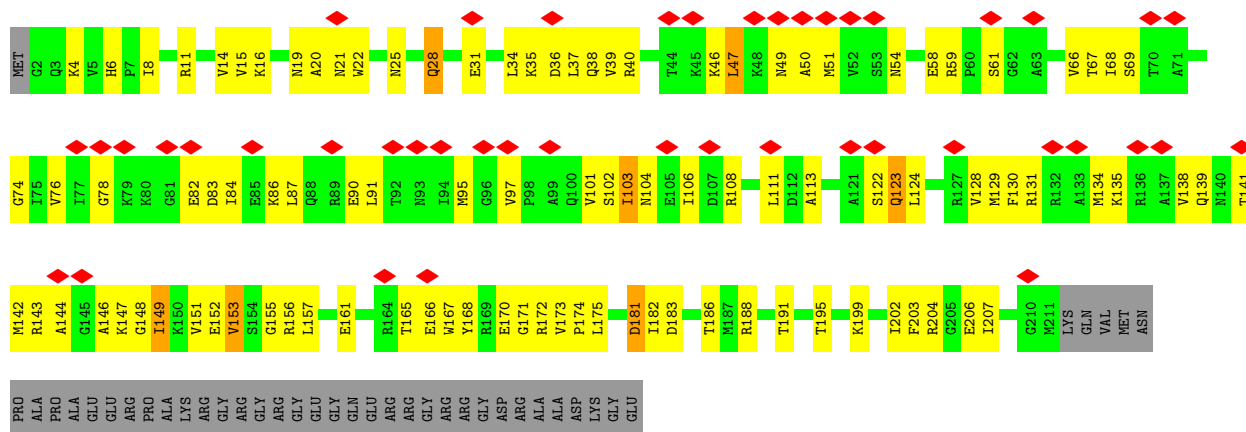
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	3	23	Total	Mg	0
			23	23	
11	n	1	Total	Mg	0
			1	1	

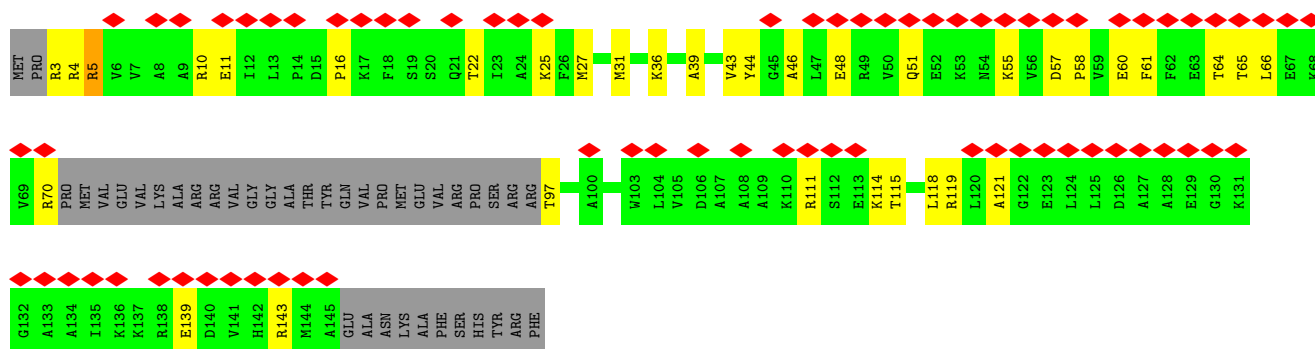
- Molecule 12 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈) (labeled as "Ligand of Interest" by depositor).



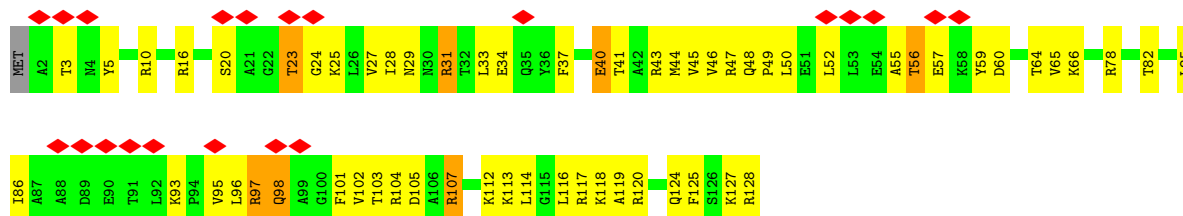
Mol	Chain	Residues	Atoms				AltConf
12	3	1	Total	C	N	O	0
			42	29	5	8	



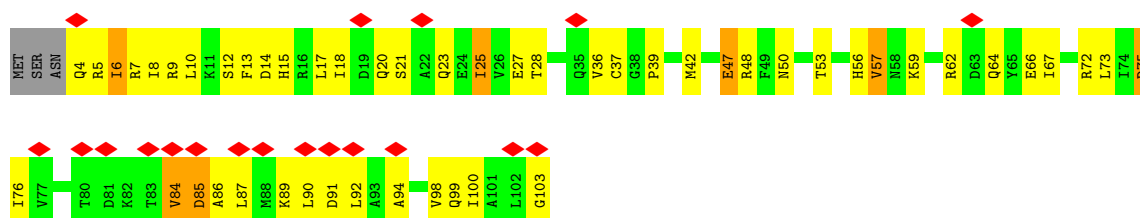
• Molecule 5: 30S ribosomal protein S7



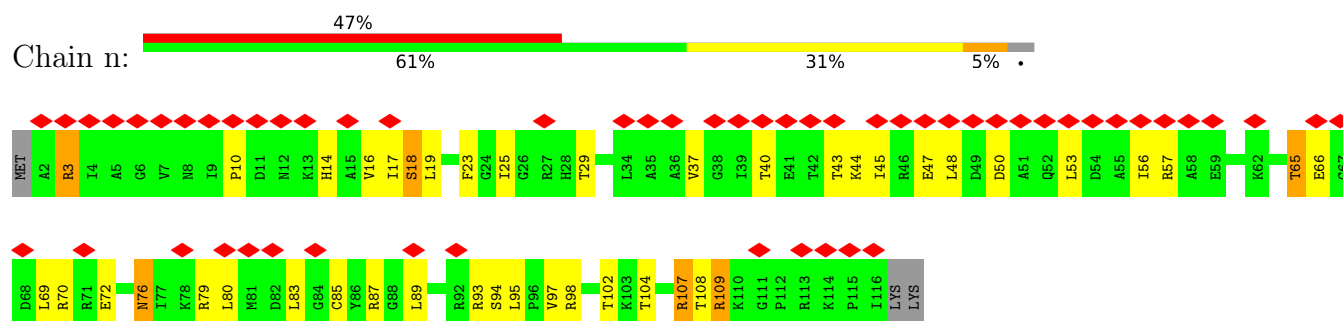
• Molecule 6: 30S ribosomal protein S9



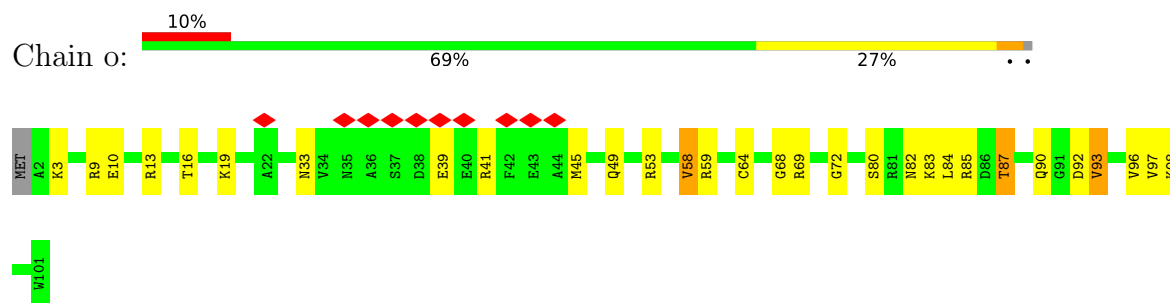
• Molecule 7: 30S ribosomal protein S10



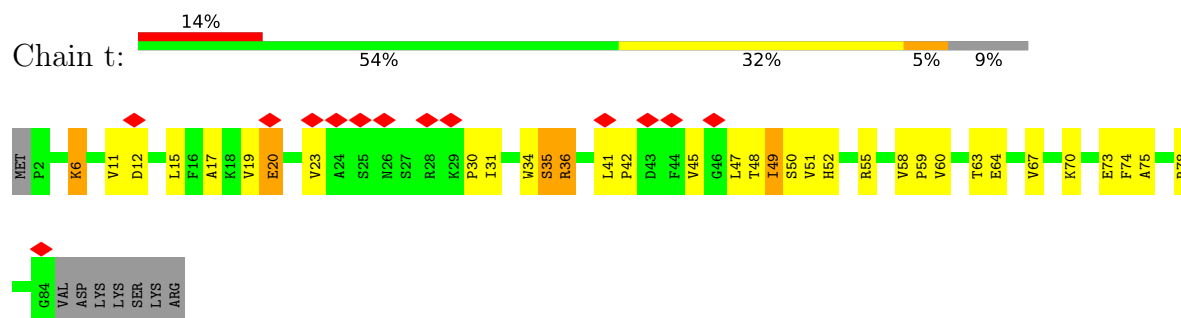
• Molecule 8: 30S ribosomal protein S13



• Molecule 9: 30S ribosomal protein S14



• Molecule 10: 30S ribosomal protein S19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	231159	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.408	Depositor
Minimum map value	-0.242	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	426.00003, 426.00003, 426.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, T1C

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	3	0.40	0/10823	0.43	0/16869
2	7	0.21	0/478	0.38	0/743
3	9	0.16	0/87	0.31	0/132
4	d	0.31	0/1673	0.57	0/2250
5	h	0.24	0/880	0.53	0/1183
6	j	0.36	0/1006	0.60	0/1346
7	k	0.37	0/807	0.56	0/1090
8	n	0.28	0/913	0.54	0/1226
9	o	0.36	0/802	0.56	0/1071
10	t	0.33	0/668	0.53	0/902
All	All	0.36	0/18137	0.48	0/26812

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	3	9676	0	4882	198	0
2	7	428	0	218	18	0
3	9	80	0	41	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	1649	0	1729	72	0
5	h	871	0	867	22	0
6	j	995	0	1053	51	0
7	k	797	0	829	40	0
8	n	903	0	962	32	0
9	o	791	0	833	25	0
10	t	650	0	666	22	0
11	3	23	0	0	0	0
11	n	1	0	0	0	0
12	3	42	0	38	4	0
All	All	16906	0	12118	432	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (432) 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)
12:3:1624:T1C:H62C	12:3:1624:T1C:H723	1.24	1.13
10:t:36:ARG:NH2	10:t:75:ALA:O	2.04	0.91
4:d:141:THR:HG21	4:d:202:ILE:HD13	1.58	0.85
12:3:1624:T1C:H62C	12:3:1624:T1C:C72	2.06	0.83
7:k:39:PRO:HA	7:k:73:LEU:O	1.79	0.83
1:3:1313:G:H4'	9:o:58:VAL:HG21	1.59	0.82
4:d:22:TRP:HB3	4:d:59:ARG:HB2	1.62	0.81
1:3:941:G:N1	1:3:1335:G:OP2	2.18	0.77
1:3:999:G:N2	1:3:1036:U:O2	2.11	0.77
1:3:1360:A:O2'	1:3:1362:G:N7	2.17	0.76
4:d:69:SER:HB2	4:d:106:ILE:HD11	1.68	0.76
9:o:64:CYS:HB3	9:o:68:GLY:H	1.50	0.76
1:3:1055:G:N2	1:3:1199:U:O4	2.16	0.73
6:j:104:ARG:NH1	6:j:105:ASP:O	2.21	0.73
1:3:1057:U:OP1	9:o:85:ARG:NH2	2.21	0.73
4:d:83:ASP:O	4:d:87:LEU:N	2.17	0.72
1:3:1311:C:H2'	1:3:1312:U:C6	2.24	0.72
6:j:97:ARG:HG2	6:j:102:VAL:HG11	1.72	0.71
1:3:1036:U:H2'	1:3:1037:A:H8	1.54	0.71
8:n:76:ASN:OD1	8:n:79:ARG:NH1	2.23	0.71
1:3:1278:U:O4	7:k:9:ARG:NH2	2.25	0.70
1:3:1052:A:O2'	4:d:156:ARG:HD2	1.91	0.70
1:3:1189:C:OP1	4:d:4:LYS:NZ	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:943:A:H2'	1:3:944:G:C8	2.27	0.70
1:3:1313:G:H22	1:3:1316:A:H5''	1.57	0.70
4:d:19:ASN:O	4:d:40:ARG:NH2	2.22	0.70
1:3:994:U:H2'	1:3:995:A:C8	2.27	0.70
5:h:114:LYS:HB3	5:h:118:LEU:HD12	1.74	0.70
4:d:129:MET:SD	4:d:129:MET:N	2.66	0.69
6:j:113:LYS:HB3	6:j:116:LEU:HD13	1.74	0.69
4:d:147:LYS:NZ	4:d:204:ARG:O	2.22	0.69
1:3:1373:U:O4	5:h:10:ARG:NH2	2.18	0.69
2:7:26:G:O6	2:7:44:A:N1	2.24	0.69
1:3:943:A:H2'	1:3:944:G:H8	1.58	0.69
10:t:31:ILE:HD11	10:t:47:LEU:HD22	1.75	0.69
5:h:46:ALA:HA	5:h:121:ALA:HB2	1.75	0.69
6:j:16:ARG:NH1	6:j:64:THR:OG1	2.27	0.68
1:3:1353:G:H2'	1:3:1354:A:C8	2.28	0.68
1:3:976:C:O2	9:o:59:ARG:NH1	2.28	0.67
1:3:1263:G:N2	1:3:1266:A:OP2	2.23	0.67
9:o:83:LYS:O	9:o:87:THR:OG1	2.13	0.67
10:t:30:PRO:HB3	10:t:48:THR:HG23	1.77	0.67
1:3:1031:G:H2'	1:3:1032:A:H8	1.59	0.66
1:3:1320:G:H2'	1:3:1321:A:C8	2.31	0.66
4:d:138:VAL:HG21	4:d:168:TYR:CE2	2.31	0.66
4:d:74:GLY:O	4:d:78:GLY:N	2.27	0.66
1:3:989:U:O2'	1:3:1039:A:N6	2.29	0.66
1:3:1001:A:OP1	1:3:1022:U:N3	2.26	0.66
1:3:1071:G:O2'	1:3:1098:A:N1	2.23	0.64
1:3:1364:C:H4'	7:k:50:ASN:ND2	2.12	0.64
1:3:1267:U:H2'	1:3:1268:G:H8	1.62	0.64
4:d:131:ARG:NH2	4:d:166:GLU:OE2	2.25	0.64
7:k:47:GLU:HG3	7:k:67:ILE:HG23	1.80	0.64
6:j:82:THR:HG21	6:j:101:PHE:HB3	1.80	0.64
1:3:1089:A:OP2	5:h:5:ARG:NH2	2.29	0.64
4:d:61:SER:HB3	7:k:92:LEU:HD11	1.80	0.64
6:j:33:LEU:HG	6:j:43:ARG:HD3	1.79	0.64
1:3:1302:G:H21	1:3:1329:A:H2	1.47	0.63
1:3:950:G:H2'	1:3:951:G:O4'	1.99	0.63
1:3:1220:C:OP2	10:t:78:ARG:NH2	2.31	0.63
4:d:122:SER:OG	4:d:123:GLN:OE1	2.15	0.63
6:j:118:LYS:O	6:j:120:ARG:N	2.28	0.63
7:k:37:CYS:HB2	7:k:75:ASP:HB2	1.79	0.63
1:3:1305:U:H2'	1:3:1306:G:H8	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:40:GLU:HA	6:j:43:ARG:HG3	1.82	0.62
1:3:1009:A:H2'	1:3:1010:G:O4'	1.98	0.62
1:3:1305:U:H2'	1:3:1306:G:C8	2.35	0.62
1:3:1310:U:H2'	1:3:1311:C:C6	2.34	0.62
1:3:1046:U:H2'	9:o:3:LYS:HD3	1.81	0.61
9:o:33:ASN:O	9:o:41:ARG:NH1	2.32	0.61
4:d:69:SER:HA	4:d:104:ASN:HB2	1.82	0.61
10:t:35:SER:OG	10:t:36:ARG:N	2.32	0.61
1:3:1127:A:H2'	1:3:1128:G:H8	1.65	0.61
4:d:108:ARG:NE	4:d:144:ALA:O	2.33	0.61
1:3:1344:G:N2	1:3:1345:U:O4	2.19	0.61
5:h:39:ALA:O	5:h:43:VAL:HG22	2.01	0.60
1:3:1008:C:H2'	1:3:1009:A:H8	1.65	0.60
1:3:1083:U:H3	1:3:1096:G:H1	1.49	0.60
1:3:1215:C:H2'	1:3:1216:A:C8	2.37	0.60
1:3:1374:A:H2	5:h:3:ARG:HD2	1.66	0.60
4:d:181:ASP:OD2	4:d:204:ARG:NH2	2.28	0.60
12:3:1624:T1C:O3	12:3:1624:T1C:H423	2.02	0.60
1:3:1255:G:H2'	1:3:1256:C:C6	2.37	0.59
8:n:23:PHE:N	8:n:66:GLU:OE2	2.30	0.59
1:3:1342:U:OP1	6:j:120:ARG:NH1	2.36	0.59
10:t:49:ILE:O	10:t:59:PRO:HA	2.02	0.59
1:3:1221:U:O2'	1:3:1319:C:OP1	2.18	0.59
1:3:1163:G:O2'	1:3:1166:A:N6	2.30	0.59
8:n:14:HIS:O	8:n:18:SER:OG	2.16	0.59
1:3:999:G:H1	1:3:1036:U:H3	1.51	0.59
1:3:1173:A:H2'	1:3:1174:G:C8	2.38	0.59
5:h:16:PRO:HB2	6:j:44:MET:HB3	1.83	0.58
2:7:43:A:H2'	2:7:44:A:C8	2.38	0.58
1:3:1310:U:OP1	10:t:6:LYS:NZ	2.33	0.58
12:3:1624:T1C:H723	12:3:1624:T1C:C6	2.14	0.58
6:j:37:PHE:O	6:j:43:ARG:NE	2.34	0.58
7:k:85:ASP:OD1	7:k:85:ASP:N	2.33	0.58
1:3:1123:U:OP1	7:k:7:ARG:NH1	2.36	0.57
1:3:1290:G:H2'	1:3:1291:A:C8	2.39	0.57
8:n:95:LEU:O	8:n:109:ARG:NH1	2.37	0.57
1:3:1364:C:H4'	7:k:50:ASN:HD21	1.69	0.57
10:t:63:THR:HG22	10:t:64:GLU:H	1.69	0.57
6:j:41:THR:HA	6:j:44:MET:HB2	1.87	0.57
4:d:108:ARG:HD2	4:d:111:LEU:HD11	1.86	0.57
1:3:1052:A:O5'	1:3:1052:A:H8	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1036:U:H2'	1:3:1037:A:C8	2.40	0.56
1:3:1140:G:H2'	1:3:1141:G:H8	1.70	0.56
1:3:1140:G:H2'	1:3:1141:G:C8	2.41	0.56
8:n:65:THR:OG1	8:n:66:GLU:N	2.26	0.56
1:3:1252:G:O2'	1:3:1255:G:H1'	2.06	0.56
1:3:974:A:O2'	1:3:976:C:OP2	2.23	0.55
8:n:37:VAL:HG21	8:n:56:ILE:HG22	1.89	0.55
10:t:15:LEU:O	10:t:19:VAL:HG23	2.05	0.55
1:3:994:U:H2'	1:3:995:A:H8	1.70	0.55
1:3:1074:G:N2	1:3:1077:A:OP2	2.35	0.55
1:3:993:A:N1	1:3:1042:C:O2'	2.32	0.55
1:3:1059:U:H2'	1:3:1060:C:C6	2.42	0.55
1:3:1306:G:OP1	8:n:87:ARG:NH2	2.32	0.55
7:k:23:GLN:O	7:k:27:GLU:HG2	2.07	0.55
1:3:930:G:O6	5:h:4:ARG:NH2	2.38	0.55
4:d:139:GLN:HB3	4:d:143:ARG:NH1	2.22	0.55
9:o:53:ARG:O	9:o:59:ARG:HD3	2.07	0.55
1:3:1019:U:H2'	1:3:1020:G:H8	1.72	0.54
1:3:1060:C:H2'	1:3:1061:G:C8	2.43	0.54
1:3:1155:C:C4	1:3:1157:G:C8	2.95	0.54
6:j:56:THR:HG23	6:j:57:GLU:HG2	1.88	0.54
1:3:1353:G:H2'	1:3:1354:A:H8	1.72	0.54
9:o:45:MET:O	9:o:49:GLN:HG2	2.07	0.54
1:3:1141:G:N2	1:3:1143:A:H62	2.06	0.54
6:j:112:LYS:NZ	6:j:113:LYS:O	2.41	0.54
1:3:1273:G:H2'	1:3:1274:C:O4'	2.08	0.54
1:3:1339:C:H2'	1:3:1340:G:C8	2.44	0.53
6:j:49:PRO:HB3	6:j:82:THR:HG22	1.90	0.53
7:k:14:ASP:OD1	7:k:17:LEU:N	2.41	0.53
1:3:947:U:H2'	1:3:948:G:H8	1.72	0.53
4:d:186:THR:OG1	4:d:199:LYS:HG2	2.09	0.53
10:t:34:TRP:CD1	10:t:52:HIS:CD2	2.96	0.53
1:3:1176:A:OP2	6:j:93:LYS:NZ	2.34	0.53
6:j:55:ALA:O	6:j:57:GLU:N	2.42	0.53
7:k:8:ILE:HG12	7:k:100:ILE:HG12	1.91	0.53
1:3:947:U:H2'	1:3:948:G:C8	2.43	0.53
1:3:964:C:OP2	1:3:965:A:O2'	2.25	0.53
1:3:1137:A:O2'	1:3:1138:U:H6	1.91	0.53
2:7:27:U:H2'	2:7:28:C:H6	1.74	0.53
7:k:48:ARG:HG2	7:k:66:GLU:HG3	1.90	0.53
1:3:954:U:O2'	1:3:956:A:N7	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1305:U:H3'	8:n:98:ARG:HH21	1.74	0.53
2:7:26:G:H1	2:7:44:A:H2	1.53	0.53
4:d:153:VAL:CG1	4:d:157:LEU:HD21	2.39	0.53
1:3:1083:U:H2'	1:3:1084:G:H8	1.74	0.53
6:j:114:LEU:HD22	7:k:64:GLN:HG3	1.90	0.52
1:3:1007:C:H2'	1:3:1008:C:C6	2.44	0.52
5:h:61:PHE:O	5:h:65:THR:HG23	2.09	0.52
1:3:1007:C:H2'	1:3:1008:C:H6	1.74	0.52
2:7:36:U:H2'	2:7:37:A:C8	2.44	0.52
1:3:1259:C:H2'	1:3:1260:A:H8	1.74	0.52
4:d:175:LEU:HD23	4:d:182:ILE:HD12	1.92	0.52
6:j:48:GLN:OE1	6:j:78:ARG:NH1	2.33	0.52
7:k:20:GLN:HA	7:k:23:GLN:HE21	1.74	0.52
1:3:1137:A:O2'	1:3:1138:U:H5'	2.09	0.52
1:3:1170:U:H2'	1:3:1171:G:O4'	2.09	0.52
5:h:66:LEU:HD13	5:h:70:ARG:NH1	2.24	0.52
1:3:1177:A:OP1	6:j:103:THR:OG1	2.22	0.52
4:d:46:LYS:NZ	4:d:90:GLU:OE1	2.41	0.52
4:d:142:MET:HG3	4:d:170:GLU:HG3	1.92	0.52
1:3:1038:G:O2'	1:3:1039:A:H5'	2.10	0.52
1:3:1335:G:H2'	1:3:1336:A:C8	2.45	0.52
4:d:183:ASP:OD1	4:d:204:ARG:NH1	2.43	0.52
6:j:23:THR:OG1	6:j:24:GLY:N	2.43	0.52
1:3:1057:U:H2'	1:3:1058:G:H8	1.75	0.52
1:3:1290:G:H2'	1:3:1291:A:H8	1.75	0.52
1:3:1323:U:H2'	1:3:1324:C:H6	1.75	0.52
1:3:962:U:OP1	1:3:1195:G:H5'	2.11	0.51
1:3:1312:U:O2'	1:3:1357:A:N3	2.39	0.51
4:d:36:ASP:OD1	4:d:59:ARG:NH2	2.29	0.51
7:k:25:ILE:HG13	7:k:90:LEU:HD23	1.92	0.51
4:d:131:ARG:O	4:d:135:LYS:HG2	2.11	0.51
1:3:1172:G:N3	1:3:1173:A:C8	2.79	0.51
4:d:8:ILE:HG23	4:d:16:LYS:HD3	1.92	0.51
6:j:86:ILE:HD12	6:j:93:LYS:HD2	1.92	0.51
4:d:174:PRO:O	4:d:182:ILE:HD11	2.11	0.51
1:3:1148:A:O2'	1:3:1149:A:O5'	2.25	0.50
4:d:47:LEU:HD22	4:d:76:VAL:HG12	1.92	0.50
1:3:1323:U:H2'	1:3:1324:C:C6	2.46	0.50
7:k:84:VAL:HA	7:k:87:LEU:HB2	1.92	0.50
1:3:1172:G:C4	1:3:1173:A:C8	2.99	0.50
4:d:181:ASP:OD1	4:d:204:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:23:PHE:CE1	8:n:70:ARG:HG3	2.47	0.50
1:3:1233:A:H4'	1:3:1301:G:H4'	1.94	0.50
4:d:152:GLU:OE2	4:d:167:TRP:HB3	2.11	0.50
6:j:114:LEU:HD13	7:k:64:GLN:NE2	2.27	0.50
1:3:1352:G:H2'	1:3:1353:G:C8	2.46	0.50
1:3:1238:G:H2'	1:3:1239:G:H8	1.77	0.50
1:3:1118:U:H2'	1:3:1119:U:C6	2.47	0.49
1:3:1259:C:H2'	1:3:1260:A:C8	2.46	0.49
4:d:86:LYS:O	4:d:86:LYS:HD3	2.12	0.49
1:3:1166:A:H2'	1:3:1167:A:C8	2.46	0.49
8:n:50:ASP:HA	8:n:53:LEU:HD13	1.94	0.49
1:3:1222:A:H2'	1:3:1223:C:C5	2.47	0.49
6:j:55:ALA:C	6:j:57:GLU:H	2.21	0.49
8:n:40:THR:HG23	8:n:43:THR:HG23	1.94	0.49
1:3:945:C:OP1	8:n:108:THR:HG22	2.13	0.49
1:3:1144:C:HO2'	6:j:5:TYR:HH	1.52	0.49
8:n:93:ARG:HB2	8:n:95:LEU:HG	1.95	0.49
1:3:1057:U:P	9:o:85:ARG:HH22	2.33	0.49
1:3:1373:U:OP2	5:h:25:LYS:NZ	2.29	0.49
2:7:41:C:H2'	2:7:42:G:C8	2.48	0.49
1:3:1019:U:H2'	1:3:1020:G:C8	2.47	0.49
4:d:146:ALA:HB1	4:d:203:PHE:O	2.13	0.49
1:3:1008:C:H2'	1:3:1009:A:C8	2.47	0.49
4:d:138:VAL:HG12	4:d:149:ILE:HD13	1.94	0.49
2:7:28:C:H2'	2:7:29:G:C8	2.48	0.48
4:d:20:ALA:HB2	4:d:40:ARG:HH21	1.78	0.48
10:t:11:VAL:HG21	10:t:41:LEU:HD11	1.94	0.48
1:3:976:C:O2	9:o:59:ARG:HG2	2.12	0.48
1:3:1220:C:P	10:t:78:ARG:HH21	2.36	0.48
8:n:16:VAL:HG13	8:n:17:ILE:HG12	1.95	0.48
1:3:1220:C:OP1	1:3:1222:A:H8	1.96	0.48
4:d:20:ALA:HB2	4:d:40:ARG:NH2	2.28	0.48
7:k:5:ARG:HE	7:k:103:GLY:HA2	1.78	0.48
1:3:1203:G:H2'	1:3:1204:G:O4'	2.14	0.48
4:d:39:VAL:HG21	4:d:95:MET:SD	2.54	0.48
4:d:54:ASN:HB3	4:d:69:SER:OG	2.13	0.48
2:7:27:U:H2'	2:7:28:C:C6	2.48	0.48
4:d:19:ASN:C	4:d:40:ARG:HH22	2.18	0.48
1:3:937:C:H2'	1:3:938:G:O4'	2.14	0.48
1:3:1369:U:H2'	1:3:1370:G:O4'	2.14	0.48
8:n:47:GLU:N	8:n:47:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:h:139:GLU:O	5:h:143:ARG:N	2.38	0.48
5:h:31:MET:SD	5:h:36:LYS:HD3	2.54	0.48
6:j:85:LEU:HD23	6:j:96:LEU:HD11	1.95	0.48
1:3:1163:G:N2	1:3:1166:A:H3'	2.29	0.48
9:o:93:VAL:HB	9:o:96:VAL:CG2	2.44	0.48
1:3:1365:G:OP1	7:k:64:GLN:NE2	2.44	0.47
5:h:3:ARG:NH1	5:h:3:ARG:HA	2.29	0.47
1:3:959:C:H1'	1:3:1198:A:C6	2.49	0.47
1:3:1127:A:H2'	1:3:1128:G:C8	2.46	0.47
2:7:39:C:H2'	2:7:40:C:H6	1.78	0.47
1:3:1285:A:H2'	1:3:1286:A:C8	2.50	0.47
2:7:33:U:N3	2:7:36:U:OP2	2.48	0.47
4:d:130:PHE:CD1	4:d:157:LEU:HD22	2.49	0.47
4:d:152:GLU:OE1	4:d:165:THR:OG1	2.32	0.47
2:7:28:C:H2'	2:7:29:G:H8	1.80	0.47
7:k:59:LYS:O	7:k:62:ARG:NE	2.41	0.47
8:n:3:ARG:O	8:n:57:ARG:NH2	2.45	0.47
1:3:1138:U:O2'	1:3:1139:G:H5''	2.15	0.47
1:3:1383:G:H2'	1:3:1384:G:C8	2.49	0.47
10:t:34:TRP:NE1	10:t:52:HIS:CD2	2.83	0.47
1:3:1157:G:H22	1:3:1173:A:H2	1.62	0.47
4:d:15:VAL:HB	4:d:207:ILE:HD12	1.96	0.47
7:k:7:ARG:HH21	7:k:73:LEU:HD21	1.80	0.47
1:3:1317:C:O2	10:t:36:ARG:NH1	2.45	0.47
7:k:15:HIS:HA	7:k:18:ILE:HG22	1.96	0.47
4:d:25:ASN:ND2	4:d:28:GLN:HE21	2.13	0.47
6:j:10:ARG:O	6:j:104:ARG:NH1	2.47	0.47
6:j:33:LEU:HD11	6:j:43:ARG:HB3	1.97	0.46
1:3:1036:U:C2	1:3:1037:A:C8	3.03	0.46
2:7:38:A:H2'	2:7:39:C:O4'	2.14	0.46
7:k:25:ILE:O	7:k:28:THR:HB	2.15	0.46
3:9:2:U:C2	3:9:3:U:C5	3.03	0.46
4:d:102:SER:OG	4:d:103:ILE:N	2.48	0.46
1:3:979:U:H4'	1:3:980:A:O4'	2.16	0.46
4:d:148:GLY:HA3	4:d:172:ARG:O	2.15	0.46
5:h:111:ARG:HD3	5:h:119:ARG:HB3	1.98	0.46
2:7:33:U:OP2	6:j:128:ARG:NH1	2.47	0.46
5:h:27:MET:HE2	5:h:43:VAL:HG21	1.97	0.46
6:j:33:LEU:HD21	6:j:47:ARG:HE	1.81	0.46
1:3:1325:C:H2'	1:3:1326:A:O4'	2.16	0.46
7:k:12:SER:OG	7:k:13:PHE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1220:C:O5'	1:3:1221:U:H5''	2.17	0.45
5:h:114:LYS:HG3	5:h:115:THR:H	1.79	0.45
1:3:972:A:N1	1:3:1363:C:O2'	2.43	0.45
1:3:1072:U:O4	1:3:1073:C:N4	2.50	0.45
6:j:29:ASN:O	6:j:31:ARG:NH2	2.49	0.45
8:n:109:ARG:HG3	8:n:109:ARG:HH11	1.81	0.45
1:3:1379:C:H2'	1:3:1380:C:H6	1.82	0.45
4:d:6:HIS:HD2	4:d:8:ILE:H	1.64	0.45
1:3:1145:U:H2'	1:3:1146:U:O4'	2.16	0.45
1:3:1292:U:H2'	1:3:1293:C:C6	2.52	0.45
4:d:39:VAL:HG21	4:d:95:MET:HG2	1.97	0.45
4:d:11:ARG:HG3	4:d:16:LYS:HG3	1.97	0.45
6:j:105:ASP:OD2	6:j:107:ARG:HG3	2.16	0.45
6:j:113:LYS:HB2	6:j:116:LEU:HD22	1.99	0.45
5:h:51:GLN:O	5:h:55:LYS:HD2	2.16	0.45
10:t:17:ALA:O	10:t:20:GLU:HG3	2.16	0.45
1:3:1016:G:H5'	1:3:1017:A:OP2	2.17	0.45
8:n:10:PRO:HG2	8:n:18:SER:HB3	1.97	0.45
1:3:1061:G:H1'	1:3:1187:G:N2	2.32	0.45
1:3:1115:U:H5'	6:j:104:ARG:HG2	1.98	0.45
1:3:1329:A:H2'	1:3:1330:A:O4'	2.17	0.45
2:7:44:A:H2'	2:7:45:G:O4'	2.17	0.45
7:k:10:LEU:HD23	7:k:98:VAL:HG22	1.98	0.45
1:3:1031:G:H2'	1:3:1032:A:C8	2.44	0.44
6:j:34:GLU:HA	6:j:43:ARG:NE	2.32	0.44
1:3:1054:G:O2'	4:d:188:ARG:HG2	2.17	0.44
1:3:1118:U:H2'	1:3:1119:U:H6	1.82	0.44
1:3:1110:C:H4'	4:d:14:VAL:HG13	1.97	0.44
7:k:42:MET:HE3	7:k:42:MET:HB3	1.62	0.44
10:t:49:ILE:HB	10:t:51:VAL:HG13	1.98	0.44
1:3:1052:A:O5'	1:3:1052:A:C8	2.70	0.44
7:k:28:THR:HG21	7:k:90:LEU:HD22	1.99	0.44
9:o:97:VAL:HG23	9:o:98:LYS:O	2.17	0.44
1:3:987:C:H2'	1:3:988:U:C6	2.53	0.44
1:3:1154:A:H4'	1:3:1155:C:O4'	2.18	0.44
1:3:1365:G:P	7:k:64:GLN:HE22	2.40	0.44
1:3:1085:G:H2'	1:3:1086:G:O4'	2.18	0.44
1:3:1117:C:C2	1:3:1118:U:C5	3.06	0.44
5:h:5:ARG:H	5:h:5:ARG:HG2	1.50	0.44
1:3:926:G:H2'	1:3:927:C:C6	2.53	0.44
6:j:40:GLU:HB3	6:j:43:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:94:SER:HA	8:n:109:ARG:NH2	2.33	0.44
4:d:66:VAL:O	4:d:101:VAL:HA	2.17	0.44
6:j:25:LYS:HB3	6:j:60:ASP:OD1	2.17	0.44
4:d:39:VAL:HG22	4:d:91:LEU:HD22	2.00	0.43
1:3:1032:A:H2'	1:3:1033:A:C8	2.53	0.43
6:j:78:ARG:O	6:j:82:THR:HG23	2.18	0.43
8:n:44:LYS:HB2	8:n:47:GLU:OE2	2.18	0.43
1:3:943:A:C2	1:3:944:G:C5	3.06	0.43
1:3:1010:G:N2	1:3:1013:A:OP2	2.27	0.43
1:3:1218:G:H5''	1:3:1318:U:O2	2.18	0.43
4:d:138:VAL:HG21	4:d:168:TYR:CD2	2.53	0.43
2:7:27:U:O2'	2:7:28:C:OP1	2.34	0.43
7:k:86:ALA:HA	7:k:89:LYS:HB3	2.00	0.43
1:3:1338:U:H2'	1:3:1339:C:C6	2.54	0.43
1:3:1357:A:C8	9:o:58:VAL:HG22	2.53	0.43
8:n:83:LEU:HA	8:n:83:LEU:HD23	1.61	0.43
1:3:972:A:H8	1:3:1354:A:HO2'	1.59	0.43
4:d:206:GLU:H	4:d:206:GLU:HG2	1.64	0.43
6:j:98:GLN:H	6:j:98:GLN:HG2	1.67	0.43
1:3:1175:G:N2	1:3:1178:G:OP2	2.52	0.43
1:3:1275:U:H5''	1:3:1276:A:O4'	2.19	0.43
5:h:44:TYR:O	5:h:48:GLU:HG2	2.19	0.43
6:j:118:LYS:HB3	6:j:118:LYS:HE3	1.80	0.43
1:3:1236:A:H62	1:3:1296:A:N6	2.17	0.43
6:j:114:LEU:HD13	7:k:64:GLN:HE21	1.84	0.43
8:n:69:LEU:HD12	8:n:72:GLU:OE2	2.19	0.43
9:o:39:GLU:H	9:o:39:GLU:CD	2.26	0.43
9:o:69:ARG:O	9:o:80:SER:OG	2.33	0.43
1:3:972:A:O2'	9:o:72:GLY:HA2	2.19	0.43
8:n:25:ILE:HG23	8:n:29:THR:HG22	2.01	0.43
1:3:1104:C:OP1	4:d:172:ARG:NH1	2.52	0.43
4:d:151:VAL:O	4:d:167:TRP:HA	2.19	0.43
6:j:20:SER:O	6:j:59:TYR:HA	2.19	0.43
1:3:1222:A:OP1	8:n:102:THR:OG1	2.29	0.42
1:3:1046:U:C2'	9:o:3:LYS:HD3	2.48	0.42
2:7:39:C:H2'	2:7:40:C:C6	2.54	0.42
4:d:50:ALA:O	4:d:51:MET:HE2	2.18	0.42
7:k:56:HIS:ND1	7:k:57:VAL:HG22	2.33	0.42
1:3:993:A:H2'	1:3:994:U:C6	2.54	0.42
6:j:40:GLU:O	6:j:44:MET:HE3	2.19	0.42
8:n:48:LEU:HD12	8:n:48:LEU:HA	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1303:A:H2'	1:3:1304:U:O4'	2.19	0.42
9:o:90:GLN:HG3	9:o:92:ASP:CG	2.44	0.42
1:3:959:C:H2'	1:3:960:G:O4'	2.20	0.42
4:d:34:LEU:O	4:d:38:GLN:HG3	2.19	0.42
4:d:124:LEU:HD23	4:d:124:LEU:HA	1.89	0.42
8:n:85:CYS:HB3	10:t:74:PHE:CE2	2.55	0.42
1:3:1382:G:H2'	1:3:1383:G:O4'	2.20	0.42
5:h:58:PRO:HA	5:h:61:PHE:HB3	2.01	0.42
7:k:10:LEU:HB2	7:k:18:ILE:HD11	2.02	0.42
1:3:973:G:H5''	1:3:1355:U:O2'	2.19	0.42
1:3:1064:A:N1	1:3:1105:G:O2'	2.46	0.42
1:3:1163:G:N2	1:3:1167:A:OP2	2.51	0.42
1:3:1339:C:H2'	1:3:1340:G:H8	1.85	0.42
9:o:64:CYS:HB2	9:o:80:SER:OG	2.19	0.42
1:3:1016:G:C5	1:3:1017:A:N7	2.88	0.42
1:3:1045:G:N3	1:3:1047:G:C8	2.88	0.42
1:3:1255:G:H2'	1:3:1256:C:H6	1.83	0.42
6:j:86:ILE:CG2	6:j:96:LEU:HD12	2.50	0.42
10:t:70:LYS:O	10:t:73:GLU:HG3	2.19	0.42
1:3:960:G:N2	7:k:57:VAL:HG11	2.35	0.42
1:3:1037:A:N1	1:3:1038:G:C6	2.87	0.42
1:3:1054:G:H5'	4:d:155:GLY:HA3	2.02	0.42
4:d:91:LEU:HD23	4:d:91:LEU:HA	1.85	0.42
6:j:40:GLU:H	6:j:40:GLU:HG2	1.72	0.42
6:j:52:LEU:HD23	6:j:96:LEU:HD23	2.01	0.42
1:3:971:A:OP1	9:o:69:ARG:NH1	2.48	0.42
1:3:1311:C:H2'	1:3:1312:U:H6	1.82	0.42
1:3:1344:G:O2'	1:3:1370:G:O6	2.32	0.42
1:3:1099:A:H2'	1:3:1100:C:C6	2.55	0.41
4:d:134:MET:O	4:d:138:VAL:HG13	2.20	0.41
1:3:1167:A:H3'	1:3:1168:A:H8	1.83	0.41
1:3:1169:C:C2	1:3:1170:U:C5	3.09	0.41
1:3:1257:U:O2'	1:3:1258:A:H5'	2.20	0.41
7:k:8:ILE:HG23	7:k:98:VAL:HG13	2.02	0.41
8:n:48:LEU:HB3	8:n:53:LEU:HD11	2.02	0.41
8:n:80:LEU:HD23	8:n:80:LEU:HA	1.89	0.41
1:3:927:C:H2'	1:3:928:C:C6	2.55	0.41
8:n:107:ARG:H	8:n:107:ARG:HG2	1.36	0.41
9:o:10:GLU:OE1	9:o:13:ARG:HD2	2.20	0.41
6:j:117:ARG:HA	6:j:117:ARG:HD3	1.75	0.41
8:n:19:LEU:HD23	8:n:19:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1048:C:H2'	1:3:1049:U:C6	2.56	0.41
2:7:26:G:C6	2:7:44:A:N1	2.88	0.41
8:n:109:ARG:HD2	8:n:109:ARG:HA	1.89	0.41
1:3:1160:A:C6	1:3:1171:G:C6	3.09	0.41
4:d:181:ASP:CG	4:d:204:ARG:HH21	2.21	0.41
4:d:87:LEU:HD23	4:d:87:LEU:HA	1.93	0.41
4:d:135:LYS:O	4:d:138:VAL:HG22	2.21	0.41
9:o:9:ARG:HG2	9:o:13:ARG:NH1	2.36	0.41
10:t:42:PRO:O	10:t:45:VAL:HG23	2.21	0.41
1:3:944:G:H2'	1:3:945:C:H6	1.86	0.41
1:3:957:U:O2'	1:3:1220:C:H4'	2.20	0.41
1:3:972:A:H5''	1:3:972:A:N3	2.36	0.41
1:3:1086:G:H2'	1:3:1087:U:O4'	2.21	0.41
1:3:1123:U:O2	1:3:1277:A:H2'	2.20	0.41
1:3:1149:A:OP1	7:k:72:ARG:NH2	2.54	0.41
1:3:1149:A:P	7:k:72:ARG:HH22	2.44	0.41
1:3:1173:A:H2'	1:3:1174:G:O4'	2.20	0.41
6:j:50:LEU:HD23	6:j:50:LEU:HA	1.88	0.41
6:j:95:VAL:O	6:j:98:GLN:HG2	2.21	0.41
8:n:23:PHE:HD1	8:n:66:GLU:HA	1.86	0.41
9:o:16:THR:O	9:o:19:LYS:N	2.53	0.41
4:d:123:GLN:HB3	4:d:128:VAL:HG21	2.02	0.41
4:d:148:GLY:HA2	4:d:171:GLY:HA3	2.02	0.41
2:7:37:A:H2'	2:7:38:A:H8	1.86	0.40
4:d:35:LYS:HB3	4:d:59:ARG:HH22	1.86	0.40
4:d:135:LYS:HD2	4:d:168:TYR:CD1	2.55	0.40
5:h:60:GLU:O	5:h:64:THR:HG22	2.20	0.40
10:t:35:SER:O	10:t:36:ARG:HB2	2.21	0.40
1:3:1021:G:H2'	1:3:1022:U:C6	2.57	0.40
1:3:1372:A:H2'	1:3:1373:U:O4'	2.21	0.40
4:d:21:ASN:O	7:k:94:ALA:HB1	2.21	0.40
7:k:6:ILE:HB	7:k:76:ILE:HB	2.03	0.40
7:k:53:THR:HG22	9:o:85:ARG:HD2	2.02	0.40
10:t:31:ILE:HB	10:t:49:ILE:HG23	2.04	0.40
1:3:944:G:H2'	1:3:945:C:C6	2.56	0.40
6:j:125:PHE:CZ	6:j:127:LYS:HG3	2.57	0.40
1:3:1176:A:O5'	6:j:97:ARG:NH2	2.54	0.40
1:3:1312:U:H2'	1:3:1313:G:O4'	2.22	0.40
4:d:113:ALA:N	4:d:183:ASP:OD2	2.54	0.40
10:t:19:VAL:O	10:t:23:VAL:HG23	2.22	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	
4	d	208/250 (83%)	189 (91%)	19 (9%)	0	100	100
5	h	113/156 (72%)	102 (90%)	11 (10%)	0	100	100
6	j	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	7	34
7	k	98/103 (95%)	88 (90%)	10 (10%)	0	100	100
8	n	113/118 (96%)	104 (92%)	9 (8%)	0	100	100
9	o	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
10	t	81/91 (89%)	75 (93%)	6 (7%)	0	100	100
All	All	836/947 (88%)	761 (91%)	73 (9%)	2 (0%)	44	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	j	119	ALA
6	j	56	THR

5.3.2 Protein sidechains [i](#)

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	
4	d	170/198 (86%)	150 (88%)	20 (12%)	5	22
5	h	82/128 (64%)	77 (94%)	5 (6%)	17	49
6	j	99/100 (99%)	85 (86%)	14 (14%)	3	16
7	k	88/91 (97%)	76 (86%)	12 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	n	95/98 (97%)	85 (90%)	10 (10%)	6	27
9	o	81/82 (99%)	76 (94%)	5 (6%)	16	49
10	t	70/78 (90%)	59 (84%)	11 (16%)	2	13
All	All	685/775 (88%)	608 (89%)	77 (11%)	8	24

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	28	GLN
4	d	31	GLU
4	d	37	LEU
4	d	47	LEU
4	d	49	ASN
4	d	58	GLU
4	d	67	THR
4	d	68	ILE
4	d	82	GLU
4	d	84	ILE
4	d	97	VAL
4	d	103	ILE
4	d	123	GLN
4	d	149	ILE
4	d	153	VAL
4	d	161	GLU
4	d	173	VAL
4	d	181	ASP
4	d	191	THR
4	d	195	THR
5	h	5	ARG
5	h	11	GLU
5	h	22	THR
5	h	57	ASP
5	h	97	THR
6	j	3	THR
6	j	23	THR
6	j	27	VAL
6	j	28	ILE
6	j	31	ARG
6	j	40	GLU
6	j	45	VAL
6	j	46	VAL

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Mol	Chain	Res	Type
6	j	65	VAL
6	j	66	LYS
6	j	97	ARG
6	j	98	GLN
6	j	107	ARG
6	j	124	GLN
7	k	4	GLN
7	k	6	ILE
7	k	21	SER
7	k	25	ILE
7	k	36	VAL
7	k	47	GLU
7	k	57	VAL
7	k	75	ASP
7	k	84	VAL
7	k	85	ASP
7	k	91	ASP
7	k	99	GLN
8	n	3	ARG
8	n	18	SER
8	n	45	ILE
8	n	65	THR
8	n	76	ASN
8	n	89	LEU
8	n	97	VAL
8	n	104	THR
8	n	107	ARG
8	n	109	ARG
9	o	58	VAL
9	o	82	ASN
9	o	84	LEU
9	o	87	THR
9	o	93	VAL
10	t	6	LYS
10	t	12	ASP
10	t	20	GLU
10	t	35	SER
10	t	36	ARG
10	t	49	ILE
10	t	50	SER
10	t	55	ARG
10	t	58	VAL

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Mol	Chain	Res	Type
10	t	60	VAL
10	t	67	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
4	d	3	GLN
4	d	6	HIS
4	d	21	ASN
4	d	28	GLN
4	d	93	ASN
4	d	104	ASN
5	h	21	GLN
5	h	29	HIS
5	h	51	GLN
6	j	29	ASN
6	j	73	GLN
6	j	79	HIS
6	j	124	GLN
7	k	23	GLN
7	k	35	GLN
7	k	64	GLN
9	o	71	HIS
9	o	82	ASN
10	t	14	HIS
10	t	52	HIS
10	t	65	HIS
10	t	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	451/1544 (29%)	108 (23%)	1 (0%)
2	7	19/77 (24%)	1 (5%)	1 (5%)
3	9	3/4 (75%)	0	0
All	All	473/1625 (29%)	109 (23%)	2 (0%)

All (109) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	931	C
1	3	932	A
1	3	939	G
1	3	942	G
1	3	957	U
1	3	960	G
1	3	961	A
1	3	963	G
1	3	966	A
1	3	971	A
1	3	972	A
1	3	973	G
1	3	974	A
1	3	975	A
1	3	978	U
1	3	981	C
1	3	984	G
1	3	989	U
1	3	990	G
1	3	1001	A
1	3	1002	A
1	3	1003	C
1	3	1015	G
1	3	1016	G
1	3	1017	A
1	3	1018	U
1	3	1041	A
1	3	1043	A
1	3	1050	G
1	3	1055	G
1	3	1061	G
1	3	1062	U
1	3	1067	U
1	3	1075	U
1	3	1078	G
1	3	1082	U
1	3	1086	G
1	3	1088	U
1	3	1091	G
1	3	1092	U
1	3	1098	A
1	3	1123	U
1	3	1128	G

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Mol	Chain	Res	Type
1	3	1130	A
1	3	1132	U
1	3	1133	U
1	3	1134	C
1	3	1136	G
1	3	1137	A
1	3	1138	U
1	3	1149	A
1	3	1154	A
1	3	1155	C
1	3	1157	G
1	3	1165	C
1	3	1167	A
1	3	1171	G
1	3	1172	G
1	3	1173	A
1	3	1180	C
1	3	1181	G
1	3	1188	A
1	3	1189	C
1	3	1193	A
1	3	1194	A
1	3	1196	U
1	3	1197	C
1	3	1209	U
1	3	1210	A
1	3	1211	C
1	3	1217	G
1	3	1221	U
1	3	1223	C
1	3	1224	A
1	3	1225	C
1	3	1235	A
1	3	1254	U
1	3	1255	G
1	3	1257	U
1	3	1259	C
1	3	1276	A
1	3	1277	A
1	3	1282	A
1	3	1284	A
1	3	1287	G

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Mol	Chain	Res	Type
1	3	1296	A
1	3	1299	C
1	3	1302	G
1	3	1314	C
1	3	1315	A
1	3	1316	A
1	3	1317	C
1	3	1319	C
1	3	1329	A
1	3	1332	U
1	3	1333	C
1	3	1337	A
1	3	1343	A
1	3	1350	G
1	3	1351	C
1	3	1360	A
1	3	1361	U
1	3	1363	C
1	3	1365	G
1	3	1367	G
1	3	1376	G
1	3	1378	U
1	3	1384	G
2	7	28	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	1154	A
2	7	27	U

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

Of 25 ligands modelled in this entry, 24 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	T1C	3	1624	11	45,45,45	1.16	4 (8%)	56,72,72	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	T1C	3	1624	11	-	7/22/80/80	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	1624	T1C	C21-N21	5.00	1.47	1.33
12	3	1624	T1C	C4-N4	2.21	1.52	1.47
12	3	1624	T1C	O11-C11	2.21	1.27	1.23
12	3	1624	T1C	C7-N7	2.10	1.48	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

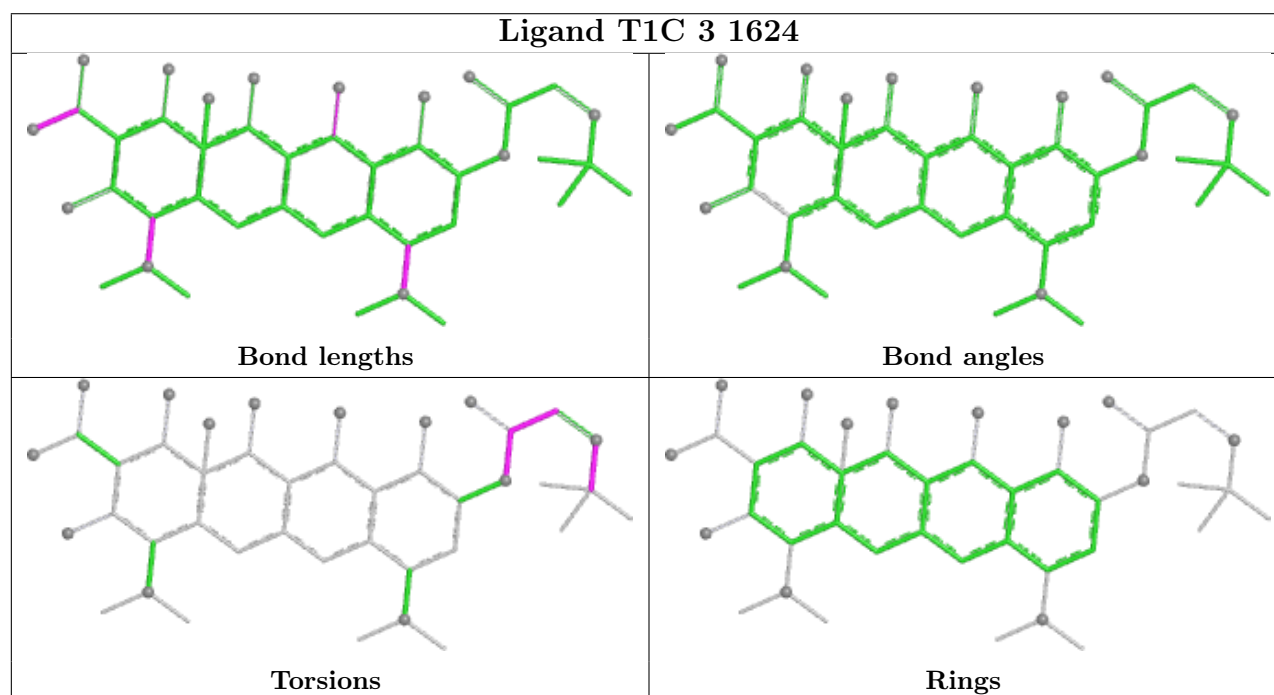
Mol	Chain	Res	Type	Atoms
12	3	1624	T1C	C95-C93-N92-C92
12	3	1624	T1C	C96-C93-N92-C92
12	3	1624	T1C	C92-C91-N9-C9
12	3	1624	T1C	C94-C93-N92-C92
12	3	1624	T1C	O91-C91-N9-C9
12	3	1624	T1C	N9-C91-C92-N92
12	3	1624	T1C	O91-C91-C92-N92

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	3	1624	T1C	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

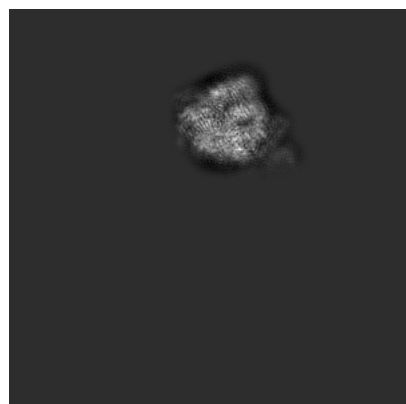
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10915. These allow visual inspection of the internal detail of the map and identification of artifacts.

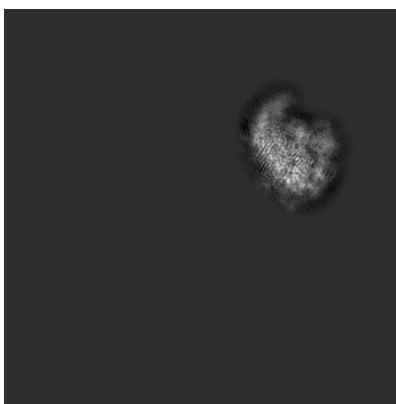
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

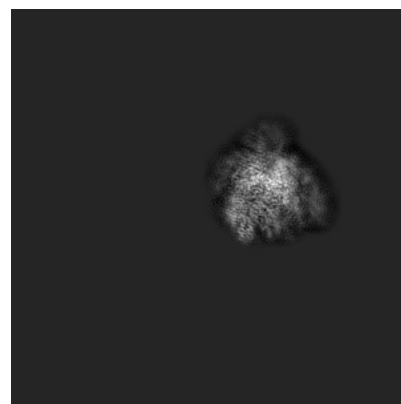
6.1.1 Primary map



X

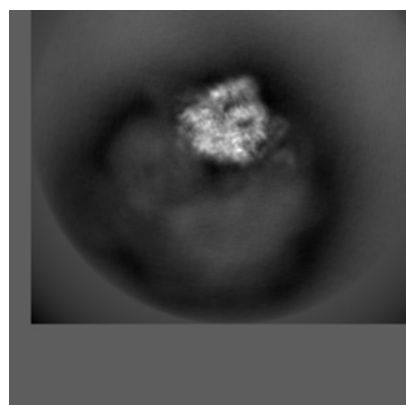


Y

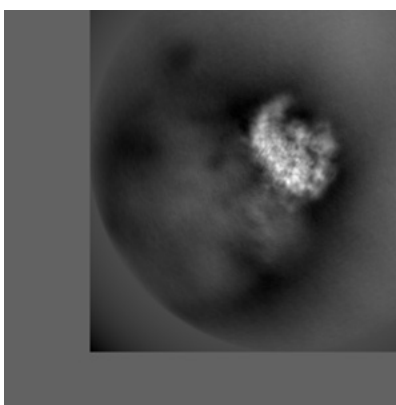


Z

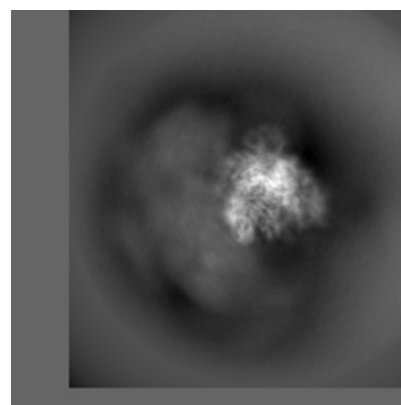
6.1.2 Raw map



X



Y

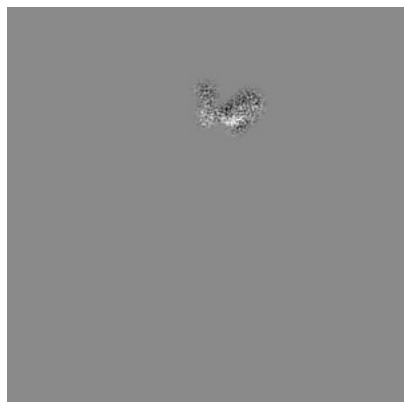


Z

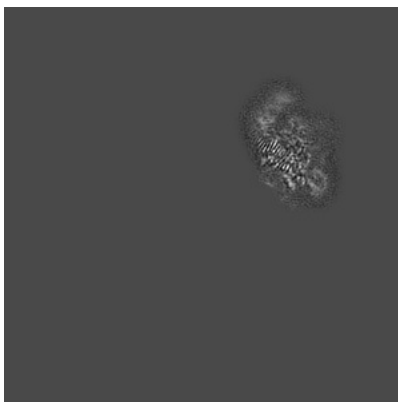
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

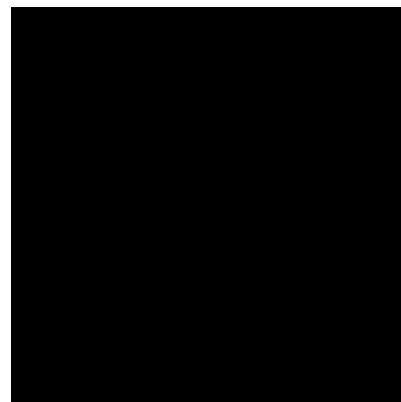
6.2.1 Primary map



X Index: 200

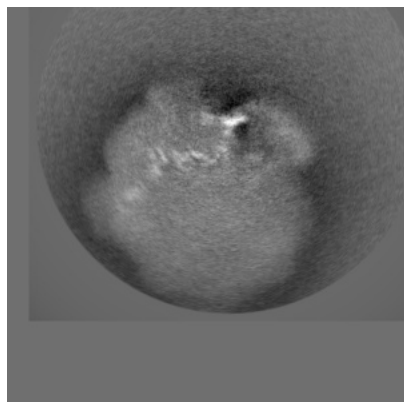


Y Index: 200

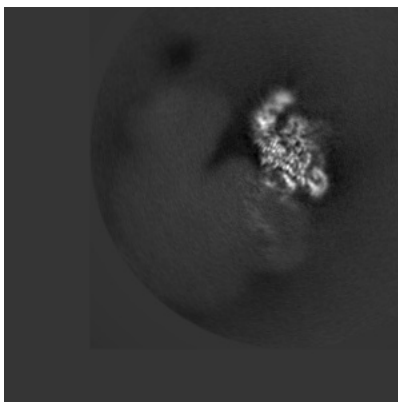


Z Index: 200

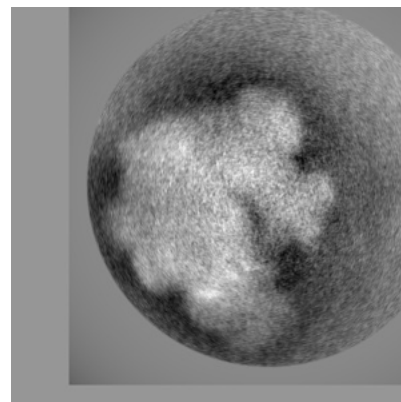
6.2.2 Raw map



X Index: 200



Y Index: 200

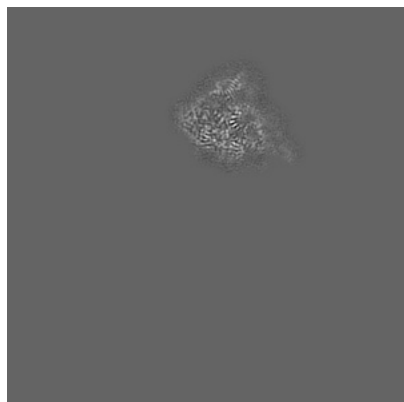


Z Index: 200

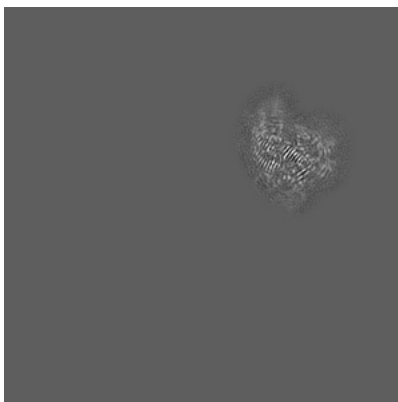
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

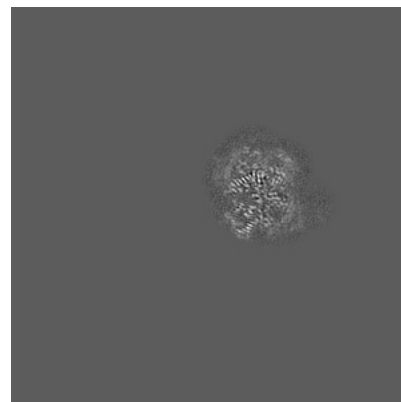
6.3.1 Primary map



X Index: 256

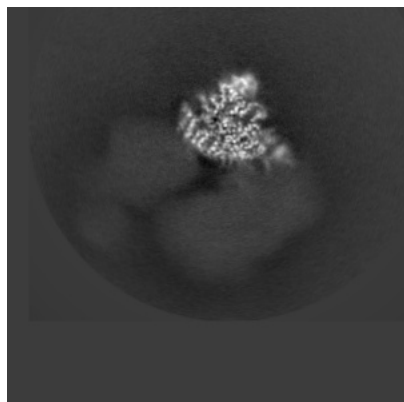


Y Index: 226

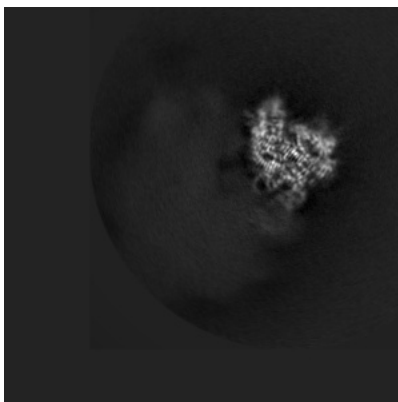


Z Index: 295

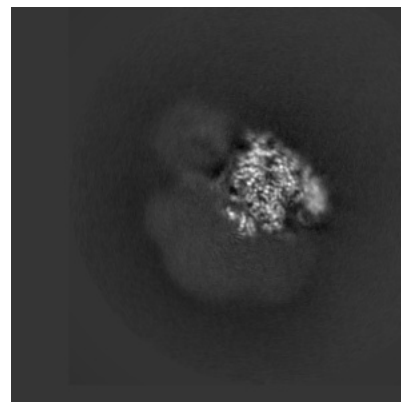
6.3.2 Raw map



X Index: 266



Y Index: 226



Z Index: 274

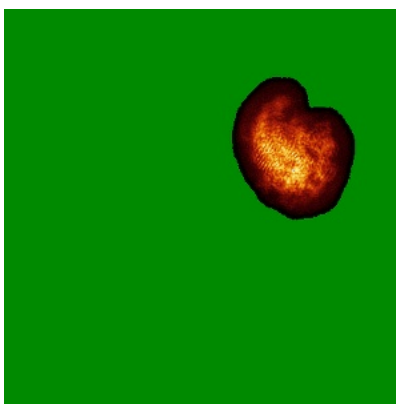
The images above show the largest variance slices of the map in three orthogonal directions.

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

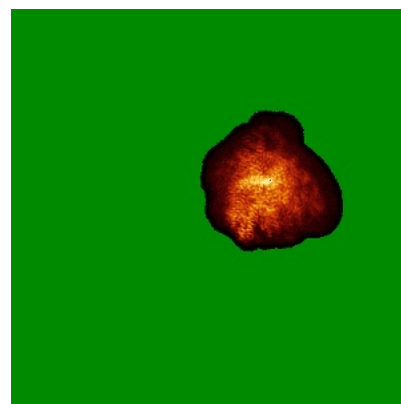
6.4.1 Primary map



X

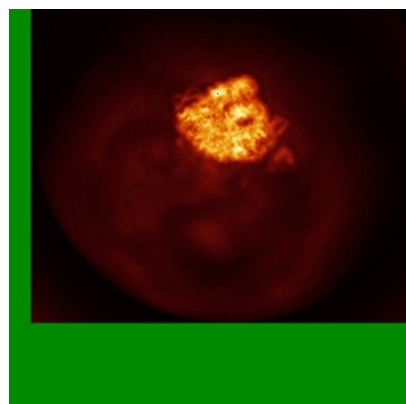


Y

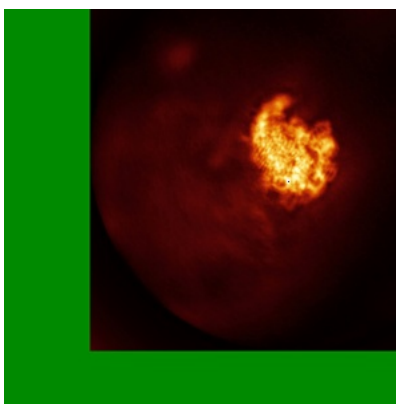


Z

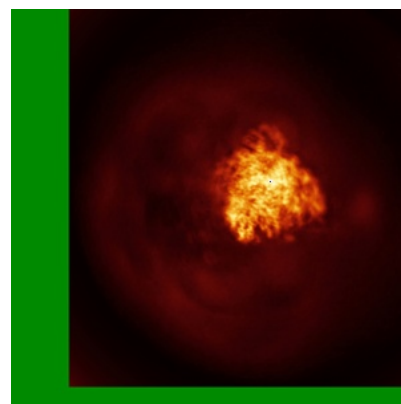
6.4.2 Raw map



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 0.05. 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.

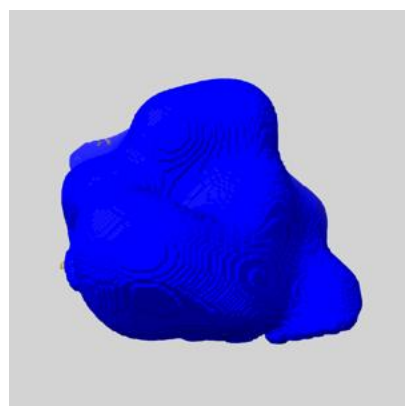
6.6 Mask visualisation [i](#)

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

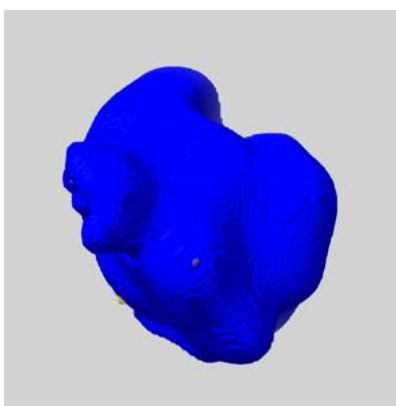
A mask typically either:

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

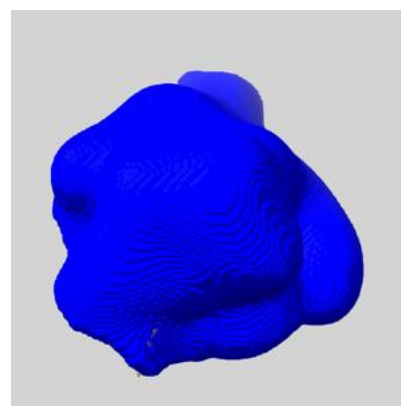
6.6.1 emd_10915_msk_1.map [i](#)



X



Y

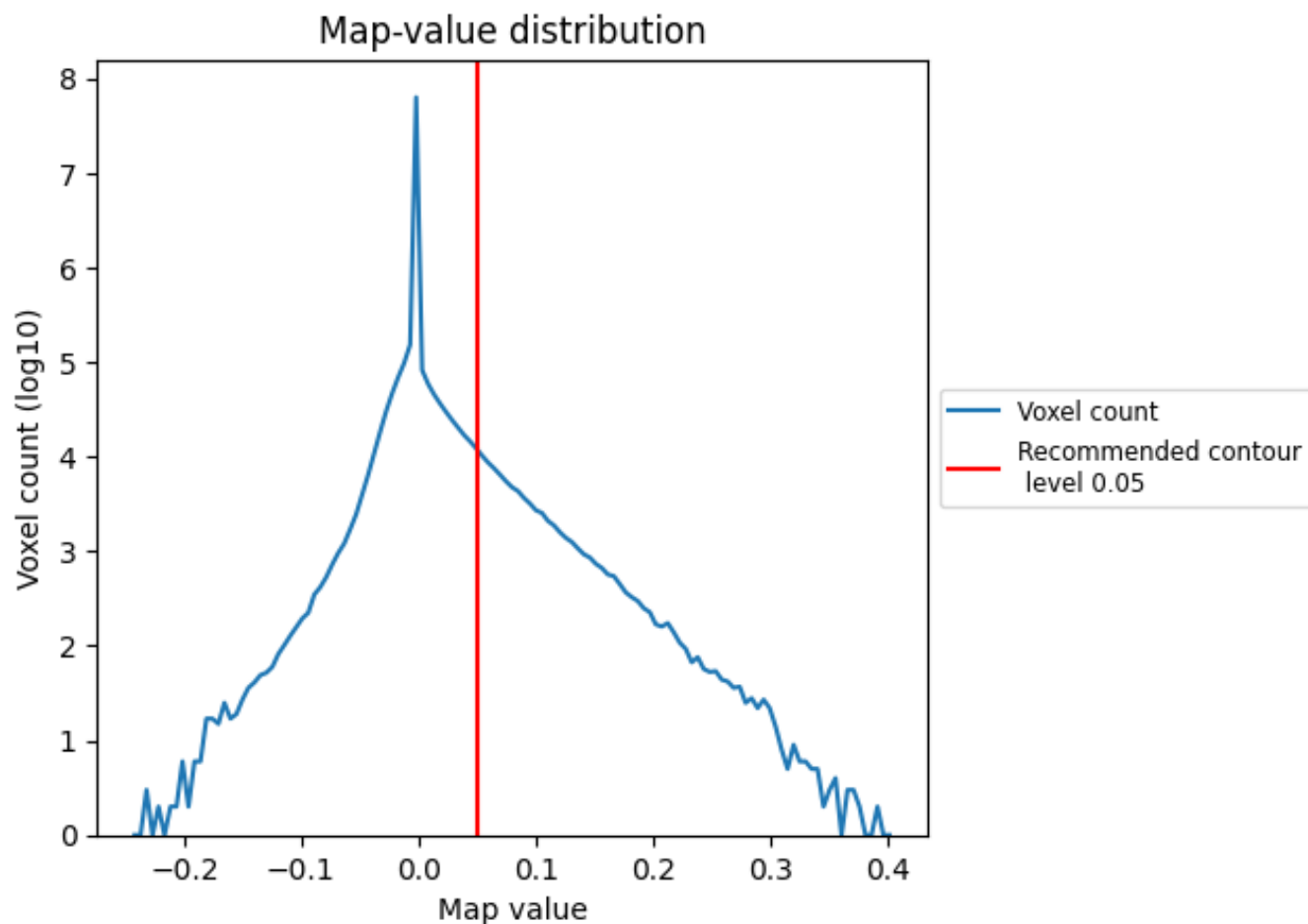


Z

7 Map analysis [i](#)

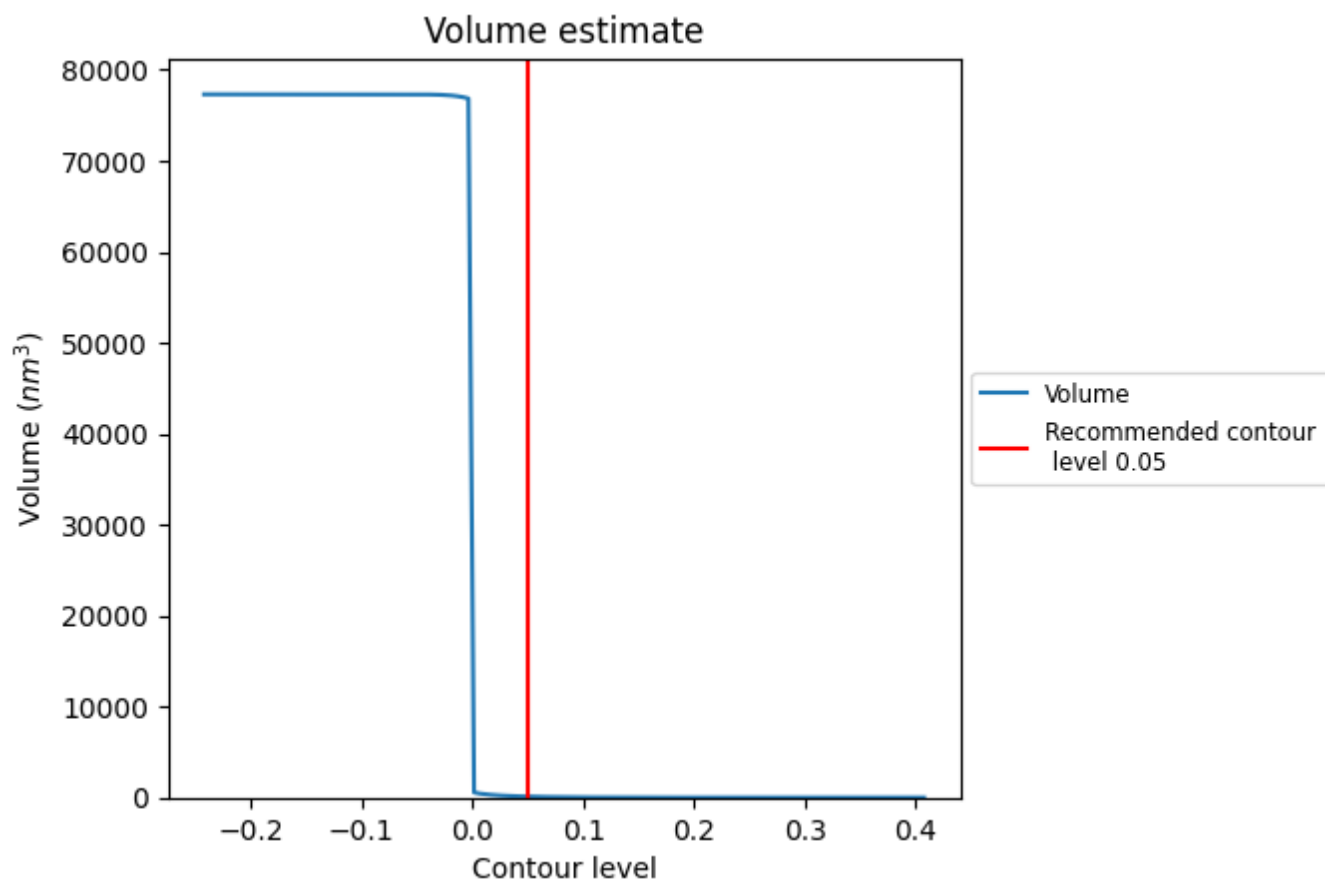
This section contains the results of statistical analysis of the map.

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.

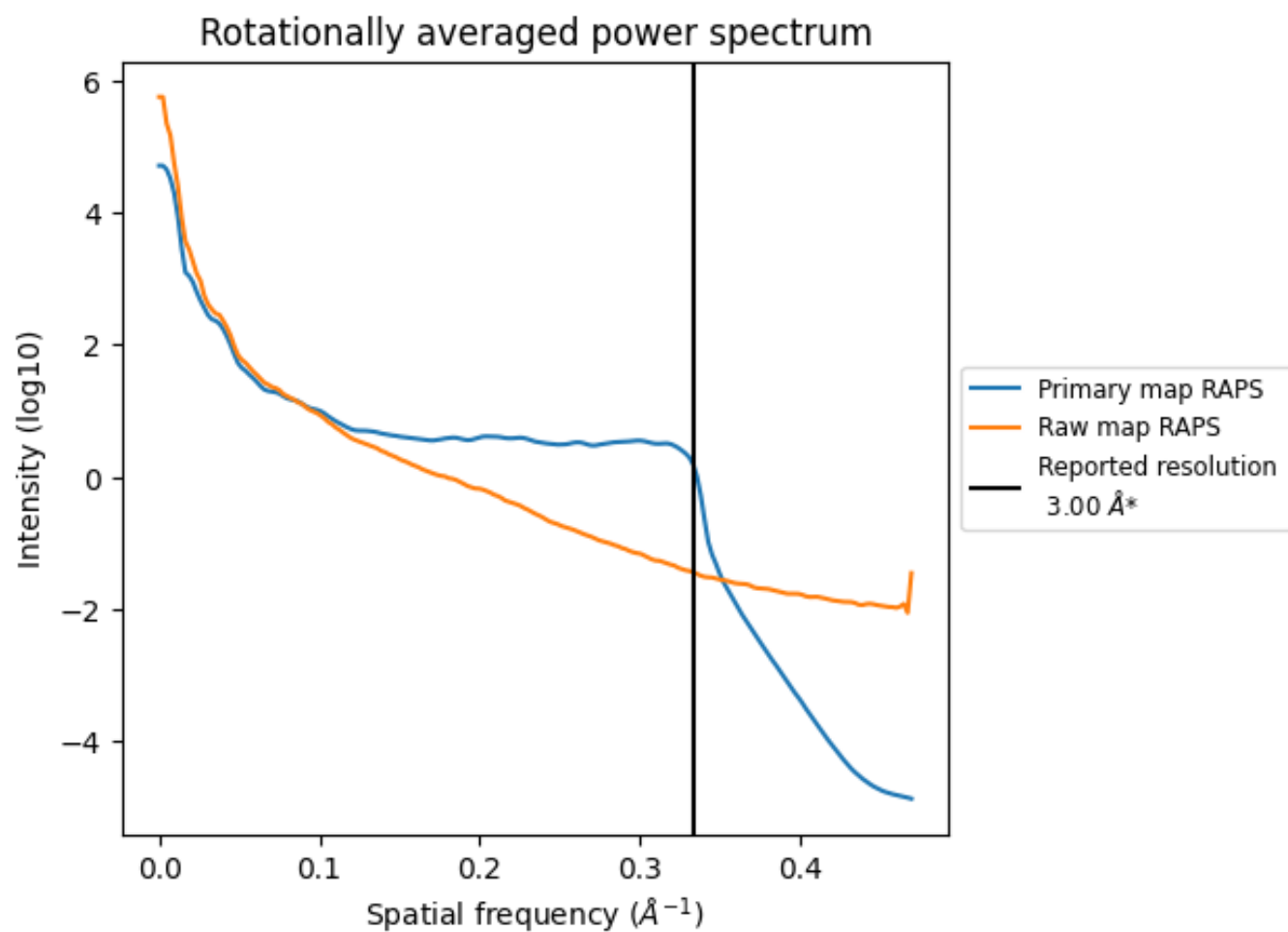
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm³; this corresponds to an approximate mass of 96 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

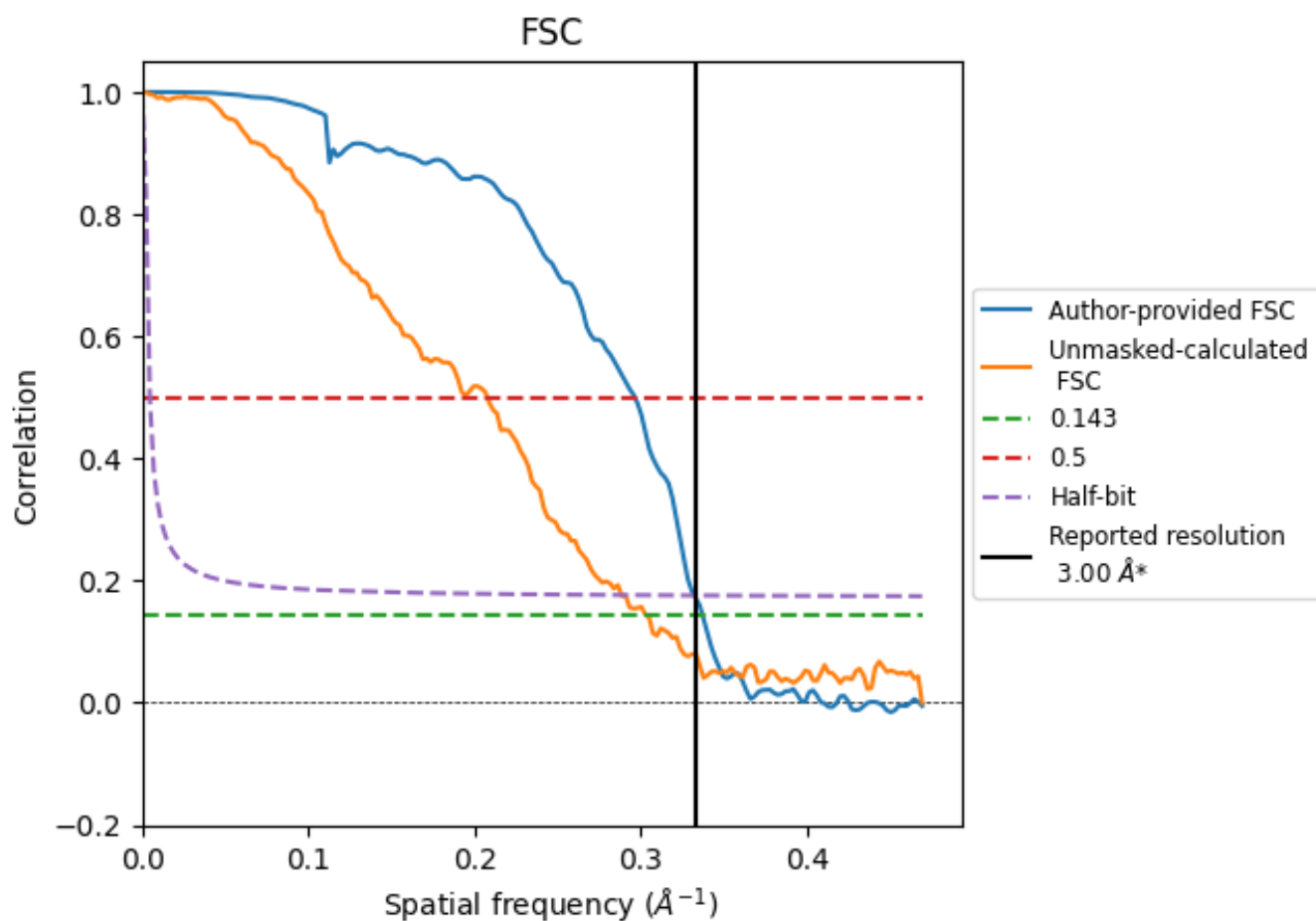


*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

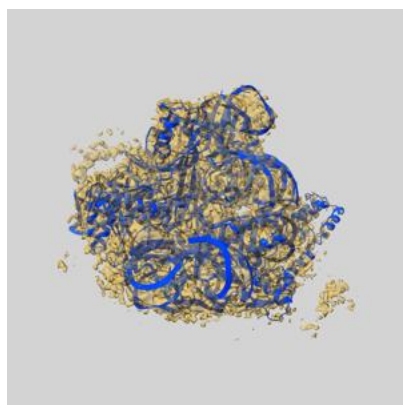
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.96	3.37	3.01
Unmasked-calculated*	3.29	4.81	3.47

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

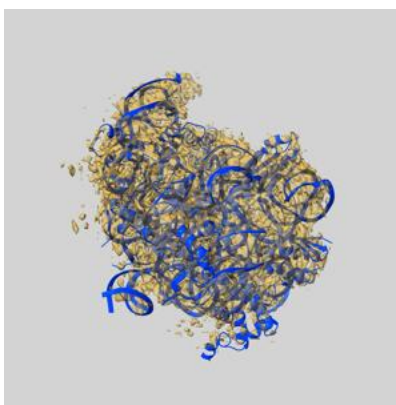
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10915 and PDB model 6YTF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

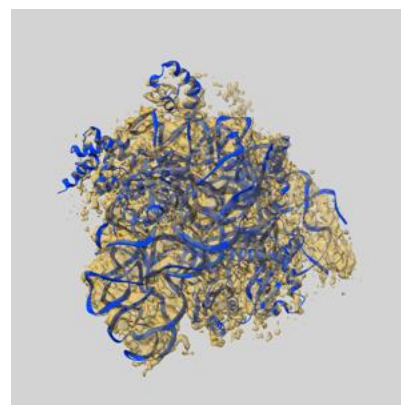
9.1 Map-model overlay [i](#)



X



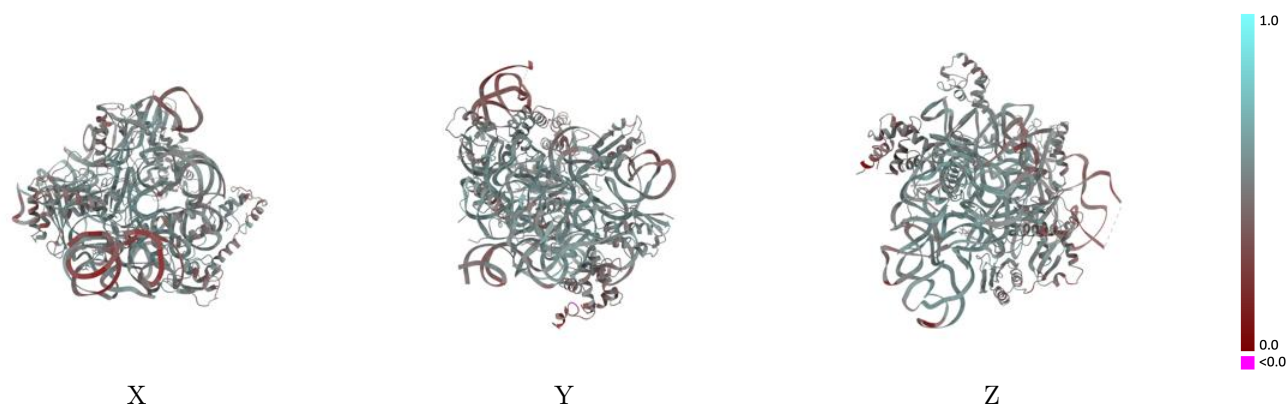
Y



Z

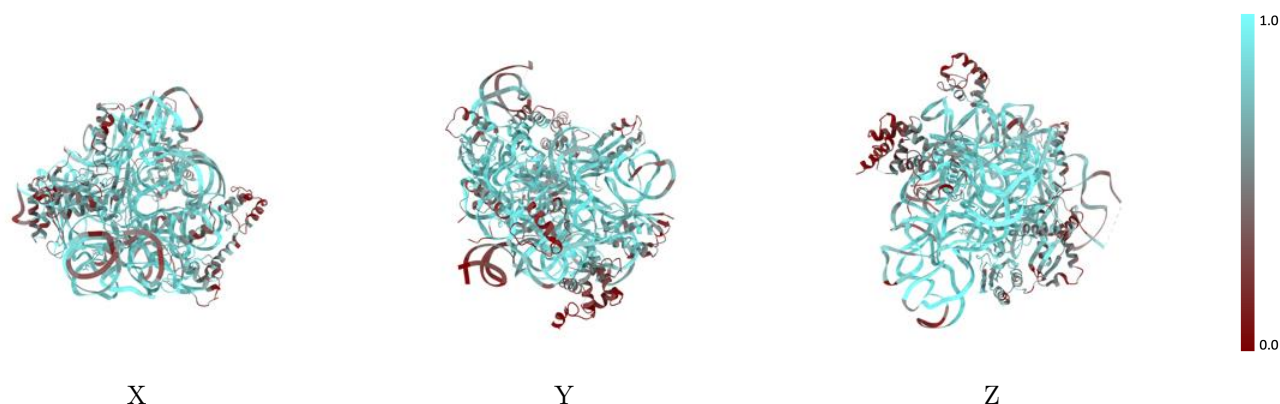
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



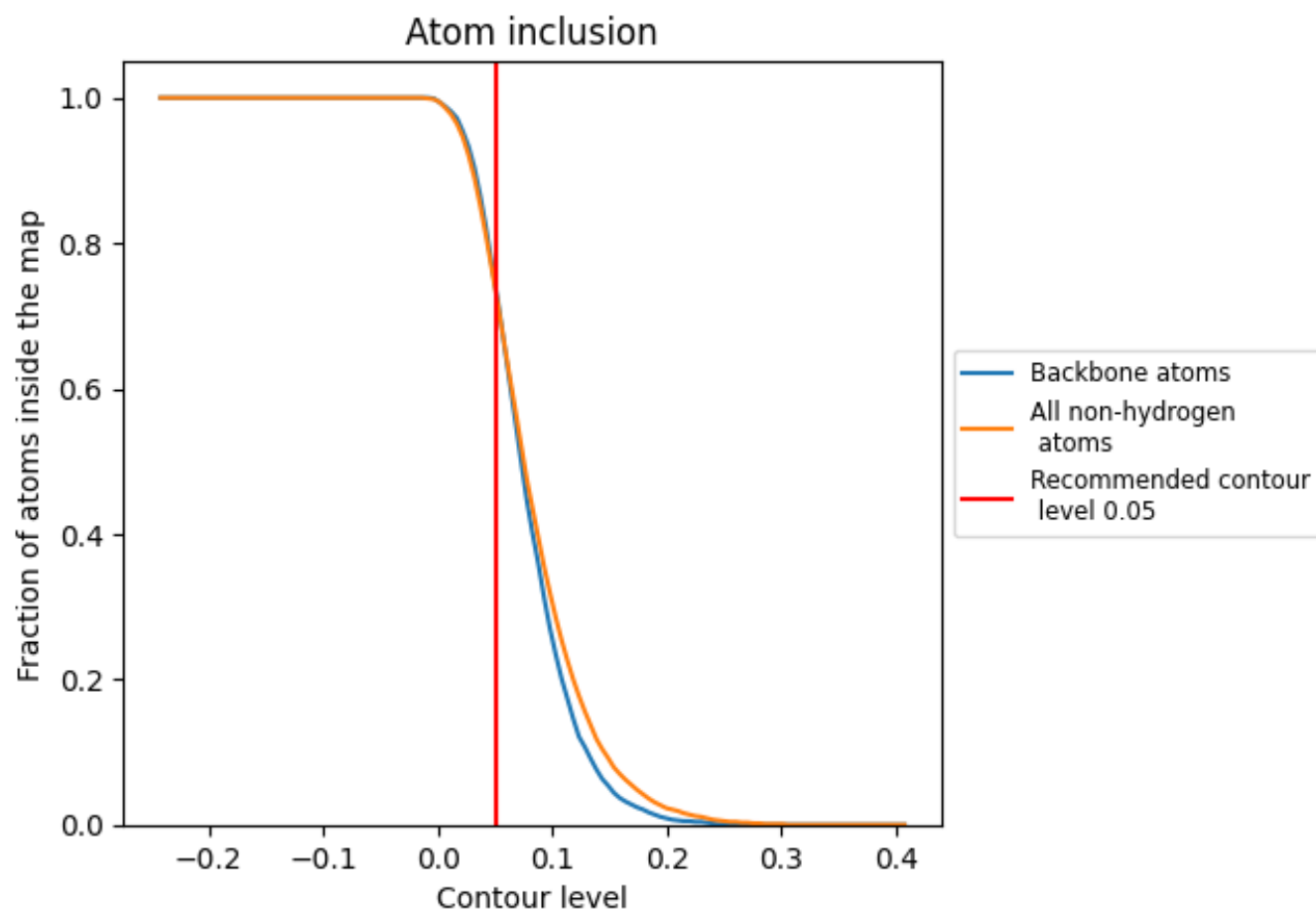
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.5110
3	0.8430	0.5220
7	0.2780	0.4470
9	0.0620	0.3160
d	0.6350	0.4920
h	0.3620	0.4410
j	0.7170	0.5360
k	0.6660	0.5010
n	0.4970	0.5010
o	0.7510	0.5190
t	0.7260	0.5230

1.0

0.0

<0.0