



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:01 PM UTC

PDB ID : 9V29 / pdb_00009v29
EMDB ID : EMD-64721
Title : Cryo- EM structure of small subunit (body) of 75S ribosome with A/P- & P/E- tRNAs from *Entamoeba histolytica* bound to antibiotic paromomycin
Authors : Sharma, S.; Mishra, S.; Gourinath, S.; Kaushal, P.S.
Deposited on : 2025-05-19
Resolution : 3.20 Å(reported)
Based on initial model : .

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:

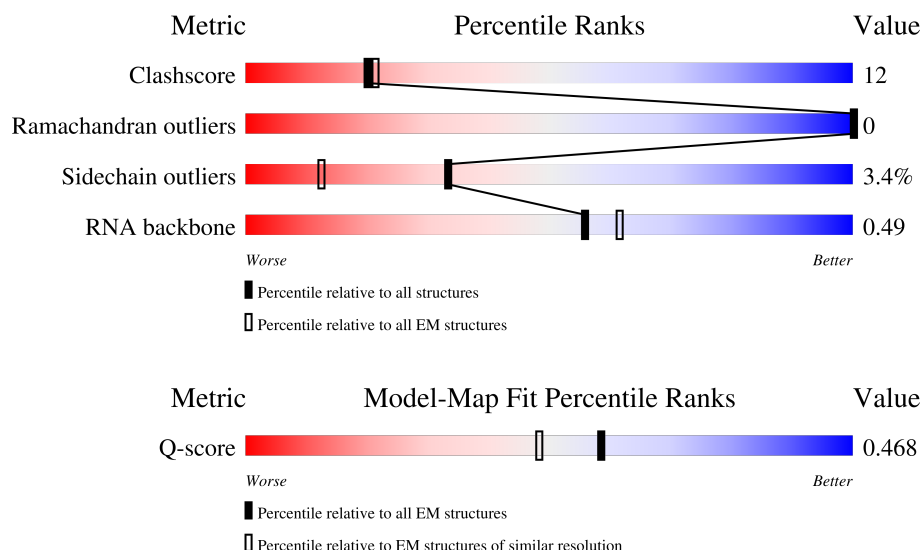
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.20 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.



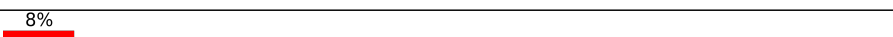
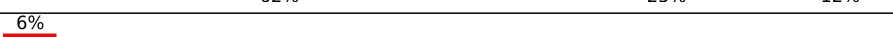
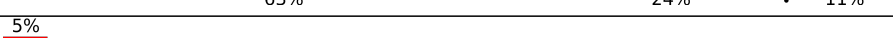
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	sB	144	 6% 51% 13% 30%
2	sC	84	 8% 8% 84%
3	sI	76	 11% 7% 82%

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Mol	Chain	Length	Quality of chain
4	sJ	77	
5	sK	10	
6	sa	1947	
7	sb	254	
8	sc	255	
9	se	256	
10	sf	326	
11	sh	266	
12	si	201	
13	sj	237	
14	sk	185	
15	sm	156	
16	so	151	
17	sp	146	
18	sr	130	
19	sy	141	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 30600 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 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	sB	94	Total	C	N	O	S	0	0
			758	459	164	129	6		

- Molecule 2 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	sC	10	Total	C	N	O	0	0
			72	43	12	17		

- Molecule 3 is a RNA chain called A/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	sI	13	Total	C	N	O	P	0	0
			272	122	44	93	13		

- Molecule 4 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	sJ	13	Total	C	N	O	P	0	0
			273	122	45	93	13		

- Molecule 5 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	sK	10	Total	C	N	O	P	0	0
			215	97	41	67	10		

- Molecule 6 is a RNA chain called 17S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	sa	930	Total	C	N	O	P	0	0
			19911	8912	3634	6435	930		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	sb	20	Total	C	N	O	0	0
			156	98	26	32		

- Molecule 8 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	sc	163	Total	C	N	O	S	0	0
			1231	782	223	219	7		

- Molecule 9 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	se	119	Total	C	N	O	S	0	0
			973	630	169	168	6		

- Molecule 10 is a protein called 40S ribosomal protein S4, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	sf	86	Total	C	N	O	S	0	0
			668	420	136	106	6		

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	sh	58	Total	C	N	O	S	0	0
			437	266	89	78	4		

- Molecule 12 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	si	19	Total	C	N	O	0	0
			151	94	31	26		

- Molecule 13 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	sj	98	Total	C	N	O	S	0	0
			772	472	159	137	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	sk	41	Total	C	N	O	S	0	0
			346	218	68	57	3		

- Molecule 15 is a protein called 40S ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	sm	136	Total	C	N	O	S	0	0
			1118	709	213	190	6		

- Molecule 16 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	so	72	Total	C	N	O	S	0	0
			604	386	113	102	3		

- Molecule 17 is a protein called Ribosomal protein S14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	sp	129	Total	C	N	O	S	0	0
			968	594	188	180	6		

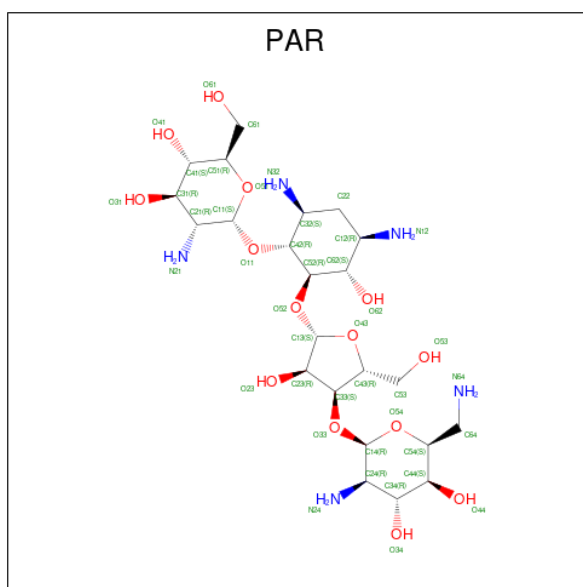
- Molecule 18 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	sr	116	Total	C	N	O	S	0	0
			919	585	168	161	5		

- Molecule 19 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	sy	91	Total	C	N	O	S	0	0
			714	446	149	116	3		

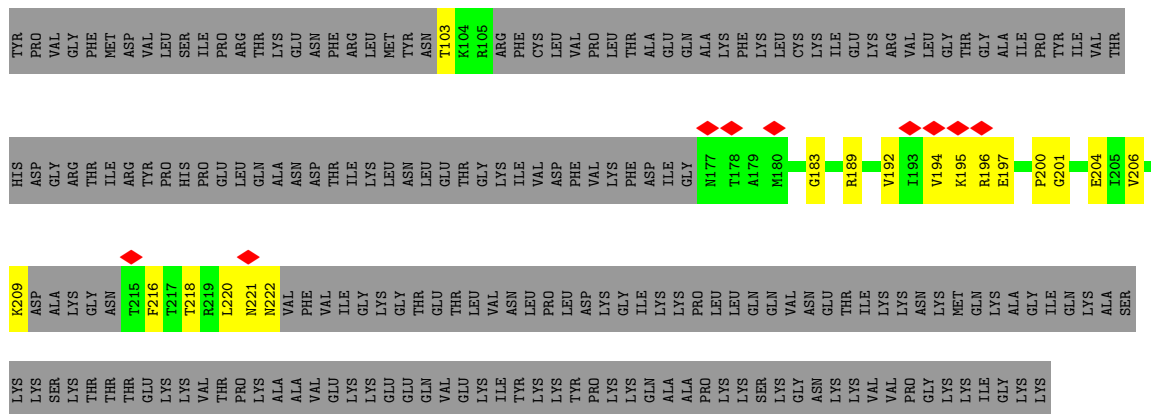
- Molecule 20 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄) (labeled as "Ligand of Interest" by depositor).



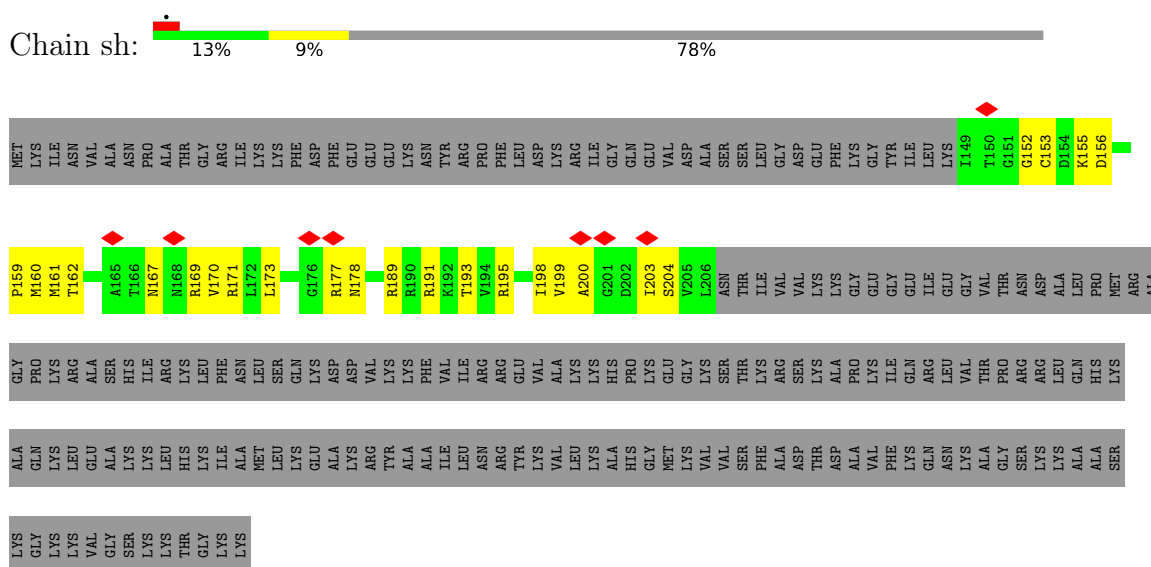
Mol	Chain	Residues	Atoms				AltConf
20	sa	1	Total	C	N	O	0
			42	23	5	14	

[illegible]

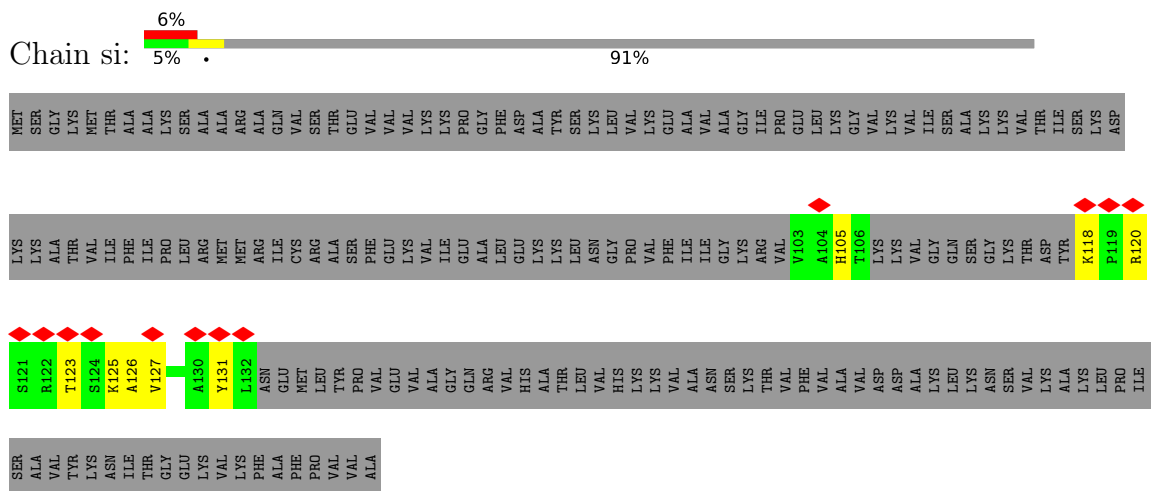




- Molecule 11: 40S ribosomal protein S6

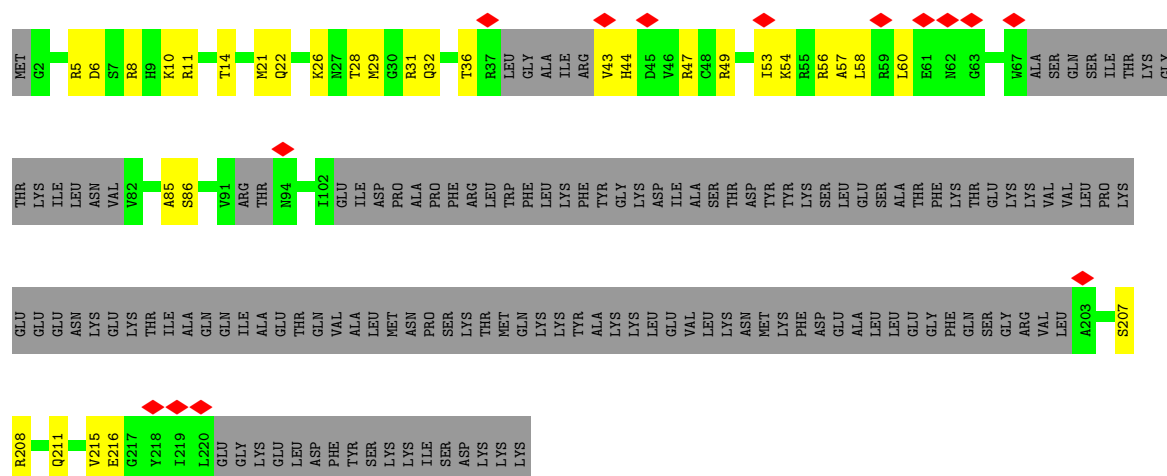


- Molecule 12: 40S ribosomal protein S7

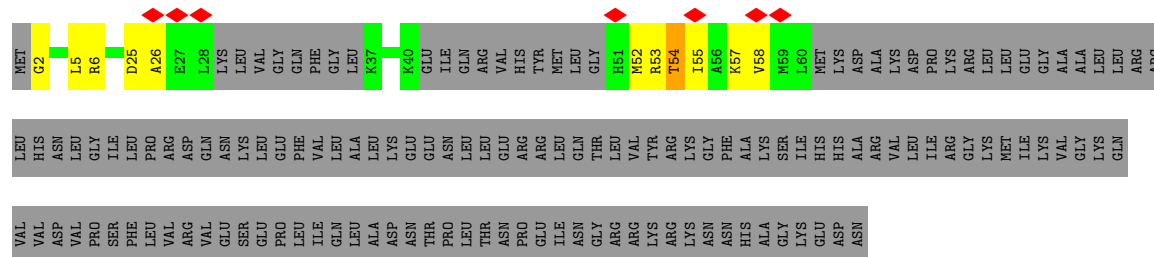


- Molecule 13: 40S ribosomal protein S8

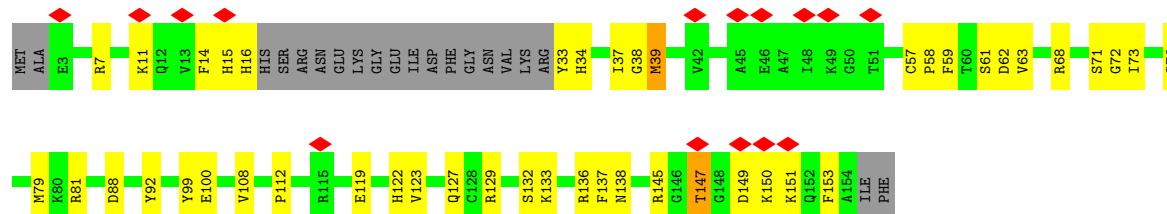




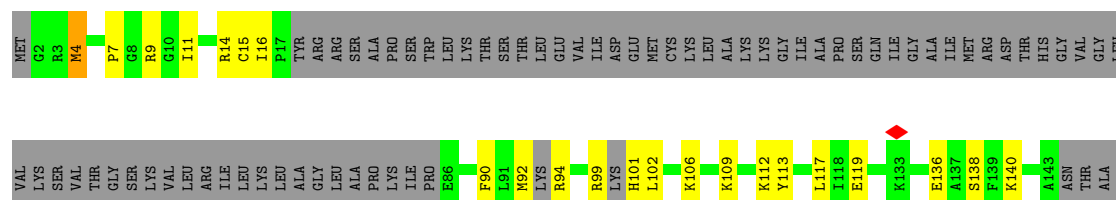
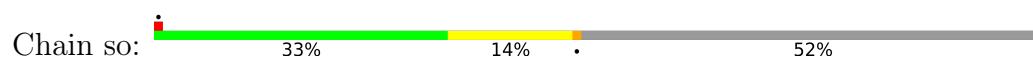
- Molecule 14: Small ribosomal subunit protein uS4



- Molecule 15: 40S ribosomal protein S11, putative

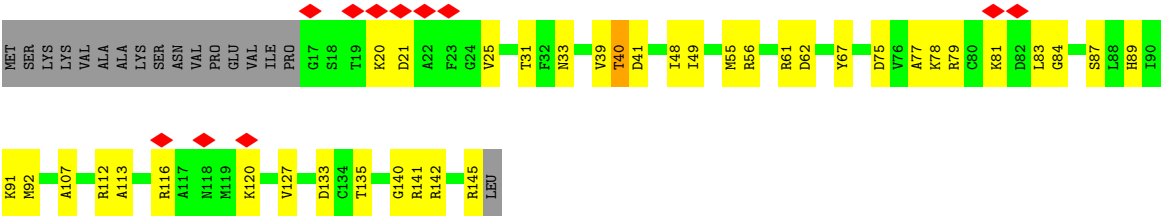


- Molecule 16: 40S ribosomal protein S13, putative

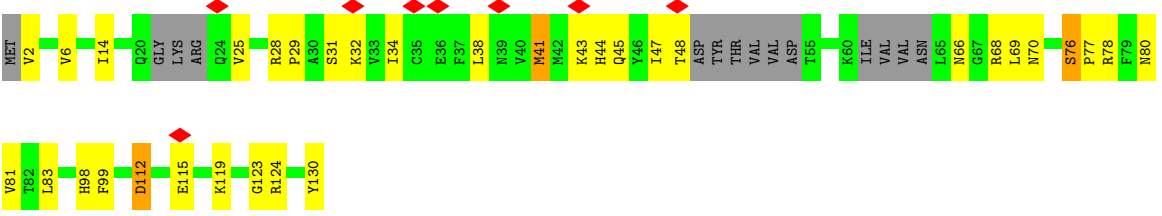


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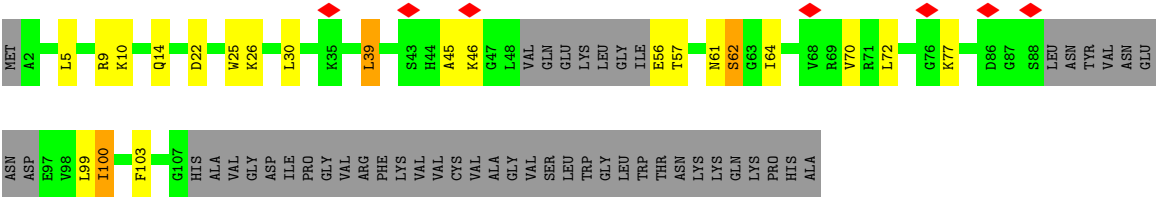
• Molecule 17: Ribosomal protein S14, putative



• Molecule 18: 40S ribosomal protein S15a, putative



• Molecule 19: 40S ribosomal protein S23, putative



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37355	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 ($e^-/\text{\AA}^2$)	1.09	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	17.330	Depositor
Minimum map value	-4.156	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	288.90002, 288.90002, 288.90002	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: PAR

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	sB	0.18	0/767	0.26	0/1020
2	sC	0.18	0/71	0.45	0/93
3	sI	0.28	0/302	0.56	0/467
4	sJ	0.16	0/303	0.27	0/469
5	sK	0.19	0/241	0.32	0/373
6	sa	0.23	3/22296 (0.0%)	0.32	2/34716 (0.0%)
7	sb	0.19	0/160	0.29	0/215
8	sc	0.20	0/1252	0.32	0/1690
9	se	0.17	0/982	0.31	0/1299
10	sf	0.17	0/684	0.34	0/914
11	sh	0.17	0/440	0.31	0/588
12	si	0.14	0/153	0.44	0/204
13	sj	0.17	0/778	0.28	0/1032
14	sk	0.14	0/350	0.29	0/462
15	sm	0.17	0/1143	0.30	0/1528
16	so	0.16	0/613	0.26	0/812
17	sp	0.16	0/981	0.31	0/1316
18	sr	0.22	0/933	0.45	0/1253
19	sy	0.16	0/723	0.34	0/958
All	All	0.21	3/33172 (0.0%)	0.33	2/49409 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
18	sr	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	sa	292	A	O3'-P	-6.62	1.51	1.61
6	sa	291	A	O3'-P	-6.27	1.51	1.61
6	sa	1089	A	C1'-N9	-5.51	1.39	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	sa	295	A	C2'-C3'-O3'	-13.63	93.25	113.70
6	sa	1090	C	C4'-C3'-O3'	6.04	122.07	113.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	sr	76	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	sB	758	0	796	18	0
2	sC	72	0	64	8	0
3	sI	272	0	139	6	0
4	sJ	273	0	140	0	0
5	sK	215	0	108	1	0
6	sa	19911	0	10007	408	0
7	sb	156	0	134	4	0
8	sc	1231	0	1282	29	0
9	se	973	0	1027	30	0
10	sf	668	0	686	36	0
11	sh	437	0	456	22	0
12	si	151	0	154	7	0
13	sj	772	0	791	27	0
14	sk	346	0	364	12	0
15	sm	1118	0	1134	34	0
16	so	604	0	624	16	0
17	sp	968	0	991	28	0
18	sr	919	0	942	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	sy	714	0	765	12	0
20	sa	42	0	45	3	0
All	All	30600	0	20649	617	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 12.

All (617) 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)
6:sa:295:A:H62	10:sf:37:LYS:HB2	1.17	1.02
6:sa:295:A:N6	10:sf:37:LYS:HB2	1.86	0.91
6:sa:1824:G:N2	6:sa:1890:U:O2	2.08	0.84
6:sa:103:U:OP2	6:sa:305:A:N6	2.15	0.80
1:sB:2:THR:OG1	1:sB:3:SER:N	2.10	0.78
6:sa:1097:C:H2'	6:sa:1098:A:H8	1.48	0.78
17:sp:75:ASP:HA	17:sp:78:LYS:HD2	1.64	0.78
6:sa:292:A:H2'	6:sa:293:U:C6	2.20	0.77
6:sa:113:A:N6	6:sa:239:U:O2	2.18	0.76
6:sa:783:A:N7	6:sa:784:U:O2'	2.19	0.75
6:sa:1824:G:H1	6:sa:1890:U:H3	0.79	0.75
6:sa:149:U:HO2'	11:sh:153:CYS:HG	1.27	0.75
6:sa:866:G:H2'	6:sa:867:A:H8	1.50	0.74
6:sa:153:U:H2'	6:sa:155:A:H5'	1.70	0.74
6:sa:438:C:O2	6:sa:440:A:N6	2.21	0.74
6:sa:295:A:N6	10:sf:38:GLU:OE1	2.21	0.74
6:sa:845:A:OP1	18:sr:28:ARG:NH2	2.22	0.72
10:sf:218:THR:OG1	10:sf:222:ASN:ND2	2.22	0.72
12:si:123:THR:O	12:si:127:VAL:HG22	1.90	0.72
6:sa:887:A:N3	6:sa:977:G:O2'	2.23	0.71
3:sI:40:C:H2'	3:sI:41:G:C8	2.25	0.71
6:sa:64:A:H2	6:sa:83:A:H62	1.38	0.71
6:sa:295:A:N7	10:sf:37:LYS:HE2	2.06	0.70
1:sB:93:ARG:NH2	6:sa:1103:U:OP1	2.24	0.70
6:sa:401:U:H2'	6:sa:402:A:H8	1.57	0.70
15:sm:108:VAL:HG12	15:sm:137:PHE:HB2	1.74	0.69
6:sa:1823:U:H5'	6:sa:1824:G:H4'	1.74	0.69
17:sp:55:MET:O	17:sp:56:ARG:NH1	2.25	0.69
6:sa:400:C:O2'	11:sh:189:ARG:O	2.11	0.69
6:sa:79:G:H2'	6:sa:80:A:C8	2.28	0.68
6:sa:332:G:O2'	13:sj:10:LYS:NZ	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:394:A:OP1	13:sj:49:ARG:NH2	2.27	0.68
6:sa:43:U:OP2	6:sa:432:A:N6	2.27	0.67
2:sC:12:THR:O	2:sC:15:SER:OG	2.09	0.67
6:sa:972:A:O2'	6:sa:1932:U:O2	2.11	0.67
6:sa:1002:U:O2'	6:sa:1151:A:N1	2.28	0.67
9:se:165:LYS:HG2	9:se:206:VAL:HG21	1.76	0.67
16:so:92:MET:O	16:so:94:ARG:N	2.28	0.67
1:sB:22:ARG:NH1	17:sp:140:GLY:O	2.26	0.66
6:sa:840:U:H2'	6:sa:841:U:C6	2.30	0.66
6:sa:585:A:H2'	6:sa:586:A:C8	2.31	0.66
10:sf:196:ARG:HG2	10:sf:206:VAL:HG22	1.77	0.66
6:sa:203:C:H5	6:sa:255:G:H21	1.44	0.66
6:sa:389:U:H3	6:sa:396:A:H62	1.43	0.66
6:sa:865:A:H2'	6:sa:866:G:C8	2.31	0.66
6:sa:880:A:H3'	6:sa:881:G:H21	1.61	0.66
20:sa:5101:PAR:O44	20:sa:5101:PAR:N64	2.27	0.65
6:sa:258:A:N6	6:sa:285:G:O2'	2.29	0.65
11:sh:153:CYS:SG	11:sh:204:SER:OG	2.54	0.65
6:sa:63:U:O2'	6:sa:163:A:N3	2.28	0.65
8:sc:228:THR:OG1	8:sc:230:ASP:OD1	2.14	0.65
18:sr:115:GLU:O	18:sr:119:LYS:N	2.23	0.65
6:sa:1808:G:OP2	20:sa:5101:PAR:O34	2.13	0.65
6:sa:1097:C:H4'	16:so:11:ILE:HD11	1.80	0.64
6:sa:788:C:H2'	6:sa:789:A:H8	1.62	0.64
6:sa:413:G:O2'	11:sh:156:ASP:OD2	2.16	0.64
6:sa:319:U:OP1	15:sm:133:LYS:NZ	2.25	0.64
6:sa:844:A:OP1	18:sr:28:ARG:NH1	2.31	0.64
6:sa:866:G:H2'	6:sa:867:A:C8	2.32	0.64
6:sa:401:U:H2'	6:sa:402:A:C8	2.33	0.63
6:sa:841:U:O2'	6:sa:842:A:O4'	2.15	0.63
6:sa:1027:G:OP1	9:se:159:LYS:NZ	2.31	0.63
6:sa:872:A:H2'	6:sa:873:A:C8	2.33	0.63
11:sh:156:ASP:OD2	11:sh:169:ARG:NH1	2.30	0.63
6:sa:794:U:H2'	6:sa:795:G:H8	1.64	0.63
6:sa:797:G:OP2	6:sa:797:G:N2	2.27	0.63
6:sa:592:U:H2'	6:sa:593:A:H8	1.62	0.63
6:sa:734:A:OP1	12:si:118:LYS:N	2.31	0.63
6:sa:158:A:H2'	6:sa:159:A:H8	1.63	0.62
6:sa:1021:G:H2'	6:sa:1022:G:C8	2.33	0.62
8:sc:175:PRO:HG3	14:sk:57:LYS:HD3	1.79	0.62
6:sa:1091:C:H5'	9:se:153:LYS:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:sj:44:HIS:N	13:sj:56:ARG:O	2.31	0.62
6:sa:138:G:H2'	6:sa:139:G:C8	2.35	0.62
6:sa:301:U:H5''	15:sm:136:ARG:HD3	1.79	0.62
6:sa:584:C:H2'	6:sa:585:A:C8	2.35	0.62
6:sa:1824:G:O6	6:sa:1890:U:O4	2.18	0.62
16:so:99:ARG:O	16:so:101:HIS:N	2.33	0.62
9:se:26:PHE:HA	9:se:29:LYS:HG3	1.82	0.62
19:sy:26:LYS:HG2	19:sy:30:LEU:HD23	1.81	0.62
15:sm:81:ARG:HH21	15:sm:112:PRO:HG2	1.64	0.61
15:sm:132:SER:OG	15:sm:133:LYS:N	2.33	0.61
13:sj:43:VAL:HA	13:sj:57:ALA:HA	1.81	0.61
6:sa:864:C:H2'	6:sa:865:A:C8	2.35	0.61
6:sa:540:U:H2'	6:sa:541:U:C6	2.35	0.61
6:sa:1097:C:H2'	6:sa:1098:A:C8	2.35	0.61
6:sa:1874:U:O2	13:sj:32:GLN:NE2	2.26	0.61
6:sa:383:G:OP2	6:sa:418:G:O2'	2.17	0.61
6:sa:328:C:OP2	13:sj:54:LYS:NZ	2.33	0.61
14:sk:52:MET:HA	14:sk:55:ILE:HD12	1.83	0.61
6:sa:746:A:H2'	6:sa:747:A:C8	2.36	0.60
6:sa:783:A:H3'	6:sa:784:U:H4'	1.82	0.60
13:sj:44:HIS:O	13:sj:56:ARG:N	2.33	0.60
6:sa:107:A:H2'	6:sa:108:G:C8	2.37	0.60
6:sa:429:G:N2	6:sa:432:A:OP2	2.35	0.60
15:sm:147:THR:HG22	15:sm:149:ASP:H	1.67	0.60
6:sa:865:A:OP1	9:se:218:LYS:NZ	2.27	0.60
6:sa:1014:C:HO2'	18:sr:2:VAL:N	1.98	0.60
6:sa:1089:A:N6	6:sa:1090:C:H42	2.00	0.60
6:sa:417:G:H2'	6:sa:418:G:C8	2.37	0.59
6:sa:1838:A:H2'	6:sa:1839:A:C8	2.37	0.59
10:sf:204:GLU:OE1	10:sf:220:LEU:HB2	2.01	0.59
17:sp:25:VAL:HG12	17:sp:89:HIS:HB2	1.83	0.59
1:sB:6:ARG:HB3	6:sa:1943:C:H5	1.68	0.59
15:sm:61:SER:OG	15:sm:62:ASP:N	2.36	0.59
6:sa:393:C:P	13:sj:47:ARG:HH22	2.25	0.59
6:sa:1816:U:H2'	6:sa:1817:A:C8	2.37	0.59
6:sa:117:U:O2	6:sa:392:A:O2'	2.20	0.59
6:sa:887:A:H2'	6:sa:888:A:H8	1.67	0.59
12:si:127:VAL:O	12:si:131:TYR:N	2.24	0.59
6:sa:1870:U:H2'	6:sa:1871:G:H8	1.69	0.58
10:sf:192:VAL:HB	10:sf:209:LYS:HE2	1.85	0.58
6:sa:781:G:H4'	6:sa:782:A:H4'	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:956:G:N1	6:sa:1003:A:O2'	2.30	0.58
6:sa:558:G:N2	6:sa:571:G:OP1	2.33	0.58
6:sa:941:C:OP2	16:so:14:ARG:NH1	2.35	0.58
6:sa:1943:C:H5'	6:sa:1944:A:C8	2.38	0.58
8:sc:69:GLN:CD	8:sc:69:GLN:H	2.11	0.58
10:sf:192:VAL:O	10:sf:209:LYS:NZ	2.35	0.58
2:sC:30:ASN:ND2	6:sa:1098:A:OP2	2.37	0.58
9:se:125:THR:HB	9:se:167:ARG:HG2	1.85	0.58
19:sy:46:LYS:HG3	19:sy:99:LEU:HD13	1.85	0.58
6:sa:345:A:H5''	6:sa:346:U:H3'	1.87	0.57
6:sa:286:U:H2'	6:sa:287:A:H8	1.69	0.57
6:sa:209:A:N6	6:sa:250:G:O6	2.38	0.57
8:sc:165:GLY:O	8:sc:168:ARG:NH1	2.38	0.57
9:se:201:ALA:O	9:se:203:CYS:N	2.36	0.57
6:sa:467:C:O2'	6:sa:760:A:N3	2.29	0.57
6:sa:402:A:H2'	6:sa:403:C:H6	1.69	0.57
6:sa:1893:A:H5''	6:sa:1894:G:H8	1.69	0.57
6:sa:1811:G:H1	20:sa:5101:PAR:H611	1.69	0.57
19:sy:10:LYS:O	19:sy:14:GLN:N	2.31	0.57
6:sa:79:G:H2'	6:sa:80:A:H8	1.68	0.56
6:sa:887:A:H2'	6:sa:888:A:C8	2.40	0.56
6:sa:243:U:OP1	15:sm:33:TYR:OH	2.23	0.56
6:sa:1846:G:O2'	6:sa:1867:A:N1	2.35	0.56
10:sf:40:LEU:HD12	10:sf:41:PRO:HD2	1.86	0.56
6:sa:5:U:OP2	8:sc:206:THR:OG1	2.19	0.56
6:sa:559:C:O3'	19:sy:62:SER:OG	2.23	0.56
6:sa:1845:G:H21	6:sa:1869:A:H62	1.53	0.56
6:sa:40:A:O2'	6:sa:432:A:O2'	2.17	0.56
15:sm:71:SER:OG	15:sm:122:HIS:NE2	2.38	0.56
16:so:102:LEU:HD21	16:so:112:LYS:HG2	1.87	0.56
6:sa:294:G:H4'	6:sa:295:A:H5''	1.87	0.56
6:sa:442:U:O2'	10:sf:25:PHE:O	2.23	0.56
6:sa:125:U:O2'	6:sa:203:C:O2	2.23	0.56
6:sa:210:U:OP1	15:sm:15:HIS:NE2	2.39	0.56
6:sa:866:G:OP1	9:se:216:LYS:NZ	2.37	0.56
6:sa:1115:C:N4	6:sa:1116:U:O4	2.39	0.56
1:sB:15:ARG:NH2	6:sa:916:G:N7	2.38	0.55
6:sa:366:G:N2	6:sa:606:U:O2	2.39	0.55
6:sa:864:C:H2'	6:sa:865:A:H8	1.72	0.55
6:sa:1126:G:H8	18:sr:76:SER:HG	1.53	0.55
6:sa:402:A:H2'	6:sa:403:C:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:584:C:H2'	6:sa:585:A:H8	1.71	0.55
6:sa:1923:A:H2'	6:sa:1924:G:C8	2.41	0.55
6:sa:1827:U:H2'	6:sa:1828:A:H8	1.71	0.55
8:sc:142:ARG:HG2	8:sc:157:PRO:HG3	1.89	0.55
6:sa:592:U:H2'	6:sa:593:A:C8	2.40	0.55
6:sa:1893:A:H5''	6:sa:1894:G:C8	2.42	0.55
8:sc:172:VAL:HB	8:sc:199:PHE:HB2	1.88	0.55
15:sm:71:SER:OG	15:sm:72:GLY:N	2.39	0.55
11:sh:155:LYS:HA	11:sh:204:SER:HB3	1.89	0.55
6:sa:61:A:H1'	6:sa:262:G:H1'	1.88	0.55
6:sa:149:U:O2'	11:sh:153:CYS:SG	2.50	0.54
6:sa:750:U:H2'	6:sa:751:A:C8	2.42	0.54
6:sa:1936:G:OP2	17:sp:141:ARG:NH2	2.40	0.54
18:sr:112:ASP:OD1	18:sr:112:ASP:N	2.37	0.54
6:sa:239:U:N3	6:sa:242:G:OP2	2.32	0.54
1:sB:5:ARG:NH2	6:sa:1942:U:OP2	2.41	0.54
6:sa:211:U:OP2	15:sm:16:HIS:ND1	2.35	0.54
6:sa:604:G:HO2'	6:sa:607:G:HO2'	1.55	0.54
6:sa:734:A:H2'	6:sa:735:U:H6	1.72	0.54
6:sa:1827:U:H2'	6:sa:1828:A:C8	2.43	0.54
15:sm:37:ILE:HG22	15:sm:38:GLY:H	1.71	0.54
6:sa:90:G:OP1	6:sa:392:A:N6	2.40	0.54
6:sa:375:A:C6	14:sk:2:GLY:HA3	2.42	0.54
11:sh:167:ASN:OD1	11:sh:198:ILE:HB	2.08	0.54
3:sI:31:A:H2'	3:sI:32:C:O4'	2.08	0.54
10:sf:194:VAL:HG13	10:sf:209:LYS:HZ2	1.73	0.54
10:sf:221:ASN:OD1	10:sf:222:ASN:N	2.41	0.54
11:sh:177:ARG:C	11:sh:178:ASN:HD22	2.16	0.54
6:sa:17:C:H2'	6:sa:18:C:C6	2.43	0.54
6:sa:443:U:H2'	6:sa:444:U:C6	2.43	0.54
6:sa:1089:A:N6	6:sa:1090:C:N4	2.56	0.54
8:sc:127:ILE:HG22	8:sc:131:MET:HE2	1.89	0.54
1:sB:85:ARG:O	6:sa:1944:A:N6	2.41	0.53
7:sb:139:GLN:O	7:sb:143:GLU:HG3	2.09	0.53
6:sa:323:A:H2'	6:sa:324:G:C8	2.44	0.53
6:sa:875:G:H2'	6:sa:876:G:C8	2.44	0.53
6:sa:867:A:H2	17:sp:135:THR:HG23	1.73	0.53
6:sa:877:G:H1	6:sa:894:G:HO2'	1.56	0.53
11:sh:171:ARG:HG2	11:sh:193:THR:HB	1.91	0.53
6:sa:395:G:H1	13:sj:29:MET:HE3	1.73	0.53
10:sf:196:ARG:HE	10:sf:206:VAL:HG22	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:sy:22:ASP:HB3	19:sy:25:TRP:HB3	1.90	0.53
8:sc:190:LEU:HD13	8:sc:198:VAL:HG11	1.90	0.53
10:sf:194:VAL:CG1	10:sf:209:LYS:HZ2	2.22	0.53
6:sa:158:A:H2'	6:sa:159:A:C8	2.42	0.53
16:so:99:ARG:NH2	16:so:119:GLU:OE2	2.41	0.53
17:sp:21:ASP:OD1	17:sp:21:ASP:N	2.38	0.53
6:sa:558:G:C5	6:sa:572:U:H1'	2.44	0.52
1:sB:97:PRO:HB2	1:sB:99:LYS:HD3	1.90	0.52
6:sa:866:G:N2	17:sp:133:ASP:O	2.41	0.52
6:sa:903:A:H2'	6:sa:904:A:C8	2.44	0.52
6:sa:555:G:H2'	6:sa:556:G:C8	2.43	0.52
7:sb:142:ARG:HG3	7:sb:142:ARG:HH11	1.74	0.52
6:sa:762:A:O2'	14:sk:6:ARG:NH1	2.42	0.52
13:sj:11:ARG:O	15:sm:133:LYS:NZ	2.43	0.52
6:sa:106:C:H2'	6:sa:107:A:H8	1.75	0.52
8:sc:82:VAL:HG22	8:sc:104:VAL:HG12	1.90	0.52
6:sa:156:U:H2'	6:sa:157:A:H8	1.74	0.52
6:sa:335:U:H2'	6:sa:336:A:C8	2.44	0.52
6:sa:1839:A:OP1	11:sh:191:ARG:NH2	2.38	0.52
8:sc:143:ARG:NH1	8:sc:194:GLY:O	2.43	0.52
6:sa:456:G:H2'	6:sa:457:G:H8	1.75	0.52
6:sa:734:A:H2'	6:sa:735:U:C6	2.45	0.52
6:sa:1030:G:C6	6:sa:1094:G:C6	2.97	0.52
6:sa:397:U:OP1	10:sf:1:ARG:NH2	2.43	0.52
6:sa:64:A:O2'	6:sa:66:A:OP2	2.25	0.51
6:sa:873:A:H2'	6:sa:874:C:C6	2.46	0.51
6:sa:599:A:OP2	6:sa:600:A:O2'	2.23	0.51
6:sa:877:G:O2'	6:sa:894:G:N2	2.43	0.51
6:sa:1923:A:H2'	6:sa:1924:G:H8	1.75	0.51
13:sj:5:ARG:NH1	13:sj:29:MET:O	2.41	0.51
9:se:200:VAL:O	9:se:204:SER:N	2.42	0.51
3:sI:34:U:HO2'	3:sI:35:U:P	2.34	0.51
6:sa:60:A:H2	6:sa:262:G:H8	1.58	0.51
6:sa:171:A:O2'	6:sa:172:G:O4'	2.19	0.51
6:sa:342:A:H5'	15:sm:79:MET:HE1	1.93	0.51
19:sy:70:VAL:HG11	19:sy:100:ILE:HD11	1.92	0.51
6:sa:867:A:H2'	6:sa:868:A:H8	1.74	0.51
17:sp:31:THR:HG23	17:sp:33:ASN:H	1.75	0.51
6:sa:287:A:H2'	6:sa:288:A:H8	1.75	0.51
6:sa:328:C:C5	13:sj:49:ARG:HD2	2.47	0.51
6:sa:555:G:H2'	6:sa:556:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:868:A:H2'	6:sa:869:A:C8	2.46	0.51
6:sa:388:C:H2'	6:sa:389:U:C6	2.46	0.50
13:sj:208:ARG:HH11	13:sj:211:GLN:HG3	1.76	0.50
19:sy:57:THR:OG1	19:sy:61:ASN:O	2.29	0.50
8:sc:75:LEU:HB3	8:sc:78:LEU:HD21	1.92	0.50
6:sa:325:U:H2'	6:sa:326:A:C8	2.46	0.50
8:sc:154:HIS:CE1	8:sc:176:ARG:HD2	2.46	0.50
13:sj:85:ALA:O	15:sm:7:ARG:NE	2.45	0.50
6:sa:295:A:N6	10:sf:37:LYS:CB	2.66	0.50
9:se:76:MET:HE2	9:se:76:MET:HA	1.93	0.50
9:se:197:LYS:N	9:se:197:LYS:HD2	2.27	0.50
14:sk:52:MET:SD	14:sk:52:MET:N	2.84	0.50
6:sa:295:A:C6	10:sf:38:GLU:OE2	2.65	0.50
6:sa:295:A:N6	10:sf:38:GLU:CD	2.69	0.50
6:sa:972:A:H2'	6:sa:973:A:H5'	1.94	0.50
8:sc:80:GLU:OE2	8:sc:81:GLU:N	2.45	0.50
6:sa:106:C:H2'	6:sa:107:A:C8	2.46	0.50
6:sa:847:G:H5'	16:so:4:MET:SD	2.52	0.50
17:sp:39:VAL:HG23	17:sp:48:ILE:HB	1.94	0.50
6:sa:619:C:H2'	6:sa:620:U:C6	2.47	0.50
6:sa:208:C:H2'	6:sa:209:A:C8	2.46	0.50
6:sa:549:A:H2'	6:sa:550:A:C8	2.47	0.50
6:sa:746:A:H2'	6:sa:747:A:H8	1.75	0.50
6:sa:839:A:H2'	6:sa:839:A:N3	2.26	0.50
1:sB:89:ARG:HH22	6:sa:1114:U:P	2.35	0.49
6:sa:867:A:H2'	6:sa:868:A:C8	2.47	0.49
10:sf:29:PRO:HB3	10:sf:41:PRO:HG3	1.93	0.49
6:sa:412:A:H5'	6:sa:413:G:C8	2.47	0.49
18:sr:45:GLN:HE22	18:sr:68:ARG:HG2	1.77	0.49
6:sa:287:A:H2'	6:sa:288:A:C8	2.46	0.49
6:sa:751:A:H2'	6:sa:752:A:O4'	2.12	0.49
18:sr:14:ILE:HG12	18:sr:25:VAL:HG11	1.94	0.49
2:sC:18:LYS:C	6:sa:1096:U:H2'	2.36	0.49
6:sa:257:C:H5''	6:sa:258:A:H5''	1.95	0.49
6:sa:860:G:H2'	6:sa:861:A:C8	2.47	0.49
13:sj:6:ASP:OD2	13:sj:8:ARG:NH1	2.41	0.49
16:so:136:GLU:OE2	16:so:138:SER:OG	2.29	0.49
3:sI:37:A:H2'	3:sI:38:A:O4'	2.13	0.49
6:sa:412:A:H4'	6:sa:413:G:O5'	2.12	0.49
6:sa:619:C:O2'	6:sa:919:A:N3	2.42	0.49
6:sa:322:U:H2'	6:sa:323:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:58:G:H4'	6:sa:448:A:H5'	1.95	0.49
6:sa:782:A:C5	6:sa:784:U:H1'	2.47	0.49
6:sa:388:C:H2'	6:sa:389:U:H6	1.77	0.48
17:sp:142:ARG:HB2	17:sp:145:ARG:HH21	1.77	0.48
2:sC:18:LYS:HB3	6:sa:1027:G:H22	1.78	0.48
6:sa:934:A:H2'	6:sa:935:C:C6	2.48	0.48
6:sa:958:A:H2'	6:sa:959:A:O4'	2.13	0.48
6:sa:151:A:H2'	6:sa:152:A:C8	2.48	0.48
6:sa:15:U:H2'	6:sa:16:G:O4'	2.13	0.48
6:sa:876:G:H2'	6:sa:877:G:C8	2.49	0.48
6:sa:1090:C:C5	6:sa:1091:C:C4	3.00	0.48
2:sC:12:THR:O	2:sC:15:SER:N	2.44	0.48
2:sC:14:ALA:HA	2:sC:17:ALA:HB3	1.94	0.48
13:sj:6:ASP:HB3	13:sj:28:THR:HG21	1.95	0.48
6:sa:150:G:N1	6:sa:155:A:C6	2.82	0.48
6:sa:301:U:O2	15:sm:68:ARG:NH2	2.39	0.48
6:sa:343:U:H4'	13:sj:14:THR:HG22	1.96	0.48
6:sa:114:G:H5'	15:sm:129:ARG:HD2	1.96	0.48
2:sC:18:LYS:HG2	6:sa:937:G:OP1	2.13	0.48
6:sa:238:G:H2'	6:sa:239:U:O4'	2.14	0.48
6:sa:1107:A:H2'	6:sa:1108:G:H8	1.79	0.48
1:sB:26:CYS:HB2	1:sB:77:CYS:SG	2.54	0.48
3:sI:34:U:O2'	3:sI:35:U:OP1	2.28	0.47
6:sa:853:U:H2'	6:sa:854:U:C6	2.49	0.47
11:sh:161:MET:HE3	11:sh:162:THR:H	1.79	0.47
18:sr:77:PRO:HB2	19:sy:5:LEU:HB2	1.95	0.47
6:sa:327:U:H5''	13:sj:31:ARG:NH1	2.30	0.47
6:sa:1007:A:OP1	6:sa:1936:G:O2'	2.25	0.47
11:sh:167:ASN:ND2	11:sh:200:ALA:HB2	2.29	0.47
14:sk:54:THR:O	14:sk:58:VAL:HG13	2.13	0.47
6:sa:23:U:H2'	6:sa:24:U:C6	2.49	0.47
6:sa:240:G:O4'	10:sf:200:PRO:HB3	2.13	0.47
6:sa:389:U:O4	6:sa:396:A:N7	2.47	0.47
6:sa:574:A:O2'	6:sa:576:U:OP1	2.32	0.47
6:sa:1089:A:C6	6:sa:1090:C:N3	2.82	0.47
6:sa:1133:A:O2'	6:sa:1134:G:H5'	2.14	0.47
6:sa:395:G:N1	13:sj:29:MET:HE3	2.29	0.47
6:sa:1090:C:H5	6:sa:1091:C:C4	2.32	0.47
9:se:31:TRP:CE2	9:se:49:VAL:HG13	2.48	0.47
15:sm:34:HIS:O	15:sm:34:HIS:ND1	2.47	0.47
6:sa:296:G:OP2	6:sa:296:G:H3'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:585:A:C6	6:sa:586:A:N6	2.82	0.47
6:sa:51:U:H2'	6:sa:52:G:C8	2.50	0.47
6:sa:51:U:H2'	6:sa:52:G:H8	1.79	0.47
6:sa:59:U:O2'	6:sa:61:A:H2	1.98	0.47
6:sa:115:U:O2'	6:sa:328:C:O2	2.25	0.47
6:sa:396:A:O2'	6:sa:397:U:H4'	2.15	0.47
6:sa:632:U:H3	12:si:120:ARG:HH12	1.63	0.47
6:sa:912:G:OP2	9:se:157:TYR:OH	2.26	0.47
6:sa:1028:A:H2'	6:sa:1029:U:C6	2.50	0.47
6:sa:1815:C:H2'	6:sa:1816:U:C6	2.48	0.47
9:se:73:ALA:O	9:se:77:GLU:N	2.46	0.47
12:si:125:LYS:HA	12:si:125:LYS:HD3	1.61	0.47
15:sm:57:CYS:O	15:sm:61:SER:HB3	2.14	0.47
6:sa:29:G:H2'	6:sa:30:C:H6	1.80	0.47
6:sa:328:C:H2'	6:sa:329:G:C8	2.49	0.47
6:sa:594:U:H2'	6:sa:595:A:C8	2.49	0.47
6:sa:1882:U:H2'	6:sa:1883:C:C6	2.50	0.47
9:se:196:PRO:HB2	9:se:197:LYS:HD2	1.97	0.47
10:sf:183:GLY:HA3	10:sf:222:ASN:OD1	2.14	0.47
17:sp:142:ARG:HB2	17:sp:145:ARG:NH2	2.30	0.47
6:sa:919:A:H2'	6:sa:920:A:C8	2.50	0.47
6:sa:1030:G:C5	6:sa:1094:G:C6	3.02	0.47
9:se:49:VAL:HG23	17:sp:41:ASP:HB3	1.97	0.47
18:sr:47:ILE:HD12	18:sr:48:THR:H	1.78	0.47
6:sa:60:A:H2	6:sa:262:G:C8	2.33	0.47
6:sa:345:A:H5''	6:sa:347:A:H5'	1.97	0.47
6:sa:581:C:H2'	6:sa:582:U:C6	2.50	0.47
6:sa:1146:U:H2'	6:sa:1147:C:C6	2.50	0.47
6:sa:609:G:O2'	6:sa:615:A:N1	2.46	0.46
6:sa:1118:G:O2'	6:sa:1119:A:H3'	2.15	0.46
6:sa:1848:U:C2'	6:sa:1849:U:H5'	2.45	0.46
10:sf:39:CYS:SG	10:sf:40:LEU:N	2.87	0.46
6:sa:456:G:H2'	6:sa:457:G:C8	2.49	0.46
8:sc:170:ARG:O	8:sc:200:THR:HA	2.15	0.46
1:sB:5:ARG:HG2	6:sa:1943:C:C2	2.50	0.46
6:sa:581:C:H2'	6:sa:582:U:H6	1.80	0.46
6:sa:841:U:HO2'	6:sa:842:A:C1'	2.28	0.46
9:se:26:PHE:CD2	17:sp:83:LEU:HD11	2.50	0.46
15:sm:119:GLU:OE1	15:sm:150:LYS:NZ	2.30	0.46
6:sa:252:C:H3'	6:sa:253:A:H8	1.80	0.46
1:sB:68:TYR:HB2	9:se:113:ARG:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:978:A:N6	6:sa:984:U:OP2	2.49	0.46
6:sa:1107:A:H2'	6:sa:1108:G:C8	2.51	0.46
6:sa:1830:A:N3	6:sa:1830:A:H2'	2.29	0.46
17:sp:83:LEU:O	17:sp:83:LEU:HD23	2.15	0.46
18:sr:70:ASN:HB2	18:sr:130:TYR:HB2	1.98	0.46
6:sa:57:U:H3	6:sa:88:G:H1	1.63	0.46
6:sa:1819:C:H2'	6:sa:1820:G:O4'	2.16	0.46
8:sc:122:GLU:OE2	8:sc:123:VAL:N	2.47	0.46
6:sa:62:G:O2'	6:sa:165:U:OP1	2.32	0.46
17:sp:113:ALA:HA	17:sp:116:ARG:HE	1.81	0.46
6:sa:16:G:H2'	6:sa:17:C:C6	2.50	0.46
6:sa:24:U:O2'	6:sa:25:A:H5'	2.15	0.46
7:sb:138:HIS:HB2	7:sb:142:ARG:NH1	2.31	0.46
18:sr:81:VAL:N	18:sr:123:GLY:O	2.39	0.46
6:sa:888:A:C2	6:sa:989:U:H1'	2.51	0.46
13:sj:21:MET:HE3	13:sj:21:MET:HB2	1.83	0.46
6:sa:323:A:H2'	6:sa:324:G:H8	1.81	0.46
6:sa:375:A:H2'	6:sa:375:A:N3	2.31	0.46
10:sf:197:GLU:O	10:sf:204:GLU:HG2	2.16	0.46
18:sr:38:LEU:HD23	18:sr:41:MET:HE3	1.97	0.46
6:sa:152:A:H2'	6:sa:153:U:H6	1.80	0.45
6:sa:570:G:H5'	6:sa:571:G:OP2	2.15	0.45
10:sf:36:MET:HG3	10:sf:37:LYS:HG3	1.98	0.45
17:sp:112:ARG:O	17:sp:116:ARG:HG3	2.15	0.45
15:sm:151:LYS:HB3	15:sm:153:PHE:HE1	1.81	0.45
8:sc:89:GLN:NE2	8:sc:96:GLN:OE1	2.49	0.45
6:sa:257:C:OP1	6:sa:258:A:H4'	2.17	0.45
6:sa:966:G:H2'	6:sa:967:G:O4'	2.17	0.45
6:sa:872:A:H2'	6:sa:873:A:H8	1.80	0.45
7:sb:134:PRO:CB	7:sb:141:LEU:HD11	2.46	0.45
14:sk:25:ASP:OD1	14:sk:26:ALA:N	2.48	0.45
6:sa:173:A:H62	6:sa:257:C:H41	1.64	0.45
6:sa:380:A:H2'	6:sa:381:G:C8	2.52	0.45
18:sr:78:ARG:O	18:sr:124:ARG:NH1	2.49	0.45
6:sa:366:G:H1	6:sa:607:G:H1	1.64	0.45
6:sa:630:A:H5''	18:sr:31:SER:HB2	1.98	0.45
6:sa:763:G:H5''	10:sf:21:LEU:HD12	1.98	0.45
17:sp:40:THR:OG1	17:sp:41:ASP:O	2.34	0.45
6:sa:31:U:O2'	6:sa:588:A:N1	2.45	0.45
6:sa:379:G:H2'	6:sa:380:A:C8	2.52	0.45
6:sa:734:A:N6	6:sa:803:G:O6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:743:A:H2	6:sa:791:G:H22	1.63	0.45
6:sa:1117:U:O2'	6:sa:1118:G:OP1	2.30	0.45
11:sh:155:LYS:HA	11:sh:155:LYS:HD3	1.85	0.45
6:sa:628:G:N1	6:sa:945:U:OP2	2.39	0.45
6:sa:792:C:H2'	6:sa:793:A:H8	1.82	0.45
6:sa:873:A:H2'	6:sa:874:C:H6	1.80	0.45
9:se:29:LYS:HB3	9:se:49:VAL:HG12	1.99	0.45
6:sa:204:A:N1	6:sa:255:G:H1'	2.32	0.45
6:sa:734:A:C6	6:sa:803:G:N1	2.85	0.45
6:sa:1015:A:C6	6:sa:1127:G:C6	3.04	0.45
6:sa:1931:C:H2'	6:sa:1932:U:C6	2.51	0.45
10:sf:10:LEU:HD21	14:sk:5:LEU:HD11	1.98	0.45
9:se:197:LYS:O	9:se:199:ILE:N	2.50	0.44
6:sa:141:U:H2'	6:sa:142:A:H8	1.82	0.44
6:sa:295:A:N7	10:sf:37:LYS:CE	2.78	0.44
6:sa:295:A:H2'	6:sa:296:G:OP1	2.15	0.44
6:sa:794:U:H2'	6:sa:795:G:C8	2.48	0.44
6:sa:870:A:H2'	6:sa:871:U:C6	2.52	0.44
9:se:30:GLU:N	9:se:50:VAL:O	2.37	0.44
6:sa:242:G:O2'	6:sa:243:U:OP1	2.26	0.44
6:sa:327:U:P	13:sj:56:ARG:HH22	2.40	0.44
6:sa:334:C:H2'	6:sa:335:U:C6	2.52	0.44
16:so:136:GLU:HG2	16:so:138:SER:H	1.82	0.44
19:sy:72:LEU:HD12	19:sy:77:LYS:O	2.18	0.44
1:sB:42:LYS:O	1:sB:67:THR:N	2.38	0.44
6:sa:3:U:H5'	8:sc:181:VAL:HG12	2.00	0.44
6:sa:585:A:C6	6:sa:586:A:C6	3.05	0.44
6:sa:744:A:OP1	10:sf:218:THR:OG1	2.35	0.44
11:sh:171:ARG:HA	11:sh:193:THR:HA	1.99	0.44
6:sa:101:U:H1'	13:sj:21:MET:HE3	1.98	0.44
6:sa:550:A:N3	6:sa:584:C:H1'	2.32	0.44
6:sa:786:U:H2'	6:sa:787:U:C2	2.52	0.44
8:sc:121:LYS:HB2	8:sc:121:LYS:HE2	1.65	0.44
9:se:143:GLY:HA2	9:se:211:ASN:O	2.18	0.44
16:so:7:PRO:O	16:so:9:ARG:NH1	2.50	0.44
16:so:140:LYS:HA	16:so:140:LYS:HD2	1.75	0.44
6:sa:29:G:H2'	6:sa:30:C:C6	2.53	0.44
8:sc:80:GLU:OE1	8:sc:106:ILE:HG22	2.17	0.44
9:se:107:LEU:HD12	9:se:215:ARG:HA	2.00	0.44
1:sB:57:SER:C	17:sp:120:LYS:HE2	2.43	0.44
6:sa:442:U:H2'	6:sa:443:U:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:1865:A:H2'	6:sa:1866:A:H8	1.83	0.44
1:sB:79:ILE:HD13	6:sa:1941:A:H1'	2.00	0.44
6:sa:402:A:OP1	11:sh:191:ARG:HD2	2.17	0.44
6:sa:785:A:H2'	6:sa:786:U:O4'	2.18	0.44
6:sa:803:G:H4'	15:sm:145:ARG:HD3	1.99	0.44
6:sa:63:U:H3'	6:sa:64:A:H5''	2.00	0.44
6:sa:113:A:N1	6:sa:241:A:H2'	2.33	0.44
6:sa:870:A:H2'	6:sa:871:U:H6	1.83	0.44
17:sp:61:ARG:HG3	17:sp:62:ASP:OD1	2.18	0.44
6:sa:416:A:HO2'	6:sa:417:G:H8	1.65	0.43
6:sa:455:A:H3'	6:sa:456:G:H8	1.83	0.43
9:se:210:ASP:OD1	9:se:210:ASP:N	2.51	0.43
14:sk:54:THR:HA	14:sk:57:LYS:HB2	2.00	0.43
15:sm:151:LYS:HB3	15:sm:153:PHE:CE1	2.53	0.43
18:sr:28:ARG:HB3	18:sr:29:PRO:HD3	2.00	0.43
6:sa:239:U:H6	6:sa:239:U:O5'	2.01	0.43
6:sa:580:G:H2'	6:sa:581:C:H6	1.83	0.43
8:sc:108:ASP:OD1	8:sc:108:ASP:C	2.62	0.43
8:sc:178:THR:HG23	14:sk:53:ARG:HH22	1.83	0.43
18:sr:31:SER:OG	18:sr:32:LYS:N	2.51	0.43
6:sa:389:U:H2'	6:sa:390:U:C6	2.53	0.43
13:sj:207:SER:HB3	13:sj:216:GLU:HB2	2.00	0.43
17:sp:20:LYS:HD3	17:sp:20:LYS:HA	1.83	0.43
6:sa:134:A:H4'	6:sa:135:C:H5'	2.00	0.43
6:sa:303:U:H2'	6:sa:304:G:C8	2.54	0.43
6:sa:839:A:C8	12:si:126:ALA:HB1	2.54	0.43
6:sa:932:C:H2'	6:sa:933:A:C8	2.54	0.43
6:sa:1089:A:C6	6:sa:1090:C:C4	3.07	0.43
8:sc:228:THR:HA	18:sr:99:PHE:CZ	2.53	0.43
9:se:108:THR:HG23	9:se:111:LYS:H	1.83	0.43
15:sm:92:TYR:HB2	15:sm:99:TYR:CE2	2.52	0.43
18:sr:69:LEU:HD12	18:sr:69:LEU:HA	1.82	0.43
6:sa:556:G:H2'	6:sa:557:U:C6	2.53	0.43
17:sp:87:SER:HB3	17:sp:120:LYS:HD2	1.99	0.43
6:sa:1840:U:P	11:sh:189:ARG:HH22	2.40	0.43
6:sa:1866:A:H2'	6:sa:1867:A:O4'	2.19	0.43
6:sa:443:U:H2'	6:sa:444:U:H6	1.80	0.43
6:sa:1111:A:H2'	6:sa:1112:A:C8	2.53	0.43
8:sc:65:ILE:HD13	8:sc:71:VAL:HG12	2.01	0.43
18:sr:6:VAL:HB	18:sr:34:ILE:HD11	2.01	0.43
6:sa:898:G:H2'	6:sa:899:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:1811:G:C2'	6:sa:1812:C:H5'	2.49	0.43
6:sa:1865:A:H2'	6:sa:1866:A:C8	2.54	0.43
8:sc:177:GLY:HA3	14:sk:53:ARG:NE	2.34	0.43
6:sa:898:G:H2'	6:sa:899:C:C6	2.54	0.43
11:sh:173:LEU:HA	11:sh:191:ARG:HA	2.01	0.43
3:sl:29:C:H2'	3:sl:30:G:C8	2.53	0.42
6:sa:849:A:H5'	16:so:90:PHE:CG	2.54	0.42
6:sa:164:A:C4	6:sa:166:A:C8	3.07	0.42
6:sa:441:C:N3	6:sa:456:G:O2'	2.50	0.42
15:sm:58:PRO:HA	15:sm:63:VAL:HG13	2.00	0.42
6:sa:208:C:H2'	6:sa:209:A:H8	1.84	0.42
6:sa:322:U:H2'	6:sa:323:A:H8	1.85	0.42
6:sa:948:U:H2'	6:sa:949:C:O4'	2.18	0.42
6:sa:335:U:H2'	6:sa:336:A:H8	1.82	0.42
10:sf:194:VAL:HG13	10:sf:209:LYS:HG3	2.01	0.42
11:sh:153:CYS:HA	11:sh:159:PRO:HA	2.01	0.42
18:sr:44:HIS:O	18:sr:45:GLN:HG3	2.20	0.42
6:sa:85:A:H1'	6:sa:143:G:H1'	2.02	0.42
6:sa:955:C:H5''	16:so:109:LYS:HD2	2.02	0.42
9:se:26:PHE:CE2	9:se:49:VAL:HG11	2.54	0.42
9:se:150:ASN:OD1	9:se:150:ASN:N	2.34	0.42
6:sa:426:C:C2	6:sa:427:G:C8	3.07	0.42
6:sa:788:C:N4	6:sa:789:A:H62	2.17	0.42
6:sa:918:G:N2	6:sa:921:A:OP2	2.42	0.42
6:sa:1893:A:H2'	6:sa:1893:A:N3	2.35	0.42
10:sf:189:ARG:HG2	10:sf:216:PHE:CZ	2.55	0.42
2:sC:13:ALA:N	16:so:15:CYS:SG	2.69	0.42
5:sK:7:A:N1	5:sK:8:A:N6	2.68	0.42
6:sa:1840:U:C2	6:sa:1841:U:C5	3.08	0.42
6:sa:1895:G:H2'	6:sa:1896:A:C8	2.55	0.42
10:sf:201:GLY:HA2	15:sm:39:MET:SD	2.59	0.42
16:so:106:LYS:HE2	16:so:106:LYS:HB2	1.72	0.42
19:sy:39:LEU:HD13	19:sy:45:ALA:HB2	2.02	0.42
6:sa:170:G:C4	6:sa:171:A:H2	2.38	0.42
6:sa:365:G:H2'	6:sa:366:G:C8	2.55	0.42
6:sa:734:A:H5'	12:si:118:LYS:N	2.35	0.42
8:sc:139:VAL:HG21	8:sc:221:ARG:HG2	2.01	0.42
17:sp:92:MET:SD	17:sp:107:ALA:HB1	2.60	0.42
1:sB:37:LYS:HE2	1:sB:37:LYS:HB2	1.76	0.42
6:sa:212:C:H2'	6:sa:213:A:O4'	2.20	0.42
6:sa:243:U:H2'	15:sm:14:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:906:A:OP1	6:sa:996:C:O2'	2.31	0.42
6:sa:1028:A:H2'	6:sa:1029:U:H6	1.85	0.42
8:sc:144:GLY:N	8:sc:155:THR:O	2.43	0.42
17:sp:21:ASP:HA	17:sp:84:GLY:O	2.20	0.42
6:sa:411:A:H5''	6:sa:412:A:N7	2.34	0.41
6:sa:444:U:H2'	6:sa:445:C:C6	2.55	0.41
6:sa:582:U:H2'	6:sa:583:C:C6	2.55	0.41
6:sa:601:G:H4'	6:sa:604:G:N2	2.34	0.41
6:sa:1089:A:N1	6:sa:1090:C:N3	2.68	0.41
18:sr:43:LYS:HD2	18:sr:43:LYS:C	2.45	0.41
18:sr:66:ASN:OD1	18:sr:66:ASN:N	2.53	0.41
6:sa:209:A:C6	6:sa:250:G:N1	2.88	0.41
6:sa:572:U:O2'	6:sa:573:A:H5''	2.20	0.41
6:sa:598:A:H2'	6:sa:599:A:O4'	2.20	0.41
6:sa:906:A:H2'	6:sa:907:U:O4'	2.20	0.41
6:sa:1018:C:H42	6:sa:1118:G:H22	1.68	0.41
14:sk:5:LEU:HD23	14:sk:5:LEU:HA	1.86	0.41
15:sm:100:GLU:OE1	19:sy:9:ARG:NH2	2.52	0.41
17:sp:120:LYS:HD3	17:sp:120:LYS:C	2.45	0.41
1:sB:84:VAL:HB	6:sa:1944:A:N6	2.35	0.41
6:sa:125:U:H2'	6:sa:256:A:N1	2.36	0.41
6:sa:389:U:C2	6:sa:399:G:N2	2.88	0.41
6:sa:558:G:C4	6:sa:572:U:H1'	2.55	0.41
6:sa:787:U:O2	6:sa:787:U:H2'	2.20	0.41
6:sa:1824:G:H2'	6:sa:1825:A:O4'	2.21	0.41
8:sc:74:LEU:HD12	8:sc:75:LEU:HG	2.02	0.41
10:sf:200:PRO:HB2	15:sm:39:MET:HB3	2.02	0.41
18:sr:47:ILE:HD12	18:sr:48:THR:N	2.36	0.41
6:sa:393:C:O2'	10:sf:1:ARG:O	2.37	0.41
6:sa:620:U:H2'	6:sa:621:C:H6	1.84	0.41
6:sa:1838:A:H2'	6:sa:1839:A:H8	1.81	0.41
11:sh:152:GLY:O	11:sh:160:MET:N	2.48	0.41
6:sa:340:A:H1'	6:sa:341:G:C8	2.56	0.41
9:se:24:GLU:OE2	17:sp:79:ARG:NH2	2.54	0.41
19:sy:64:ILE:HD13	19:sy:64:ILE:HA	1.95	0.41
6:sa:295:A:C2'	6:sa:296:G:OP1	2.66	0.41
6:sa:622:G:H21	6:sa:951:A:H62	1.69	0.41
6:sa:933:A:H2'	6:sa:934:A:C8	2.55	0.41
10:sf:9:ARG:HE	10:sf:18:LEU:HB3	1.85	0.41
10:sf:195:LYS:HE2	10:sf:197:GLU:HG3	2.03	0.41
11:sh:195:ARG:HH22	11:sh:203:ILE:HD11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:sp:77:ALA:O	17:sp:81:LYS:HE2	2.21	0.41
6:sa:416:A:O2'	6:sa:417:G:H8	2.03	0.41
6:sa:1805:C:H2'	6:sa:1806:C:O4'	2.21	0.41
6:sa:1844:A:H2'	6:sa:1845:G:H8	1.85	0.41
13:sj:36:THR:HA	13:sj:58:LEU:O	2.21	0.41
17:sp:91:LYS:HD3	17:sp:127:VAL:HG11	2.02	0.41
6:sa:121:U:H2'	6:sa:122:G:H8	1.86	0.41
6:sa:169:U:H2'	6:sa:170:G:O4'	2.21	0.41
6:sa:380:A:H2'	6:sa:381:G:H8	1.85	0.41
6:sa:607:G:OP2	6:sa:1125:U:O2'	2.37	0.41
6:sa:1926:U:H2'	6:sa:1928:A:OP2	2.21	0.41
13:sj:60:LEU:HD21	13:sj:215:VAL:HG23	2.02	0.41
13:sj:86:SER:C	15:sm:7:ARG:HH21	2.29	0.41
18:sr:66:ASN:O	18:sr:68:ARG:N	2.54	0.41
6:sa:42:A:H2'	6:sa:43:U:C6	2.56	0.41
6:sa:134:A:N6	6:sa:171:A:N3	2.69	0.41
6:sa:286:U:H2'	6:sa:287:A:C8	2.53	0.41
6:sa:298:A:H2'	6:sa:299:U:C6	2.56	0.41
6:sa:299:U:H2'	6:sa:300:U:O4'	2.20	0.41
6:sa:367:G:O2'	6:sa:605:C:N3	2.53	0.41
6:sa:373:A:H2'	6:sa:374:C:O4'	2.21	0.41
6:sa:413:G:O2'	11:sh:169:ARG:NH1	2.41	0.41
6:sa:911:C:O2'	9:se:120:CYS:O	2.34	0.41
6:sa:966:G:C2	6:sa:967:G:H1'	2.56	0.41
16:so:113:TYR:CZ	16:so:117:LEU:HD11	2.55	0.41
6:sa:169:U:H2'	6:sa:170:G:C8	2.56	0.41
6:sa:566:C:H2'	6:sa:567:C:C6	2.56	0.41
6:sa:960:G:H4'	6:sa:1923:A:H4'	2.03	0.41
6:sa:983:A:H1'	6:sa:985:A:N7	2.36	0.41
6:sa:585:A:N6	6:sa:586:A:N6	2.69	0.40
6:sa:1899:G:H2'	6:sa:1900:A:H8	1.85	0.40
15:sm:58:PRO:HG3	15:sm:138:ASN:HB3	2.03	0.40
1:sB:89:ARG:NH2	6:sa:1114:U:OP1	2.54	0.40
6:sa:293:U:O5'	6:sa:293:U:H6	2.04	0.40
6:sa:381:G:H2'	6:sa:382:A:C8	2.57	0.40
6:sa:391:U:O4	13:sj:26:LYS:NZ	2.53	0.40
6:sa:410:U:O2'	6:sa:413:G:O6	2.37	0.40
6:sa:606:U:OP2	6:sa:607:G:O2'	2.39	0.40
6:sa:990:C:H2'	6:sa:991:G:C8	2.56	0.40
6:sa:1816:U:H2'	6:sa:1817:A:H8	1.82	0.40
6:sa:301:U:O4'	15:sm:127:GLN:NE2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sa:1821:A:C8	6:sa:1893:A:N6	2.89	0.40
9:se:125:THR:OG1	9:se:126:SER:N	2.54	0.40
6:sa:574:A:C5	6:sa:577:C:C4	3.09	0.40
6:sa:744:A:H2'	6:sa:745:U:O4'	2.22	0.40
6:sa:751:A:N1	6:sa:785:A:N6	2.69	0.40
6:sa:1129:C:H2'	6:sa:1130:U:H6	1.86	0.40
15:sm:76:SER:HA	15:sm:119:GLU:OE2	2.21	0.40
6:sa:762:A:C4	6:sa:763:G:C8	3.09	0.40
6:sa:762:A:H3'	6:sa:763:G:H8	1.86	0.40
6:sa:1029:U:H3	6:sa:1094:G:H1	1.68	0.40
6:sa:1906:C:H2'	6:sa:1907:G:C8	2.56	0.40
8:sc:222:GLN:H	8:sc:222:GLN:HG2	1.79	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	sB	90/144 (62%)	88 (98%)	2 (2%)	0	100	100
2	sC	6/84 (7%)	6 (100%)	0	0	100	100
7	sb	16/254 (6%)	15 (94%)	1 (6%)	0	100	100
8	sc	159/255 (62%)	146 (92%)	13 (8%)	0	100	100
9	se	101/256 (40%)	98 (97%)	3 (3%)	0	100	100
10	sf	78/326 (24%)	77 (99%)	1 (1%)	0	100	100
11	sh	56/266 (21%)	50 (89%)	6 (11%)	0	100	100
12	si	15/201 (8%)	14 (93%)	1 (7%)	0	100	100
13	sj	88/237 (37%)	87 (99%)	1 (1%)	0	100	100
14	sk	35/185 (19%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	sm	132/156 (85%)	120 (91%)	12 (9%)	0	100	100
16	so	64/151 (42%)	62 (97%)	2 (3%)	0	100	100
17	sp	127/146 (87%)	119 (94%)	8 (6%)	0	100	100
18	sr	108/130 (83%)	96 (89%)	12 (11%)	0	100	100
19	sy	85/141 (60%)	78 (92%)	7 (8%)	0	100	100
All	All	1160/2932 (40%)	1090 (94%)	70 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	sB	84/127 (66%)	83 (99%)	1 (1%)	63	79
2	sC	7/73 (10%)	7 (100%)	0	100	100
7	sb	17/218 (8%)	17 (100%)	0	100	100
8	sc	128/199 (64%)	127 (99%)	1 (1%)	73	82
9	se	110/225 (49%)	106 (96%)	4 (4%)	31	63
10	sf	71/283 (25%)	69 (97%)	2 (3%)	38	68
11	sh	46/220 (21%)	44 (96%)	2 (4%)	26	59
12	si	16/167 (10%)	15 (94%)	1 (6%)	16	48
13	sj	82/205 (40%)	80 (98%)	2 (2%)	43	70
14	sk	38/164 (23%)	37 (97%)	1 (3%)	40	69
15	sm	121/138 (88%)	114 (94%)	7 (6%)	18	51
16	so	64/129 (50%)	62 (97%)	2 (3%)	35	66
17	sp	99/114 (87%)	96 (97%)	3 (3%)	36	66
18	sr	100/113 (88%)	95 (95%)	5 (5%)	22	55
19	sy	72/114 (63%)	67 (93%)	5 (7%)	14	45
All	All	1055/2489 (42%)	1019 (97%)	36 (3%)	33	64

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	sB	2	THR
8	sc	81	GLU
9	se	49	VAL
9	se	62	GLN
9	se	105	LEU
9	se	150	ASN
10	sf	36	MET
10	sf	103	THR
11	sh	170	VAL
11	sh	199	VAL
12	si	105	HIS
13	sj	22	GLN
13	sj	53	ILE
14	sk	54	THR
15	sm	11	LYS
15	sm	39	MET
15	sm	59	PHE
15	sm	73	ILE
15	sm	88	ASP
15	sm	123	VAL
15	sm	147	THR
16	so	4	MET
16	so	16	ILE
17	sp	40	THR
17	sp	49	ILE
17	sp	67	TYR
18	sr	41	MET
18	sr	80	ASN
18	sr	83	LEU
18	sr	98	HIS
18	sr	112	ASP
19	sy	39	LEU
19	sy	56	GLU
19	sy	62	SER
19	sy	100	ILE
19	sy	103	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	sB	94	ASN

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Mol	Chain	Res	Type
8	sc	112	HIS
8	sc	227	GLN
9	se	47	GLN
9	se	62	GLN
11	sh	178	ASN
15	sm	10	GLN
15	sm	91	HIS
15	sm	127	GLN
15	sm	138	ASN
17	sp	108	GLN
18	sr	45	GLN
18	sr	98	HIS
18	sr	120	HIS
19	sy	14	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	sI	12/76 (15%)	8 (66%)	0
4	sJ	12/77 (15%)	0	0
5	sK	9/10 (90%)	0	0
6	sa	913/1947 (46%)	188 (20%)	0
All	All	946/2110 (44%)	196 (20%)	0

All (196) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	sI	30	G
3	sI	32	C
3	sI	33	U
3	sI	34	U
3	sI	35	U
3	sI	36	U
3	sI	38	A
3	sI	39	U
6	sa	4	C
6	sa	17	C
6	sa	24	U
6	sa	33	A
6	sa	41	G
6	sa	42	A

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Mol	Chain	Res	Type
6	sa	44	U
6	sa	46	A
6	sa	56	G
6	sa	61	A
6	sa	62	G
6	sa	64	A
6	sa	65	U
6	sa	79	G
6	sa	80	A
6	sa	100	U
6	sa	103	U
6	sa	113	A
6	sa	114	G
6	sa	115	U
6	sa	135	C
6	sa	136	A
6	sa	137	A
6	sa	139	G
6	sa	141	U
6	sa	148	G
6	sa	154	G
6	sa	171	A
6	sa	173	A
6	sa	204	A
6	sa	243	U
6	sa	244	U
6	sa	246	G
6	sa	252	C
6	sa	253	A
6	sa	254	C
6	sa	259	A
6	sa	260	U
6	sa	262	G
6	sa	295	A
6	sa	296	G
6	sa	299	U
6	sa	311	C
6	sa	313	A
6	sa	317	G
6	sa	324	G
6	sa	328	C
6	sa	332	G

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Mol	Chain	Res	Type
6	sa	333	A
6	sa	345	A
6	sa	347	A
6	sa	354	A
6	sa	355	A
6	sa	356	C
6	sa	383	G
6	sa	385	G
6	sa	394	A
6	sa	395	G
6	sa	397	U
6	sa	399	G
6	sa	411	A
6	sa	412	A
6	sa	413	G
6	sa	417	G
6	sa	419	C
6	sa	420	A
6	sa	421	G
6	sa	423	A
6	sa	430	U
6	sa	432	A
6	sa	434	U
6	sa	439	C
6	sa	440	A
6	sa	447	A
6	sa	448	A
6	sa	449	U
6	sa	455	A
6	sa	456	G
6	sa	463	A
6	sa	470	A
6	sa	548	C
6	sa	549	A
6	sa	551	G
6	sa	553	C
6	sa	555	G
6	sa	559	C
6	sa	561	A
6	sa	562	G
6	sa	568	G
6	sa	572	U

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Mol	Chain	Res	Type
6	sa	576	U
6	sa	579	A
6	sa	580	G
6	sa	584	C
6	sa	588	A
6	sa	589	G
6	sa	600	A
6	sa	602	U
6	sa	604	G
6	sa	613	A
6	sa	614	A
6	sa	616	A
6	sa	617	C
6	sa	628	G
6	sa	742	G
6	sa	746	A
6	sa	782	A
6	sa	783	A
6	sa	784	U
6	sa	785	A
6	sa	786	U
6	sa	787	U
6	sa	790	A
6	sa	804	C
6	sa	840	U
6	sa	843	A
6	sa	844	A
6	sa	845	A
6	sa	856	G
6	sa	879	G
6	sa	893	U
6	sa	894	G
6	sa	902	U
6	sa	904	A
6	sa	913	A
6	sa	915	A
6	sa	922	G
6	sa	924	A
6	sa	927	U
6	sa	940	U
6	sa	946	A
6	sa	968	A

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Mol	Chain	Res	Type
6	sa	972	A
6	sa	973	A
6	sa	977	G
6	sa	983	A
6	sa	984	U
6	sa	985	A
6	sa	1006	A
6	sa	1008	C
6	sa	1012	G
6	sa	1027	G
6	sa	1090	C
6	sa	1091	C
6	sa	1096	U
6	sa	1097	C
6	sa	1101	A
6	sa	1106	A
6	sa	1117	U
6	sa	1118	G
6	sa	1122	U
6	sa	1123	U
6	sa	1135	G
6	sa	1140	G
6	sa	1164	A
6	sa	1797	A
6	sa	1800	C
6	sa	1801	A
6	sa	1812	C
6	sa	1821	A
6	sa	1822	U
6	sa	1823	U
6	sa	1824	G
6	sa	1825	A
6	sa	1826	A
6	sa	1831	G
6	sa	1832	A
6	sa	1849	U
6	sa	1878	A
6	sa	1883	C
6	sa	1886	U
6	sa	1887	A
6	sa	1892	G
6	sa	1894	G

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Mol	Chain	Res	Type
6	sa	1895	G
6	sa	1902	A
6	sa	1907	G
6	sa	1909	A
6	sa	1913	A
6	sa	1916	U
6	sa	1927	G
6	sa	1929	A
6	sa	1930	C
6	sa	1939	G
6	sa	1940	G
6	sa	1941	A
6	sa	1942	U
6	sa	1943	C

There are no RNA pucker outliers to report.

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	PAR	sa	5101	-	44,45,45	0.79	0	63,67,67	1.01	2 (3%)

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
20	PAR	sa	5101	-	-	6/18/94/94	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	sa	5101	PAR	C34-C24-N24	-2.16	106.63	111.05
20	sa	5101	PAR	C62-C12-N12	-2.09	106.81	110.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	sa	5101	PAR	O54-C14-O33-C33
20	sa	5101	PAR	O51-C51-C61-O61
20	sa	5101	PAR	O51-C11-O11-C42
20	sa	5101	PAR	C52-C42-O11-C11
20	sa	5101	PAR	C24-C14-O33-C33
20	sa	5101	PAR	C44-C54-C64-N64

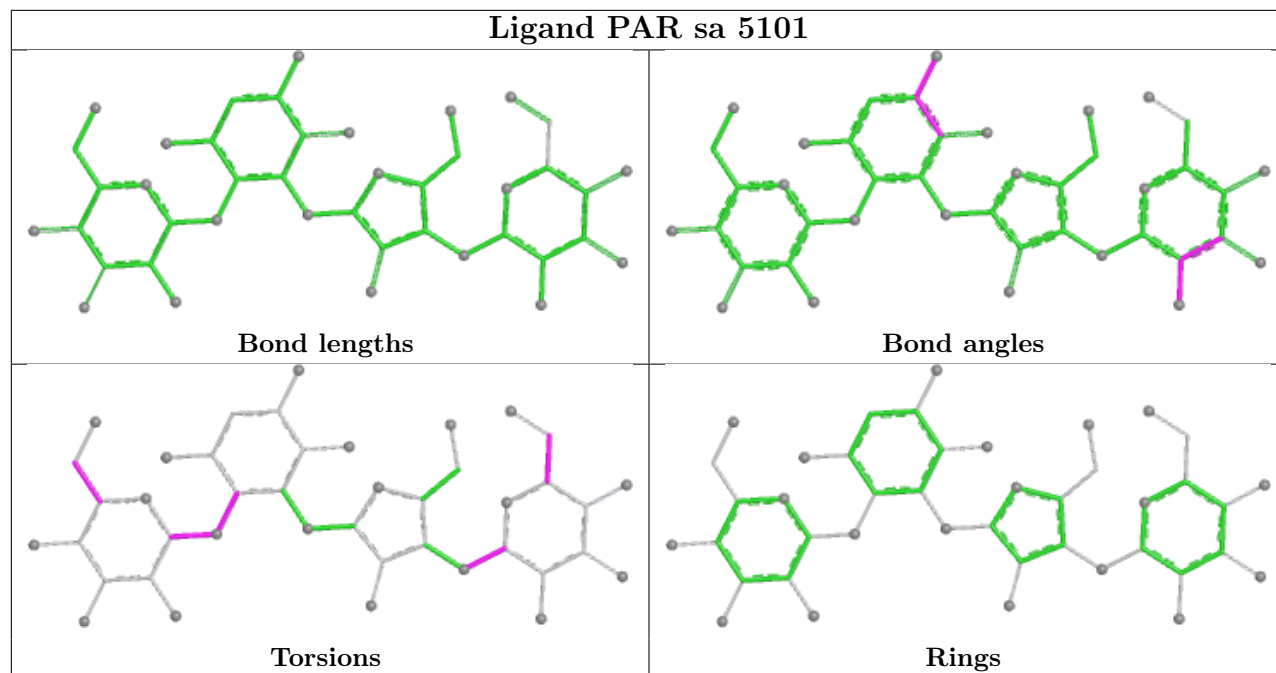
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	sa	5101	PAR	3	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.

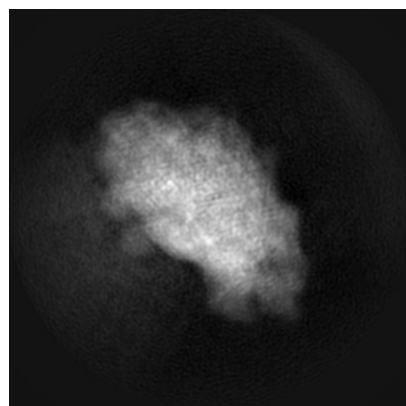
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64721. These allow visual inspection of the internal detail of the map and identification of artifacts.

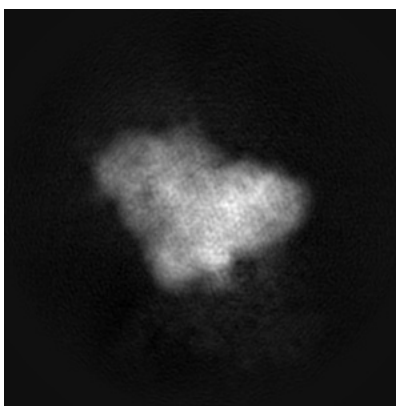
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

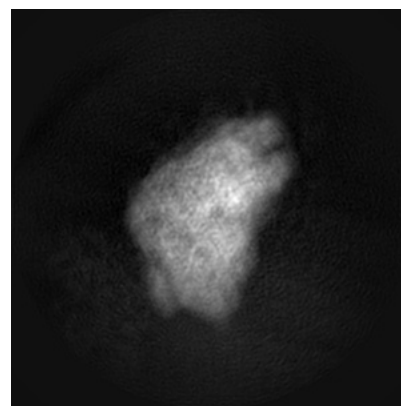
6.1.1 Primary map



X

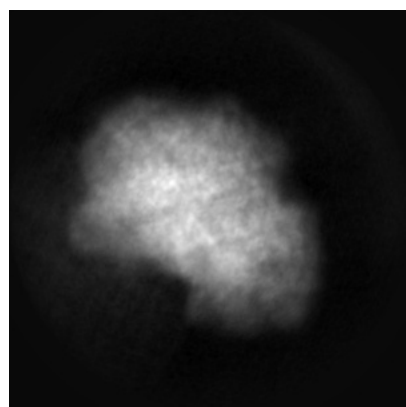


Y

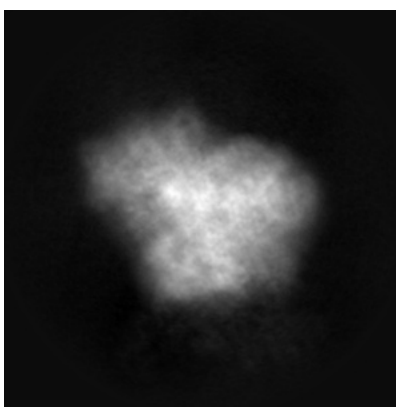


Z

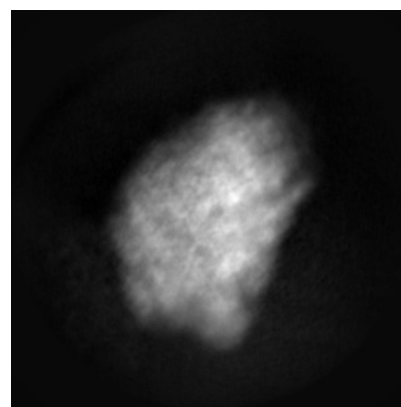
6.1.2 Raw map



X



Y

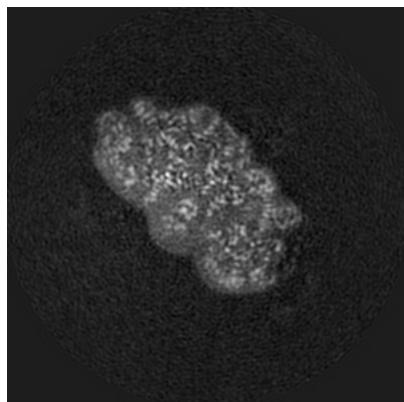


Z

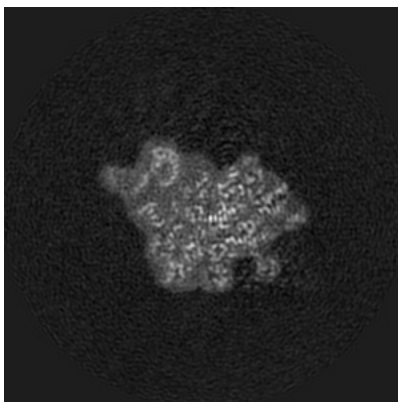
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

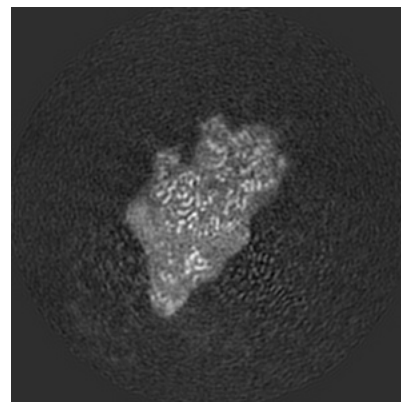
6.2.1 Primary map



X Index: 135

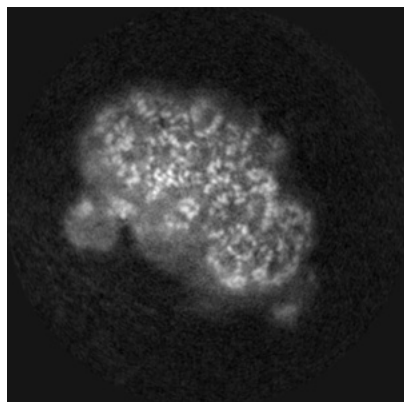


Y Index: 135

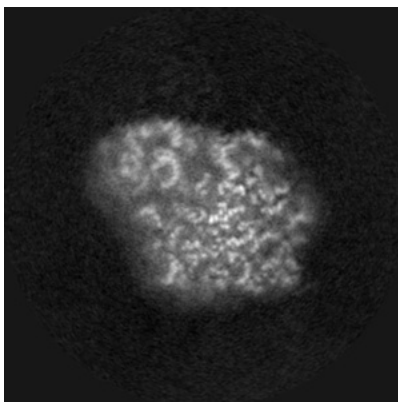


Z Index: 135

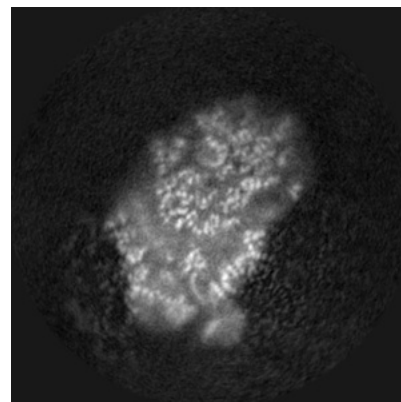
6.2.2 Raw map



X Index: 135



Y Index: 135

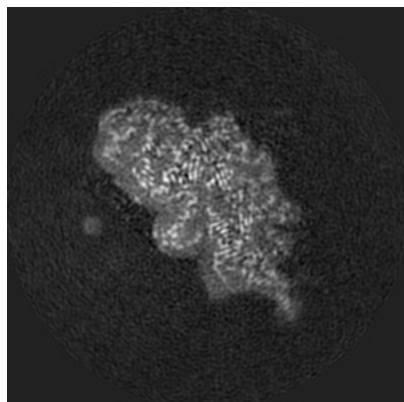


Z Index: 135

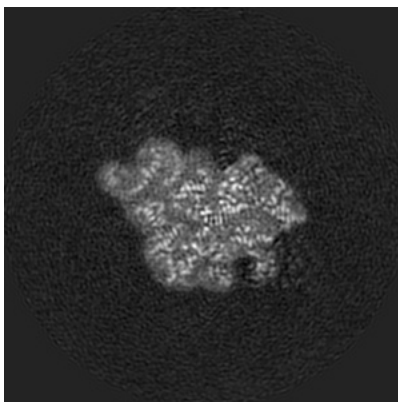
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

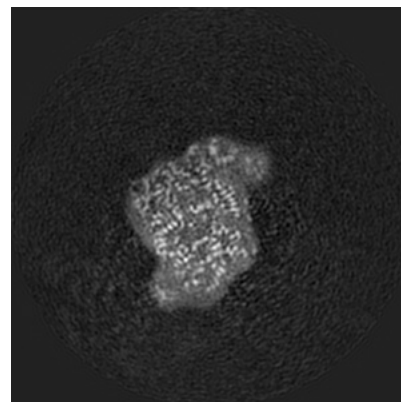
6.3.1 Primary map



X Index: 142

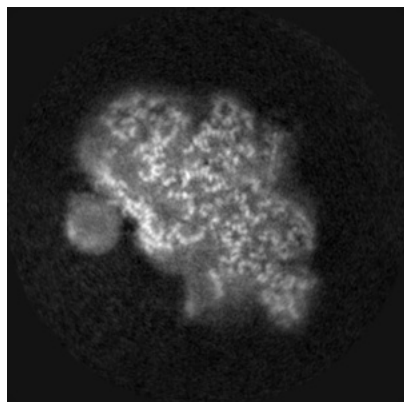


Y Index: 137

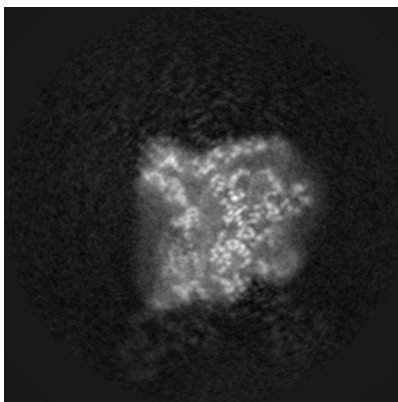


Z Index: 149

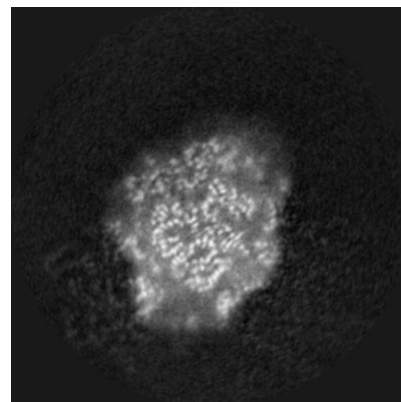
6.3.2 Raw map



X Index: 145



Y Index: 112

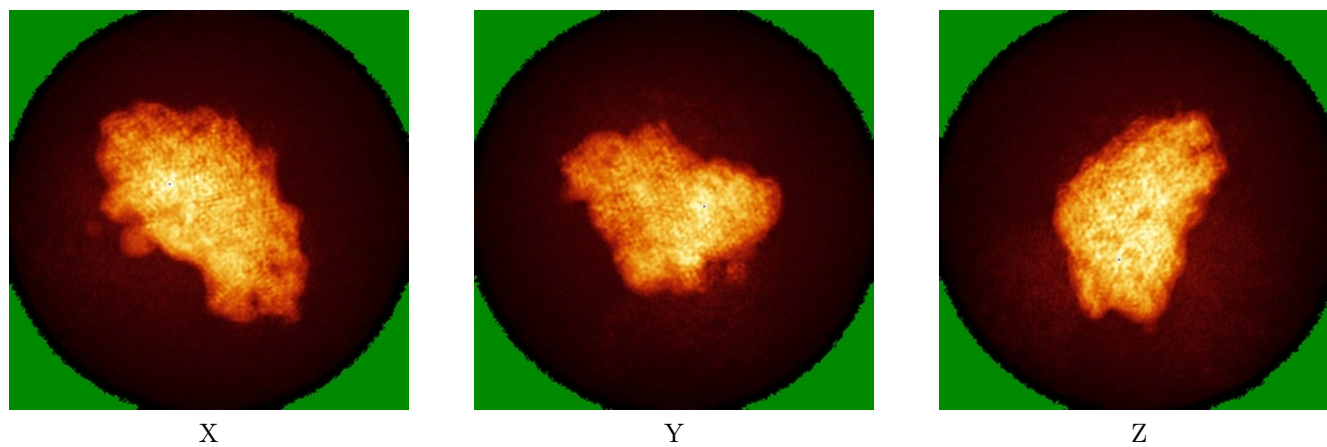


Z Index: 152

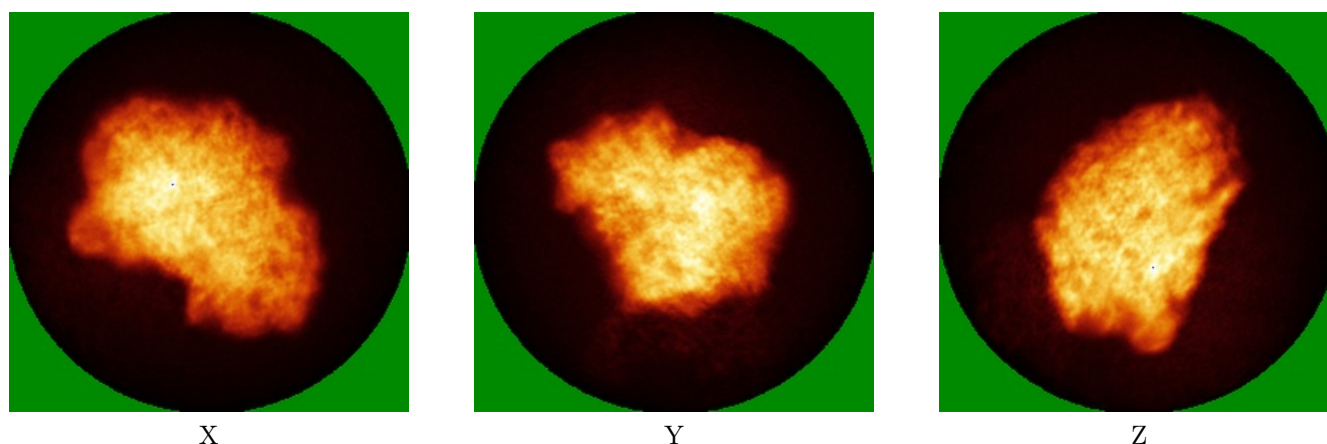
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

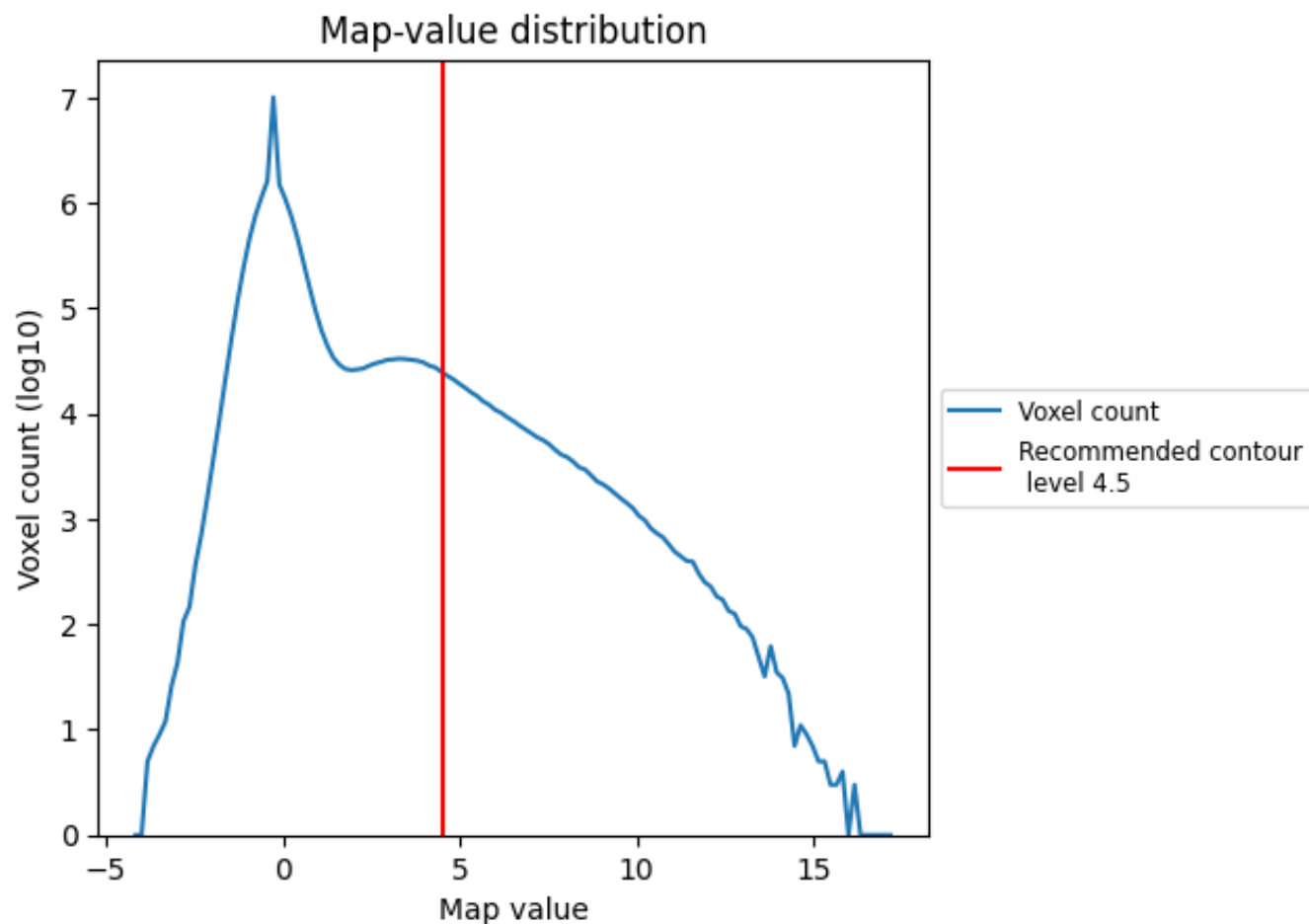
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

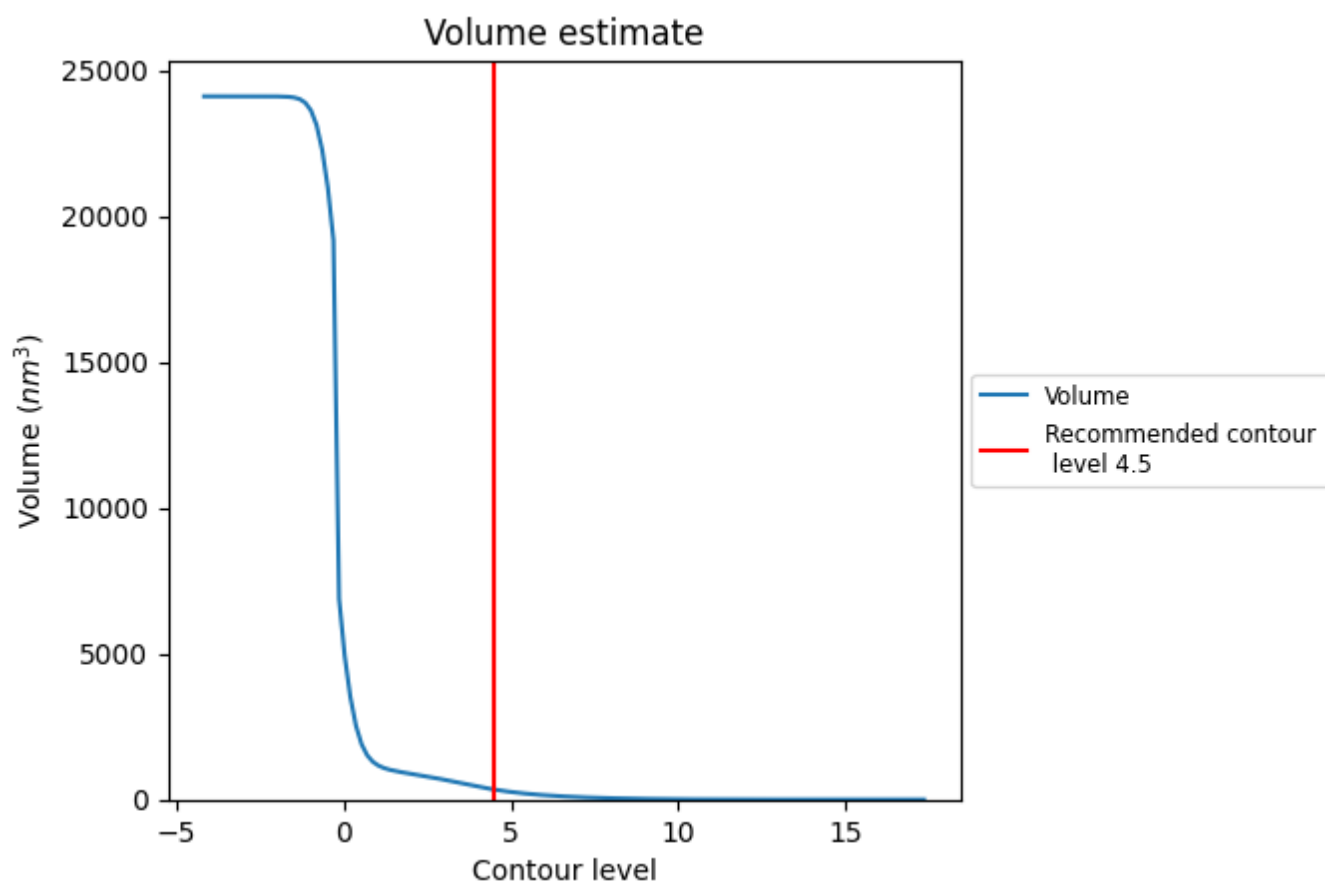
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

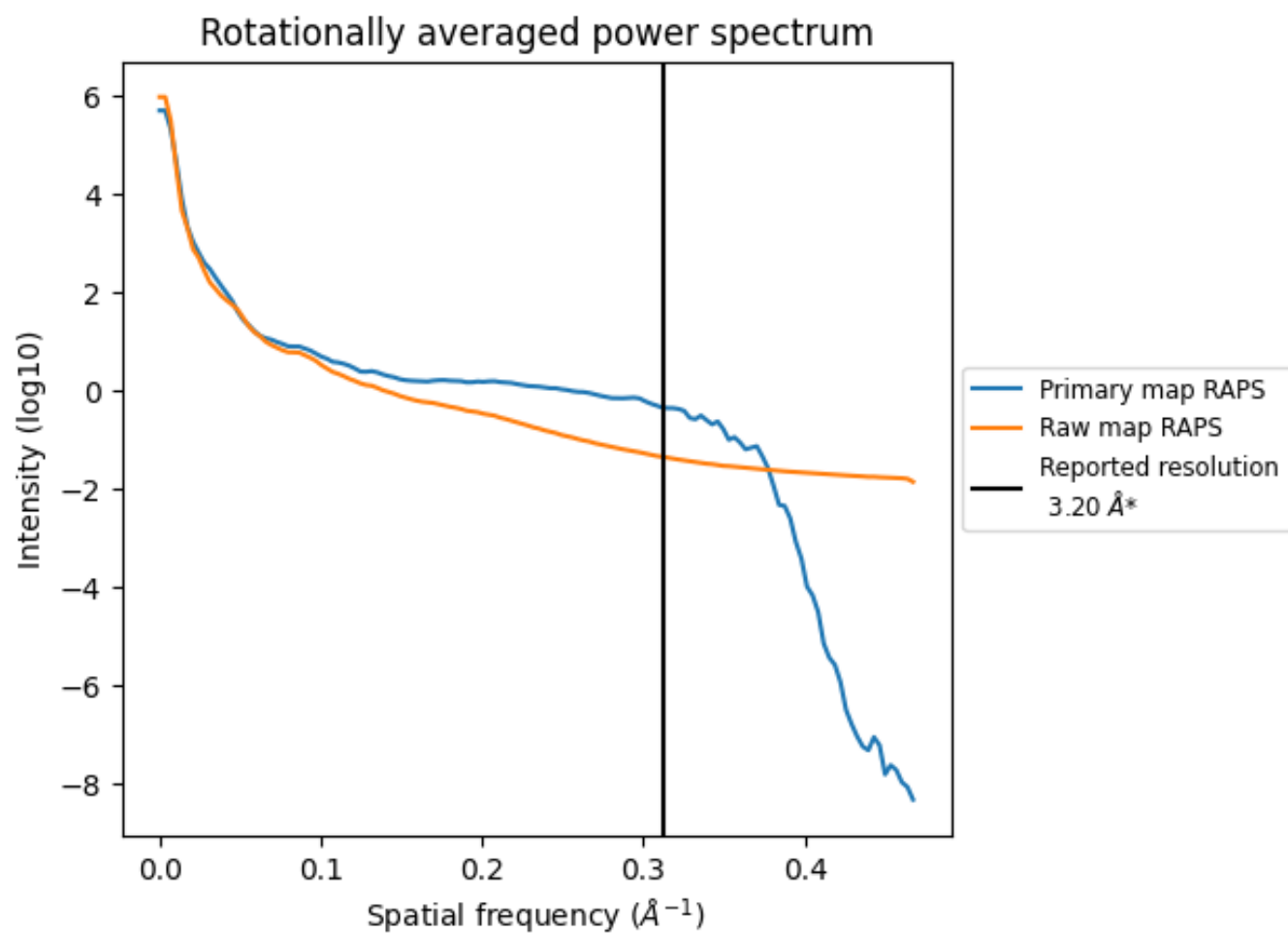
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm³; this corresponds to an approximate mass of 310 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 ⓘ

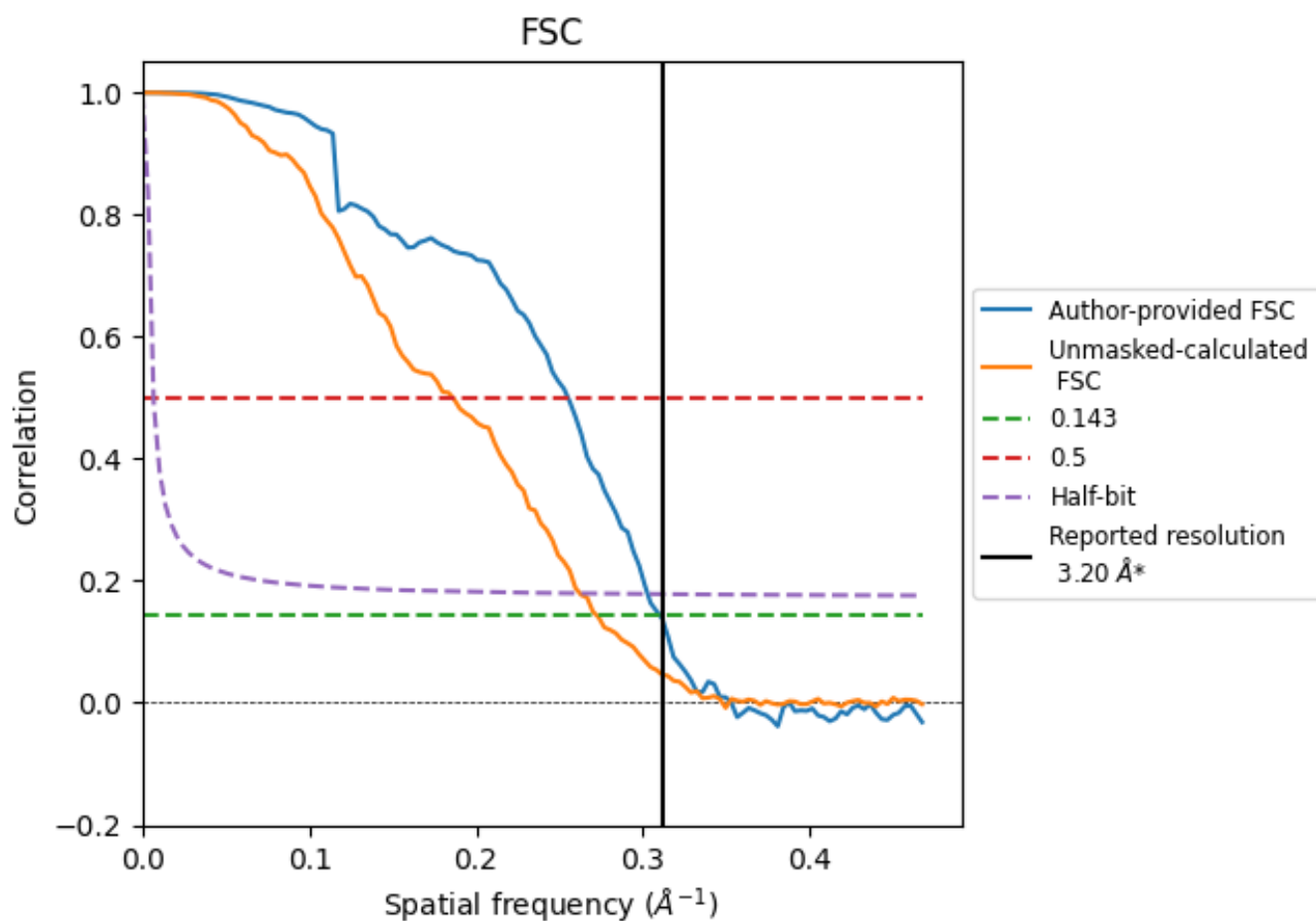


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.92	3.30
Unmasked-calculated*	3.67	5.37	3.81

*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 3.67 differs from the reported value 3.2 by more than 10 %

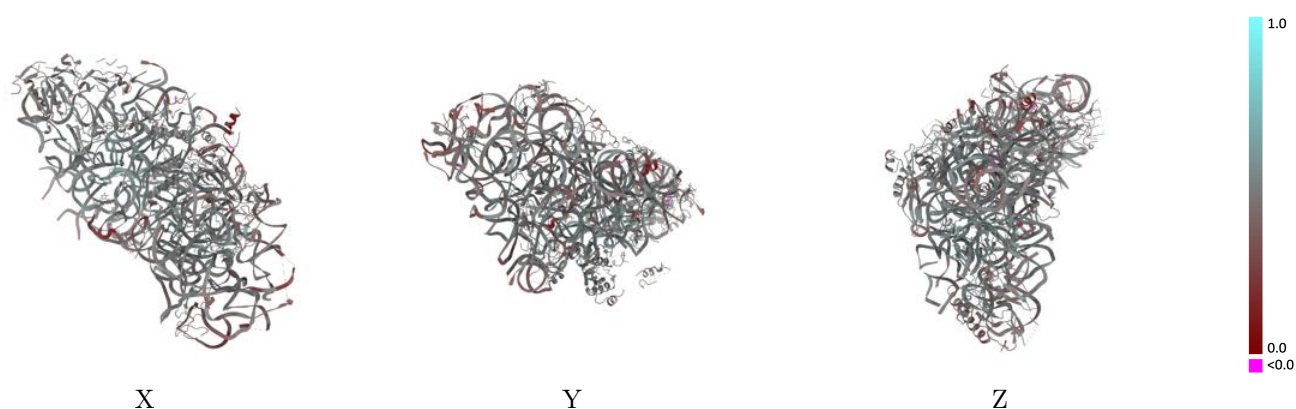
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-64721 and PDB model 9V29. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

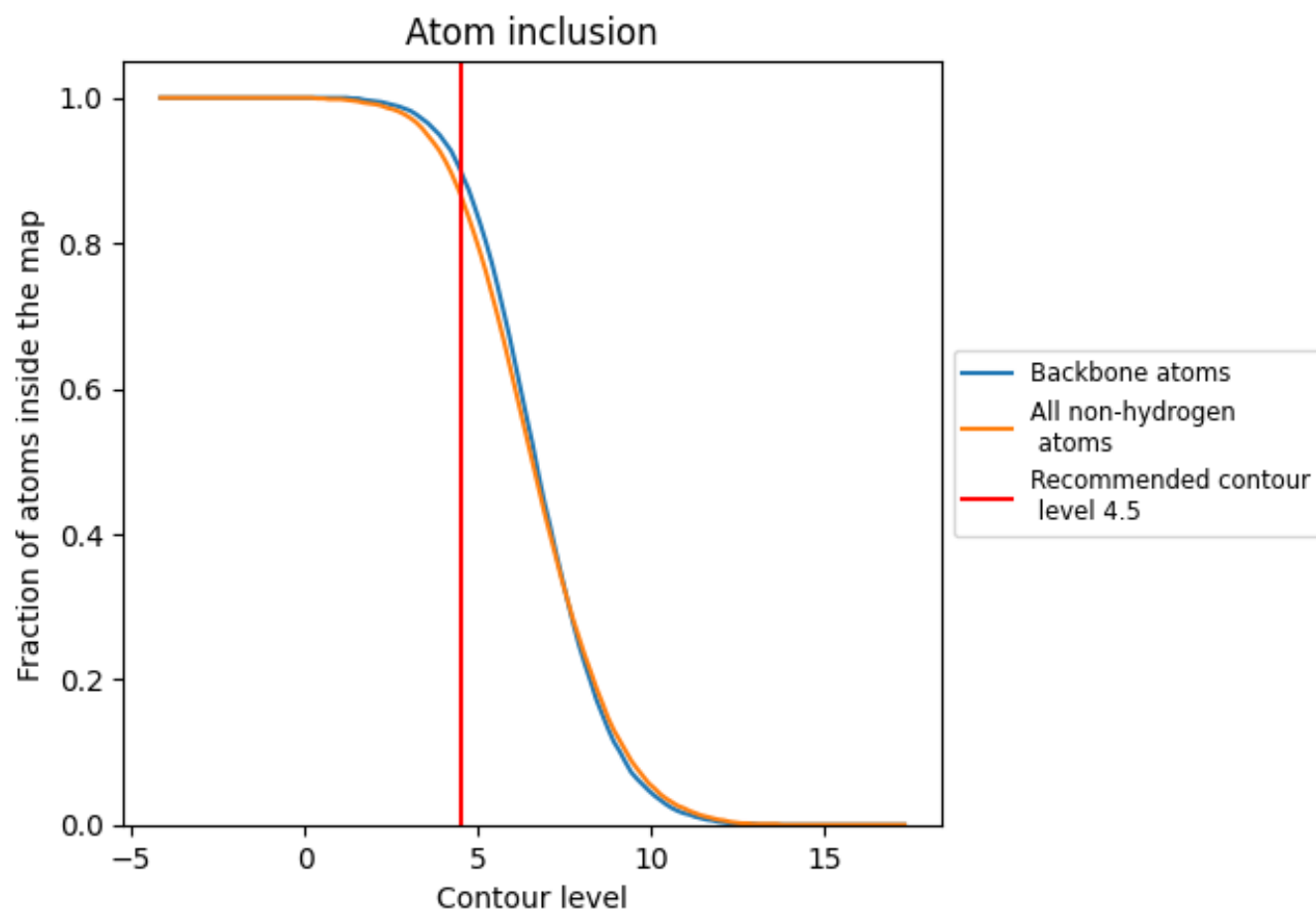


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.4680
sB	 0.8520	 0.4890
sC	 0.2960	 0.1890
sI	 0.9630	 0.4230
sJ	 0.9850	 0.4640
sK	 0.9950	 0.4900
sa	 0.9280	 0.4720
sb	 0.4710	 0.4260
sc	 0.7720	 0.4830
se	 0.6820	 0.4570
sf	 0.6600	 0.4590
sh	 0.7210	 0.4480
si	 0.2940	 0.1870
sj	 0.7100	 0.4830
sk	 0.6530	 0.4440
sm	 0.7520	 0.4520
so	 0.8230	 0.4710
sp	 0.7850	 0.4550
sr	 0.7460	 0.4760
sy	 0.7630	 0.4570

