Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 01:54 pm BST

PDB ID	:	9QEH / pdb_00009qeh
EMDB ID	:	EMD-53067
Title	:	Cryo-EM structure of the A2085-methylated 50S ribosome of a MLSb resistant S. aureus strain "MNY196" in complex with solithromycin
Authors	:	Rivalta, A.; Yonath, A.
Deposited on	:	2025-03-10
Resolution	:	2.08 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

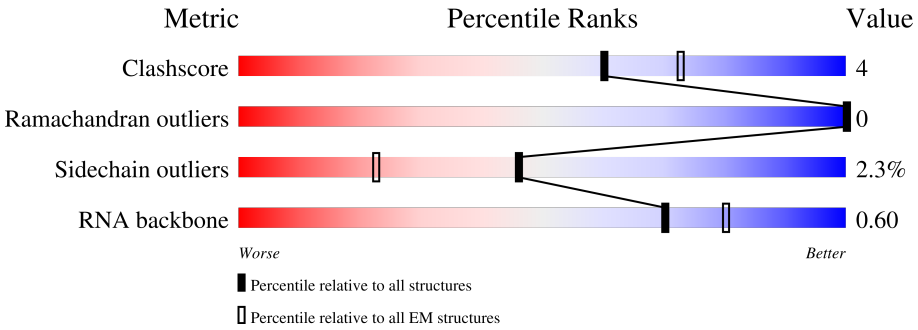
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.08 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	1	52	69% 21% • 8%
2	2	45	89% 9% •
3	3	66	98% •
4	4	37	84% 16%
5	L	122	89% 10% •
6	A	2923	63% 25% • 11%
7	B	115	55% 38% 5% •

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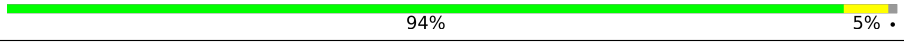
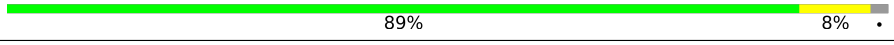
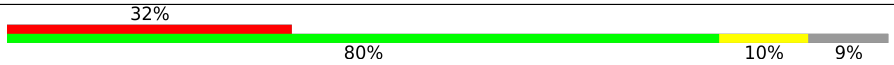
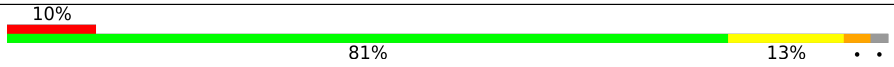
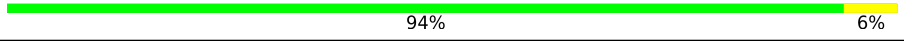
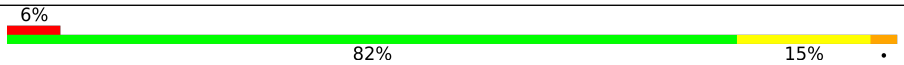
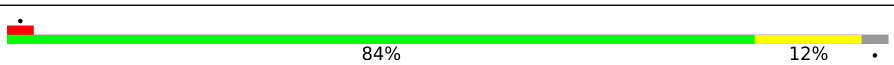
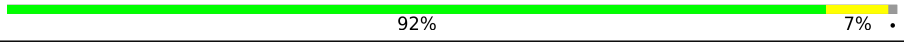
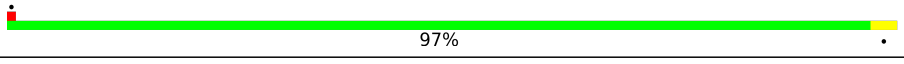
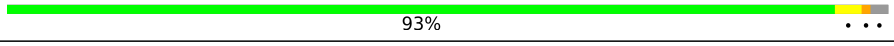
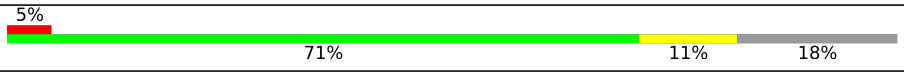
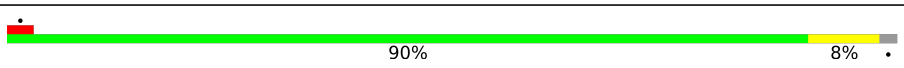
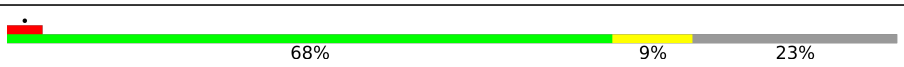
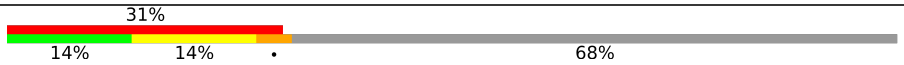
Mol	Chain	Length	Quality of chain
8	C	277	
9	D	220	
10	E	207	
11	F	179	
12	G	178	
13	H	145	
14	I	122	
15	J	146	
16	K	144	
17	M	119	
18	N	116	
19	O	118	
20	P	102	
21	Q	117	
22	R	91	
23	S	105	
24	T	217	
25	U	94	
26	V	62	
27	W	73	
28	X	59	
29	Z	57	
30	8	71	
31	11	13	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 82317 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	48	Total	C	N	O	S	0	0
			359	221	68	66	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	44	Total	C	N	O	S	0	0
			368	225	89	53	1		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	65	Total	C	N	O	S	0	0
			518	321	112	83	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	37	Total	C	N	O	S	0	0
			292	183	59	45	5		

- Molecule 5 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	120	Total	C	N	O	S	0	0
			908	563	182	162	1		

- Molecule 6 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	2616	Total	C	N	O	P	2	0
			56161	25076	10304	18163	2618		

- Molecule 7 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 8 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	274	Total	C	N	O	S	0	0
			2043	1274	405	359	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	215	Total	C	N	O	S	0	0
			1559	982	294	278	5		

- Molecule 10 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	206	Total	C	N	O	S	0	0
			1517	957	284	274	2		

- Molecule 11 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	162	Total	C	N	O	S	0	0
			937	582	179	174	2		

- Molecule 12 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	175	Total	C	N	O	S	0	0
			1165	724	230	208	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	145	Total	C	N	O	S	0	0
			1088	686	203	196	3		

- Molecule 14 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	122	Total 908	C 566	N 173	O 165	S 4	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	J	146	Total 1024	C 637	N 209	O 178	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	137	Total 1040	C 668	N 197	O 172	S 3	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	119	Total 813	C 507	N 163	O 143	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	N	112	Total 860	C 544	N 172	O 144	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	117	Total 910	C 576	N 184	O 146	S 4	0	0

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	102	Total 757	C 484	N 138	O 134	S 1	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	111	Total	C	N	O	S	0	0
			802	506	157	137	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	89	Total	C	N	O	S	0	0
			650	416	116	114	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	94	Total	C	N	O	S	0	0
			664	421	124	118	1		

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	T	94	Total	C	N	O	0	0
			624	401	113	110		

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	U	78	Total	C	N	O	0	0
			566	352	114	100		

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	V	51	Total	C	N	O	0	0
			370	229	80	61		

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	W	64	Total	C	N	O	0	0
			480	299	97	84		

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	58	Total 434	C 271	N 84	O 79	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	44	Total 344	C 212	N 73	O 55	S 4	0	0

- Molecule 30 is a RNA chain called P_site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	23	Total 497	C 221	N 94	O 159	P 23	0	0

- Molecule 31 is a RNA chain called E_site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	11	13	Total 280	C 124	N 53	O 90	P 13	0	0

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	1	1	Total 1	Zn 1	0
32	4	1	Total 1	Zn 1	0
32	Z	1	Total 1	Zn 1	0

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	L	1	Total 1	Mg 1	0
33	A	227	Total 227	Mg 227	0
33	D	1	Total 1	Mg 1	0
33	J	1	Total 1	Mg 1	0

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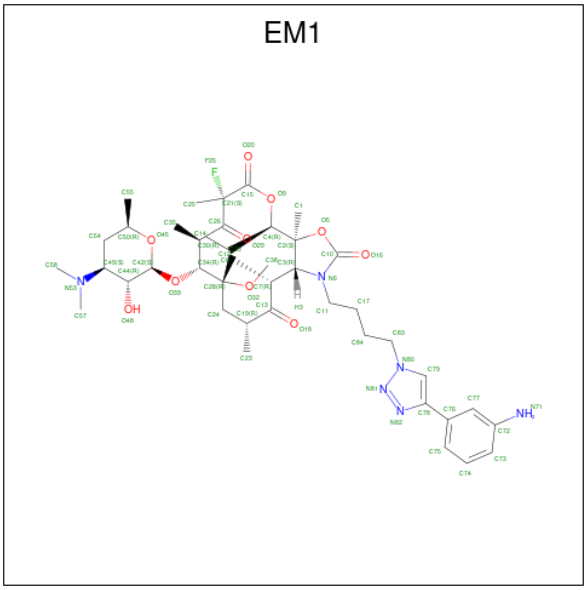
Mol	Chain	Residues	Atoms	AltConf
33	U	1	Total Mg 1 1	0

- Molecule 34 is (3aS,4R,7S,9R,10R,11R,13R,15R,15aR)-1-{4-[4-(3-aminophenyl)-1H-1,2,3-triazol-1-yl]butyl}-4-ethyl-7-fluoro-11-methoxy-3a ,7,9,11,13,15-hexamethyl-2,6,8,14-tetraoxotetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-10-yl 3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranoside (CCD ID: EM1) (formula: $C_{43}H_{65}FN_6O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C F N O 60 43 1 6 10	0

- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
35	A	11	Total K 11 11	0
35	C	1	Total K 1 1	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	3	1	Total O 1 1	0

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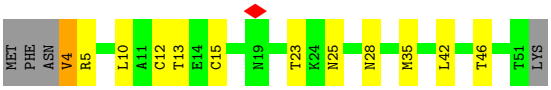
Mol	Chain	Residues	Atoms	AltConf
36	A	626	Total O 626 626	0
36	C	21	Total O 21 21	0
36	D	3	Total O 3 3	0
36	E	1	Total O 1 1	0
36	H	1	Total O 1 1	0
36	J	6	Total O 6 6	0
36	N	2	Total O 2 2	0
36	O	2	Total O 2 2	0
36	R	1	Total O 1 1	0
36	X	1	Total O 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

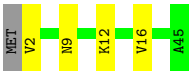
• Molecule 1: Large ribosomal subunit protein bL33A

Chain 1:



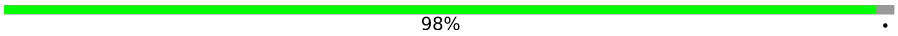
• Molecule 2: Large ribosomal subunit protein bL34

Chain 2:



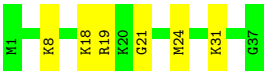
• Molecule 3: Large ribosomal subunit protein bL35

Chain 3:



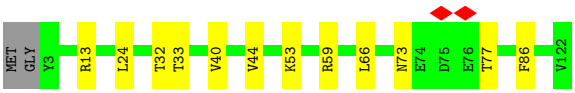
• Molecule 4: Large ribosomal subunit protein bL36

Chain 4:



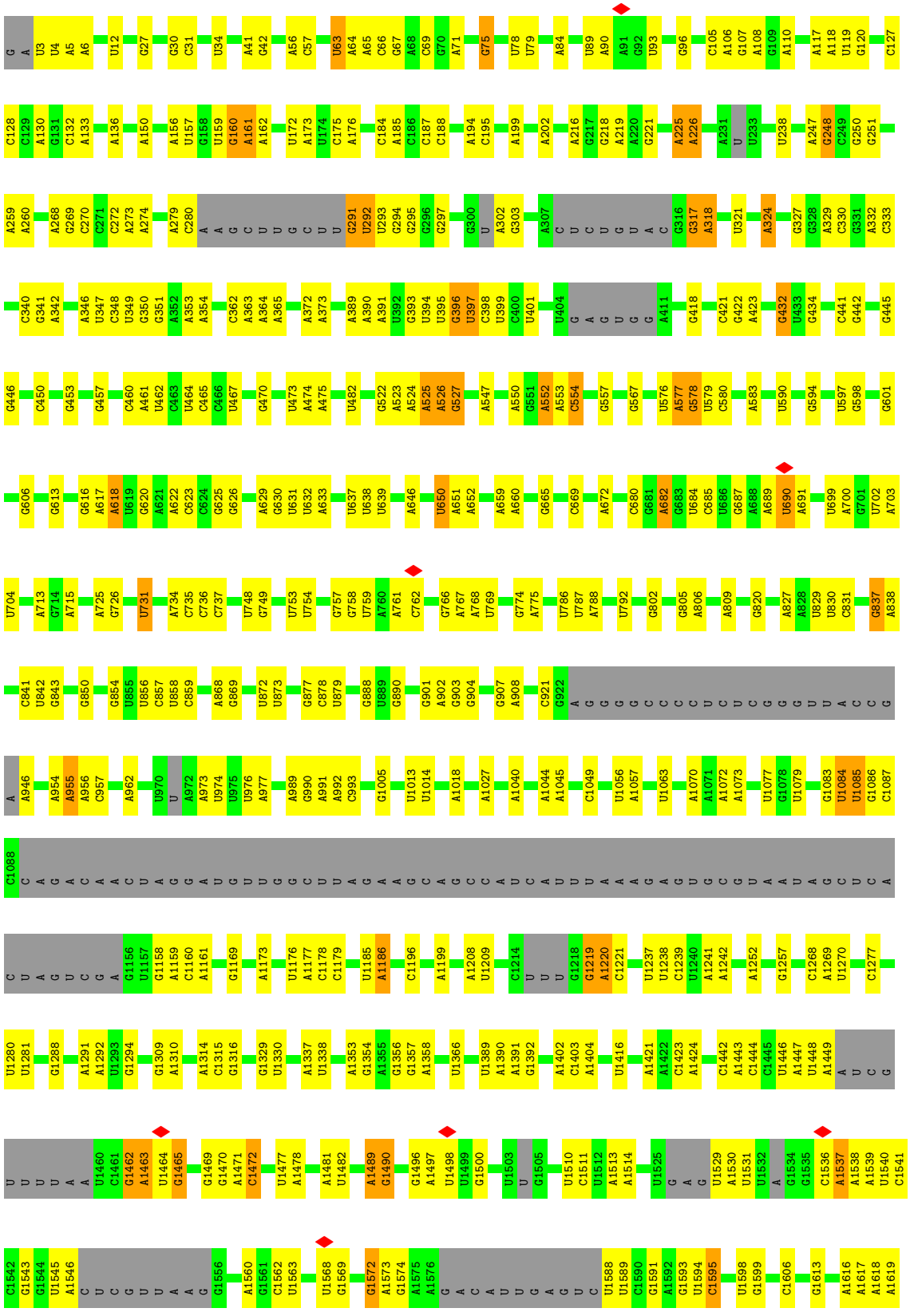
• Molecule 5: Large ribosomal subunit protein bL17

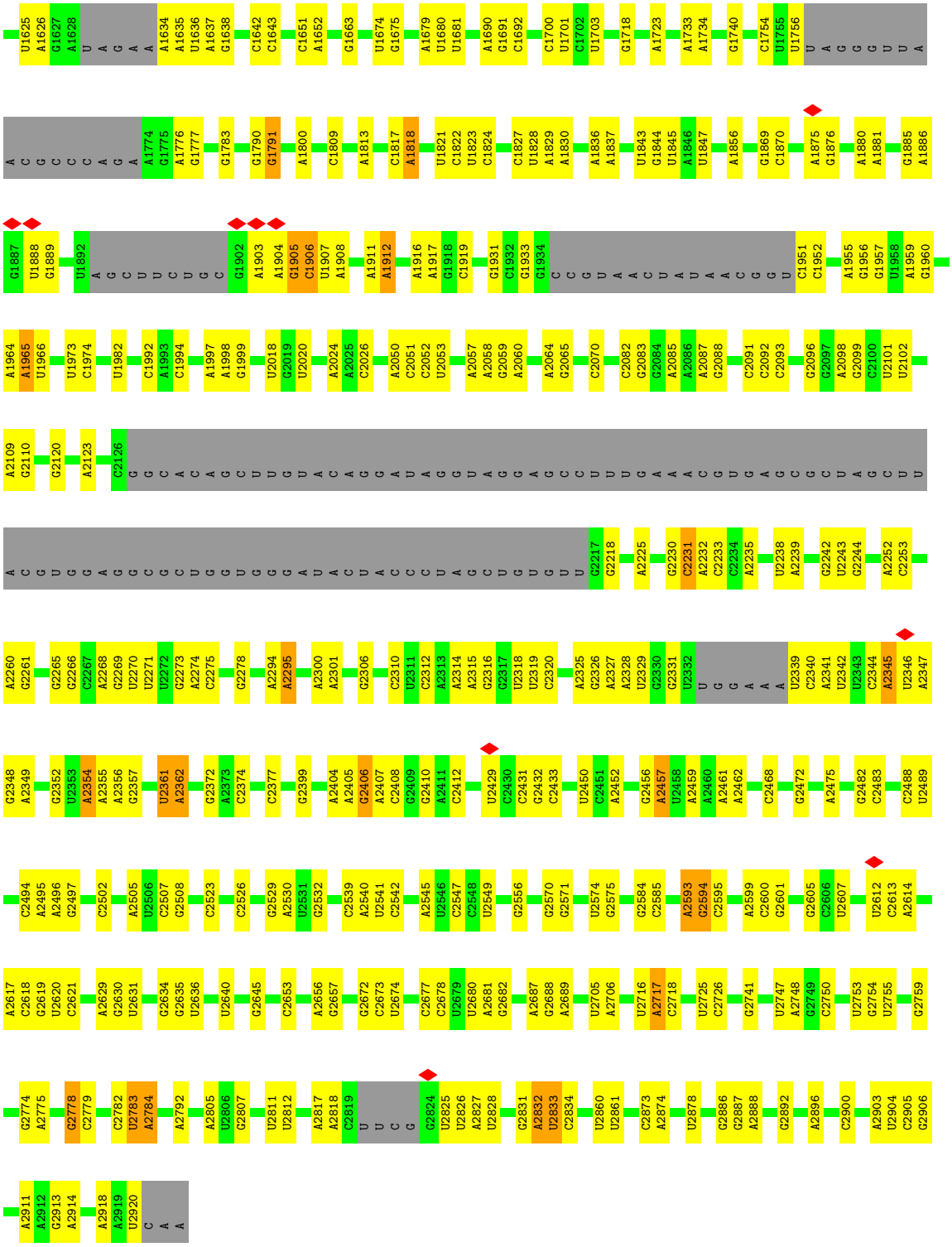
Chain L:



• Molecule 6: 23S rRNA

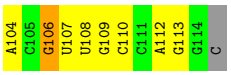
Chain A:





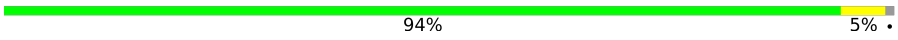
• Molecule 7: 5S rRNA

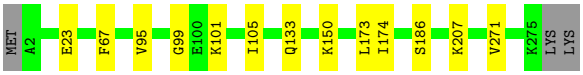
Chain B:



• Molecule 8: Large ribosomal subunit protein uL2

Chain C:





• Molecule 9: Large ribosomal subunit protein uL3

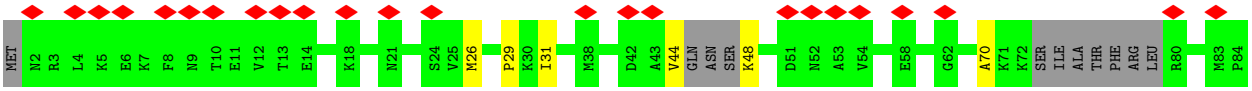
Chain D:

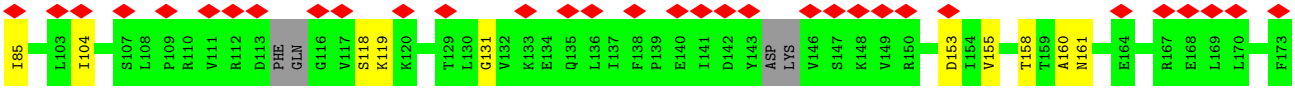
• Molecule 10: Large ribosomal subunit protein uL4

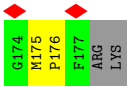
Chain E:

• Molecule 11: Large ribosomal subunit protein uL5

Chain F:

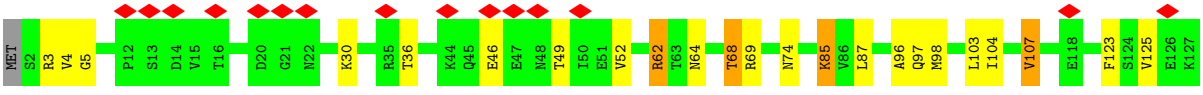






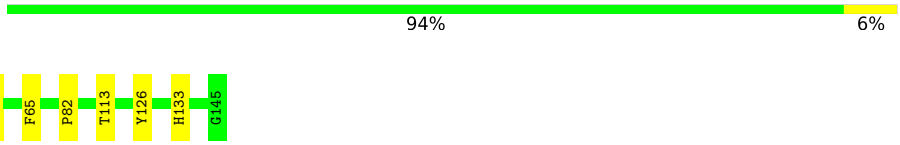
• Molecule 12: Large ribosomal subunit protein uL6

Chain G:



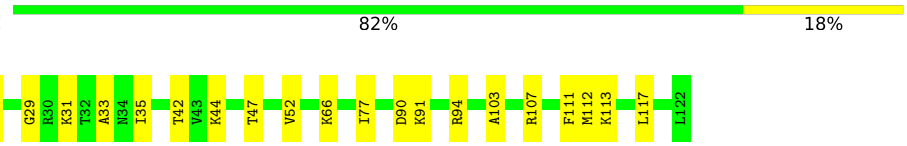
• Molecule 13: Large ribosomal subunit protein uL13

Chain H:



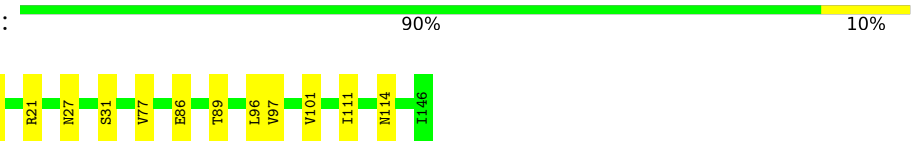
• Molecule 14: Large ribosomal subunit protein uL14

Chain I:



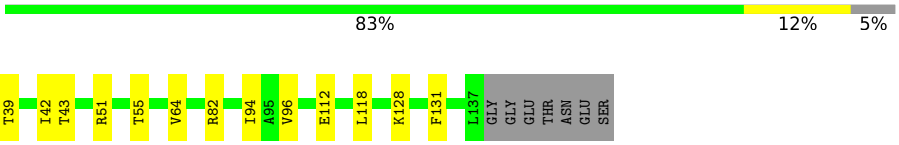
• Molecule 15: Large ribosomal subunit protein uL15

Chain J:



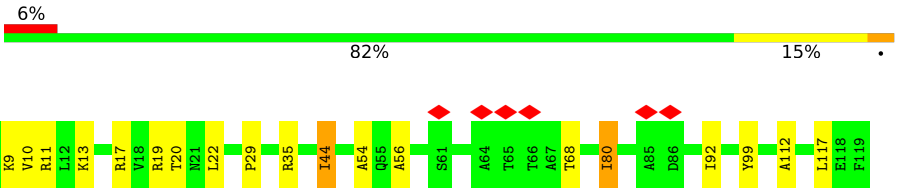
• Molecule 16: Large ribosomal subunit protein uL16

Chain K:



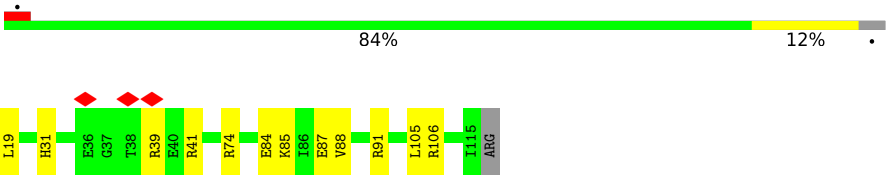
• Molecule 17: Large ribosomal subunit protein uL18

Chain M:



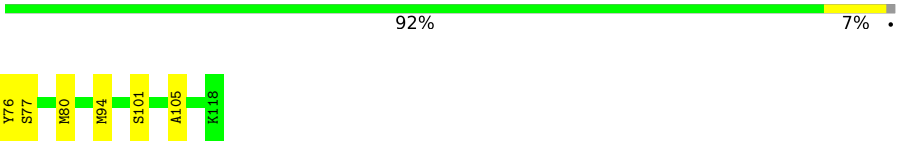
• Molecule 18: Large ribosomal subunit protein bL19

Chain N:



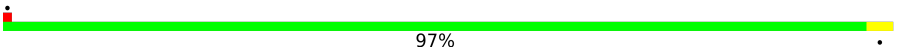
• Molecule 19: Large ribosomal subunit protein bL20

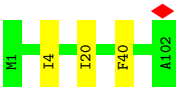
Chain O:



• Molecule 20: Large ribosomal subunit protein bL21

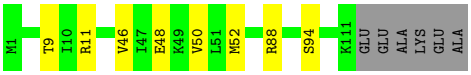
Chain P:





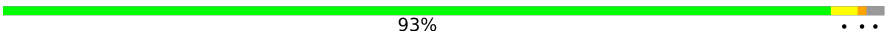
• Molecule 21: Large ribosomal subunit protein uL22

Chain Q:



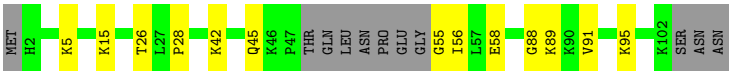
• Molecule 22: Large ribosomal subunit protein uL23

Chain R:



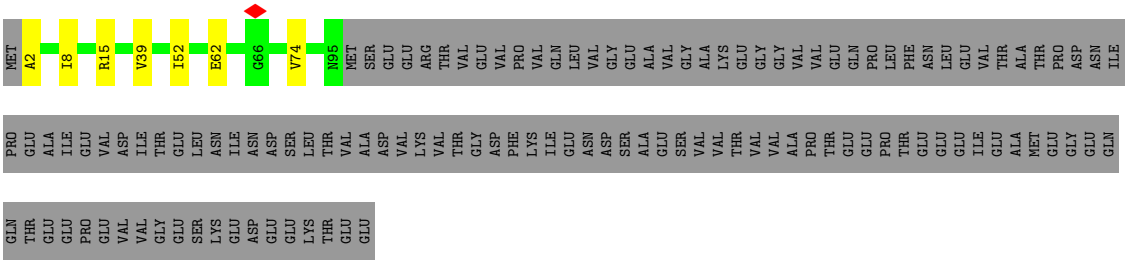
• Molecule 23: Large ribosomal subunit protein uL24

Chain S:



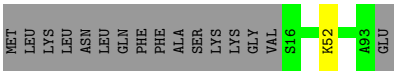
• Molecule 24: 50S ribosomal protein L25

Chain T:



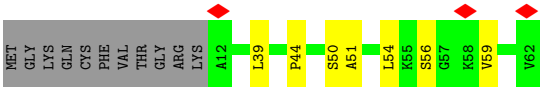
• Molecule 25: Large ribosomal subunit protein bL27

Chain U:



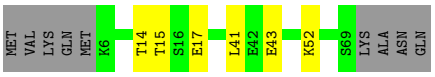
• Molecule 26: Large ribosomal subunit protein bL28

Chain V:



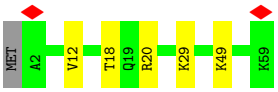
• Molecule 27: Large ribosomal subunit protein uL29

Chain W:



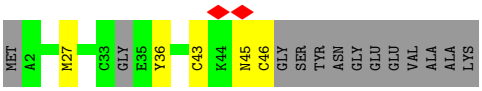
• Molecule 28: Large ribosomal subunit protein uL30

Chain X:



• Molecule 29: Large ribosomal subunit protein bL32

Chain Z:

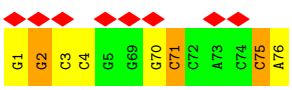


• Molecule 30: P_site tRNA

Chain 8:

• Molecule 31: E_site tRNA

Chain 11:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	263087	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.298	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	362.56, 362.56, 362.56	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	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: 2MG, H2U, OMG, K, ZN, G7M, 2MA, 5MU, MG, EM1, MA6, PSU

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	1	0.16	0/364	0.32	0/495
2	2	0.20	0/372	0.34	0/487
3	3	0.18	0/523	0.35	0/689
4	4	0.22	0/295	0.33	0/389
5	L	0.17	0/912	0.34	0/1223
6	A	0.23	0/62614	0.36	0/97606
7	B	0.17	0/2692	0.33	0/4193
8	C	0.18	0/2078	0.32	0/2799
9	D	0.18	0/1583	0.38	0/2131
10	E	0.16	0/1540	0.30	0/2087
11	F	0.13	0/945	0.32	0/1293
12	G	0.13	0/1179	0.27	0/1603
13	H	0.17	0/1110	0.35	0/1502
14	I	0.18	0/915	0.34	0/1230
15	J	0.18	0/1038	0.33	0/1395
16	K	0.19	0/1064	0.36	0/1438
17	M	0.14	0/822	0.28	0/1117
18	N	0.16	0/872	0.31	0/1172
19	O	0.21	0/922	0.35	0/1227
20	P	0.17	0/767	0.27	0/1032
21	Q	0.19	0/810	0.40	0/1097
22	R	0.17	0/657	0.30	0/886
23	S	0.17	0/671	0.30	0/904
24	T	0.13	0/631	0.30	0/863
25	U	0.16	0/572	0.33	0/764
26	V	0.16	0/375	0.33	0/506
27	W	0.14	0/481	0.29	0/645
28	X	0.18	0/436	0.35	0/589
29	Z	0.19	0/349	0.38	0/464
30	8	0.13	0/553	0.26	0/854
31	11	0.15	0/311	0.27	0/479
All	All	0.22	0/88453	0.35	0/133159

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	1	359	0	328	9	0
2	2	368	0	409	4	0
3	3	518	0	566	0	0
4	4	292	0	328	4	0
5	L	908	0	948	7	0
6	A	56161	0	28241	390	0
7	B	2408	0	1218	22	0
8	C	2043	0	2117	8	0
9	D	1559	0	1573	11	0
10	E	1517	0	1544	13	0
11	F	937	0	619	12	0
12	G	1165	0	1024	14	0
13	H	1088	0	1066	6	0
14	I	908	0	964	14	0
15	J	1024	0	1014	9	0
16	K	1040	0	1055	9	0
17	M	813	0	746	16	0
18	N	860	0	889	9	0
19	O	910	0	956	6	0
20	P	757	0	769	4	0
21	Q	802	0	839	3	0
22	R	650	0	650	2	0
23	S	664	0	658	7	0
24	T	624	0	569	2	0
25	U	566	0	555	1	0
26	V	370	0	360	3	0
27	W	480	0	491	4	0
28	X	434	0	468	4	0
29	Z	344	0	350	4	0
30	8	497	0	254	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	11	280	0	145	7	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	227	0	0	0	0
33	D	1	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	U	1	0	0	0	0
34	A	60	0	65	0	0
35	A	11	0	0	0	0
35	C	1	0	0	0	0
36	3	1	0	0	0	0
36	A	626	0	0	1	0
36	C	21	0	0	0	0
36	D	3	0	0	0	0
36	E	1	0	0	0	0
36	H	1	0	0	0	0
36	J	6	0	0	0	0
36	N	2	0	0	0	0
36	O	2	0	0	0	0
36	R	1	0	0	0	0
36	X	1	0	0	0	0
All	All	82317	0	51778	563	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 4.

All (563) 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:A:1219:G:HO2'	6:A:1220:A:H8	1.31	0.79
13:H:126:TYR:HH	13:H:133:HIS:HE2	1.28	0.79
29:Z:43:CYS:HB3	29:Z:46:CYS:SG	2.23	0.78
1:1:5:ARG:HB3	1:1:25:ASN:HA	1.69	0.75
6:A:788:A:O2'	6:A:1703:U:OP1	2.05	0.75
14:I:52:VAL:HG22	14:I:94:ARG:HH21	1.53	0.73
7:B:52:G:H21	11:F:26:MET:HE1	1.57	0.69
17:M:56:ALA:HB3	17:M:80:ILE:HG12	1.74	0.69
6:A:1634:A:H2'	6:A:1635:A:C8	2.29	0.68
6:A:2355:A:H2'	6:A:2356:A:C8	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1513:A:H2'	6:A:1514:A:C8	2.31	0.66
16:K:55:THR:HG22	16:K:64:VAL:HG21	1.77	0.66
6:A:1463:A:H2'	6:A:1465:G:N7	2.11	0.66
26:V:39:LEU:HA	26:V:44:PRO:HA	1.75	0.65
6:A:1462:G:H8	6:A:1626:A:H62	1.42	0.65
6:A:759:U:H1'	6:A:762:C:H41	1.62	0.65
6:A:901:G:H2'	6:A:902:A:C8	2.31	0.65
5:L:73:ASN:HB2	5:L:77:THR:HG23	1.79	0.65
6:A:650:U:OP1	10:E:102:PRO:HA	1.97	0.65
7:B:53:U:H1'	11:F:26:MET:HE3	1.78	0.64
12:G:64:ASN:O	12:G:68:THR:OG1	2.12	0.64
6:A:2825:U:H2'	6:A:2826:U:C6	2.33	0.64
5:L:13:ARG:NH2	6:A:2717:A:OP2	2.31	0.64
10:E:17:ILE:HD12	10:E:196:GLU:HG2	1.80	0.64
11:F:104:ILE:HD11	11:F:176:PRO:HD3	1.80	0.64
6:A:921:C:H42	6:A:946:A:H61	1.43	0.64
6:A:1538:A:N3	6:A:1625:U:O2'	2.31	0.64
11:F:29:PRO:HB3	11:F:160:ALA:HB2	1.80	0.64
6:A:2318:U:OP1	6:A:2407:A:O2'	2.15	0.63
6:A:221:G:H22	6:A:238:U:H4'	1.64	0.63
9:D:38:LYS:HD2	9:D:96:VAL:HG22	1.81	0.63
6:A:1442:C:H2'	6:A:1443:A:H8	1.64	0.62
6:A:2318:U:H2'	6:A:2319:U:C6	2.33	0.62
6:A:1588:U:H2'	6:A:1589:U:C6	2.34	0.62
6:A:1675:G:H1'	6:A:1679:A:N6	2.15	0.62
23:S:42:LYS:HG2	23:S:58:GLU:HG3	1.81	0.62
1:1:12:CYS:HB3	1:1:15:CYS:SG	2.39	0.62
6:A:159:U:H2'	6:A:160:G:C8	2.35	0.62
10:E:5:ASP:OD1	10:E:13:LYS:NZ	2.33	0.62
23:S:26:THR:HG22	23:S:28:PRO:HD3	1.81	0.61
7:B:58:C:OP1	17:M:9:LYS:NZ	2.28	0.61
6:A:1888:U:H2'	6:A:1889:G:H8	1.66	0.61
6:A:1911:A:H2'	6:A:1912:A:H5"	1.81	0.61
6:A:684:U:H2'	6:A:685:C:C6	2.36	0.61
6:A:1447:A:H2'	6:A:1448:U:C6	2.36	0.61
6:A:2231:C:H2'	6:A:2232:A:H8	1.65	0.60
6:A:1442:C:H2'	6:A:1443:A:C8	2.35	0.60
6:A:858:U:H2'	6:A:859:C:C6	2.36	0.60
6:A:317:G:O2'	6:A:318:A:H8	1.84	0.60
6:A:78:U:H2'	6:A:79:U:C6	2.37	0.60
10:E:115:SER:O	10:E:119:GLN:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1880:A:H2'	6:A:1881:A:C8	2.36	0.60
30:8:13:C:H2'	30:8:14:A:H5"	1.85	0.59
6:A:687:G:N2	6:A:690:U:OP2	2.31	0.59
6:A:1829:A:H2'	6:A:1830:A:C8	2.38	0.59
6:A:901:G:H2'	6:A:902:A:H8	1.65	0.58
6:A:1931:G:O2'	6:A:1955:A:N1	2.34	0.58
6:A:1823:U:H2'	6:A:1824:C:C6	2.39	0.58
6:A:2270:U:H2'	6:A:2271:U:C6	2.38	0.58
6:A:620:G:O2'	6:A:1292:A:OP1	2.21	0.58
6:A:787:U:H2'	6:A:788:A:C8	2.38	0.58
14:I:91:LYS:HG2	14:I:111:PHE:CE2	2.39	0.58
18:N:31:HIS:NE2	18:N:87:GLU:OE1	2.36	0.58
1:1:25:ASN:HB3	1:1:28:ASN:HB2	1.85	0.58
12:G:87:LEU:HD12	12:G:162:ILE:HG22	1.85	0.58
6:A:1916:A:H2'	6:A:1917:A:C8	2.40	0.57
7:B:27:A:H2'	7:B:28:C:C6	2.39	0.57
11:F:31:ILE:HA	11:F:158:THR:HA	1.85	0.57
11:F:44:VAL:O	11:F:48:LYS:N	2.36	0.57
6:A:259:A:H2'	6:A:260:A:C8	2.40	0.57
31:11:70:G:H2'	31:11:71:C:C6	2.40	0.57
6:A:268:A:N1	6:A:473:U:O2'	2.37	0.56
6:A:830:U:H2'	6:A:831:C:C6	2.40	0.56
6:A:5:A:H2'	6:A:6:A:C8	2.40	0.56
6:A:156:A:HO2'	6:A:157:U:H6	1.53	0.56
6:A:1572:G:N2	6:A:1593:G:O6	2.38	0.56
6:A:702:U:H2'	6:A:703:A:C8	2.41	0.56
6:A:1357:G:C2	6:A:1366:U:H5"	2.40	0.56
6:A:759:U:O2'	6:A:761:A:N7	2.36	0.56
6:A:2341:A:H2'	6:A:2342:U:C6	2.41	0.56
7:B:38:U:N3	7:B:42:G:OP2	2.30	0.56
6:A:766:G:H2'	6:A:767:A:C8	2.41	0.56
6:A:2705:U:H2'	6:A:2706:A:C8	2.40	0.56
6:A:2050:A:H2'	6:A:2051:C:C6	2.41	0.55
6:A:631:U:H2'	6:A:632:U:C6	2.40	0.55
6:A:2232:A:H2'	6:A:2233:C:C6	2.41	0.55
6:A:525:A:H1'	6:A:526:A:H5"	1.88	0.55
6:A:577:A:H4'	6:A:578:G:C8	2.41	0.55
6:A:156:A:O2'	6:A:157:U:H5"	2.06	0.55
6:A:1617:A:H2'	6:A:1618:A:C8	2.41	0.55
4:4:31:LYS:HE2	6:A:2505:A:H5'	1.87	0.55
6:A:2231:C:H2'	6:A:2232:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:85:LYS:HE3	18:N:87:GLU:OE1	2.07	0.55
6:A:1530:A:H2'	6:A:1531:U:C6	2.42	0.54
6:A:2052:C:H2'	6:A:2053:U:C6	2.43	0.54
6:A:2687:A:H2'	6:A:2688:G:O4'	2.07	0.54
6:A:2109:A:H2'	6:A:2110:G:O4'	2.07	0.54
6:A:2231:C:H4'	8:C:150:LYS:HD2	1.87	0.54
6:A:259:A:H2'	6:A:260:A:H8	1.73	0.54
6:A:2618:C:H2'	6:A:2619:G:C8	2.42	0.54
7:B:27:A:H2'	7:B:28:C:H6	1.70	0.54
6:A:302:A:H2'	6:A:303:G:C8	2.43	0.54
6:A:954:A:H2'	6:A:957:C:C5	2.43	0.54
6:A:1219:G:O2'	6:A:1220:A:H8	1.90	0.54
6:A:422:G:H2'	6:A:423:A:C8	2.43	0.53
6:A:579:U:H2'	6:A:580:C:C6	2.43	0.53
17:M:44:ILE:HG13	17:M:54:ALA:HB3	1.90	0.53
19:O:105:ALA:HB1	20:P:40:PHE:HZ	1.73	0.53
6:A:291:G:O2'	6:A:292:U:OP1	2.26	0.53
6:A:332:A:H2'	6:A:333:C:C6	2.44	0.53
6:A:2331:G:H22	6:A:2339:U:H3	1.56	0.53
6:A:2495:A:HO2'	6:A:2496:A:H8	1.56	0.53
6:A:75:G:H22	6:A:110:A:H2	1.57	0.53
6:A:2341:A:H1'	11:F:155:VAL:HG11	1.89	0.53
6:A:2406:G:H2'	6:A:2407:A:C8	2.44	0.53
6:A:2361:U:H3'	6:A:2362:A:H4'	1.90	0.53
24:T:52:ILE:HD11	24:T:74:VAL:HG21	1.91	0.53
6:A:66:C:H2'	6:A:67:G:H8	1.73	0.53
6:A:618:A:OP2	6:A:2526:C:O2'	2.27	0.53
6:A:1072:A:N6	6:A:1169:G:H2'	2.25	0.52
6:A:1537:A:H2'	6:A:1538:A:C8	2.43	0.52
6:A:2372:G:N3	6:A:2408:C:H2'	2.24	0.52
6:A:250:G:H4'	6:A:432:G:C5	2.44	0.52
6:A:221:G:N2	6:A:238:U:H4'	2.23	0.52
6:A:766:G:H2'	6:A:767:A:H8	1.75	0.52
6:A:632:U:H2'	6:A:633:A:C8	2.44	0.52
6:A:2091:C:H2'	6:A:2092:C:C6	2.44	0.52
6:A:2356:A:H2'	6:A:2357:G:C8	2.44	0.52
6:A:2361:U:H1'	17:M:20:THR:HG21	1.91	0.52
15:J:86:GLU:O	15:J:89:THR:OG1	2.21	0.52
6:A:2672:G:H4'	6:A:2759:G:O2'	2.10	0.52
6:A:279:A:H2'	6:A:280:C:C6	2.45	0.51
6:A:976:U:OP1	28:X:29:LYS:NZ	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2347:A:H4'	6:A:2348:G:C4	2.45	0.51
6:A:2300:A:H2'	6:A:2301:A:C8	2.46	0.51
6:A:324:A:N1	6:A:401:U:O2'	2.33	0.51
7:B:45:C:OP2	17:M:7:LYS:NZ	2.40	0.51
6:A:629:A:N1	6:A:854:G:O2'	2.41	0.51
6:A:1241:A:H2'	6:A:1242:A:C8	2.45	0.51
6:A:1680:U:H2'	6:A:1681:U:C6	2.46	0.51
6:A:2584:G:H2'	6:A:2585:C:C6	2.45	0.51
6:A:2594:G:H2'	6:A:2595:C:C6	2.46	0.51
6:A:774:G:C6	8:C:207:LYS:HB2	2.46	0.51
6:A:2260:A:H2'	6:A:2261:G:C8	2.45	0.51
10:E:153:LEU:HD23	10:E:192:LEU:HD11	1.93	0.51
30:8:14:A:H2'	30:8:15:G:O4'	2.10	0.51
6:A:903:G:N3	6:A:2295:A:H2'	2.26	0.51
6:A:1073:A:OP1	16:K:128:LYS:NZ	2.42	0.51
6:A:2325:A:N6	6:A:2345:A:O2'	2.44	0.51
6:A:1905:G:H2'	6:A:1906:C:C6	2.46	0.51
6:A:441:C:H2'	6:A:442:G:H8	1.76	0.51
6:A:2098:A:H2'	6:A:2099:G:C8	2.46	0.51
6:A:460:C:H2'	6:A:461:A:C8	2.46	0.51
6:A:2680:U:OP2	6:A:2681:A:O2'	2.28	0.51
10:E:123:LEU:HD23	10:E:192:LEU:HB3	1.93	0.51
6:A:69:C:H4'	6:A:75:G:N7	2.26	0.50
6:A:291:G:H2'	6:A:292:U:C6	2.46	0.50
6:A:78:U:H2'	6:A:79:U:H6	1.75	0.50
6:A:1966:5MU:OP1	6:A:2631:U:O2'	2.30	0.50
6:A:2404:A:H2'	6:A:2405:A:C8	2.46	0.50
14:I:107:ARG:HG2	14:I:112:MET:HE1	1.93	0.50
2:2:2:VAL:N	6:A:1663:G:HO2'	2.09	0.50
6:A:247:A:H2'	6:A:248:G:O4'	2.12	0.50
6:A:2273:G:H2'	6:A:2274:A:C8	2.47	0.50
6:A:2599:A:N7	9:D:158:SER:OG	2.40	0.50
6:A:632:U:H2'	6:A:633:A:H8	1.76	0.50
6:A:954:A:H2'	6:A:957:C:H5	1.76	0.50
10:E:153:LEU:HB3	10:E:192:LEU:HD12	1.93	0.50
14:I:17:ARG:HG3	14:I:47:THR:HG23	1.94	0.50
23:S:45:GLN:N	23:S:55:GLY:O	2.41	0.50
6:A:398:C:H2'	6:A:399:U:O4'	2.11	0.50
6:A:2340:C:H2'	6:A:2341:A:H8	1.75	0.50
7:B:55:A:H2'	7:B:56:A:H8	1.76	0.50
14:I:35:ILE:HG21	14:I:103:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:422:G:H2'	6:A:423:A:H8	1.77	0.49
18:N:84:GLU:HG2	18:N:85:LYS:HG2	1.94	0.49
6:A:651:A:H2'	6:A:652:A:C8	2.47	0.49
6:A:858:U:H2'	6:A:859:C:H6	1.77	0.49
6:A:1390:A:H2'	6:A:1391:A:C8	2.47	0.49
10:E:17:ILE:HD11	10:E:200:LYS:HD3	1.94	0.49
11:F:131:GLY:HA2	11:F:153:ASP:HA	1.94	0.49
14:I:112:MET:HA	14:I:112:MET:HE3	1.95	0.49
6:A:613:G:H2'	6:A:2057:A:N7	2.27	0.49
6:A:1513:A:H2'	6:A:1514:A:H8	1.74	0.49
6:A:2050:A:H2'	6:A:2051:C:H6	1.77	0.49
12:G:98:MET:HE1	12:G:123:PHE:HB2	1.95	0.49
6:A:346:A:H2'	6:A:347:U:C6	2.48	0.49
6:A:396:G:H2'	6:A:397:U:C6	2.47	0.49
6:A:1014:U:OP1	28:X:20:ARG:NH2	2.45	0.49
6:A:2618:C:H2'	6:A:2619:G:H8	1.76	0.49
7:B:108:U:H2'	7:B:109:G:H8	1.78	0.49
13:H:42:LYS:NZ	13:H:51:THR:O	2.40	0.49
14:I:29:GLY:O	14:I:31:LYS:HD3	2.13	0.49
17:M:13:LYS:O	17:M:17:ARG:HG2	2.13	0.49
2:2:9:ASN:HB3	2:2:12:LYS:HB3	1.94	0.49
6:A:2354:A:H2'	6:A:2355:A:C8	2.47	0.49
7:B:2:C:H2'	7:B:3:U:C6	2.47	0.49
12:G:96:ALA:HB1	12:G:103:LEU:HD11	1.95	0.49
17:M:29:PRO:HD2	17:M:92:ILE:HG22	1.94	0.49
26:V:51:ALA:HA	26:V:54:LEU:HD12	1.95	0.49
6:A:638:U:H2'	6:A:639:U:C6	2.48	0.49
6:A:2101:U:H2'	6:A:2102:U:C6	2.48	0.49
6:A:672:A:H61	6:A:682:A:H5"	1.78	0.48
6:A:2341:A:H2'	6:A:2342:U:H6	1.77	0.48
6:A:1477:U:H2'	6:A:1478:A:C8	2.48	0.48
6:A:1353:A:H2'	6:A:1354:G:C8	2.48	0.48
6:A:2570:G:H2'	6:A:2571:G:C8	2.49	0.48
10:E:181:LEU:HD22	10:E:186:ILE:HD11	1.95	0.48
6:A:461:A:H2'	6:A:462:U:C6	2.49	0.48
6:A:2431:C:H2'	6:A:2432:G:O4'	2.14	0.48
9:D:191:GLU:C	9:D:193:LYS:H	2.21	0.48
6:A:2574:U:H5'	6:A:2593:A:C2	2.49	0.48
6:A:877:G:H2'	6:A:878:C:C6	2.48	0.48
6:A:1314:A:H2'	6:A:1315:C:C6	2.49	0.48
6:A:1529:U:H2'	6:A:1530:A:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2688:G:H2'	6:A:2689:A:C8	2.49	0.48
6:A:441:C:H2'	6:A:442:G:C8	2.49	0.48
6:A:703:A:H2'	6:A:704:U:C6	2.48	0.48
17:M:5:ILE:HD12	17:M:10:VAL:HG21	1.95	0.48
6:A:395:U:H2'	6:A:396:G:C8	2.49	0.48
6:A:1280:U:H2'	6:A:1281:U:C6	2.49	0.48
6:A:1329:G:H2'	6:A:1330:U:C6	2.49	0.48
6:A:2361:U:O3'	17:M:17:ARG:HD2	2.13	0.48
17:M:92:ILE:HD13	17:M:117:LEU:HD22	1.95	0.48
6:A:172:U:H2'	6:A:173:A:C8	2.49	0.48
6:A:2319:U:H2'	6:A:2320:C:C6	2.49	0.48
6:A:684:U:H2'	6:A:685:C:H6	1.77	0.47
6:A:1238:U:H2'	6:A:1239:C:C6	2.49	0.47
6:A:1836:A:H2'	6:A:1837:A:C8	2.48	0.47
27:W:41:LEU:C	27:W:43:GLU:H	2.22	0.47
6:A:66:C:H2'	6:A:67:G:C8	2.48	0.47
6:A:132:C:H2'	6:A:133:A:C8	2.50	0.47
6:A:390:A:H2'	6:A:391:A:C8	2.49	0.47
6:A:418:G:H8	26:V:56:SER:HA	1.79	0.47
6:A:1618:A:H2'	6:A:1619:A:C8	2.49	0.47
27:W:14:THR:HG22	27:W:17:GLU:HG3	1.95	0.47
6:A:175:C:H2'	6:A:176:A:O4'	2.14	0.47
6:A:957:C:OP1	16:K:8:LYS:NZ	2.43	0.47
6:A:2326:G:H2'	6:A:2327:A:C8	2.49	0.47
18:N:88:VAL:HG11	18:N:91:ARG:CZ	2.44	0.47
6:A:2488:C:H2'	6:A:2489:U:C6	2.49	0.47
6:A:273:A:OP2	6:A:297:G:N1	2.39	0.47
6:A:907:G:H2'	6:A:908:A:O4'	2.15	0.47
13:H:1:MET:HE1	20:P:20:ILE:HA	1.96	0.47
6:A:302:A:H2'	6:A:303:G:H8	1.78	0.47
6:A:590:U:OP1	6:A:1257:G:O2'	2.25	0.47
6:A:5:A:H2'	6:A:6:A:H8	1.77	0.47
6:A:597:U:H2'	6:A:598:G:O4'	2.14	0.47
6:A:890:G:OP2	6:A:890:G:N2	2.22	0.47
6:A:1423:C:H2'	6:A:1424:A:C8	2.50	0.47
6:A:1823:U:H2'	6:A:1824:C:H6	1.78	0.47
6:A:1959:A:H2'	6:A:1960:G:O4'	2.14	0.47
6:A:2457:A:H2'	6:A:2457:A:N3	2.29	0.47
11:F:118:SER:OG	11:F:119:LYS:N	2.48	0.47
18:N:39:ARG:NH1	18:N:41:ARG:HB3	2.30	0.47
6:A:394:U:H2'	6:A:395:U:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1813:A:H1'	6:A:1965:A:N6	2.30	0.47
4:4:19:ARG:HB2	4:4:24:MET:SD	2.55	0.47
6:A:89:U:H3'	6:A:90:A:H2'	1.96	0.47
6:A:274:A:N6	6:A:297:G:H1'	2.30	0.47
6:A:1238:U:H2'	6:A:1239:C:H6	1.80	0.47
10:E:4:TYR:CE1	10:E:19:LEU:HB2	2.50	0.47
5:L:24:LEU:HD23	5:L:44:VAL:HG21	1.97	0.47
6:A:1481:A:H2'	6:A:1482:U:C6	2.50	0.47
6:A:27:G:N2	6:A:557:G:H1'	2.30	0.46
6:A:194:A:H2'	6:A:195:C:C6	2.50	0.46
6:A:1539:A:H2'	6:A:1541:C:C5	2.50	0.46
7:B:12:U:OP2	7:B:68:U:O2'	2.32	0.46
12:G:144:LEU:HD13	12:G:144:LEU:HA	1.78	0.46
15:J:27:ASN:O	15:J:31:SER:HA	2.15	0.46
22:R:3:ALA:HA	22:R:6:ILE:HD12	1.98	0.46
6:A:1700:C:H2'	6:A:1701:U:H6	1.80	0.46
14:I:24:VAL:HG13	14:I:33:ALA:HB2	1.98	0.46
30:8:44:A:H2'	30:8:45:A:C8	2.50	0.46
1:1:12:CYS:SG	1:1:46:THR:OG1	2.62	0.46
6:A:622:A:H2'	6:A:623:C:C6	2.51	0.46
6:A:768:A:H2'	6:A:769:U:O4'	2.16	0.46
6:A:1268:C:H2'	6:A:1269:A:C8	2.51	0.46
6:A:1443:A:H2'	6:A:1444:C:C6	2.51	0.46
6:A:1919:C:O2'	31:11:71:C:H5'	2.15	0.46
10:E:81:PRO:HB3	10:E:89:VAL:HG23	1.97	0.46
6:A:187:C:H2'	6:A:188:C:H6	1.81	0.46
6:A:1160:C:H2'	6:A:1161:A:H8	1.79	0.46
6:A:2274:A:H2'	6:A:2275:C:H6	1.81	0.46
6:A:2494:C:H2'	6:A:2495:A:O4'	2.16	0.46
6:A:12:U:O2	6:A:2653:C:H4'	2.16	0.46
6:A:734:A:H2'	6:A:735:C:C6	2.51	0.46
6:A:2294:A:H5"	6:A:2295:A:H5'	1.97	0.46
6:A:1593:G:OP2	6:A:1593:G:N2	2.41	0.45
6:A:2811:U:H2'	6:A:2812:U:C6	2.51	0.45
15:J:2:LYS:HE3	15:J:4:HIS:CE1	2.51	0.45
6:A:2326:G:H2'	6:A:2327:A:H8	1.80	0.45
6:A:64:A:H2'	6:A:65:A:C8	2.52	0.45
6:A:955:A:H2'	6:A:956:A:C8	2.52	0.45
12:G:3:ARG:NH1	12:G:5:GLY:H	2.14	0.45
15:J:2:LYS:HE3	15:J:4:HIS:HE1	1.81	0.45
6:A:162:A:N1	6:A:2244:G:O2'	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:525:A:N3	6:A:527:G:H5”	2.31	0.45
6:A:1072:A:H2’	6:A:1073:A:C8	2.51	0.45
6:A:1268:C:H2’	6:A:1269:A:H8	1.81	0.45
6:A:1489:A:H8	6:A:1490:G:N7	2.14	0.45
6:A:2270:U:H2’	6:A:2271:U:H6	1.80	0.45
7:B:64:A:N6	7:B:104:A:H2’	2.31	0.45
8:C:173:LEU:HD11	8:C:271:VAL:HG21	1.99	0.45
17:M:19:ARG:NH1	17:M:22:LEU:O	2.47	0.45
18:N:105:LEU:O	18:N:106:ARG:NH1	2.44	0.45
5:L:53:LYS:HB2	5:L:53:LYS:HE2	1.83	0.45
6:A:187:C:H2’	6:A:188:C:C6	2.51	0.45
6:A:342:A:N3	6:A:362:C:O2’	2.48	0.45
6:A:363:A:H4’	6:A:365:A:N7	2.32	0.45
6:A:868:A:H2’	6:A:869:G:C8	2.51	0.45
6:A:1572:G:C6	6:A:1591:G:C6	3.04	0.45
6:A:1973:U:H2’	6:A:1974:C:C6	2.52	0.45
6:A:2482:G:H2’	6:A:2483:C:C6	2.52	0.45
6:A:2747:U:H2’	6:A:2748:A:C8	2.52	0.45
15:J:96:LEU:HD22	15:J:101:VAL:HG11	1.98	0.45
5:L:66:LEU:HD23	5:L:66:LEU:HA	1.84	0.45
6:A:659:A:H2’	6:A:660:A:C8	2.52	0.45
6:A:1562:C:H2’	6:A:1563:U:C6	2.51	0.45
7:B:33:U:H2’	7:B:34:C:C6	2.52	0.45
30:8:9:G:O2’	30:8:10:G:N7	2.44	0.45
6:A:3:U:H2’	6:A:4:U:C6	2.52	0.45
6:A:637:U:H2’	6:A:638:U:C6	2.52	0.45
6:A:1545:U:H2’	6:A:1546:A:C8	2.52	0.45
6:A:2778:G:H4’	12:G:4:VAL:HG23	1.98	0.45
7:B:103:A:H2’	7:B:104:A:O4’	2.16	0.45
11:F:161:ASN:OD1	11:F:161:ASN:N	2.50	0.45
12:G:107:VAL:HG11	12:G:162:ILE:HD11	1.97	0.45
17:M:11:ARG:HD3	17:M:99:TYR:CE1	2.51	0.45
6:A:172:U:H2’	6:A:173:A:H8	1.81	0.45
6:A:372:A:N6	23:S:15:LYS:H	2.15	0.45
6:A:2268:A:H2’	6:A:2269:G:C8	2.51	0.45
6:A:2705:U:H2’	6:A:2706:A:H8	1.80	0.45
7:B:26:C:H2’	7:B:27:A:O4’	2.17	0.45
7:B:46:A:P	17:M:35:ARG:HH22	2.40	0.45
12:G:125:VAL:HG23	12:G:130:VAL:O	2.17	0.45
1:1:10:LEU:HD11	1:1:35:MET:HE3	1.99	0.44
6:A:30:G:H2’	6:A:31:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:725:A:H2'	6:A:726:G:C8	2.52	0.44
6:A:2539:C:H2'	6:A:2540:A:O4'	2.16	0.44
6:A:2860:U:H2'	6:A:2861:U:C6	2.51	0.44
14:I:23:LYS:HE2	14:I:23:LYS:HB2	1.75	0.44
16:K:2:LEU:HB3	16:K:3:LEU:HD23	1.99	0.44
31:11:2:G:H2'	31:11:3:C:C6	2.52	0.44
6:A:4:U:H2'	6:A:5:A:H8	1.81	0.44
6:A:1598:U:H2'	6:A:1599:G:O4'	2.17	0.44
19:O:105:ALA:HB1	20:P:40:PHE:CZ	2.53	0.44
6:A:2896:A:H5'	18:N:4:HIS:CG	2.52	0.44
9:D:4:GLY:HA2	9:D:211:ILE:O	2.18	0.44
1:1:42:LEU:HD13	1:1:46:THR:HG21	1.98	0.44
6:A:669:C:O2'	6:A:702:U:OP1	2.32	0.44
6:A:753:U:H2'	6:A:754:U:C6	2.53	0.44
6:A:1510:U:O2'	6:A:1593:G:H1'	2.17	0.44
6:A:1636:U:H2'	6:A:1637:A:C8	2.52	0.44
6:A:2774:G:OP1	12:G:74:ASN:ND2	2.41	0.44
17:M:112:ALA:HB1	17:M:117:LEU:HD12	1.99	0.44
23:S:55:GLY:C	23:S:56:ILE:HD13	2.43	0.44
6:A:787:U:H2'	6:A:788:A:H8	1.80	0.44
6:A:1674:U:H2'	6:A:1675:G:O4'	2.16	0.44
8:C:133:GLN:HG2	8:C:186:SER:HB3	1.98	0.44
1:1:4:VAL:HG12	6:A:2312:C:OP2	2.17	0.44
2:2:12:LYS:HE2	6:A:731:U:C2	2.53	0.44
6:A:805:G:H2'	6:A:806:A:O4'	2.18	0.44
6:A:1821:U:H2'	6:A:1822:C:C6	2.53	0.44
12:G:85:LYS:HD3	12:G:85:LYS:HA	1.81	0.44
6:A:350:G:N1	6:A:353:A:OP2	2.39	0.44
6:A:1044:A:H2'	6:A:1045:A:C8	2.53	0.44
9:D:159:ASP:HA	9:D:160:ALA:HA	1.82	0.44
22:R:46:PHE:CG	22:R:87:ILE:HD13	2.53	0.44
6:A:127:C:H2'	6:A:128:C:C6	2.53	0.43
6:A:1185:U:H4'	6:A:1186:A:O4'	2.17	0.43
19:O:94:MET:SD	20:P:4:ILE:HD12	2.58	0.43
6:A:1013:U:H2'	6:A:1014:U:C6	2.53	0.43
6:A:1160:C:H2'	6:A:1161:A:C8	2.53	0.43
6:A:1869:G:H2'	6:A:1870:C:C6	2.53	0.43
6:A:2319:U:H2'	6:A:2320:C:H6	1.83	0.43
28:X:18:THR:HG1	28:X:49:LYS:HZ1	1.58	0.43
29:Z:27:MET:HG3	29:Z:36:TYR:CD2	2.53	0.43
6:A:767:A:H2'	6:A:768:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1754:C:H4'	6:A:2878:U:O2	2.18	0.43
6:A:2634:G:H2'	6:A:2635:G:O4'	2.18	0.43
6:A:2677:C:H2'	6:A:2678:C:H6	1.84	0.43
8:C:23:GLU:H	8:C:23:GLU:HG2	1.61	0.43
6:A:736:C:H2'	6:A:737:C:H6	1.82	0.43
6:A:1844:G:H2'	6:A:1845:U:H5'	2.01	0.43
6:A:1642:C:H2'	6:A:1643:C:H6	1.83	0.43
6:A:1904:A:H3'	6:A:1905:G:H8	1.83	0.43
6:A:2831:G:H2'	6:A:2832:A:O4'	2.18	0.43
4:4:8:LYS:NZ	6:A:2494:C:OP1	2.35	0.43
6:A:464:U:H2'	6:A:465:C:C6	2.53	0.43
6:A:748:U:H2'	6:A:749:G:O4'	2.18	0.43
6:A:991:A:H2'	6:A:992:A:C8	2.54	0.43
6:A:1208:A:H2'	6:A:1209:U:C6	2.53	0.43
9:D:52:GLY:HA3	9:D:85:LYS:HG3	2.00	0.43
10:E:22:ALA:O	10:E:111:ARG:HD3	2.19	0.43
6:A:625:G:H2'	6:A:626:G:C8	2.53	0.43
6:A:842:U:H2'	6:A:843:G:H8	1.84	0.43
6:A:1353:A:H2'	6:A:1354:G:H8	1.84	0.43
6:A:1907:U:H2'	6:A:1908:A:C8	2.53	0.43
6:A:2459:A:H1'	31:11:75:C:O4'	2.18	0.43
6:A:2523:C:OP2	16:K:82:ARG:HD3	2.18	0.43
8:C:95:VAL:HG22	8:C:101:LYS:HG2	2.01	0.43
19:O:15:LYS:HB3	19:O:15:LYS:HE3	1.74	0.43
4:4:18:LYS:HE2	4:4:21:GLY:HA2	2.01	0.43
6:A:1562:C:H2'	6:A:1563:U:H6	1.83	0.43
6:A:2645:G:H21	9:D:163:VAL:HG21	1.83	0.43
6:A:2774:G:O6	6:A:2782:C:H5"	2.18	0.43
7:B:60:C:H2'	7:B:61:C:H6	1.84	0.43
16:K:51:ARG:O	16:K:55:THR:HG23	2.18	0.43
6:A:132:C:H2'	6:A:133:A:H8	1.84	0.43
6:A:522:G:H4'	6:A:547:A:N1	2.34	0.43
6:A:552:A:H1'	6:A:554:C:N3	2.34	0.43
6:A:878:C:H2'	6:A:879:U:C6	2.54	0.43
6:A:1269:A:H2'	6:A:1270:U:C6	2.54	0.43
11:F:104:ILE:HD11	11:F:175:MET:HA	2.00	0.43
1:1:4:VAL:HG13	6:A:2312:C:C5	2.53	0.43
6:A:291:G:H2'	6:A:292:U:H6	1.82	0.43
6:A:973:A:H2'	6:A:974:U:C6	2.53	0.43
6:A:1403:C:H2'	6:A:1404:A:O4'	2.19	0.43
6:A:2051:C:H2'	6:A:2052:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Z:27:MET:HG3	29:Z:36:TYR:HD2	1.84	0.43
6:A:226:A:N1	6:A:453:G:O2'	2.51	0.42
6:A:329:A:H2'	6:A:330:C:C6	2.54	0.42
6:A:856:U:H2'	15:J:21:ARG:HA	2.01	0.42
6:A:1463:A:O2'	6:A:1465:G:OP2	2.34	0.42
6:A:2886:G:C2	6:A:2888:A:H1'	2.54	0.42
18:N:19:LEU:HD23	18:N:19:LEU:HA	1.89	0.42
6:A:4:U:H2'	6:A:5:A:C8	2.54	0.42
6:A:90:A:OP1	6:A:90:A:H8	2.01	0.42
6:A:601:G:OP1	13:H:113:THR:HB	2.19	0.42
6:A:2782:C:O2'	6:A:2783:U:H2'	2.18	0.42
6:A:2826:U:H2'	6:A:2827:A:O4'	2.19	0.42
31:11:3:C:H2'	31:11:4:C:H6	1.84	0.42
6:A:1529:U:H2'	6:A:1530:A:C8	2.54	0.42
6:A:2673:C:H2'	6:A:2674:U:O4'	2.19	0.42
6:A:1196:C:H4'	19:O:77:SER:HA	2.01	0.42
6:A:2260:A:H2'	6:A:2261:G:H8	1.83	0.42
7:B:112:A:H2'	7:B:113:G:C8	2.54	0.42
21:Q:88:ARG:HG3	21:Q:94:SER:HB2	2.01	0.42
6:A:523:A:H2'	6:A:524:A:C8	2.55	0.42
6:A:1821:U:H2'	6:A:1822:C:H6	1.84	0.42
6:A:2507:C:H2'	6:A:2508:G:O4'	2.19	0.42
10:E:202:VAL:HG13	10:E:206:LEU:HD12	2.01	0.42
14:I:44:LYS:HA	14:I:44:LYS:HD2	1.81	0.42
6:A:75:G:O2'	27:W:52:LYS:NZ	2.30	0.42
6:A:2026:C:H5"	6:A:2750:C:O2'	2.19	0.42
6:A:2092:C:H2'	6:A:2093:C:C6	2.55	0.42
6:A:2340:C:C2	6:A:2341:A:C8	3.07	0.42
16:K:112:GLU:H	16:K:112:GLU:CD	2.24	0.42
6:A:1356:G:O2'	6:A:1357:G:H5'	2.19	0.42
6:A:1594:U:O2'	6:A:1595:C:H6	2.02	0.42
6:A:2613:C:H2'	6:A:2614:A:C8	2.54	0.42
12:G:164:TYR:HB2	12:G:167:GLU:HG3	2.01	0.42
19:O:76:TYR:CZ	19:O:80:MET:HG3	2.55	0.42
6:A:340:C:H2'	6:A:341:G:O4'	2.19	0.42
6:A:2232:A:H2'	6:A:2233:C:H6	1.84	0.42
11:F:70:ALA:HB2	11:F:85:ILE:HG13	2.02	0.42
6:A:291:G:HO2'	6:A:292:U:P	2.43	0.42
6:A:1315:C:H2'	6:A:1316:G:H8	1.85	0.42
6:A:1869:G:H2'	6:A:1870:C:H6	1.84	0.42
6:A:2541:U:H2'	6:A:2542:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:41:A:H2'	6:A:42:G:C8	2.54	0.42
6:A:1472:C:H5	36:A:3613:HOH:O	2.02	0.42
6:A:1637:A:H2'	6:A:1638:G:C8	2.55	0.41
6:A:2064:A:H2'	6:A:2065:G:C8	2.55	0.41
6:A:2274:A:H2'	6:A:2275:C:C6	2.55	0.41
6:A:2482:G:H2'	6:A:2483:C:H6	1.84	0.41
30:8:27:G:H2'	30:8:28:U:H6	1.85	0.41
6:A:107:G:H2'	6:A:108:A:O4'	2.19	0.41
6:A:161:A:N3	6:A:2235:A:O2'	2.45	0.41
6:A:842:U:H2'	6:A:843:G:C8	2.55	0.41
6:A:1446:U:H2'	6:A:1447:A:C8	2.55	0.41
6:A:2725:U:H2'	6:A:2726:C:C6	2.55	0.41
12:G:46:GLU:N	12:G:49:THR:O	2.52	0.41
25:U:52:LYS:HB2	25:U:52:LYS:HE2	1.77	0.41
1:1:4:VAL:HG23	1:1:23:THR:HB	2.02	0.41
2:2:12:LYS:HE3	2:2:16:VAL:HG21	2.02	0.41
6:A:2778:G:H3'	6:A:2779:C:H6	1.86	0.41
6:A:225:A:H5"	6:A:467:U:OP1	2.19	0.41
6:A:841:C:H2'	6:A:842:U:C6	2.55	0.41
6:A:1776:A:H2'	6:A:1777:G:O4'	2.20	0.41
7:B:90:U:H2'	7:B:91:C:C6	2.56	0.41
16:K:43:THR:HG22	16:K:94:ILE:HG22	2.02	0.41
23:S:88:GLY:O	23:S:89:LYS:HG2	2.20	0.41
28:X:12:VAL:HB	28:X:20:ARG:HG2	2.01	0.41
6:A:56:A:H2'	6:A:57:C:O4'	2.21	0.41
6:A:348:C:H2'	6:A:349:U:C6	2.56	0.41
6:A:2833:U:H2'	6:A:2834:C:H6	1.86	0.41
7:B:48:A:H5'	17:M:68:THR:HG22	2.02	0.41
8:C:67:PHE:HE1	8:C:105:ILE:HD11	1.86	0.41
5:L:32:THR:OG1	5:L:33:THR:N	2.54	0.41
6:A:682:A:H2'	15:J:114:ASN:OD1	2.21	0.41
6:A:758:G:H2'	6:A:759:U:C6	2.55	0.41
9:D:164:PHE:HB3	13:H:82:PRO:HG3	2.01	0.41
14:I:66:LYS:HE2	14:I:66:LYS:HB3	1.96	0.41
6:A:1084:U:H2'	6:A:1085:U:O4'	2.21	0.41
15:J:77:VAL:HB	15:J:111:ILE:HD13	2.01	0.41
21:Q:46:VAL:O	21:Q:50:VAL:HG23	2.20	0.41
31:11:1:G:C2'	31:11:2:G:H5'	2.50	0.41
6:A:1237:U:H2'	6:A:1238:U:C6	2.56	0.41
6:A:1723:A:H2	6:A:1791:G:C8	2.38	0.41
6:A:2617:A:H2'	6:A:2618:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:42:THR:HG23	14:I:44:LYS:HD3	2.03	0.41
15:J:13:ARG:HA	15:J:13:ARG:HD2	1.95	0.41
24:T:2:ALA:O	24:T:62:GLU:N	2.43	0.41
5:L:59:ARG:HA	5:L:86:PHE:CZ	2.55	0.41
6:A:120:G:H4'	6:A:150:A:H5'	2.02	0.41
6:A:578:G:H2'	6:A:579:U:C6	2.56	0.41
6:A:689:A:H2'	6:A:691:A:C8	2.56	0.41
6:A:786:U:H2'	6:A:787:U:C6	2.55	0.41
6:A:1391:A:H2'	6:A:1392:G:O4'	2.20	0.41
6:A:1469:G:H2'	6:A:1470:G:C8	2.56	0.41
6:A:1733:A:H2'	6:A:1734:A:C8	2.56	0.41
6:A:2242:G:H2'	6:A:2243:U:C6	2.55	0.41
6:A:2599:A:OP1	9:D:157:ALA:HB3	2.20	0.41
12:G:62:ARG:H	12:G:62:ARG:HG2	1.51	0.41
14:I:77:ILE:HD12	18:N:74:ARG:HD3	2.02	0.41
21:Q:48:GLU:O	21:Q:52:MET:HG2	2.20	0.41
23:S:5:LYS:HE2	23:S:5:LYS:HB3	1.74	0.41
30:8:25:U:H2'	30:8:26:C:C6	2.56	0.41
6:A:63:U:HO2'	6:A:64:A:H8	1.68	0.41
6:A:421:C:H2'	6:A:422:G:H8	1.86	0.41
6:A:1063:U:OP1	6:A:1079:U:O2'	2.26	0.41
6:A:1424:A:H5'	6:A:1513:A:H1'	2.03	0.41
6:A:1817:C:H2'	6:A:1818:A:C5	2.56	0.41
6:A:2085:MA6:O5'	6:A:2085:MA6:H8	2.21	0.41
6:A:2620:U:H2'	6:A:2621:C:C6	2.56	0.41
7:B:61:C:H2'	7:B:62:U:C6	2.55	0.41
9:D:139:GLY:HA3	9:D:147:PHE:HD1	1.85	0.41
13:H:26:LEU:HD22	13:H:65:PHE:HE1	1.86	0.41
6:A:2340:C:H2'	6:A:2341:A:C8	2.56	0.40
6:A:2601:G7M:O2'	9:D:156:MET:HB3	2.20	0.40
14:I:113:LYS:HD3	14:I:117:LEU:HG	2.03	0.40
6:A:292:U:H2'	6:A:293:U:H6	1.87	0.40
6:A:650:U:C5	6:A:665:G:C5	3.09	0.40
6:A:680:C:O2'	6:A:684:U:OP1	2.33	0.40
6:A:992:A:H2'	6:A:993:C:C6	2.56	0.40
6:A:1086:G:H2'	6:A:1087:C:C6	2.56	0.40
6:A:1252:A:H4'	6:A:1277:C:H4'	2.03	0.40
6:A:1951:C:H2'	6:A:1952:C:C6	2.55	0.40
6:A:2783:U:H4'	6:A:2784:A:OP1	2.21	0.40
6:A:2873:C:H2'	6:A:2874:A:H8	1.86	0.40
6:A:105:C:H2'	6:A:106:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1543:G:O2'	8:C:99:GLY:O	2.34	0.40
6:A:2318:U:H2'	6:A:2319:U:H6	1.80	0.40
6:A:2904:U:H2'	6:A:2905:C:O4'	2.21	0.40
7:B:106:G:H2'	7:B:107:U:C6	2.56	0.40
6:A:349:U:H2'	6:A:350:G:O4'	2.21	0.40
6:A:418:G:O2'	6:A:446:G:O6	2.36	0.40
6:A:713:A:H2'	6:A:715:A:H62	1.86	0.40
6:A:2549:U:O2'	6:A:2674:U:OP1	2.37	0.40
6:A:2747:U:H2'	6:A:2748:A:H8	1.86	0.40
16:K:118:LEU:HD12	16:K:131:PHE:CD1	2.57	0.40
31:11:3:C:H2'	31:11:4:C:C6	2.56	0.40
6:A:837:G:H4'	6:A:838:A:C4	2.57	0.40
6:A:1220:A:HO2'	6:A:1221:C:H6	1.69	0.40
6:A:2328:A:H2'	6:A:2329:U:O4'	2.21	0.40
6:A:2356:A:H2'	6:A:2357:G:H8	1.86	0.40
6:A:2601:G7M:H8	6:A:2601:G7M:O5'	2.22	0.40
6:A:2754:G:H2'	6:A:2755:U:C6	2.57	0.40
17:M:80:ILE:HD13	17:M:80:ILE:HA	2.00	0.40
27:W:14:THR:HG23	27:W:17:GLU:H	1.87	0.40
29:Z:43:CYS:C	29:Z:45:ASN:H	2.30	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	1	46/52 (88%)	43 (94%)	3 (6%)	0	100	100
2	2	42/45 (93%)	42 (100%)	0	0	100	100
3	3	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
4	4	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	L	118/122 (97%)	114 (97%)	4 (3%)	0	100	100
8	C	272/277 (98%)	270 (99%)	2 (1%)	0	100	100
9	D	213/220 (97%)	204 (96%)	9 (4%)	0	100	100
10	E	204/207 (99%)	201 (98%)	3 (2%)	0	100	100
11	F	152/179 (85%)	142 (93%)	10 (7%)	0	100	100
12	G	173/178 (97%)	165 (95%)	8 (5%)	0	100	100
13	H	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
14	I	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
15	J	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
16	K	135/144 (94%)	131 (97%)	4 (3%)	0	100	100
17	M	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
18	N	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
19	O	115/118 (98%)	115 (100%)	0	0	100	100
20	P	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
21	Q	109/117 (93%)	106 (97%)	3 (3%)	0	100	100
22	R	87/91 (96%)	87 (100%)	0	0	100	100
23	S	90/105 (86%)	88 (98%)	2 (2%)	0	100	100
24	T	92/217 (42%)	85 (92%)	7 (8%)	0	100	100
25	U	76/94 (81%)	74 (97%)	2 (3%)	0	100	100
26	V	49/62 (79%)	48 (98%)	1 (2%)	0	100	100
27	W	62/73 (85%)	59 (95%)	3 (5%)	0	100	100
28	X	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
29	Z	40/57 (70%)	36 (90%)	4 (10%)	0	100	100
All	All	2963/3270 (91%)	2881 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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
1	1	36/50 (72%)	34 (94%)	2 (6%)	17 15
2	2	38/40 (95%)	38 (100%)	0	100 100
3	3	53/57 (93%)	53 (100%)	0	100 100
4	4	34/35 (97%)	34 (100%)	0	100 100
5	L	88/102 (86%)	87 (99%)	1 (1%)	70 76
8	C	209/224 (93%)	208 (100%)	1 (0%)	86 90
9	D	154/177 (87%)	151 (98%)	3 (2%)	52 57
10	E	153/169 (90%)	150 (98%)	3 (2%)	50 55
11	F	39/158 (25%)	39 (100%)	0	100 100
12	G	89/155 (57%)	75 (84%)	14 (16%)	2 1
13	H	108/123 (88%)	108 (100%)	0	100 100
14	I	97/100 (97%)	96 (99%)	1 (1%)	73 78
15	J	91/112 (81%)	90 (99%)	1 (1%)	70 76
16	K	100/119 (84%)	96 (96%)	4 (4%)	27 27
17	M	61/95 (64%)	58 (95%)	3 (5%)	21 19
18	N	86/102 (84%)	85 (99%)	1 (1%)	67 73
19	O	86/98 (88%)	84 (98%)	2 (2%)	45 49
20	P	74/86 (86%)	74 (100%)	0	100 100
21	Q	76/94 (81%)	74 (97%)	2 (3%)	41 44
22	R	62/82 (76%)	61 (98%)	1 (2%)	58 64
23	S	62/90 (69%)	60 (97%)	2 (3%)	34 36
24	T	51/190 (27%)	48 (94%)	3 (6%)	16 13
25	U	50/75 (67%)	50 (100%)	0	100 100
26	V	32/52 (62%)	30 (94%)	2 (6%)	15 12
27	W	45/66 (68%)	44 (98%)	1 (2%)	47 51
28	X	48/53 (91%)	48 (100%)	0	100 100
29	Z	37/50 (74%)	37 (100%)	0	100 100
All	All	2059/2754 (75%)	2012 (98%)	47 (2%)	46 49

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	4	VAL

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Mol	Chain	Res	Type
1	1	13	THR
5	L	40	VAL
8	C	174	ILE
9	D	96	VAL
9	D	137	SER
9	D	200	ASN
10	E	58	SER
10	E	77	THR
10	E	123	LEU
12	G	30	LYS
12	G	36	THR
12	G	52	VAL
12	G	62	ARG
12	G	68	THR
12	G	69	ARG
12	G	85	LYS
12	G	97	GLN
12	G	104	ILE
12	G	107	VAL
12	G	130	VAL
12	G	136	ILE
12	G	144	LEU
12	G	169	VAL
14	I	90	ASP
15	J	97	VAL
16	K	38	THR
16	K	39	THR
16	K	42	ILE
16	K	96	VAL
17	M	5	ILE
17	M	44	ILE
17	M	80	ILE
18	N	7	ILE
19	O	51	ARG
19	O	101	SER
21	Q	9	THR
21	Q	11	ARG
22	R	87	ILE
23	S	91	VAL
23	S	95	LYS
24	T	8	ILE
24	T	15	ARG

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Mol	Chain	Res	Type
24	T	39	VAL
26	V	50	SER
26	V	59	VAL
27	W	15	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	27	ASN
8	C	133	GLN
8	C	228	ASN
9	D	134	HIS
9	D	136	GLN
9	D	192	ASN
10	E	119	GLN
13	H	81	HIS
16	K	35	GLN
19	O	52	GLN
20	P	101	ASN
23	S	69	GLN
25	U	86	GLN
27	W	40	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	8	19/71 (26%)	5 (26%)	0
31	11	11/13 (84%)	4 (36%)	0
6	A	2590/2923 (88%)	295 (11%)	10 (0%)
7	B	112/115 (97%)	22 (19%)	2 (1%)
All	All	2732/3122 (87%)	326 (11%)	12 (0%)

All (326) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	34	U
6	A	63	U
6	A	71	A
6	A	75	G
6	A	84	A

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Mol	Chain	Res	Type
6	A	93	U
6	A	96	G
6	A	117	A
6	A	118	A
6	A	119	U
6	A	130	A
6	A	136	A
6	A	160	G
6	A	161	A
6	A	184	C
6	A	185	A
6	A	199	A
6	A	202	A
6	A	216	A
6	A	218	G
6	A	219	A
6	A	225	A
6	A	226	A
6	A	248	G
6	A	251	G
6	A	269	G
6	A	270	C
6	A	272	C
6	A	292	U
6	A	294	G
6	A	295	G
6	A	317	G
6	A	318	A
6	A	321	U
6	A	324	A
6	A	327	G
6	A	351	G
6	A	354	A
6	A	364	A
6	A	373	A
6	A	389	A
6	A	393	G
6	A	397	U
6	A	432	G
6	A	434	G
6	A	445	G
6	A	450	C

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Mol	Chain	Res	Type
6	A	457	G
6	A	470	G
6	A	474	A
6	A	475	A
6	A	482	U
6	A	526	A
6	A	527	G
6	A	550	A
6	A	552	A
6	A	553	A
6	A	554	C
6	A	567	G
6	A	576	U
6	A	577	A
6	A	578	G
6	A	583	A
6	A	594	G
6	A	606	G
6	A	616	G
6	A	617	A
6	A	618	A
6	A	630	G
6	A	646	A
6	A	650	U
6	A	682	A
6	A	690	U
6	A	699	U
6	A	700	A
6	A	731	U
6	A	757	G
6	A	775	A
6	A	792	5MU
6	A	802	G
6	A	809	A
6	A	820	G
6	A	827	A
6	A	829	U
6	A	837	G
6	A	850	G
6	A	857	C
6	A	872	U
6	A	873	U

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Mol	Chain	Res	Type
6	A	888	G
6	A	904	G
6	A	955	A
6	A	962	A
6	A	977	A
6	A	989	A
6	A	990	G
6	A	1005	G
6	A	1018	A
6	A	1027	A
6	A	1040	A
6	A	1049	C
6	A	1056	U
6	A	1057	A
6	A	1070	A
6	A	1077	U
6	A	1083	G
6	A	1084	U
6	A	1085	U
6	A	1158	G
6	A	1159	A
6	A	1173	A
6	A	1176	U
6	A	1177	A
6	A	1178	C
6	A	1179	C
6	A	1186	A
6	A	1199	A
6	A	1219	G
6	A	1220	A
6	A	1288	G
6	A	1291	A
6	A	1294	G
6	A	1309	G
6	A	1310	A
6	A	1337	A
6	A	1338	U
6	A	1358	A
6	A	1389	U
6	A	1402	A
6	A	1416	U
6	A	1421	A

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Mol	Chain	Res	Type
6	A	1449	A
6	A	1462	G
6	A	1463	A
6	A	1464	U
6	A	1465	G
6	A	1471	A
6	A	1472	C
6	A	1489	A
6	A	1490	G
6	A	1496	G
6	A	1497	A
6	A	1498	U
6	A	1500	G
6	A	1511	C
6	A	1536	C
6	A	1537	A
6	A	1540	U
6	A	1560	A
6	A	1568	U
6	A	1569	G
6	A	1572	G
6	A	1573	A
6	A	1574	G
6	A	1595	C
6	A	1606	C
6	A	1613	G
6	A	1616	A
6	A	1651	C
6	A	1652	A
6	A	1690	A
6	A	1691	G
6	A	1692	C
6	A	1718	G
6	A	1740	G
6	A	1756	U
6	A	1783	G
6	A	1790	G
6	A	1791	G
6	A	1800	A
6	A	1809	C
6	A	1818	A
6	A	1827	C

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Mol	Chain	Res	Type
6	A	1828	U
6	A	1843	U
6	A	1847	U
6	A	1856	A
6	A	1875	A
6	A	1876	G
6	A	1885	G
6	A	1886	A
6	A	1903	A
6	A	1906	C
6	A	1912	A
6	A	1933	G
6	A	1956	G
6	A	1957	G
6	A	1964	A
6	A	1965	A
6	A	1982	U
6	A	1992	C
6	A	1994	C
6	A	1997	A
6	A	1998	A
6	A	1999	G
6	A	2018	U
6	A	2020	U
6	A	2024	A
6	A	2058	A
6	A	2059	G
6	A	2060	A
6	A	2070	C
6	A	2082	C
6	A	2083	G
6	A	2087	A
6	A	2088	G
6	A	2096	G
6	A	2120	G
6	A	2123	A
6	A	2218	G
6	A	2225	A
6	A	2230	G
6	A	2231	C
6	A	2238	U
6	A	2239	A

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Mol	Chain	Res	Type
6	A	2252	A
6	A	2253	C
6	A	2265	G
6	A	2266	G
6	A	2295	A
6	A	2306	G
6	A	2310	C
6	A	2314	A
6	A	2315	A
6	A	2316	G
6	A	2344	C
6	A	2345	A
6	A	2346	U
6	A	2349	A
6	A	2352	G
6	A	2354	A
6	A	2361	U
6	A	2362	A
6	A	2374	C
6	A	2377	C
6	A	2399	G
6	A	2406	G
6	A	2410	G
6	A	2412	C
6	A	2429	U
6	A	2433	C
6	A	2450	U
6	A	2452	A
6	A	2456	G
6	A	2457	A
6	A	2461	A
6	A	2462	A
6	A	2468	C
6	A	2475	A
6	A	2497	G
6	A	2502	C
6	A	2529	G
6	A	2532	G
6	A	2545	A
6	A	2547	C
6	A	2556	G
6	A	2575	G

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Mol	Chain	Res	Type
6	A	2593	A
6	A	2594	G
6	A	2600	C
6	A	2605	G
6	A	2612	U
6	A	2629	A
6	A	2630	G
6	A	2636	U
6	A	2640	U
6	A	2656	A
6	A	2657	G
6	A	2682	G
6	A	2716	U
6	A	2717	A
6	A	2718	C
6	A	2741	G
6	A	2753	U
6	A	2775	A
6	A	2778	G
6	A	2784	A
6	A	2792	A
6	A	2805	A
6	A	2807	G
6	A	2817	A
6	A	2818	A
6	A	2828	U
6	A	2832	A
6	A	2833	U
6	A	2887	G
6	A	2892	G
6	A	2900	C
6	A	2903	A
6	A	2906	G
6	A	2911	A
6	A	2913	G
6	A	2914	A
6	A	2918	A
6	A	2920	U
7	B	10	U
7	B	11	A
7	B	19	G
7	B	23	U

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Mol	Chain	Res	Type
7	B	24	C
7	B	30	U
7	B	33	U
7	B	39	G
7	B	40	C
7	B	43	A
7	B	49	G
7	B	50	A
7	B	52	G
7	B	54	U
7	B	55	A
7	B	56	A
7	B	59	U
7	B	64	A
7	B	87	C
7	B	88	G
7	B	106	G
7	B	110	C
30	8	9	G
30	8	10	G
30	8	14	A
30	8	76	C
30	8	77	A
31	11	2	G
31	11	71	C
31	11	75	C
31	11	76	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	291	G
6	A	396	G
6	A	525	A
6	A	809	A
6	A	1158	G
6	A	1463	A
6	A	1905	G
6	A	2344	C
6	A	2457	A
6	A	2783	U
7	B	9	C

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Mol	Chain	Res	Type
7	B	55	A

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

11 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
6	5MU	A	1966	6,35	19,22,23	0.32	0	28,32,35	0.40	0
6	5MU	A	792	6	19,22,23	0.31	0	28,32,35	0.33	0
6	H2U	A	2476	6	18,21,22	0.35	0	21,30,33	0.43	0
6	PSU	A	2484	6	18,21,22	0.53	0	22,30,33	0.59	0
6	2MA	A	2530	33,6,35	19,25,26	1.06	2 (10%)	21,37,40	3.03	4 (19%)
6	G7M	A	2601	33,6	20,26,27	0.58	0	17,39,42	0.33	0
6	PSU	A	2607	6	18,21,22	0.63	1 (5%)	22,30,33	0.71	1 (4%)
6	2MG	A	2472	6	18,26,27	1.09	3 (16%)	16,38,41	0.62	0
6	MA6	A	2085	6	18,26,27	0.75	0	19,38,41	0.71	0
6	OMG	A	2278	30,6	18,26,27	0.95	2 (11%)	19,38,41	0.57	0
6	PSU	A	2632	6	18,21,22	0.49	0	22,30,33	0.63	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
6	5MU	A	1966	6,35	-	0/7/25/26	0/2/2/2
6	5MU	A	792	6	-	0/7/25/26	0/2/2/2
6	H2U	A	2476	6	-	0/7/38/39	0/2/2/2
6	PSU	A	2484	6	-	0/7/25/26	0/2/2/2
6	2MA	A	2530	33,6,35	-	1/3/25/26	0/3/3/3
6	G7M	A	2601	33,6	-	0/3/25/26	0/3/3/3
6	PSU	A	2607	6	-	0/7/25/26	0/2/2/2
6	2MG	A	2472	6	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MA6	A	2085	6	-	0/7/29/30	0/3/3/3
6	OMG	A	2278	30,6	-	1/5/27/28	0/3/3/3
6	PSU	A	2632	6	-	0/7/25/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2472	2MG	C5-C6	-2.88	1.41	1.47
6	A	2530	2MA	C6-N6	-2.36	1.25	1.34
6	A	2472	2MG	C8-N7	-2.29	1.31	1.35
6	A	2278	OMG	C5-C6	-2.21	1.42	1.47
6	A	2607	PSU	O4'-C1'	-2.15	1.40	1.43
6	A	2278	OMG	C8-N7	-2.10	1.31	1.35
6	A	2472	2MG	C5-C4	-2.10	1.37	1.43
6	A	2530	2MA	C6-N1	2.04	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2530	2MA	C5-C6-N1	-12.18	113.01	121.01
6	A	2530	2MA	C2-N1-C6	3.89	124.15	118.08
6	A	2530	2MA	C2-N3-C4	-3.72	112.50	115.52
6	A	2530	2MA	N6-C6-N1	2.61	124.15	117.07
6	A	2607	PSU	O4'-C1'-C2'	2.45	108.60	105.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2278	OMG	C1'-C2'-O2'-CM2
6	A	2472	2MG	C3'-C4'-C5'-O5'
6	A	2530	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1966	5MU	1	0
6	A	2601	G7M	2	0
6	A	2085	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 247 ligands modelled in this entry, 246 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	$\#\|Z\| > 2$
34	EM1	A	3001	-	58,64,64	0.51	0	71,97,97	0.45	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
34	EM1	A	3001	-	-	1/71/112/112	0/4/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	3001	EM1	C84-C83-N80-N81

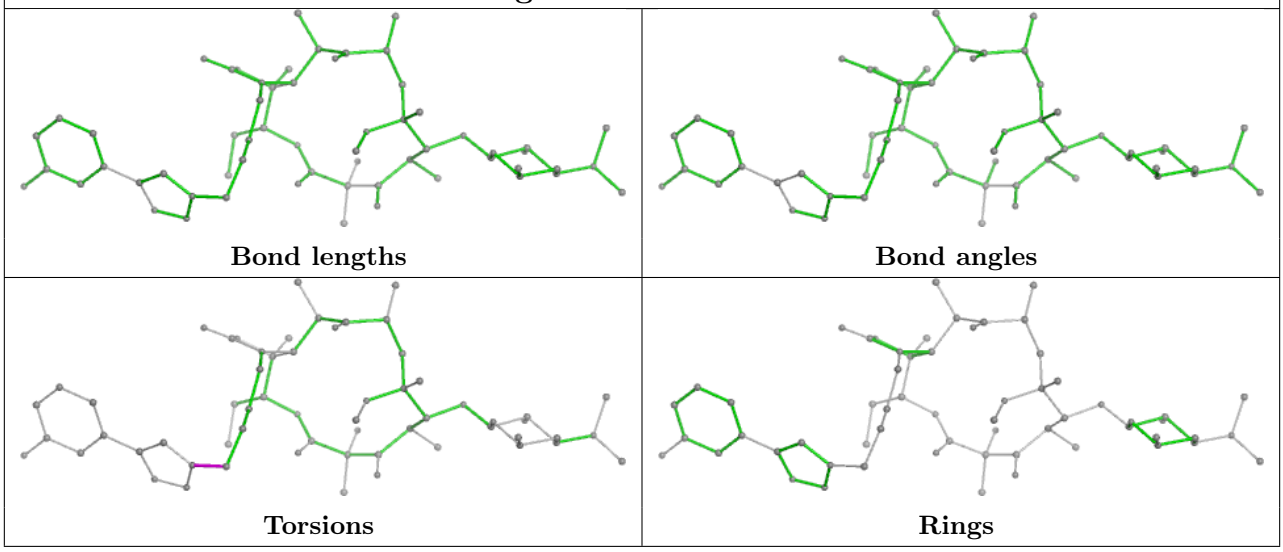
There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand EM1 A 3001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
31	11	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	11	5:G	O3'	69:G	P	13.84

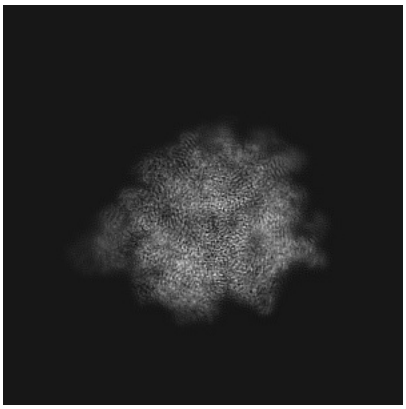
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53067. These allow visual inspection of the internal detail of the map and identification of artifacts.

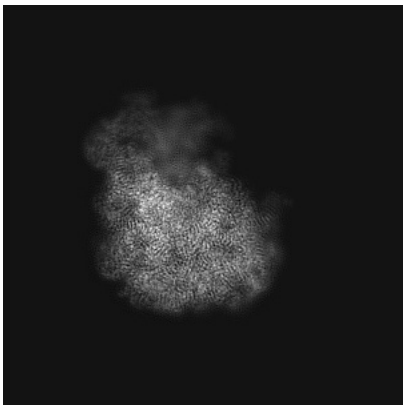
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

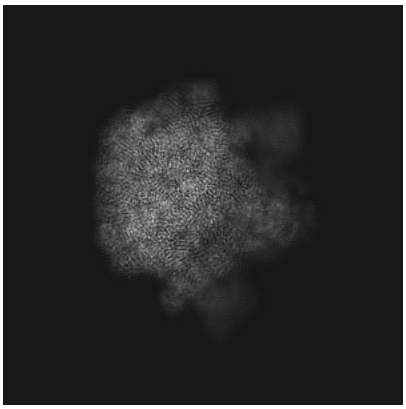
6.1.1 Primary map



X

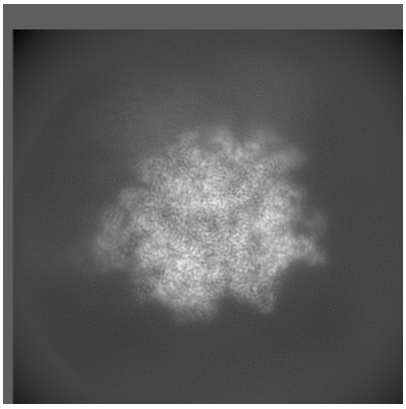


Y

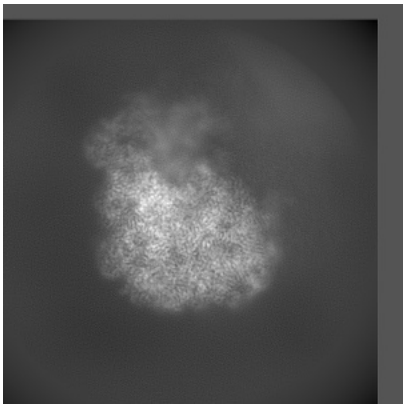


Z

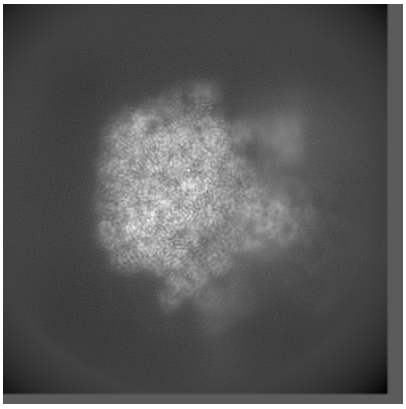
6.1.2 Raw map



X



Y

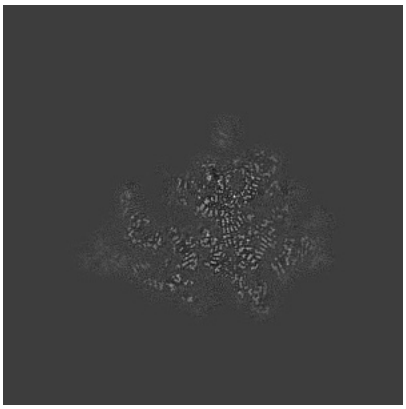


Z

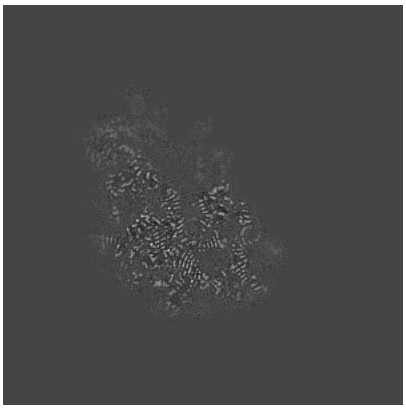
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

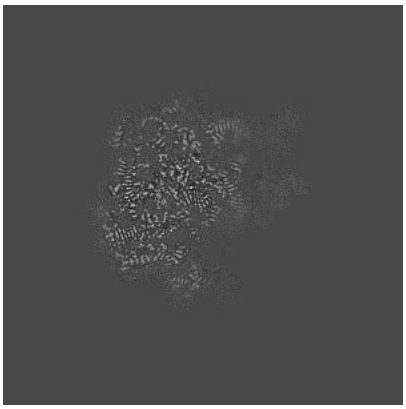
6.2.1 Primary map



X Index: 220

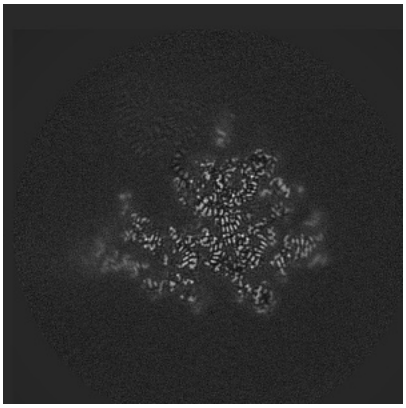


Y Index: 220

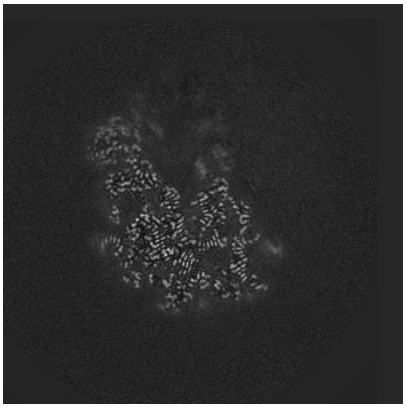


Z Index: 220

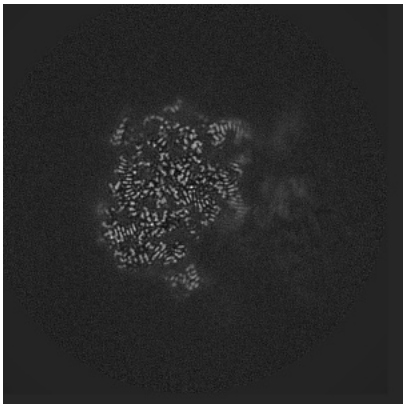
6.2.2 Raw map



X Index: 220



Y Index: 220

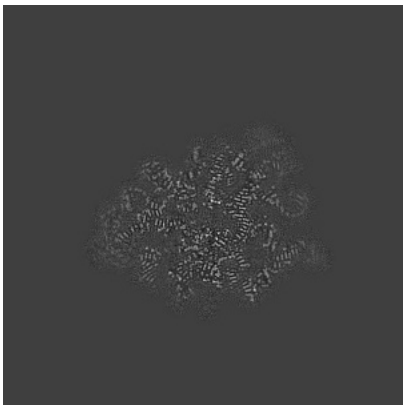


Z Index: 220

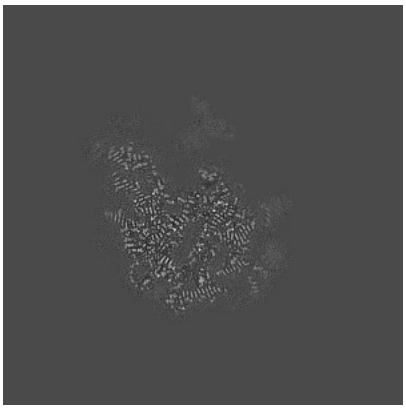
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

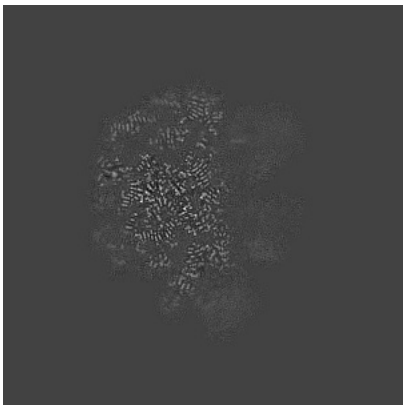
6.3.1 Primary map



X Index: 192

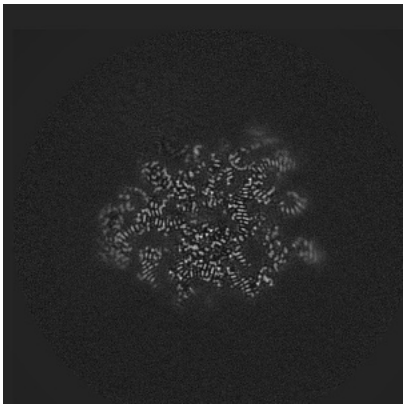


Y Index: 237

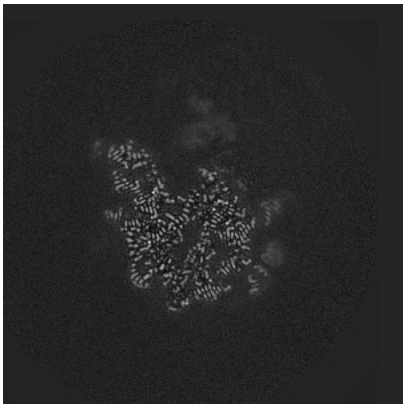


Z Index: 177

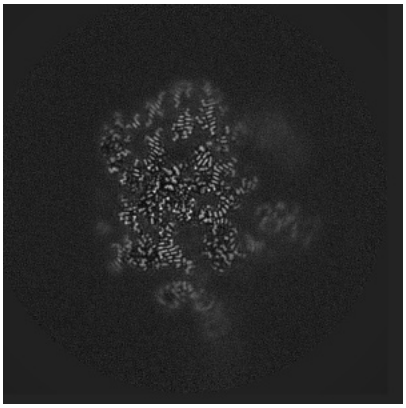
6.3.2 Raw map



X Index: 191



Y Index: 236

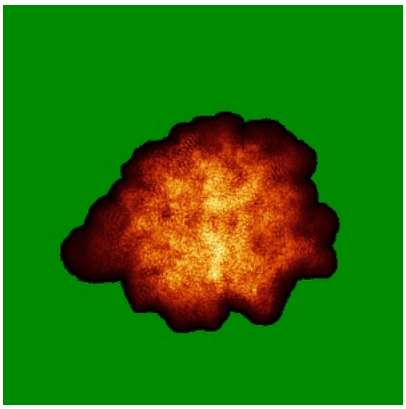


Z Index: 164

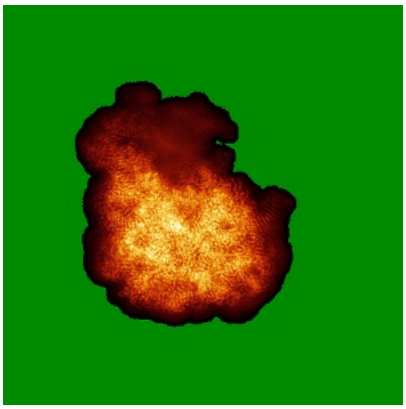
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

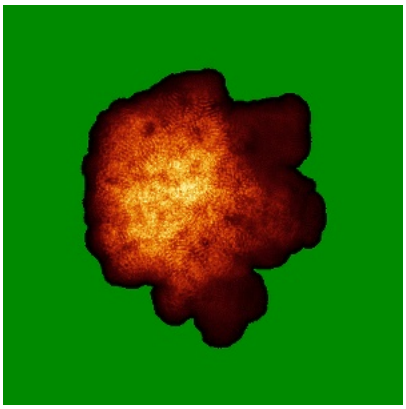
6.4.1 Primary map



X

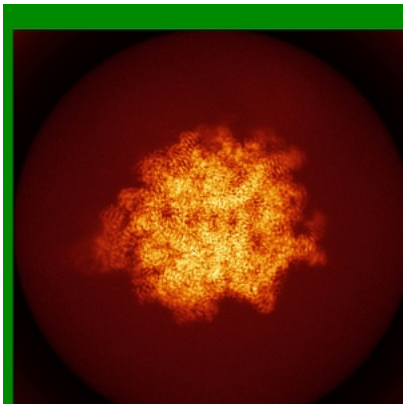


Y

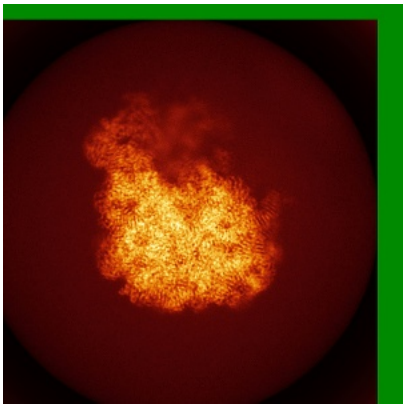


Z

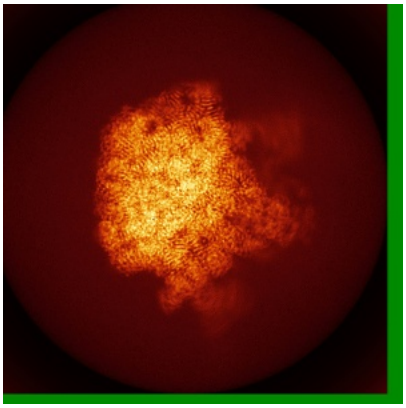
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

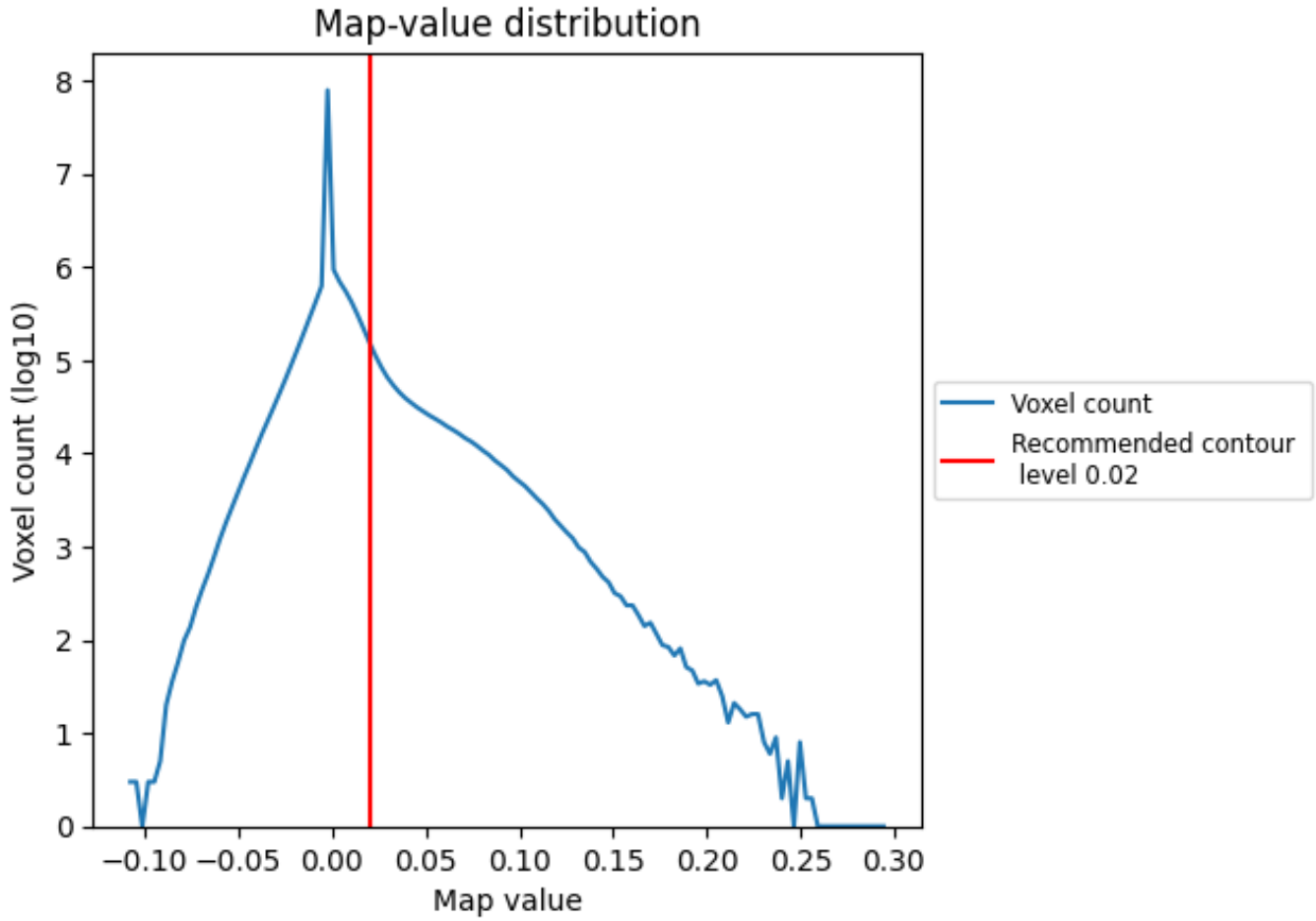
6.6 Mask visualisation (i)

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

7 Map analysis

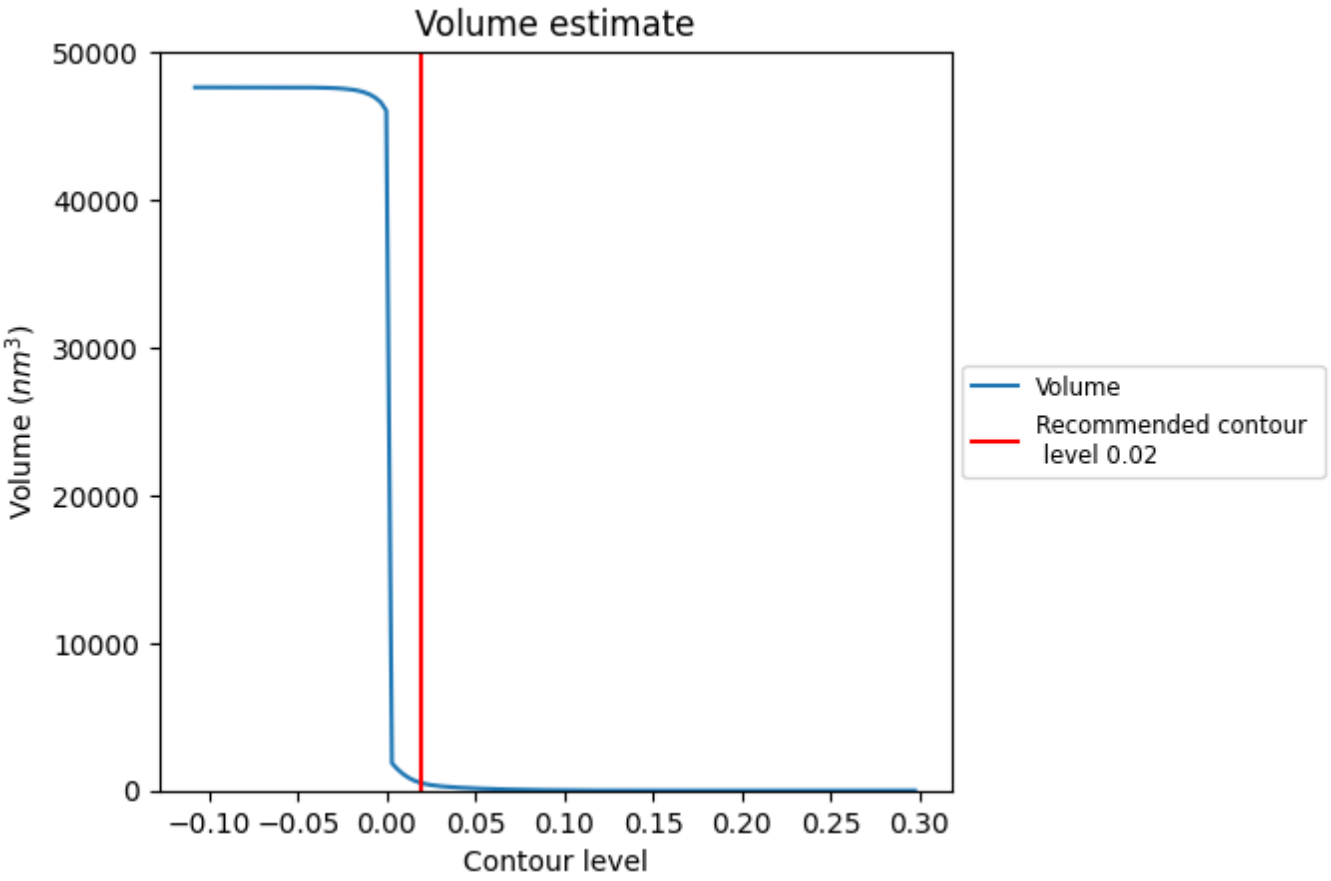
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

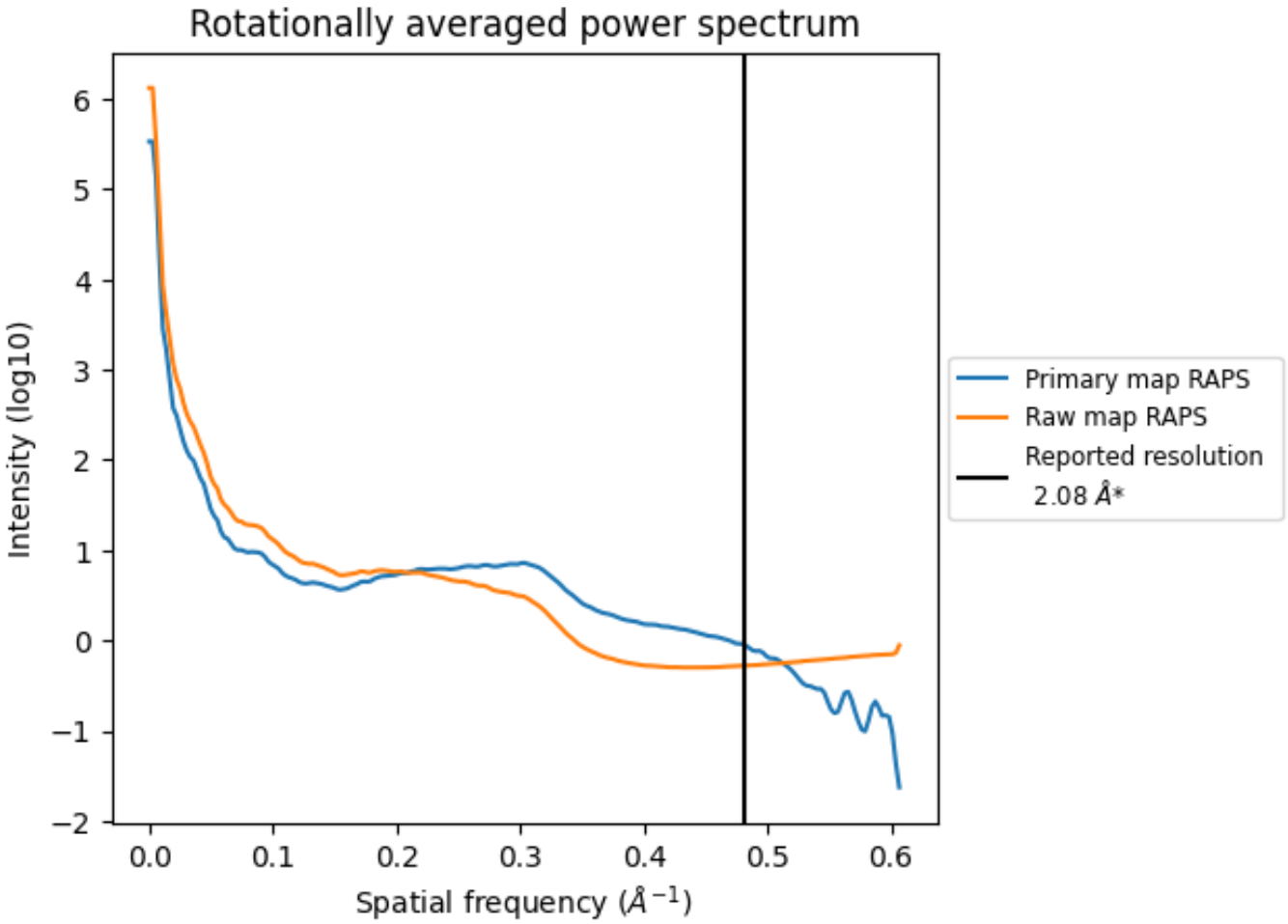
7.2 Volume estimate (i)



The volume at the recommended contour level is 503 nm^3; this corresponds to an approximate mass of 455 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 (i)

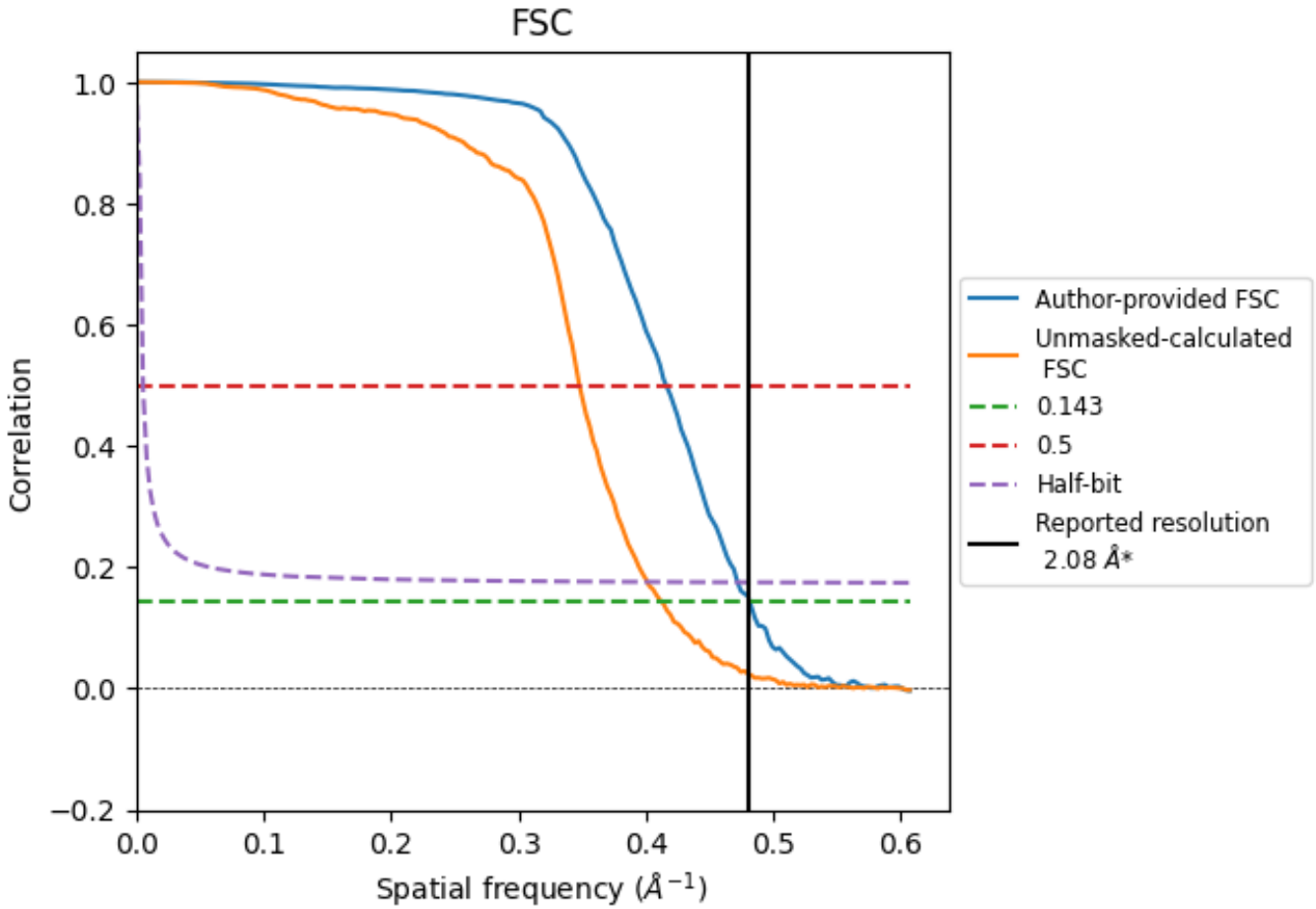


*Reported resolution corresponds to spatial frequency of 0.481 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.481 $Å^{-1}$

8.2 Resolution estimates (i)

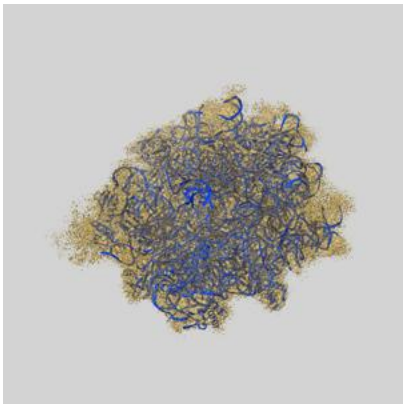
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.08	2.41	2.12
Unmasked-calculated*	2.43	2.88	2.49

*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 2.43 differs from the reported value 2.08 by more than 10 %

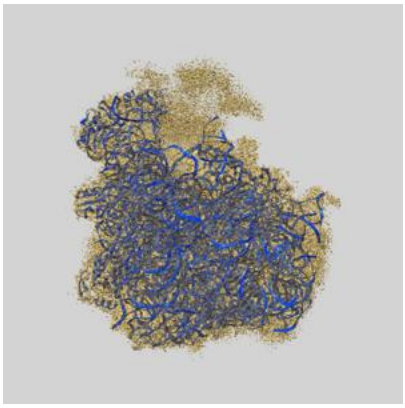
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-53067 and PDB model 9QEH. Per-residue inclusion information can be found in section 3 on page 11.

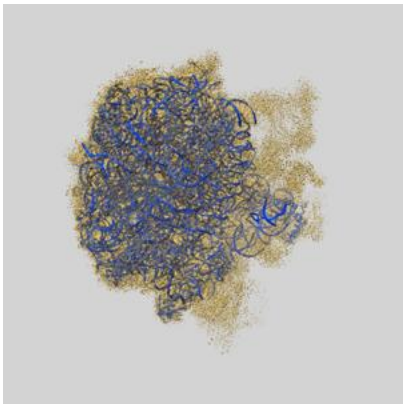
9.1 Map-model overlay



X



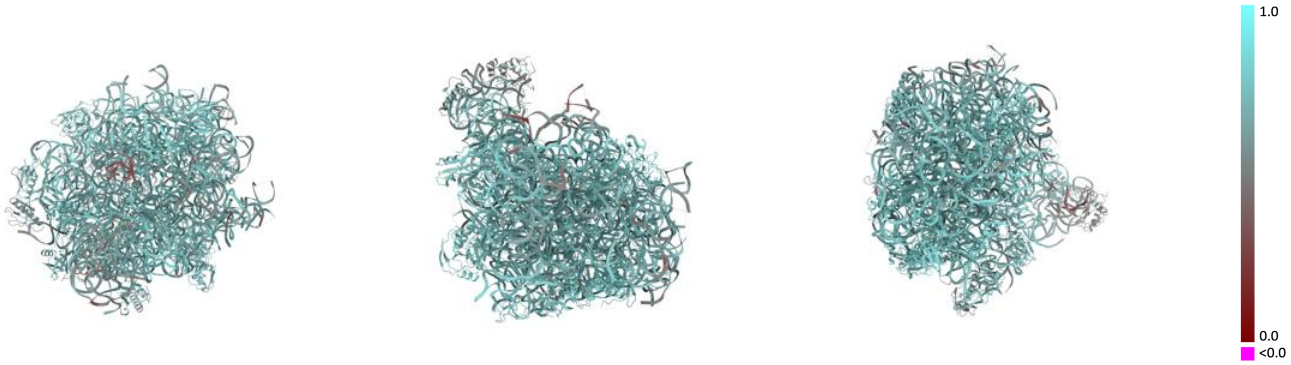
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

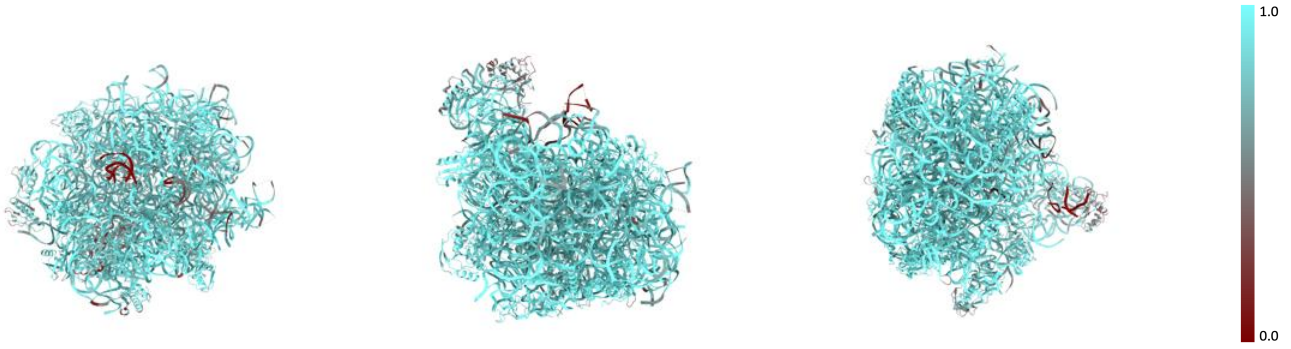
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

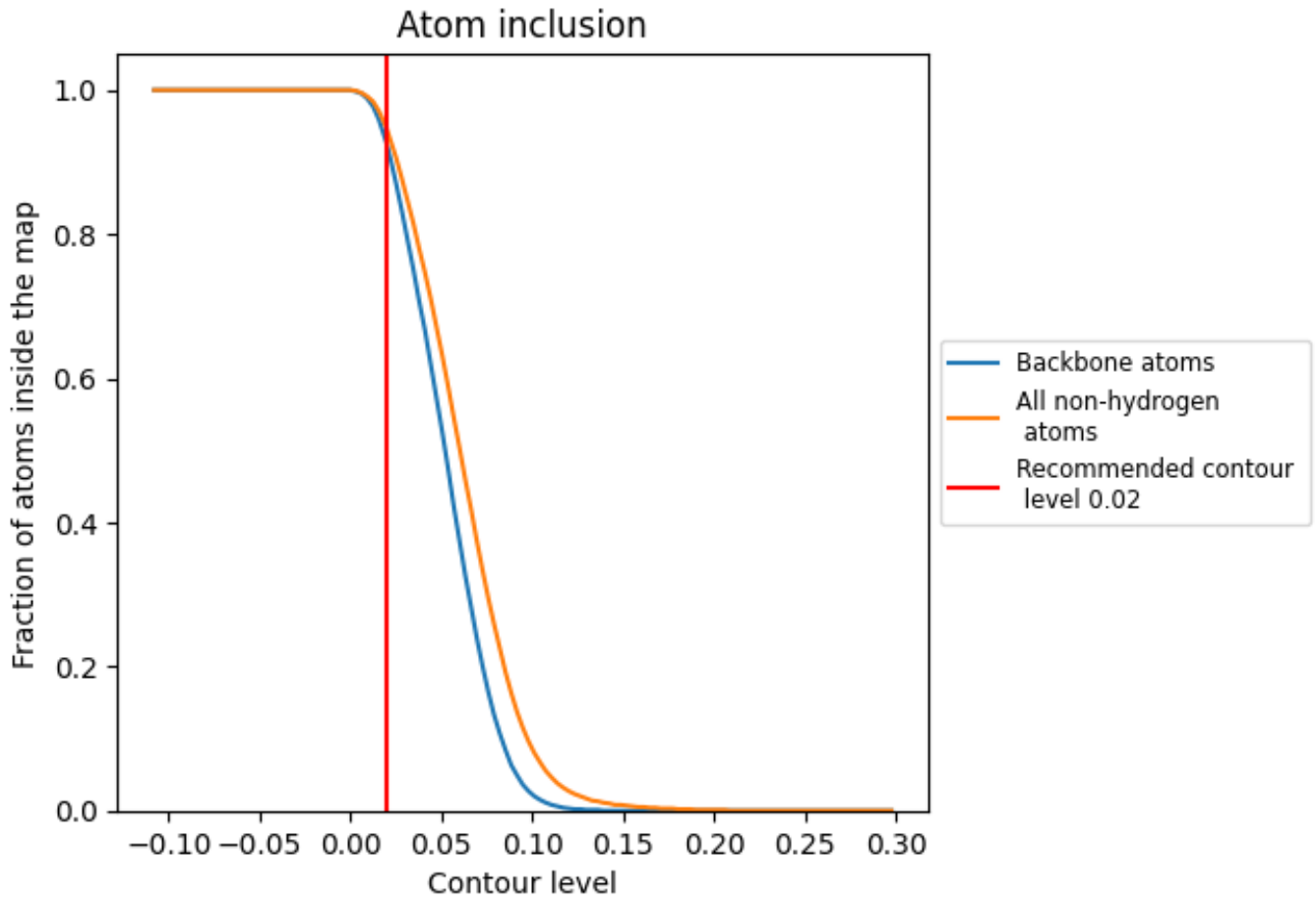
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 95% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9470	0.7230
1	0.8690	0.6740
11	0.4390	0.5190
2	0.9940	0.7960
3	0.9980	0.7910
4	0.9790	0.7610
8	0.0660	0.3650
A	0.9640	0.7270
B	0.8890	0.6240
C	0.9820	0.7760
D	0.9920	0.7750
E	0.9550	0.7590
F	0.5520	0.5050
G	0.7620	0.6150
H	0.9880	0.7730
I	0.9730	0.7610
J	0.9780	0.7510
K	0.9770	0.7580
L	0.9750	0.7700
M	0.8530	0.6410
N	0.9580	0.7430
O	0.9950	0.7880
P	0.9710	0.7600
Q	0.9860	0.7870
R	0.9780	0.7420
S	0.9120	0.6940
T	0.9150	0.6870
U	0.9890	0.7720
V	0.9020	0.7000
W	0.9420	0.7110
X	0.9580	0.7620
Z	0.9370	0.7380