



Full wwPDB EM Validation Report ⓘ

Jun 26, 2026 – 08:38 AM EDT

PDB ID : 6U48 / pdb_00006u48
EMDB ID : EMD-20638
Title : E. coli 50S with phazolicin (PHZ) bound in exit tunnel
Authors : Watson, Z.L.; Cate, J.H.D.; Polikanov, Y.S.; Severinov, K.
Deposited on : 2019-08-23
Resolution : 2.87 Å(reported)
Based on initial model : 4YBB

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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

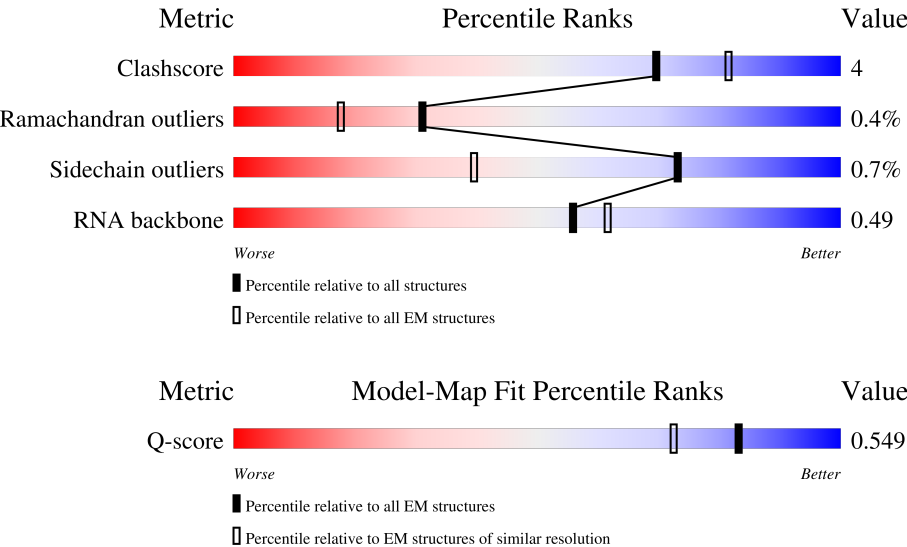
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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	12062 (2.37 - 3.37)

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	CA	2904	31% 71% 26% .
2	CB	118	77% 71% 26% .
3	CC	271	35% 78% 21% .

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Mol	Chain	Length	Quality of chain
4	CD	209	
5	CE	201	
6	CF	177	
7	CG	176	
8	CH	149	
9	CJ	134	
10	CK	142	
11	CL	122	
12	CM	144	
13	CN	136	
14	CO	120	
15	CP	116	
16	CQ	114	
17	CR	117	
18	CS	103	
19	CT	110	
20	CU	93	
21	CV	102	
22	CW	94	
23	CX	75	
24	CY	77	
25	CZ	62	
26	C0	58	
27	C1	56	
28	C2	50	

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Mol	Chain	Length	Quality of chain
29	C3	46	9% 80% 20%
30	C4	64	11% 86% 9% • •
31	C5	38	55% 76% 16% 5% •
32	A	22	64% 32% 5%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CA	2898	Total	C	N	O	P	0	0
			62229	27768	11448	20115	2898		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 3 is a protein called 50S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CC	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 4 is a protein called 50S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein uL4.

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

- Molecule 6 is a protein called 50S ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CF	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 7 is a protein called 50S ribosomal protein uL6.

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

- Molecule 8 is a protein called 50S ribosomal protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CH	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CJ	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 10 is a protein called 50S ribosomal protein uL13.

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

- Molecule 11 is a protein called 50S ribosomal protein uL14.

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

- Molecule 12 is a protein called 50S ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CM	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 13 is a protein called 50S ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CN	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 14 is a protein called 50S ribosomal protein bL17.

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

- Molecule 15 is a protein called 50S ribosomal protein uL18.

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

- Molecule 16 is a protein called 50S ribosomal protein bL19.

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

- Molecule 17 is a protein called 50S ribosomal protein bL20.

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

- Molecule 18 is a protein called 50S ribosomal protein bL21.

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

- Molecule 19 is a protein called 50S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CT	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 20 is a protein called 50S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CU	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 21 is a protein called 50S ribosomal protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	CV	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 22 is a protein called 50S ribosomal protein bL25.

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

- Molecule 23 is a protein called 50S ribosomal protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CX	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 24 is a protein called 50S ribosomal protein bL28.

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

- Molecule 25 is a protein called 50S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CZ	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 26 is a protein called 50S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C0	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 27 is a protein called 50S ribosomal protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C1	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	C2	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 29 is a protein called 50S ribosomal protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	C3	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C4	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	C5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called phazolicin.

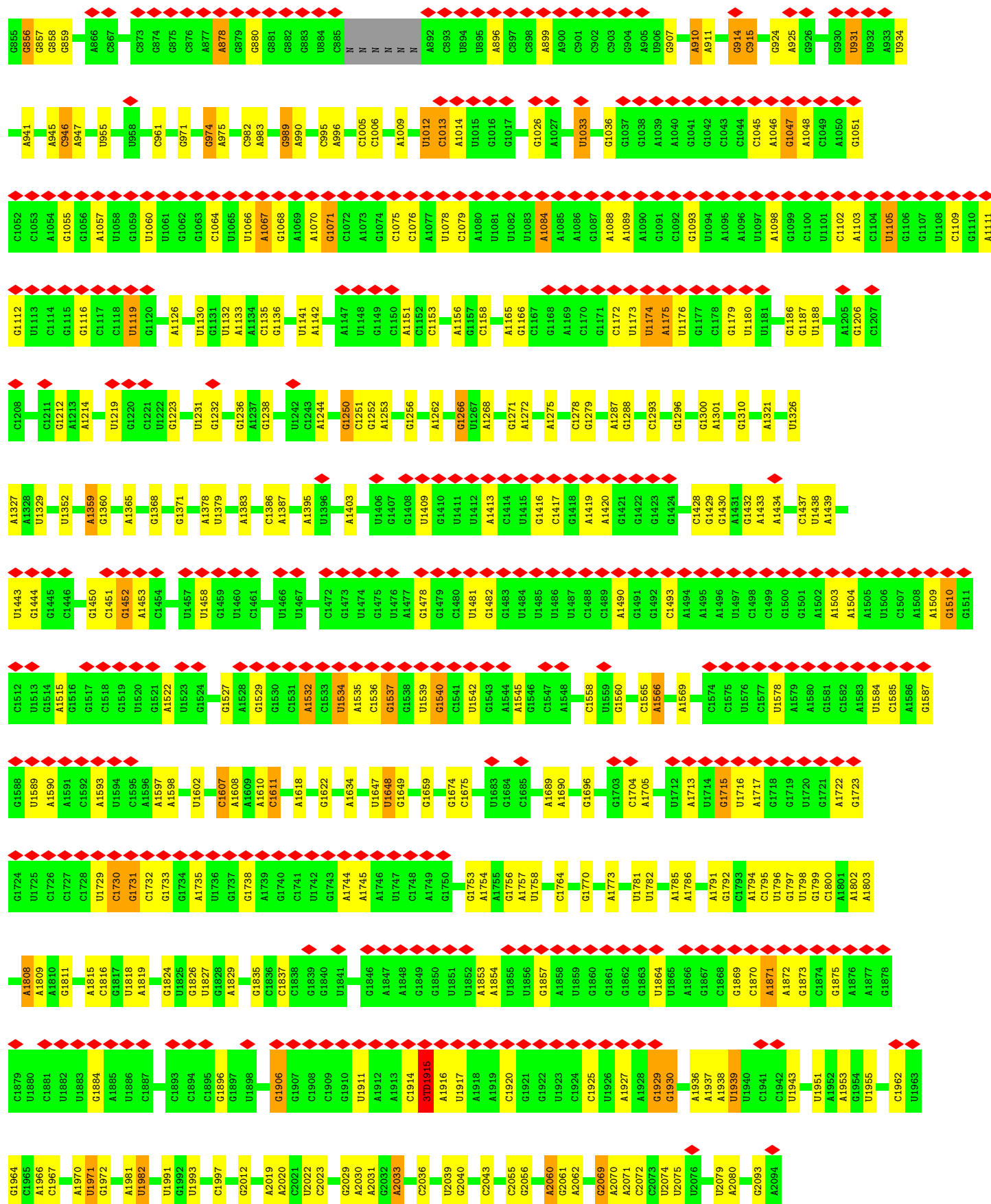
Mol	Chain	Residues	Atoms					AltConf	Trace
32	A	22	Total	C	N	O	S	0	0
			132	74	29	26	3		

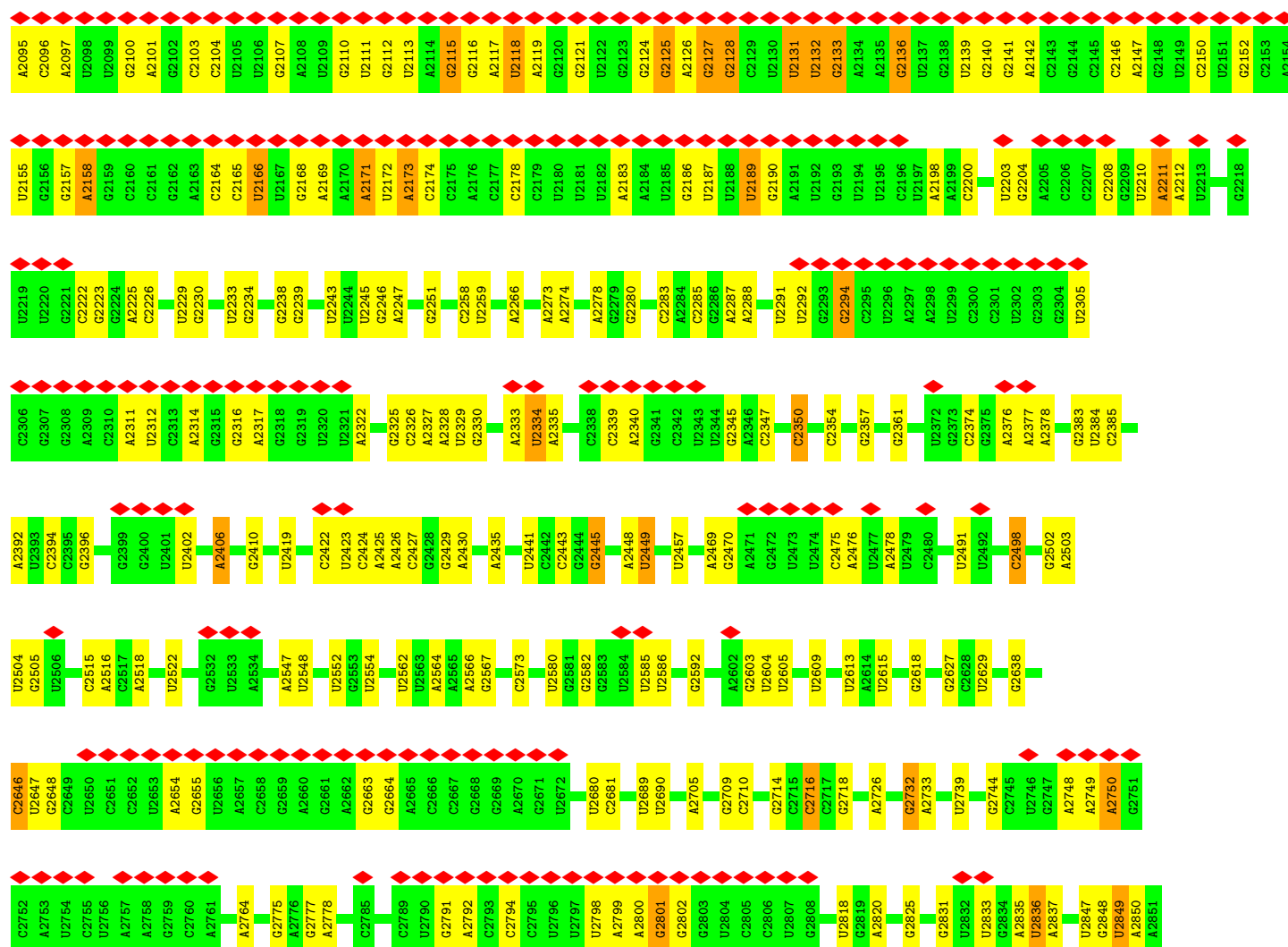
3 Residue-property plots

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

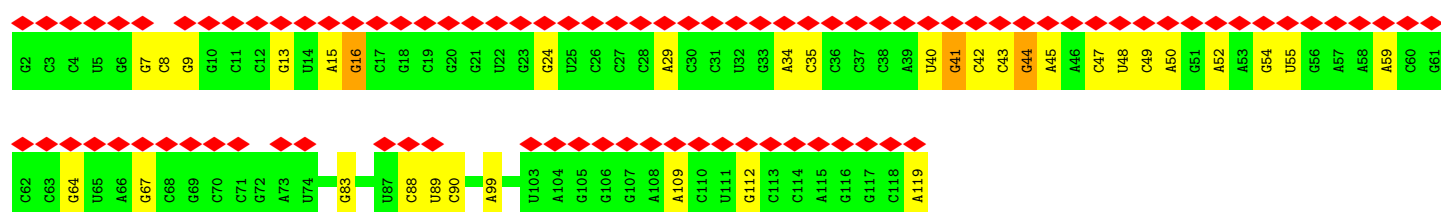
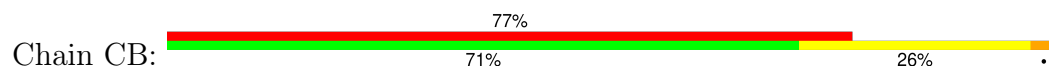
• Molecule 1: 23S rRNA



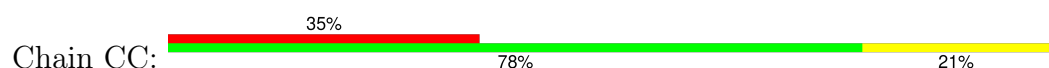


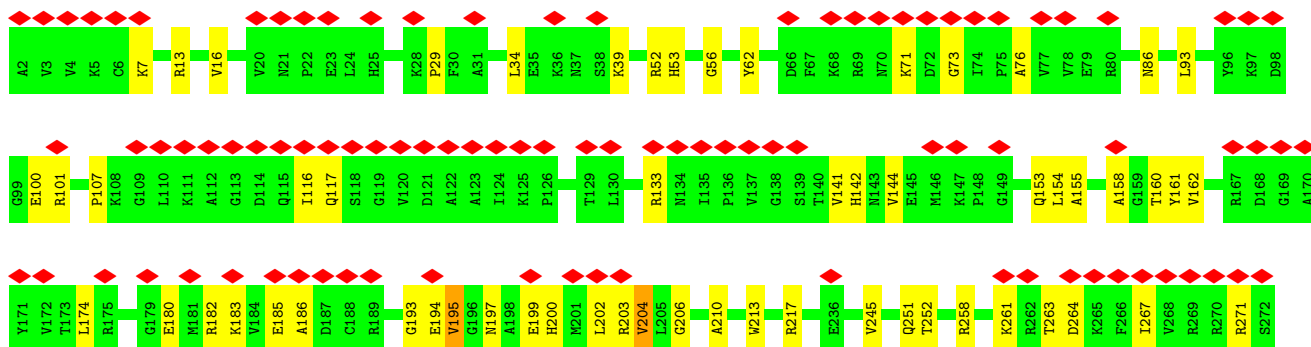


• Molecule 2: 5S rRNA

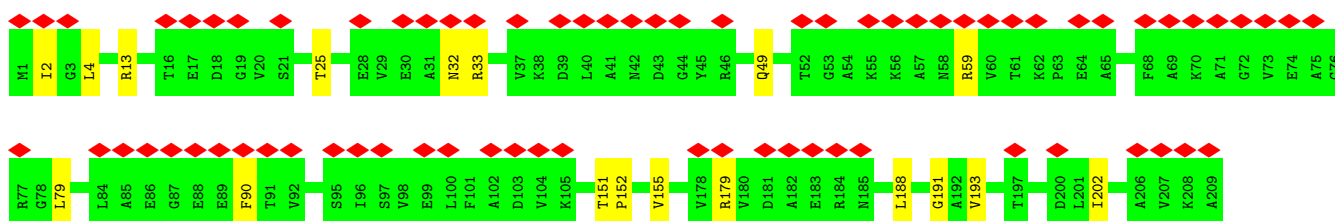


• Molecule 3: 50S ribosomal protein uL2

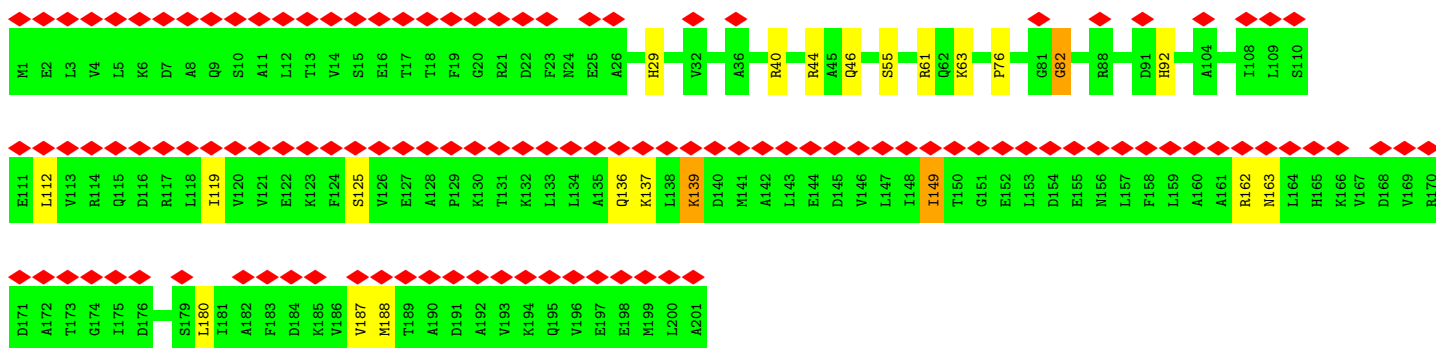
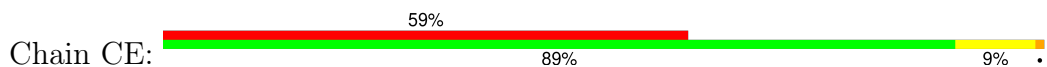




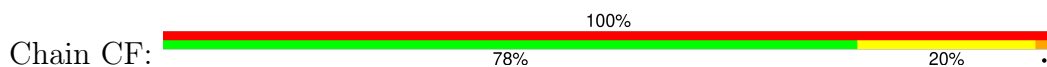
• Molecule 4: 50S ribosomal protein uL3



• Molecule 5: 50S ribosomal protein uL4

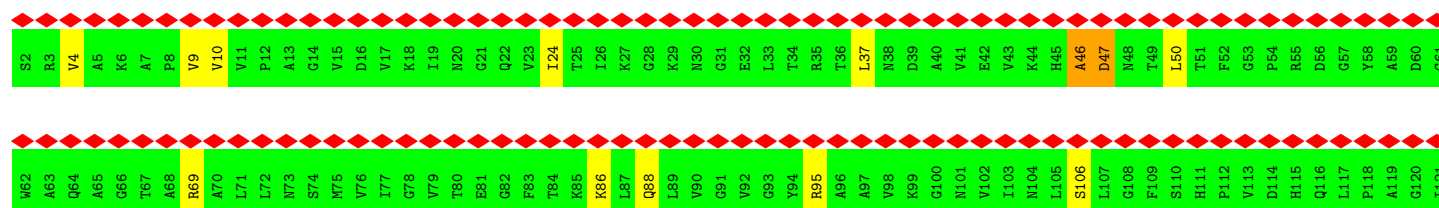
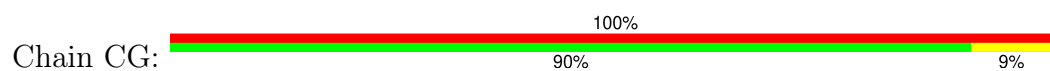


• Molecule 6: 50S ribosomal protein uL5

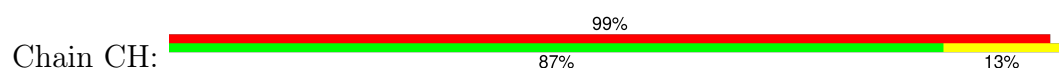




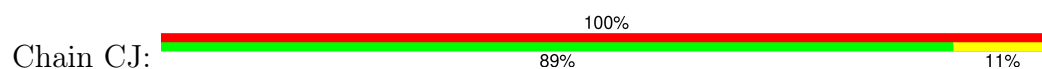
• Molecule 7: 50S ribosomal protein uL6



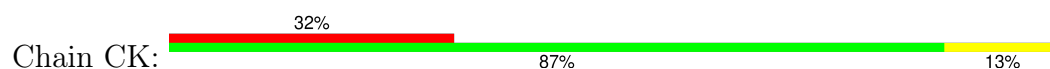
• Molecule 8: 50S ribosomal protein bL9

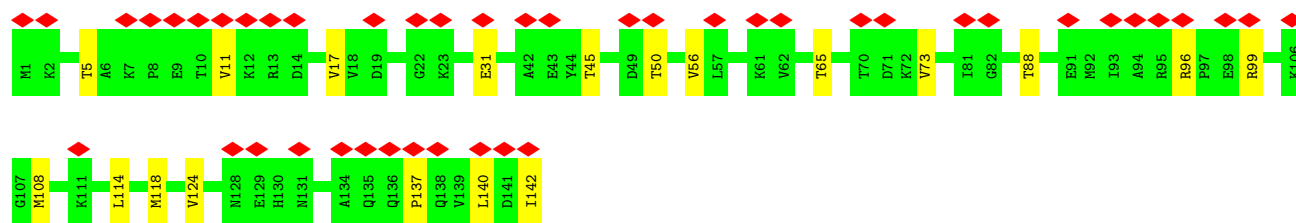


• Molecule 9: 50S ribosomal protein uL11

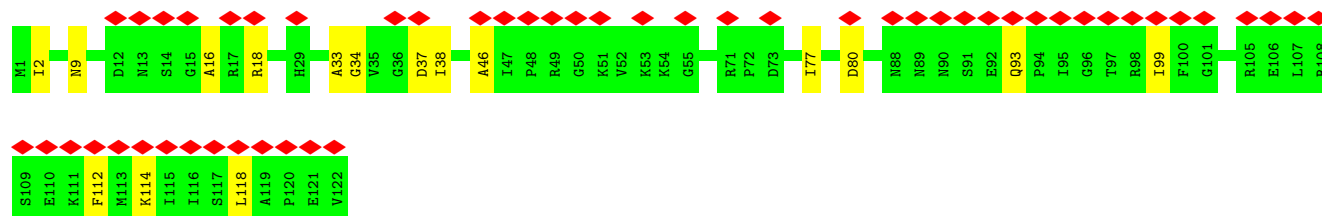
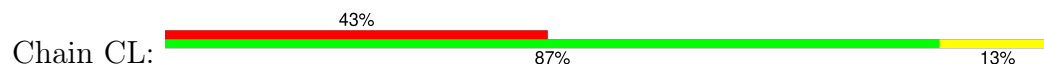


• Molecule 10: 50S ribosomal protein uL13

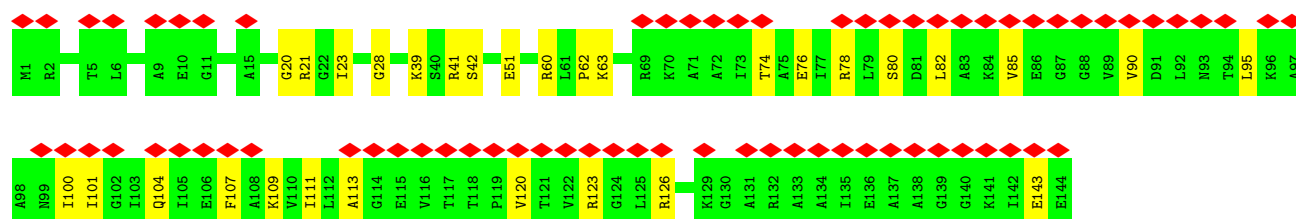
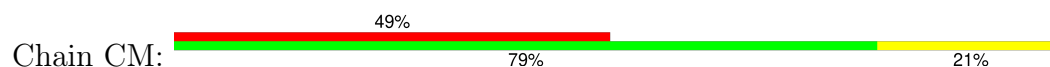




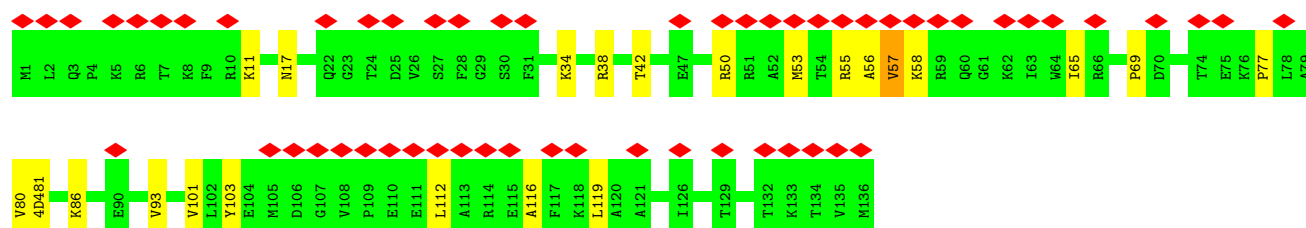
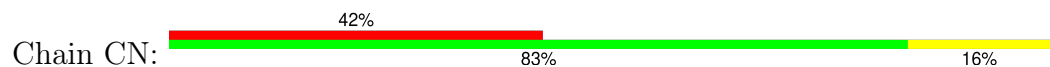
- Molecule 11: 50S ribosomal protein uL14



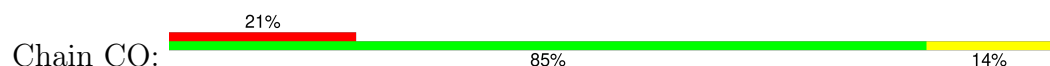
- Molecule 12: 50S ribosomal protein uL15



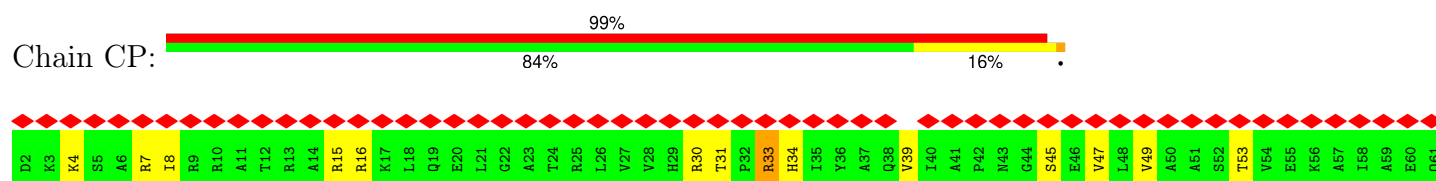
- Molecule 13: 50S ribosomal protein uL16



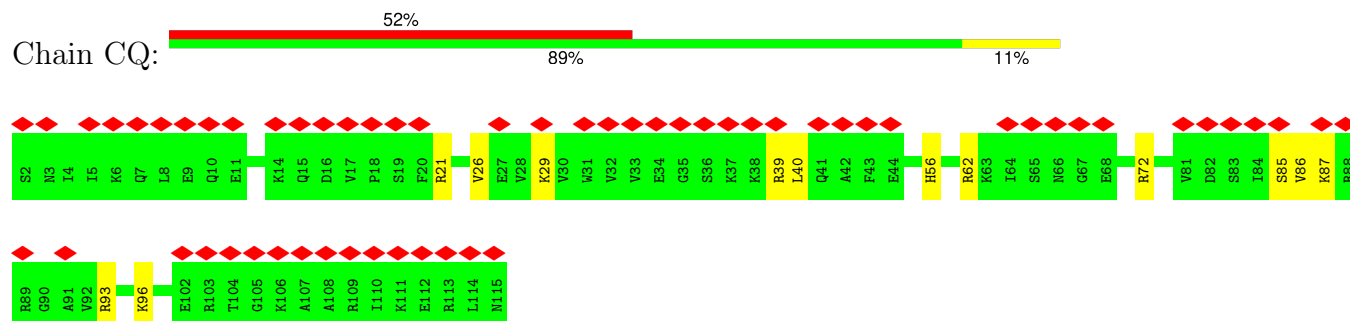
- Molecule 14: 50S ribosomal protein bL17



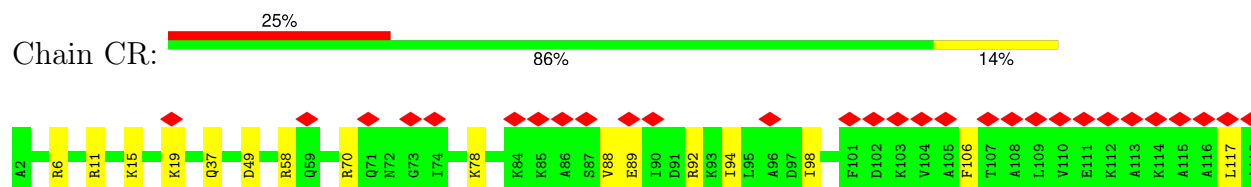
- Molecule 15: 50S ribosomal protein uL18



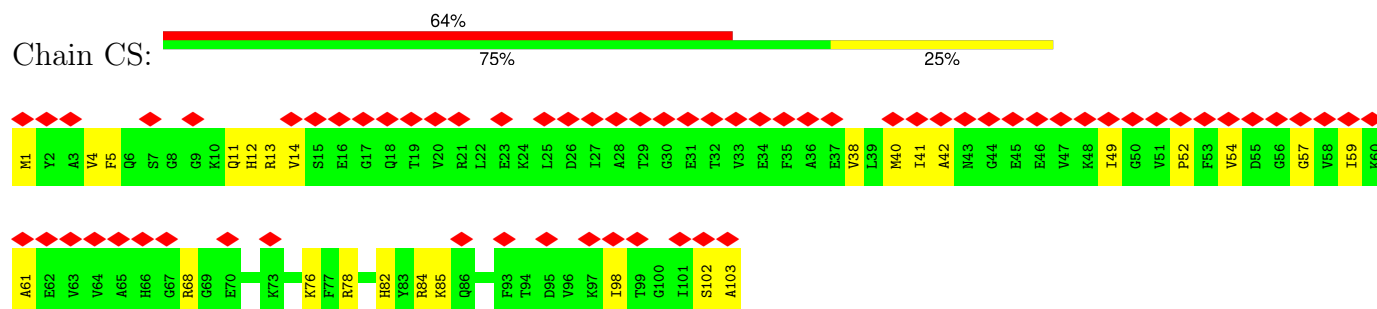
• Molecule 16: 50S ribosomal protein bL19



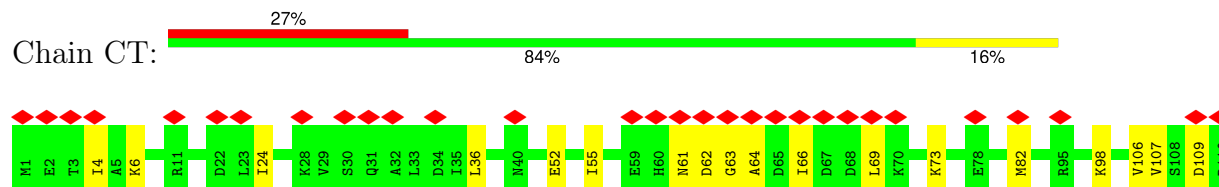
• Molecule 17: 50S ribosomal protein bL20



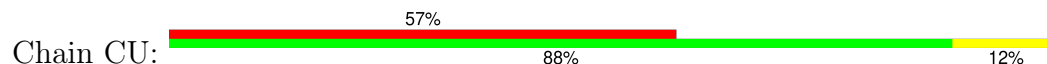
• Molecule 18: 50S ribosomal protein bL21

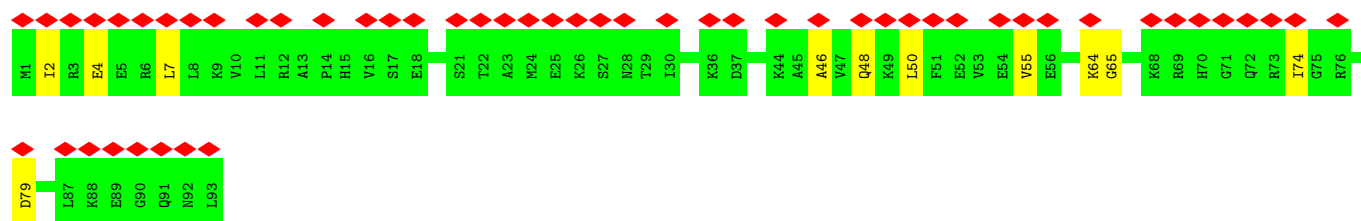


• Molecule 19: 50S ribosomal protein uL22

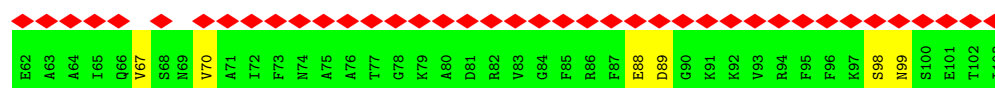
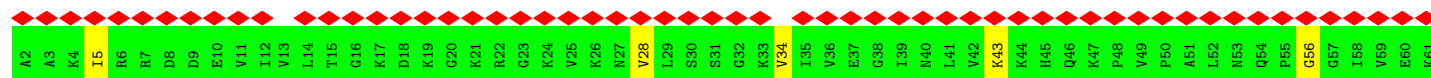
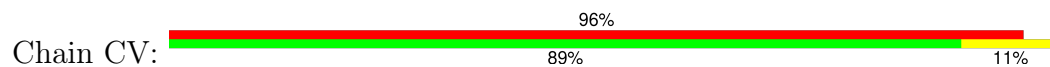


• Molecule 20: 50S ribosomal protein uL23

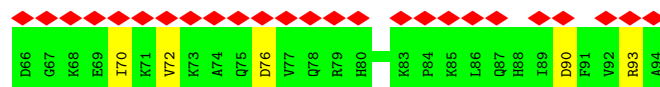
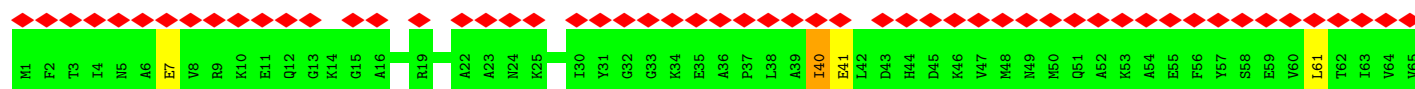
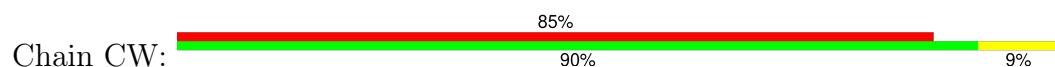




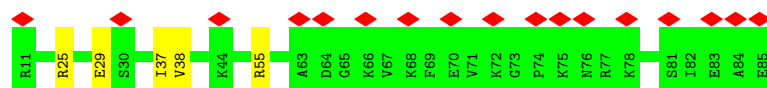
- Molecule 21: 50S ribosomal protein uL24



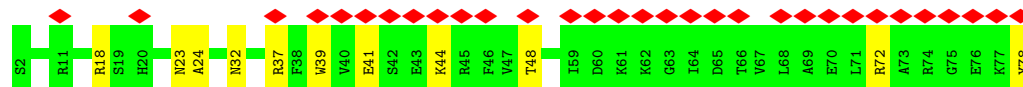
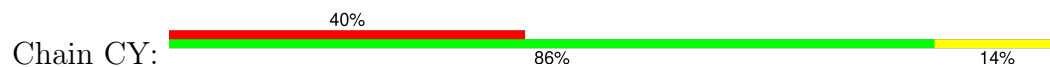
- Molecule 22: 50S ribosomal protein bL25



- Molecule 23: 50S ribosomal protein bL27

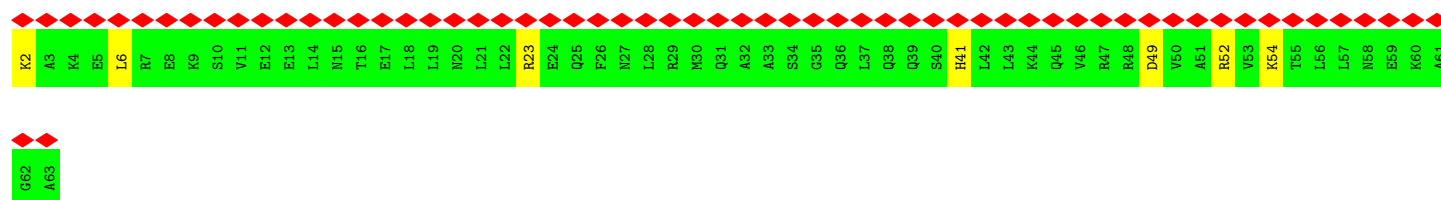


- Molecule 24: 50S ribosomal protein bL28

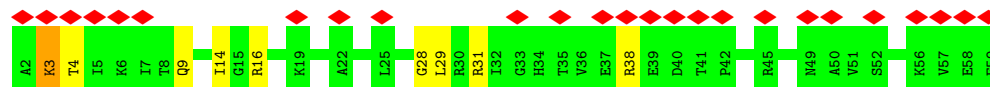
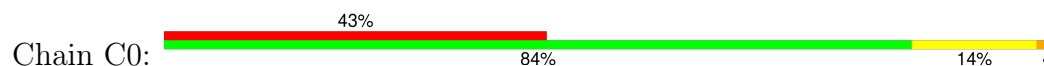


- Molecule 25: 50S ribosomal protein uL29

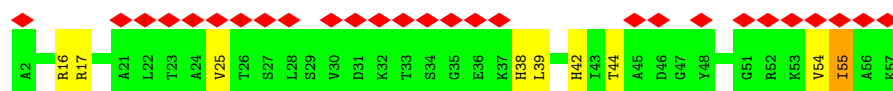
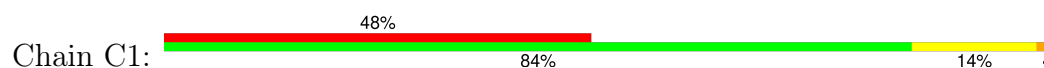




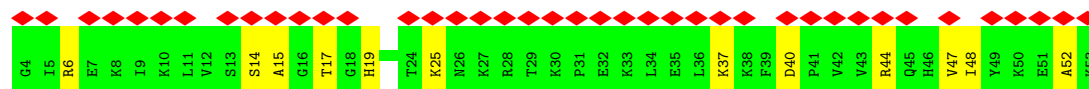
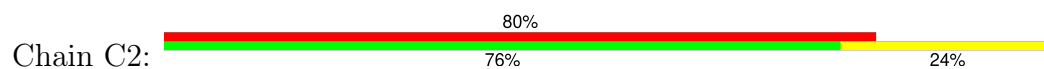
- Molecule 26: 50S ribosomal protein uL30



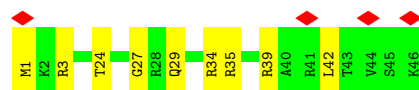
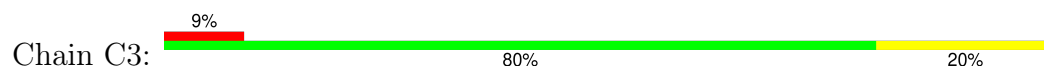
- Molecule 27: 50S ribosomal protein bL32



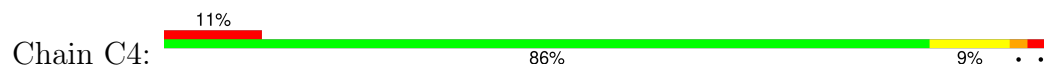
- Molecule 28: 50S ribosomal protein bL33



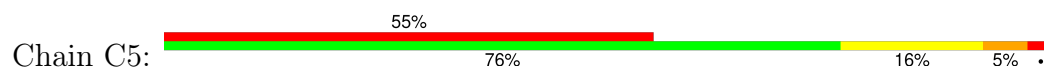
- Molecule 29: 50S ribosomal protein bL34

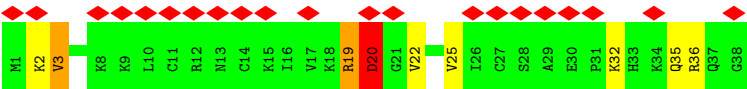


- Molecule 30: 50S ribosomal protein bL35

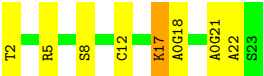


- Molecule 31: 50S ribosomal protein bL36





• Molecule 32: phazolicin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.141	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	356.352, 356.352, 356.352	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1136, 1.1136, 1.1136	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BB9, PSU, A0G, 6MZ, OMG, 1MG, 2MA, 5MU, H2U, MEQ, 2MG, G7M, 5MC, 4D4, 3TD, OMC, OMU

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	CA	0.27	0/69143	0.41	0/107862
2	CB	0.20	0/2828	0.35	0/4410
3	CC	0.27	0/2122	0.59	0/2852
4	CD	0.29	0/1576	0.61	0/2119
5	CE	0.26	0/1571	0.56	0/2113
6	CF	0.26	0/1435	0.69	0/1926
7	CG	0.20	0/1343	0.61	2/1816 (0.1%)
8	CH	0.27	1/1121 (0.1%)	0.58	0/1515
9	CJ	0.29	0/993	0.60	0/1341
10	CK	0.26	0/1152	0.55	0/1551
11	CL	0.29	0/947	0.60	0/1268
12	CM	0.29	0/1062	0.70	0/1413
13	CN	0.27	0/1081	0.58	0/1443
14	CO	0.31	0/973	0.69	0/1301
15	CP	0.23	0/902	0.63	0/1209
16	CQ	0.23	0/929	0.51	0/1242
17	CR	0.28	0/960	0.56	0/1278
18	CS	0.27	0/829	0.57	0/1107
19	CT	0.28	0/864	0.64	0/1156
20	CU	0.24	0/745	0.62	0/994
21	CV	0.29	0/788	0.77	2/1051 (0.2%)
22	CW	0.21	0/766	0.53	0/1025
23	CX	0.29	0/576	0.49	0/762
24	CY	0.25	0/635	0.51	0/848
25	CZ	0.20	0/502	0.52	0/667
26	C0	0.27	0/453	0.62	0/605
27	C1	0.32	0/450	0.77	0/599
28	C2	0.26	0/416	0.63	0/554
29	C3	0.33	0/380	0.68	0/498
30	C4	0.33	0/513	0.80	3/676 (0.4%)
31	C5	0.31	0/303	0.85	3/397 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	A	0.31	0/82	0.51	0/97
All	All	0.27	1/98440 (0.0%)	0.46	10/147695 (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
4	CD	0	1
5	CE	0	1
6	CF	0	1
7	CG	0	2
8	CH	0	1
11	CL	0	1
13	CN	0	1
15	CP	0	1
19	CT	0	1
21	CV	0	1
26	C0	0	1
27	C1	0	1
30	C4	0	1
31	C5	0	3
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	CH	31	VAL	C-N	5.64	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C5	20	ASP	N-CA-C	-8.31	93.11	110.80
21	CV	98	SER	CA-C-N	8.15	137.11	121.54
21	CV	98	SER	C-N-CA	8.15	137.11	121.54
7	CG	46	ALA	CA-C-N	6.07	133.13	121.54
7	CG	46	ALA	C-N-CA	6.07	133.13	121.54
30	C4	32	ILE	N-CA-C	5.52	120.83	109.34
30	C4	31	HIS	CA-C-N	5.45	131.79	121.97
30	C4	31	HIS	C-N-CA	5.45	131.79	121.97
31	C5	20	ASP	CA-C-N	-5.13	111.35	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C5	20	ASP	C-N-CA	-5.13	111.35	121.41

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	C0	3	LYS	Peptide
27	C1	54	VAL	Peptide
30	C4	31	HIS	Peptide
31	C5	19	ARG	Peptide,Mainchain
31	C5	20	ASP	Peptide
4	CD	151	THR	Peptide
5	CE	82	GLY	Peptide
6	CF	174	ASP	Peptide
7	CG	46	ALA	Peptide
7	CG	47	ASP	Peptide
8	CH	8	LYS	Peptide
11	CL	93	GLN	Peptide
13	CN	57	VAL	Peptide
15	CP	33	ARG	Peptide
19	CT	64	ALA	Peptide
21	CV	88	GLU	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	CA	62229	0	31320	267	0
2	CB	2529	0	1281	14	0
3	CC	2083	0	2154	35	0
4	CD	1566	0	1618	9	0
5	CE	1552	0	1619	16	0
6	CF	1411	0	1444	22	0
7	CG	1323	0	1371	8	0
8	CH	1110	0	1148	11	0
9	CJ	979	0	1028	9	0
10	CK	1129	0	1162	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CL	938	0	1012	8	0
12	CM	1053	0	1129	20	0
13	CN	1075	0	1155	11	0
14	CO	960	0	1000	11	0
15	CP	892	0	923	16	0
16	CQ	917	0	962	10	0
17	CR	947	0	1019	15	0
18	CS	816	0	839	18	0
19	CT	857	0	922	12	0
20	CU	739	0	807	6	0
21	CV	780	0	831	5	0
22	CW	753	0	780	6	0
23	CX	569	0	581	3	0
24	CY	625	0	652	8	0
25	CZ	501	0	531	5	0
26	C0	449	0	488	7	0
27	C1	444	0	458	6	0
28	C2	409	0	440	7	0
29	C3	377	0	418	8	0
30	C4	504	0	572	8	0
31	C5	302	0	343	4	0
32	A	132	0	99	3	0
All	All	90950	0	60106	507	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 (507) 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)
1:CA:1093:G:H21	1:CA:1098:A:H62	1.01	0.99
1:CA:1093:G:N2	1:CA:1098:A:H62	1.64	0.95
1:CA:284:U:H3	1:CA:356:G:H1	1.25	0.81
1:CA:1607:C:N4	1:CA:1622:G:OP2	2.15	0.79
1:CA:1715:G:N2	1:CA:1744:A:OP2	2.15	0.79
1:CA:1093:G:H21	1:CA:1098:A:N6	1.81	0.79
1:CA:630:G:N2	1:CA:633:A:OP2	2.18	0.76
1:CA:500:G:N1	1:CA:503:A:OP2	2.19	0.75
20:CU:4:GLU:OE2	25:CZ:23:ARG:NH2	2.21	0.74
20:CU:46:ALA:O	20:CU:50:LEU:HB2	1.88	0.73
1:CA:2646:C:OP2	1:CA:2732:G:O2'	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1012:U:OP2	17:CR:70:ARG:NH1	2.24	0.71
1:CA:2200:C:OP2	24:CY:37:ARG:NH1	2.24	0.71
4:CD:13:ARG:HH12	16:CQ:56:HIS:HA	1.57	0.70
1:CA:1798:U:OP2	3:CC:271:ARG:NH2	2.25	0.69
1:CA:1252:G:H1	17:CR:37:GLN:HE21	1.38	0.69
5:CE:61:ARG:NH1	32:A:22:ALA:O	2.26	0.68
1:CA:307:G:N1	1:CA:310:A:OP2	2.20	0.68
11:CL:34:GLY:N	11:CL:37:ASP:OD2	2.25	0.68
1:CA:2171:A:O2'	1:CA:2173:A:OP1	2.11	0.67
2:CB:55:U:HO2'	6:CF:24:SER:HG	1.37	0.67
1:CA:494:G:H4'	19:CT:6:LYS:HB2	1.77	0.67
6:CF:29:PRO:HB2	6:CF:169:LEU:HD22	1.78	0.65
14:CO:56:LYS:NZ	14:CO:87:PHE:O	2.30	0.65
12:CM:62:PRO:HB2	30:C4:30:ARG:HH11	1.63	0.64
6:CF:108:VAL:HG11	6:CF:176:PRO:HG2	1.78	0.64
1:CA:254:G:N7	30:C4:5:LYS:NZ	2.46	0.64
19:CT:4:ILE:HG12	19:CT:106:VAL:HG22	1.80	0.64
1:CA:298:G:N1	1:CA:339:U:OP2	2.26	0.64
1:CA:2392:A:OP2	1:CA:2422:C:N4	2.29	0.64
1:CA:971:G:OP2	1:CA:974:G:N2	2.32	0.63
1:CA:2258:C:O2'	1:CA:2427:C:OP2	2.16	0.63
8:CH:128:HIS:O	8:CH:143:ILE:HA	1.99	0.62
1:CA:2376:A:N3	15:CP:111:ARG:NH1	2.47	0.62
3:CC:142:HIS:ND1	3:CC:193:GLY:O	2.33	0.62
6:CF:112:ARG:NH2	6:CF:113:ASP:OD2	2.33	0.62
24:CY:41:GLU:OE2	24:CY:44:LYS:NZ	2.33	0.62
1:CA:1250:G:OP2	12:CM:21:ARG:NH2	2.32	0.61
12:CM:123:ARG:NE	12:CM:143:GLU:OE2	2.28	0.61
1:CA:466:A:OP1	29:C3:34:ARG:NH1	2.33	0.61
30:C4:15:LYS:HD2	30:C4:23:LYS:HE2	1.83	0.61
1:CA:1819:A:H5''	3:CC:160:THR:HG21	1.82	0.60
2:CB:48:U:OP2	15:CP:30:ARG:NH2	2.28	0.60
1:CA:2133:G:N2	1:CA:2158:A:N1	2.51	0.59
1:CA:2394:C:H5''	12:CM:63:LYS:HE2	1.83	0.59
1:CA:2848:G:HO2'	1:CA:2867:G:H22	1.49	0.59
1:CA:2127:G:H21	1:CA:2173:A:H1'	1.68	0.59
1:CA:2125:G:H21	1:CA:2174:C:H42	1.51	0.58
6:CF:111:ILE:HG12	6:CF:137:ILE:HD12	1.85	0.58
18:CS:61:ALA:HB2	18:CS:98:ILE:HD13	1.84	0.58
3:CC:62:TYR:HA	3:CC:86:ASN:HD21	1.67	0.58
19:CT:66:ILE:HA	19:CT:69:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2857:G:N2	1:CA:2860:A:OP2	2.28	0.58
1:CA:2831:G:OP2	4:CD:59:ARG:NH1	2.29	0.58
1:CA:1824:G:H5'	3:CC:52:ARG:HH11	1.69	0.58
2:CB:8:C:OP1	15:CP:15:ARG:NH2	2.36	0.57
5:CE:125:SER:O	5:CE:137:LYS:NZ	2.36	0.57
14:CO:22:ARG:HG3	14:CO:70:THR:HA	1.85	0.57
9:CJ:24:VAL:HG22	9:CJ:28:LEU:HD22	1.86	0.57
29:C3:24:THR:HG23	29:C3:27:GLY:H	1.69	0.57
1:CA:728:G:H4'	3:CC:13:ARG:HD3	1.86	0.57
1:CA:1102:C:H2'	1:CA:1103:A:H8	1.70	0.57
6:CF:52:ASN:O	6:CF:56:ASP:N	2.36	0.57
8:CH:12:LEU:HD13	8:CH:19:VAL:HG21	1.87	0.57
8:CH:135:HIS:HD2	8:CH:137:GLU:HG2	1.69	0.57
17:CR:78:LYS:HE3	17:CR:117:LEU:HD21	1.87	0.57
8:CH:78:VAL:HG21	8:CH:103:VAL:HG22	1.87	0.57
1:CA:210:C:OP1	29:C3:29:GLN:NE2	2.35	0.56
1:CA:739:A:H1'	1:CA:740:C:H5	1.70	0.56
3:CC:258:ARG:NH1	3:CC:264:ASP:OD1	2.37	0.56
14:CO:101:GLY:H	27:C1:42:HIS:HD2	1.52	0.56
1:CA:711:G:H1	1:CA:720:U:H3	1.53	0.56
3:CC:144:VAL:HB	3:CC:154:LEU:HB2	1.86	0.56
13:CN:57:VAL:HG12	13:CN:112:LEU:HG	1.87	0.56
1:CA:975:A:H5'	18:CS:78:ARG:HH22	1.71	0.56
18:CS:38:VAL:HG13	18:CS:54:VAL:HB	1.87	0.56
29:C3:34:ARG:HE	29:C3:39:ARG:HG3	1.69	0.56
25:CZ:2:LYS:HB3	25:CZ:6:LEU:HD23	1.88	0.56
3:CC:258:ARG:NH2	3:CC:263:THR:OG1	2.39	0.56
12:CM:76:GLU:HB2	12:CM:111:ILE:HD13	1.87	0.56
8:CH:73:ASN:ND2	8:CH:141:LYS:O	2.39	0.56
1:CA:1527:G:H21	1:CA:1545:A:H62	1.54	0.56
3:CC:39:LYS:NZ	3:CC:56:GLY:O	2.39	0.55
3:CC:158:ALA:HB1	3:CC:197:ASN:HB3	1.88	0.55
1:CA:355:U:H2'	1:CA:356:G:H8	1.70	0.55
1:CA:1792:G:H5'	3:CC:204:VAL:HG23	1.87	0.55
12:CM:78:ARG:NH2	12:CM:80:SER:OG	2.39	0.55
12:CM:100:ILE:HG13	12:CM:101:ILE:HG23	1.87	0.55
9:CJ:100:LYS:HD3	9:CJ:141:GLU:HG3	1.86	0.55
1:CA:631:A:OP2	30:C4:23:LYS:NZ	2.29	0.55
18:CS:76:LYS:O	18:CS:84:ARG:HA	2.06	0.55
31:C5:2:LYS:NZ	31:C5:32:LYS:O	2.39	0.55
7:CG:24:ILE:HD12	7:CG:37:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:CO:49:GLU:OE2	14:CO:95:THR:HG22	2.06	0.55
1:CA:2285:C:OP2	28:C2:6:ARG:NH1	2.39	0.54
8:CH:129:GLU:HB3	8:CH:141:LYS:HD3	1.89	0.54
24:CY:18:ARG:HH21	24:CY:24:ALA:HB2	1.72	0.54
1:CA:1781:U:O2	32:A:5:ARG:NH2	2.41	0.54
1:CA:713:G:H21	1:CA:718:A:H62	1.56	0.54
1:CA:320:A:N3	5:CE:163:ASN:ND2	2.55	0.54
1:CA:706:A:OP1	3:CC:7:LYS:NZ	2.38	0.54
1:CA:651:G:H5'	30:C4:19:LYS:HG2	1.90	0.54
9:CJ:73:THR:HG23	9:CJ:116:ASP:OD2	2.08	0.54
13:CN:42:THR:HG22	13:CN:93:VAL:HG12	1.90	0.54
19:CT:69:LEU:HA	19:CT:109:ASP:HA	1.90	0.54
1:CA:2316:G:H2'	1:CA:2317:A:H8	1.73	0.54
9:CJ:59:ILE:HD12	9:CJ:69:PHE:HB3	1.90	0.54
1:CA:1047:G:O2'	1:CA:1109:C:N4	2.38	0.54
1:CA:1288:G:OP2	1:CA:1288:G:N2	2.26	0.54
1:CA:675:A:N3	1:CA:2443:C:O2'	2.40	0.54
3:CC:162:VAL:HG11	3:CC:174:LEU:HD23	1.90	0.54
12:CM:109:LYS:HG2	12:CM:126:ARG:HB2	1.90	0.54
1:CA:2849:U:O4	16:CQ:21:ARG:NH2	2.38	0.54
1:CA:1770:G:H1	1:CA:1982:U:H3	1.56	0.53
18:CS:41:ILE:HD13	18:CS:103:ALA:HA	1.89	0.53
19:CT:82:MET:HB2	19:CT:98:LYS:HB2	1.90	0.53
12:CM:20:GLY:HA2	12:CM:28:GLY:HA2	1.89	0.53
1:CA:467:G:OP2	29:C3:34:ARG:HD3	2.08	0.53
1:CA:1158:C:H5''	26:C0:31:ARG:HD3	1.90	0.53
3:CC:29:PRO:HG2	3:CC:34:LEU:HD11	1.90	0.53
1:CA:340:A:O2'	5:CE:162:ARG:NH1	2.42	0.53
12:CM:95:LEU:HD22	12:CM:100:ILE:HD11	1.90	0.53
1:CA:1084:A:N3	1:CA:1105:U:O2'	2.38	0.53
15:CP:7:ARG:NH1	15:CP:95:SER:O	2.41	0.53
31:C5:19:ARG:O	31:C5:22:VAL:HB	2.09	0.53
5:CE:44:ARG:HH11	5:CE:46:GLN:HE22	1.57	0.53
5:CE:61:ARG:NH2	5:CE:63:LYS:O	2.42	0.53
21:CV:5:ILE:HD13	21:CV:70:VAL:HG23	1.90	0.53
29:C3:35:ARG:HG3	29:C3:42:LEU:HD11	1.91	0.53
12:CM:51:GLU:OE1	12:CM:60:ARG:NH1	2.41	0.52
1:CA:468:G:N7	29:C3:39:ARG:NH2	2.45	0.52
17:CR:94:ILE:HD12	18:CS:13:ARG:HB2	1.91	0.52
1:CA:160:A:N3	1:CA:2208:C:O2'	2.40	0.52
1:CA:1925:C:O2	1:CA:1929:G:N2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1826:G:O2'	1:CA:1971:U:OP2	2.27	0.52
3:CC:182:ARG:NH2	3:CC:183:LYS:O	2.42	0.52
15:CP:34:HIS:ND1	15:CP:53:THR:OG1	2.35	0.52
1:CA:2314:A:OP1	6:CF:88:LYS:NZ	2.40	0.52
12:CM:78:ARG:NH1	12:CM:113:ALA:O	2.42	0.52
1:CA:931:U:O4	1:CA:1166:G:N2	2.42	0.52
1:CA:1006:C:O2'	10:CK:108:MET:O	2.28	0.52
11:CL:77:ILE:HG12	16:CQ:72:ARG:HG2	1.92	0.52
5:CE:136:GLN:OE1	5:CE:139:LYS:NZ	2.42	0.52
28:C2:17:THR:HG22	28:C2:19:HIS:H	1.75	0.52
1:CA:641:U:O2'	1:CA:2350:C:OP1	2.28	0.51
1:CA:284:U:O2	1:CA:356:G:N2	2.36	0.51
1:CA:2029:G:N1	1:CA:2033:A:OP2	2.36	0.51
7:CG:88:GLN:HE21	7:CG:163:ARG:HD2	1.75	0.51
1:CA:2291:U:O2'	1:CA:2374:C:O2	2.29	0.51
1:CA:2131:U:H5'	1:CA:2132:U:H5''	1.92	0.51
13:CN:77:PRO:HG2	13:CN:80:VAL:HG21	1.91	0.51
1:CA:358:U:H2'	1:CA:359:G:H8	1.75	0.51
1:CA:1438:U:H2'	1:CA:1439:A:H8	1.75	0.51
15:CP:4:LYS:HE2	15:CP:8:ILE:HD11	1.92	0.51
15:CP:4:LYS:HE3	15:CP:7:ARG:HH21	1.76	0.51
1:CA:2140:G:H2'	1:CA:2141:G:H8	1.75	0.51
1:CA:1360:G:N7	1:CA:1371:G:N2	2.59	0.51
19:CT:62:ASP:OD1	19:CT:62:ASP:N	2.44	0.51
19:CT:69:LEU:HD12	19:CT:107:VAL:HG22	1.91	0.51
1:CA:1266:G:OP2	27:C1:17:ARG:NE	2.36	0.50
19:CT:52:GLU:HA	19:CT:55:ILE:HD12	1.92	0.50
1:CA:743:A:O2'	1:CA:1659:G:OP1	2.29	0.50
1:CA:1266:G:OP1	27:C1:16:ARG:NE	2.40	0.50
9:CJ:113:LYS:HB3	9:CJ:117:MET:HE3	1.93	0.50
11:CL:2:ILE:HB	11:CL:33:ALA:HB3	1.93	0.50
11:CL:9:ASN:OD1	11:CL:18:ARG:NH1	2.41	0.50
3:CC:161:TYR:HB3	3:CC:194:GLU:HG3	1.94	0.50
3:CC:210:ALA:HA	3:CC:213:TRP:CE2	2.47	0.50
1:CA:483:A:O2'	21:CV:56:GLY:O	2.24	0.50
1:CA:2233:U:H2'	1:CA:2234:G:H8	1.75	0.50
23:CX:25:ARG:NH1	23:CX:29:GLU:OE2	2.44	0.50
1:CA:2627:G:N2	1:CA:2777:G:OP2	2.42	0.50
26:C0:9:GLN:HB2	26:C0:29:LEU:HD13	1.93	0.50
1:CA:444:C:OP2	5:CE:44:ARG:NH2	2.45	0.50
1:CA:2469:A:H4'	13:CN:55:ARG:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C0:4:THR:HA	26:C0:38:ARG:O	2.12	0.50
1:CA:2229:U:H2'	1:CA:2230:G:H8	1.76	0.49
21:CV:34:VAL:HG13	21:CV:67:VAL:HG22	1.94	0.49
11:CL:80:ASP:OD2	16:CQ:62:ARG:NH2	2.44	0.49
14:CO:33:ILE:HD11	27:C1:55:ILE:HD12	1.93	0.49
1:CA:2100:G:O6	1:CA:2189:U:O4	2.30	0.49
2:CB:83:G:H5''	26:C0:16:ARG:HH12	1.76	0.49
4:CD:25:THR:HG21	4:CD:193:VAL:HG22	1.94	0.49
24:CY:37:ARG:HG2	24:CY:48:THR:HG22	1.93	0.49
28:C2:40:ASP:O	28:C2:44:ARG:HA	2.13	0.49
1:CA:1857:G:N2	1:CA:1884:G:O2'	2.39	0.49
1:CA:1936:A:H2	1:CA:1943:U:H3	1.60	0.49
1:CA:2210:U:H4'	1:CA:2211:A:H5'	1.94	0.49
14:CO:114:GLU:HB2	14:CO:118:ARG:HD2	1.93	0.49
29:C3:1:MET:HB2	29:C3:3:ARG:HH11	1.78	0.49
1:CA:373:U:H2'	1:CA:374:A:H8	1.77	0.49
1:CA:1906:G:OP2	1:CA:1930:G:H8	1.96	0.49
14:CO:65:LEU:HG	14:CO:69:ARG:HH22	1.77	0.49
22:CW:72:VAL:HG12	22:CW:93:ARG:HA	1.93	0.49
28:C2:25:LYS:NZ	28:C2:52:ALA:O	2.44	0.49
1:CA:184:C:H2'	1:CA:185:G:C8	2.48	0.49
2:CB:40:U:O2'	2:CB:43:C:OP2	2.17	0.49
1:CA:95:A:O2'	25:CZ:41:HIS:ND1	2.43	0.48
6:CF:123:ASP:OD2	6:CF:127:ASN:HB2	2.12	0.48
7:CG:86:LYS:HG2	7:CG:132:VAL:HG22	1.95	0.48
1:CA:1250:G:H5''	17:CR:6:ARG:HD3	1.95	0.48
1:CA:1310:G:H1'	1:CA:1611:C:H5''	1.94	0.48
1:CA:1602:U:OP2	20:CU:64:LYS:NZ	2.44	0.48
17:CR:89:GLU:O	18:CS:11:GLN:NE2	2.41	0.48
1:CA:672:C:OP2	12:CM:42:SER:OG	2.28	0.48
1:CA:1141:U:OP2	10:CK:65:THR:OG1	2.27	0.48
3:CC:180:GLU:OE2	3:CC:267:ILE:HD12	2.12	0.48
31:C5:3:VAL:HG21	31:C5:36:ARG:HH21	1.79	0.48
1:CA:807:U:O2'	1:CA:2060:A:N1	2.42	0.48
14:CO:28:LEU:HD23	14:CO:48:VAL:HG21	1.96	0.48
3:CC:133:ARG:HB3	3:CC:186:ALA:HB1	1.96	0.48
18:CS:14:VAL:HG21	18:CS:98:ILE:HG13	1.94	0.48
22:CW:76:ASP:HB3	22:CW:90:ASP:OD2	2.14	0.48
1:CA:463:G:N2	1:CA:466:A:OP2	2.35	0.48
1:CA:2419:U:OP2	30:C4:33:LEU:HD13	2.13	0.48
8:CH:104:THR:HG22	8:CH:109:GLU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:692:C:H5''	3:CC:39:LYS:HB2	1.96	0.47
10:CK:114:LEU:HG	10:CK:118:MET:HE3	1.96	0.47
10:CK:140:LEU:HG	10:CK:142:ILE:HG12	1.95	0.47
9:CJ:20:PRO:HB2	9:CJ:23:PRO:HD2	1.95	0.47
1:CA:239:C:HO2'	1:CA:622:G:HO2'	1.62	0.47
1:CA:2848:G:O2'	1:CA:2867:G:N2	2.36	0.47
12:CM:82:LEU:HD12	12:CM:120:VAL:HG11	1.95	0.47
27:C1:38:HIS:ND1	27:C1:39:LEU:O	2.38	0.47
1:CA:45:G:H5''	1:CA:46:G:H5'	1.95	0.47
1:CA:280:U:H2'	1:CA:281:C:H6	1.78	0.47
1:CA:1036:G:O6	1:CA:1119:U:O2	2.32	0.47
28:C2:37:LYS:HG2	28:C2:48:ILE:HG13	1.97	0.47
1:CA:1153:C:OP1	17:CR:92:ARG:NH1	2.35	0.47
1:CA:414:C:H2'	1:CA:415:A:C8	2.50	0.47
1:CA:581:C:H2'	1:CA:582:A:C8	2.49	0.47
1:CA:974:G:H8	1:CA:990:A:H62	1.62	0.47
1:CA:1266:G:O2'	1:CA:2012:G:O6	2.28	0.47
1:CA:1716:U:H2'	1:CA:1717:A:H8	1.78	0.47
6:CF:105:THR:HG22	6:CF:106:ILE:HG23	1.95	0.47
8:CH:1:MET:N	8:CH:21:VAL:O	2.48	0.47
1:CA:2419:U:OP1	30:C4:41:LYS:NZ	2.48	0.47
19:CT:24:ILE:HD13	19:CT:36:LEU:HD11	1.96	0.47
16:CQ:29:LYS:HB3	16:CQ:40:LEU:HD23	1.97	0.47
17:CR:11:ARG:HE	17:CR:15:LYS:HG3	1.80	0.47
18:CS:57:GLY:HA2	18:CS:102:SER:O	2.14	0.47
1:CA:1013:C:H2'	1:CA:1014:A:H8	1.80	0.46
1:CA:2618:G:H21	4:CD:155:VAL:HG21	1.79	0.46
9:CJ:79:LEU:HA	9:CJ:82:LYS:HG2	1.96	0.46
1:CA:324:A:N6	1:CA:338:G:O2'	2.48	0.46
1:CA:534:U:O2'	17:CR:49:ASP:OD2	2.17	0.46
1:CA:1066:U:H2'	1:CA:1067:A:H3'	1.96	0.46
1:CA:1174:U:H5'	1:CA:1175:A:OP2	2.15	0.46
3:CC:16:VAL:HG22	3:CC:206:GLY:HA3	1.98	0.46
6:CF:48:LYS:HA	6:CF:51:ASP:HB2	1.97	0.46
20:CU:2:ILE:HG13	20:CU:7:LEU:HD11	1.96	0.46
1:CA:2334:U:O4	15:CP:16:ARG:NH2	2.48	0.46
3:CC:261:LYS:HA	3:CC:264:ASP:OD2	2.15	0.46
22:CW:7:GLU:O	22:CW:40:ILE:HA	2.16	0.46
24:CY:72:ARG:NH2	24:CY:78:TYR:OH	2.48	0.46
5:CE:149:ILE:HG23	5:CE:188:MET:HA	1.96	0.46
13:CN:34:LYS:HA	13:CN:101:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:589:U:H2'	1:CA:590:A:C8	2.51	0.46
1:CA:1864:U:OP1	1:CA:2410:G:O2'	2.29	0.46
1:CA:1296:G:OP1	1:CA:2709:G:O2'	2.26	0.46
1:CA:1386:C:H2'	1:CA:1387:A:C8	2.50	0.46
1:CA:1869:G:N2	1:CA:1871:A:O2'	2.48	0.46
3:CC:199:GLU:HA	3:CC:202:LEU:HD13	1.97	0.46
23:CX:37:ILE:HG22	23:CX:38:VAL:HG23	1.97	0.46
1:CA:1359:A:OP2	1:CA:1371:G:N1	2.39	0.46
1:CA:1713:A:H61	1:CA:1745:A:H61	1.63	0.46
1:CA:2245:U:H5''	1:CA:2246:G:H5'	1.98	0.46
1:CA:2705:A:O2'	1:CA:2852:G:OP1	2.31	0.46
1:CA:458:G:O2'	1:CA:469:G:O6	2.32	0.46
1:CA:946:C:H2'	1:CA:947:A:H8	1.81	0.46
10:CK:11:VAL:HG11	10:CK:50:THR:HA	1.98	0.46
10:CK:56:VAL:HB	10:CK:124:VAL:HG12	1.97	0.46
19:CT:109:ASP:OD1	19:CT:109:ASP:N	2.49	0.46
32:A:8:SER:HB3	32:A:17:LYS:HD2	1.98	0.46
1:CA:807:U:OP2	12:CM:41:ARG:NH1	2.48	0.46
1:CA:910:A:H2'	1:CA:911:A:C8	2.51	0.46
1:CA:1429:G:H2'	1:CA:1430:G:H8	1.81	0.46
1:CA:1443:U:H2'	1:CA:1444:G:C8	2.51	0.46
1:CA:1443:U:H2'	1:CA:1444:G:H8	1.80	0.46
1:CA:2229:U:H2'	1:CA:2230:G:C8	2.51	0.46
1:CA:1326:U:H2'	1:CA:1327:A:H8	1.81	0.45
1:CA:2547:A:H2'	1:CA:2548:U:C6	2.51	0.45
1:CA:2564:A:OP1	1:CA:2648:G:O2'	2.32	0.45
6:CF:134:GLU:OE2	6:CF:149:VAL:HG12	2.16	0.45
1:CA:1165:A:H2'	1:CA:1166:G:H8	1.82	0.45
1:CA:1589:U:H2'	1:CA:1590:A:H8	1.81	0.45
1:CA:1409:U:H3	1:CA:1593:A:H61	1.63	0.45
28:C2:14:SER:OG	28:C2:48:ILE:O	2.33	0.45
1:CA:258:G:H1'	12:CM:104:GLN:HE21	1.82	0.45
2:CB:34:A:N6	2:CB:44:G:O2'	2.49	0.45
5:CE:76:PRO:HA	5:CE:82:GLY:HA2	1.98	0.45
28:C2:15:ALA:HB2	28:C2:47:VAL:HG11	1.99	0.45
1:CA:1481:U:O2	1:CA:1510:G:O6	2.34	0.45
13:CN:53:MET:HE1	13:CN:103:TYR:CG	2.52	0.45
1:CA:1071:G:N2	1:CA:1089:A:N3	2.64	0.45
1:CA:2142:A:N1	1:CA:2150:C:N4	2.65	0.45
6:CF:142:ASP:HB3	6:CF:145:LYS:HB2	1.98	0.45
1:CA:1287:A:N1	1:CA:1648:U:O2'	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:CN:17:ASN:O	13:CN:38:ARG:NH1	2.44	0.45
10:CK:17:VAL:HG23	10:CK:137:PRO:HB2	1.98	0.45
13:CN:11:LYS:HD3	13:CN:86:LYS:HD3	1.98	0.45
15:CP:39:VAL:HB	15:CP:49:VAL:HB	1.99	0.45
1:CA:72:U:H5'	25:CZ:54:LYS:HD2	1.97	0.44
1:CA:1244:A:O2'	5:CE:29:HIS:NE2	2.46	0.44
1:CA:1529:G:H1	1:CA:1542:U:H3	1.65	0.44
1:CA:1785:A:OP2	1:CA:1982:U:H5''	2.18	0.44
1:CA:2222:C:H4'	3:CC:185:GLU:OE2	2.17	0.44
2:CB:52:A:H2'	15:CP:33:ARG:HH22	1.82	0.44
3:CC:155:ALA:HB2	3:CC:162:VAL:HG23	1.99	0.44
14:CO:44:LEU:HD23	14:CO:113:ILE:HD13	1.98	0.44
15:CP:83:LEU:HD11	15:CP:114:GLY:HA3	1.99	0.44
1:CA:1013:C:H2'	1:CA:1014:A:C8	2.53	0.44
1:CA:1796:U:H2'	1:CA:1797:G:C8	2.52	0.44
1:CA:2079:U:O2'	24:CY:23:ASN:OD1	2.29	0.44
1:CA:322:A:OP2	5:CE:163:ASN:HB2	2.17	0.44
1:CA:468:G:H5''	5:CE:55:SER:HB3	2.00	0.44
1:CA:579:G:O2'	1:CA:2019:A:OP1	2.36	0.44
1:CA:1532:A:N6	1:CA:1540:G:O6	2.50	0.44
1:CA:1730:C:O2'	1:CA:1731:G:N3	2.49	0.44
1:CA:2139:U:O2	1:CA:2152:G:O6	2.34	0.44
1:CA:2140:G:H2'	1:CA:2141:G:C8	2.52	0.44
1:CA:2801:G:H2'	1:CA:2802:G:C8	2.52	0.44
17:CR:88:VAL:HG13	18:CS:49:ILE:HD11	2.00	0.44
1:CA:721:A:H2'	1:CA:722:A:C8	2.51	0.44
1:CA:1219:U:OP2	17:CR:19:LYS:NZ	2.51	0.44
7:CG:9:VAL:HB	7:CG:50:LEU:HB2	1.99	0.44
10:CK:5:THR:HG23	10:CK:45:THR:HG21	1.99	0.44
10:CK:96:ARG:HH21	10:CK:99:ARG:HG2	1.81	0.44
18:CS:4:VAL:HA	18:CS:12:HIS:O	2.16	0.44
1:CA:135:U:H3	1:CA:144:A:H61	1.65	0.44
1:CA:1534:U:O2'	1:CA:1537:G:O6	2.35	0.44
1:CA:1539:U:H2'	1:CA:1540:G:C8	2.53	0.44
1:CA:2847:U:OP1	16:CQ:96:LYS:NZ	2.40	0.44
1:CA:30:G:O2'	1:CA:1214:A:N3	2.46	0.44
1:CA:914:G:H5'	1:CA:915:C:OP2	2.17	0.44
1:CA:1432:G:H2'	1:CA:1433:A:C8	2.52	0.44
1:CA:2339:C:H2'	1:CA:2340:A:H8	1.81	0.44
3:CC:200:HIS:CE1	3:CC:203:ARG:HH11	2.36	0.44
4:CD:2:ILE:HD13	4:CD:90:PHE:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CS:40:MET:HE2	18:CS:42:ALA:HB2	1.99	0.44
1:CA:495:G:O2'	19:CT:61:ASN:ND2	2.51	0.44
1:CA:989:G:H5''	26:C0:14:ILE:HD11	1.99	0.44
1:CA:1796:U:H2'	1:CA:1797:G:H8	1.83	0.44
1:CA:2110:G:H5'	1:CA:2118:U:H1'	2.00	0.44
4:CD:49:GLN:HE21	4:CD:79:LEU:HB3	1.83	0.44
12:CM:74:THR:HG22	12:CM:107:PHE:HB2	1.99	0.44
1:CA:397:U:H5''	24:CY:32:ASN:HB2	1.98	0.44
1:CA:685:A:O2'	1:CA:773:U:O4	2.30	0.44
1:CA:1187:G:N2	1:CA:1188:U:O4	2.51	0.44
1:CA:1837:C:O2'	1:CA:1927:A:N3	2.41	0.44
1:CA:2339:C:H2'	1:CA:2340:A:C8	2.53	0.44
19:CT:73:LYS:HB3	19:CT:106:VAL:HB	1.99	0.44
1:CA:585:G:N7	17:CR:6:ARG:NH1	2.63	0.44
1:CA:1827:U:H5'	1:CA:1971:U:H4'	1.99	0.44
1:CA:2136:G:H8	1:CA:2136:G:OP2	2.01	0.44
3:CC:245:VAL:HG12	3:CC:251:GLN:HA	1.98	0.44
8:CH:96:THR:HG22	8:CH:115:VAL:HB	1.99	0.44
1:CA:581:C:H2'	1:CA:582:A:H8	1.83	0.43
1:CA:668:A:H2'	1:CA:670:A:H62	1.82	0.43
1:CA:833:A:OP2	12:CM:39:LYS:NZ	2.39	0.43
1:CA:1696:G:H8	1:CA:1696:G:OP2	2.00	0.43
1:CA:2070:A:H2'	1:CA:2071:A:C8	2.53	0.43
1:CA:856:G:H2'	1:CA:857:G:C8	2.53	0.43
20:CU:65:GLY:N	20:CU:79:ASP:OD1	2.42	0.43
1:CA:2273:A:H2'	1:CA:2274:A:C8	2.53	0.43
4:CD:4:LEU:HD12	4:CD:32:ASN:HD22	1.83	0.43
1:CA:639:U:H2'	1:CA:640:C:C6	2.52	0.43
1:CA:815:C:OP2	18:CS:85:LYS:HE2	2.19	0.43
3:CC:107:PRO:HA	3:CC:195:VAL:HA	2.00	0.43
6:CF:64:LYS:HA	6:CF:65:PRO:HD3	1.78	0.43
1:CA:362:A:H5'	1:CA:363:G:OP2	2.18	0.43
1:CA:414:C:H2'	1:CA:415:A:H8	1.83	0.43
1:CA:586:A:N1	1:CA:809:G:O2'	2.44	0.43
1:CA:818:G:N1	1:CA:1188:U:OP2	2.28	0.43
1:CA:1915:3TD:H5'	1:CA:1916:A:OP2	2.18	0.43
1:CA:1981:A:H5''	1:CA:1982:U:OP2	2.18	0.43
4:CD:179:ARG:HB3	4:CD:188:LEU:HD12	2.00	0.43
1:CA:361:G:H8	1:CA:361:G:OP2	2.02	0.43
2:CB:41:G:H5'	2:CB:42:C:H5''	2.00	0.43
1:CA:9:G:O2'	1:CA:2800:A:N6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:589:U:H2'	1:CA:590:A:H8	1.82	0.43
1:CA:833:A:H2'	1:CA:834:G:C8	2.52	0.43
1:CA:1794:A:H2'	1:CA:1795:C:C6	2.54	0.43
1:CA:2039:U:H2'	1:CA:2040:G:C8	2.53	0.43
1:CA:2115:G:O5'	1:CA:2166:U:O2'	2.35	0.43
3:CC:73:GLY:HA2	3:CC:117:GLN:HE21	1.83	0.43
6:CF:56:ASP:OD2	6:CF:135:GLN:HG3	2.19	0.43
10:CK:31:GLU:HG2	10:CK:142:ILE:HD12	2.01	0.43
30:C4:31:HIS:C	30:C4:33:LEU:H	2.26	0.43
1:CA:1223:G:OP1	18:CS:68:ARG:NH2	2.52	0.43
1:CA:1951:U:H2'	1:CA:1953:A:OP2	2.19	0.43
1:CA:2329:U:H2'	1:CA:2330:G:C8	2.53	0.43
5:CE:40:ARG:HD2	5:CE:92:HIS:CD2	2.54	0.43
5:CE:119:ILE:HB	5:CE:187:VAL:HG22	2.01	0.43
6:CF:116:GLY:HA3	6:CF:178:ARG:HD3	2.01	0.43
11:CL:16:ALA:HA	11:CL:46:ALA:HA	1.99	0.43
1:CA:1433:A:H2'	1:CA:1434:A:C8	2.54	0.43
1:CA:1503:A:H2'	1:CA:1504:A:C8	2.54	0.43
1:CA:2859:G:H2'	1:CA:2860:A:C8	2.53	0.43
22:CW:7:GLU:HB2	22:CW:41:GLU:OE2	2.18	0.43
1:CA:5:A:H2'	1:CA:6:A:C8	2.54	0.42
1:CA:117:G:OP2	1:CA:119:A:O2'	2.27	0.42
6:CF:175:PHE:O	6:CF:177:PHE:N	2.51	0.42
13:CN:57:VAL:HG13	13:CN:116:ALA:HB2	2.01	0.42
16:CQ:26:VAL:HG22	16:CQ:86:VAL:HG22	2.01	0.42
1:CA:1386:C:H2'	1:CA:1387:A:H8	1.84	0.42
1:CA:1853:A:H2'	1:CA:1854:A:C8	2.54	0.42
18:CS:49:ILE:HD12	18:CS:52:PRO:HA	2.01	0.42
1:CA:1915:3TD:O5'	1:CA:1915:3TD:H6	2.19	0.42
1:CA:2638:G:O2'	1:CA:2775:G:N2	2.45	0.42
6:CF:80:ARG:HD3	6:CF:83:TYR:HE2	1.84	0.42
1:CA:362:A:H3'	1:CA:363:G:H8	1.84	0.42
1:CA:1231:U:H2'	1:CA:1232:G:H8	1.85	0.42
1:CA:2246:G:H2'	1:CA:2247:A:C8	2.54	0.42
1:CA:2377:A:H2'	1:CA:2378:A:C8	2.55	0.42
6:CF:57:LEU:HD13	6:CF:89:VAL:HG23	2.01	0.42
1:CA:20:C:H2'	1:CA:21:A:H8	1.85	0.42
1:CA:302:C:H2'	1:CA:303:G:H8	1.84	0.42
1:CA:411:G:OP2	1:CA:2406:A:O2'	2.34	0.42
1:CA:1689:A:H2'	1:CA:1690:A:C8	2.54	0.42
1:CA:2074:U:H2'	1:CA:2075:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CJ:113:LYS:O	9:CJ:117:MET:N	2.53	0.42
22:CW:61:LEU:HB2	22:CW:72:VAL:O	2.19	0.42
3:CC:53:HIS:HA	3:CC:217:ARG:HB2	2.01	0.42
7:CG:4:VAL:HG12	7:CG:69:ARG:HD2	2.00	0.42
1:CA:878:A:N6	1:CA:899:A:O2'	2.44	0.42
6:CF:16:LEU:HD11	6:CF:169:LEU:HA	2.02	0.42
16:CQ:85:SER:OG	16:CQ:87:LYS:NZ	2.53	0.42
1:CA:184:C:H2'	1:CA:185:G:H8	1.84	0.42
1:CA:2294:G:H5'	15:CP:98:GLN:HE21	1.84	0.42
2:CB:7:G:OP1	15:CP:4:LYS:NZ	2.39	0.42
12:CM:23:ILE:HG13	18:CS:82:HIS:CD2	2.55	0.42
21:CV:28:VAL:HB	21:CV:34:VAL:HG12	2.01	0.42
1:CA:1033:U:O2'	1:CA:2750:A:N6	2.53	0.42
1:CA:1565:C:O2	1:CA:1566:A:O2'	2.35	0.42
1:CA:2655:G:O2'	1:CA:2664:G:O6	2.35	0.42
3:CC:93:LEU:HD11	3:CC:101:ARG:HB3	2.01	0.42
12:CM:85:VAL:HG11	12:CM:90:VAL:HG22	2.02	0.42
20:CU:48:GLN:HE21	20:CU:55:VAL:H	1.67	0.42
1:CA:2710:C:OP1	14:CO:15:SER:OG	2.31	0.41
3:CC:71:LYS:NZ	3:CC:100:GLU:OE1	2.48	0.41
3:CC:76:ALA:HB3	3:CC:116:ILE:HG13	2.02	0.41
8:CH:124:THR:OG1	8:CH:128:HIS:NE2	2.42	0.41
9:CJ:58:VAL:O	9:CJ:69:PHE:HA	2.19	0.41
22:CW:70:ILE:HG22	22:CW:72:VAL:HG13	2.02	0.41
1:CA:1278:C:H2'	1:CA:1279:G:H8	1.85	0.41
1:CA:593:U:H2'	1:CA:594:U:C6	2.55	0.41
1:CA:1754:A:N1	1:CA:2716:C:O2'	2.44	0.41
16:CQ:39:ARG:HE	16:CQ:40:LEU:H	1.68	0.41
1:CA:1597:A:H5''	1:CA:1598:A:H5'	2.02	0.41
1:CA:2291:U:H2'	1:CA:2292:U:C6	2.56	0.41
2:CB:29:A:OP2	15:CP:31:THR:HG23	2.20	0.41
2:CB:112:G:N2	15:CP:45:SER:O	2.46	0.41
11:CL:38:ILE:HD11	11:CL:112:PHE:HZ	1.84	0.41
1:CA:2328:A:H2'	1:CA:2329:U:C6	2.55	0.41
2:CB:47:C:O2'	15:CP:98:GLN:OE1	2.38	0.41
7:CG:95:ARG:HB2	7:CG:106:SER:HB2	2.03	0.41
1:CA:499:U:H5''	21:CV:43:LYS:HE2	2.02	0.41
1:CA:1704:C:H2'	1:CA:1705:A:C8	2.55	0.41
1:CA:1808:A:H3'	1:CA:1809:A:C8	2.55	0.41
1:CA:353:C:H2'	1:CA:354:A:H8	1.85	0.41
7:CG:86:LYS:NZ	7:CG:130:GLU:OE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:CN:56:ALA:HB2	13:CN:119:LEU:HD12	2.03	0.41
1:CA:155:A:H2'	1:CA:156:A:H8	1.84	0.41
1:CA:1450:G:N2	1:CA:1452:G:O6	2.48	0.41
7:CG:155:GLU:OE2	7:CG:157:TYR:HB2	2.21	0.41
18:CS:5:PHE:HB3	18:CS:59:ILE:HD12	2.03	0.41
1:CA:151:C:H2'	1:CA:152:A:H8	1.86	0.41
1:CA:171:U:H2'	1:CA:172:A:H8	1.86	0.41
1:CA:2384:U:OP2	23:CX:55:ARG:NH2	2.54	0.41
1:CA:2522:U:O2'	1:CA:2647:U:OP1	2.31	0.41
2:CB:15:A:H3'	2:CB:16:G:H8	1.86	0.41
2:CB:49:C:H2'	2:CB:50:A:C8	2.56	0.41
4:CD:25:THR:OG1	4:CD:191:GLY:O	2.36	0.41
10:CK:73:VAL:HG22	10:CK:88:THR:HG22	2.02	0.41
11:CL:114:LYS:HE3	11:CL:118:LEU:HD11	2.03	0.41
18:CS:1:MET:HA	18:CS:42:ALA:O	2.20	0.41
24:CY:39:TRP:NE1	24:CY:41:GLU:OE1	2.46	0.41
31:C5:25:VAL:HB	31:C5:35:GLN:HB2	2.02	0.41
1:CA:1251:C:OP2	17:CR:6:ARG:HD2	2.20	0.41
1:CA:1503:A:H2'	1:CA:1504:A:H8	1.85	0.41
1:CA:1753:G:H5''	16:CQ:93:ARG:HD3	2.03	0.40
1:CA:2316:G:H2'	1:CA:2317:A:C8	2.55	0.40
1:CA:2515:C:H2'	1:CA:2516:A:H8	1.86	0.40
1:CA:2836:U:H2'	1:CA:2837:A:C8	2.56	0.40
8:CH:129:GLU:OE2	8:CH:143:ILE:HG12	2.21	0.40
1:CA:347:A:H2'	1:CA:348:A:C8	2.57	0.40
1:CA:514:A:N3	1:CA:581:C:O2'	2.51	0.40
1:CA:1939:5MU:OP1	1:CA:2604:U:O2'	2.37	0.40
6:CF:64:LYS:HD2	6:CF:64:LYS:H	1.86	0.40
25:CZ:49:ASP:OD1	25:CZ:52:ARG:NH2	2.53	0.40
27:C1:38:HIS:HB3	27:C1:44:THR:HG22	2.02	0.40
1:CA:742:A:H2'	1:CA:743:A:C8	2.56	0.40
1:CA:924:G:H2'	1:CA:925:A:C8	2.57	0.40
1:CA:2096:C:H2'	1:CA:2097:A:C8	2.56	0.40
6:CF:148:ARG:HB2	6:CF:150:ARG:HG3	2.03	0.40
6:CF:170:LEU:HA	6:CF:173:PHE:HD2	1.87	0.40
14:CO:28:LEU:HD13	14:CO:34:ILE:HG12	2.03	0.40
17:CR:98:ILE:HG22	17:CR:106:PHE:HB2	2.02	0.40
1:CA:1802:A:H2'	1:CA:1803:A:C8	2.56	0.40
1:CA:2128:G:H1'	1:CA:2174:C:H5'	2.03	0.40
17:CR:58:ARG:HH21	17:CR:92:ARG:NH1	2.19	0.40
26:C0:3:LYS:HD2	26:C0:3:LYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1818:U:O2'	3:CC:153:GLN:O	2.35	0.40
5:CE:112:LEU:HD11	5:CE:180:LEU:HB3	2.03	0.40
13:CN:50:ARG:HG3	13:CN:65:ILE:HD11	2.03	0.40
26:C0:28:GLY:HA3	26:C0:38:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CC	269/271 (99%)	254 (94%)	15 (6%)	0	100	100
4	CD	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	51
5	CE	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
6	CF	175/177 (99%)	155 (89%)	17 (10%)	3 (2%)	7	23
7	CG	174/176 (99%)	155 (89%)	18 (10%)	1 (1%)	21	48
8	CH	147/149 (99%)	134 (91%)	13 (9%)	0	100	100
9	CJ	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
10	CK	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	CL	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
12	CM	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
13	CN	133/136 (98%)	127 (96%)	4 (3%)	2 (2%)	8	26
14	CO	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
15	CP	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
16	CQ	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
17	CR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
18	CS	101/103 (98%)	93 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CT	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	14	38
20	CU	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
21	CV	100/102 (98%)	80 (80%)	18 (18%)	2 (2%)	6	20
22	CW	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
23	CX	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
24	CY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
25	CZ	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
26	C0	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
27	C1	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	6	21
28	C2	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
29	C3	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
30	C4	62/64 (97%)	56 (90%)	4 (6%)	2 (3%)	3	11
31	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	14
32	A	13/22 (59%)	11 (85%)	2 (15%)	0	100	100
All	All	3309/3378 (98%)	3087 (93%)	208 (6%)	14 (0%)	31	56

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	CG	47	ASP
13	CN	58	LYS
21	CV	89	ASP
30	C4	32	ILE
30	C4	33	LEU
31	C5	20	ASP
4	CD	152	PRO
6	CF	176	PRO
27	C1	55	ILE
13	CN	69	PRO
21	CV	99	ASN
6	CF	175	PHE
19	CT	63	GLY
6	CF	123	ASP

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	
3	CC	216/216 (100%)	212 (98%)	4 (2%)	50	77
4	CD	163/163 (100%)	161 (99%)	2 (1%)	63	84
5	CE	165/165 (100%)	163 (99%)	2 (1%)	63	84
6	CF	148/148 (100%)	148 (100%)	0	100	100
7	CG	137/137 (100%)	136 (99%)	1 (1%)	76	90
8	CH	114/114 (100%)	113 (99%)	1 (1%)	70	88
9	CJ	104/104 (100%)	104 (100%)	0	100	100
10	CK	116/116 (100%)	116 (100%)	0	100	100
11	CL	103/103 (100%)	102 (99%)	1 (1%)	68	87
12	CM	103/103 (100%)	103 (100%)	0	100	100
13	CN	108/108 (100%)	108 (100%)	0	100	100
14	CO	100/100 (100%)	99 (99%)	1 (1%)	68	87
15	CP	86/86 (100%)	85 (99%)	1 (1%)	63	84
16	CQ	99/99 (100%)	99 (100%)	0	100	100
17	CR	89/89 (100%)	89 (100%)	0	100	100
18	CS	84/84 (100%)	84 (100%)	0	100	100
19	CT	93/93 (100%)	93 (100%)	0	100	100
20	CU	80/80 (100%)	79 (99%)	1 (1%)	61	84
21	CV	83/83 (100%)	83 (100%)	0	100	100
22	CW	78/78 (100%)	77 (99%)	1 (1%)	61	84
23	CX	56/57 (98%)	56 (100%)	0	100	100
24	CY	67/67 (100%)	67 (100%)	0	100	100
25	CZ	54/54 (100%)	54 (100%)	0	100	100
26	C0	48/48 (100%)	48 (100%)	0	100	100
27	C1	47/47 (100%)	46 (98%)	1 (2%)	47	75
28	C2	45/45 (100%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	C3	38/38 (100%)	38 (100%)	0	100	100
30	C4	51/51 (100%)	50 (98%)	1 (2%)	48	76
31	C5	34/34 (100%)	33 (97%)	1 (3%)	37	68
32	A	9/9 (100%)	7 (78%)	2 (22%)	1	2
All	All	2718/2719 (100%)	2698 (99%)	20 (1%)	73	90

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CC	141	VAL
3	CC	195	VAL
3	CC	204	VAL
3	CC	252	THR
4	CD	33	ARG
4	CD	202	ILE
5	CE	139	LYS
5	CE	149	ILE
7	CG	10	VAL
8	CH	12	LEU
11	CL	99	ILE
14	CO	70	THR
15	CP	47	VAL
20	CU	74	ILE
22	CW	40	ILE
27	C1	25	VAL
30	C4	32	ILE
31	C5	3	VAL
32	A	2	THR
32	A	17	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	CC	25	HIS
3	CC	86	ASN
3	CC	117	GLN
3	CC	153	GLN
3	CC	197	ASN
3	CC	200	HIS
4	CD	49	GLN

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Mol	Chain	Res	Type
5	CE	97	ASN
5	CE	115	GLN
6	CF	5	HIS
6	CF	52	ASN
7	CG	30	ASN
7	CG	88	GLN
8	CH	20	ASN
8	CH	135	HIS
8	CH	145	ASN
10	CK	80	HIS
11	CL	93	GLN
12	CM	99	ASN
12	CM	104	GLN
14	CO	3	HIS
14	CO	31	HIS
17	CR	37	GLN
17	CR	81	ASN
18	CS	82	HIS
19	CT	9	HIS
19	CT	61	ASN
20	CU	28	ASN
20	CU	70	HIS
24	CY	16	ASN
24	CY	17	ASN
24	CY	36	HIS
25	CZ	25	GLN
25	CZ	58	ASN
27	C1	6	ASN
27	C1	42	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	2896/2904 (99%)	518 (17%)	12 (0%)
2	CB	117/118 (99%)	18 (15%)	0
All	All	3013/3022 (99%)	536 (17%)	12 (0%)

All (536) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	CA	10	A

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Mol	Chain	Res	Type
1	CA	15	G
1	CA	23	G
1	CA	34	U
1	CA	35	G
1	CA	43	G
1	CA	46	G
1	CA	49	A
1	CA	51	G
1	CA	58	G
1	CA	63	A
1	CA	71	A
1	CA	72	U
1	CA	74	A
1	CA	75	G
1	CA	83	A
1	CA	84	A
1	CA	91	A
1	CA	100	U
1	CA	101	A
1	CA	102	U
1	CA	103	A
1	CA	118	A
1	CA	119	A
1	CA	120	U
1	CA	125	A
1	CA	138	U
1	CA	139	U
1	CA	141	G
1	CA	142	A
1	CA	162	U
1	CA	165	A
1	CA	181	A
1	CA	196	A
1	CA	199	A
1	CA	215	G
1	CA	216	A
1	CA	222	A
1	CA	226	A
1	CA	233	A
1	CA	239	C
1	CA	248	G
1	CA	264	C

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Mol	Chain	Res	Type
1	CA	265	A
1	CA	266	G
1	CA	272	A
1	CA	275	C
1	CA	276	U
1	CA	280	U
1	CA	282	A
1	CA	283	G
1	CA	287	G
1	CA	294	A
1	CA	299	A
1	CA	302	C
1	CA	305	C
1	CA	308	G
1	CA	311	A
1	CA	317	G
1	CA	329	G
1	CA	330	A
1	CA	333	G
1	CA	335	C
1	CA	336	C
1	CA	344	A
1	CA	352	A
1	CA	353	C
1	CA	354	A
1	CA	362	A
1	CA	367	G
1	CA	370	G
1	CA	371	A
1	CA	372	G
1	CA	383	C
1	CA	386	G
1	CA	396	G
1	CA	399	U
1	CA	405	U
1	CA	411	G
1	CA	412	A
1	CA	424	G
1	CA	426	C
1	CA	457	A
1	CA	467	G
1	CA	475	C

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Mol	Chain	Res	Type
1	CA	481	G
1	CA	490	C
1	CA	491	G
1	CA	501	A
1	CA	504	A
1	CA	505	A
1	CA	508	A
1	CA	509	C
1	CA	513	A
1	CA	529	A
1	CA	530	G
1	CA	532	A
1	CA	544	C
1	CA	546	U
1	CA	547	A
1	CA	548	G
1	CA	563	A
1	CA	573	U
1	CA	575	A
1	CA	586	A
1	CA	603	A
1	CA	613	A
1	CA	614	A
1	CA	615	U
1	CA	621	A
1	CA	627	A
1	CA	634	C
1	CA	637	A
1	CA	645	C
1	CA	647	G
1	CA	648	G
1	CA	654	A
1	CA	655	A
1	CA	668	A
1	CA	677	A
1	CA	686	U
1	CA	710	U
1	CA	717	C
1	CA	718	A
1	CA	721	A
1	CA	726	G
1	CA	730	A

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Mol	Chain	Res	Type
1	CA	738	G
1	CA	747	5MU
1	CA	748	G
1	CA	762	U
1	CA	764	A
1	CA	770	G
1	CA	775	G
1	CA	776	G
1	CA	782	A
1	CA	783	A
1	CA	784	G
1	CA	785	G
1	CA	788	A
1	CA	789	A
1	CA	791	C
1	CA	792	A
1	CA	800	A
1	CA	805	G
1	CA	811	U
1	CA	812	C
1	CA	819	A
1	CA	827	U
1	CA	828	U
1	CA	845	A
1	CA	846	U
1	CA	847	U
1	CA	856	G
1	CA	858	G
1	CA	859	G
1	CA	878	A
1	CA	880	G
1	CA	896	A
1	CA	907	G
1	CA	910	A
1	CA	914	G
1	CA	915	C
1	CA	931	U
1	CA	934	U
1	CA	941	A
1	CA	945	A
1	CA	946	C
1	CA	961	C

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Mol	Chain	Res	Type
1	CA	974	G
1	CA	982	C
1	CA	983	A
1	CA	989	G
1	CA	995	C
1	CA	996	A
1	CA	1005	C
1	CA	1009	A
1	CA	1012	U
1	CA	1013	C
1	CA	1026	G
1	CA	1033	U
1	CA	1045	C
1	CA	1046	A
1	CA	1047	G
1	CA	1048	A
1	CA	1051	G
1	CA	1055	G
1	CA	1057	A
1	CA	1060	U
1	CA	1064	C
1	CA	1067	A
1	CA	1068	G
1	CA	1070	A
1	CA	1071	G
1	CA	1075	C
1	CA	1076	C
1	CA	1079	C
1	CA	1084	A
1	CA	1088	A
1	CA	1105	U
1	CA	1111	A
1	CA	1112	G
1	CA	1116	G
1	CA	1119	U
1	CA	1126	A
1	CA	1130	U
1	CA	1132	U
1	CA	1133	A
1	CA	1135	C
1	CA	1136	G
1	CA	1142	A

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Mol	Chain	Res	Type
1	CA	1151	A
1	CA	1156	A
1	CA	1172	C
1	CA	1173	U
1	CA	1174	U
1	CA	1175	A
1	CA	1176	U
1	CA	1179	G
1	CA	1180	U
1	CA	1186	G
1	CA	1206	G
1	CA	1212	G
1	CA	1236	G
1	CA	1238	G
1	CA	1250	G
1	CA	1253	A
1	CA	1256	G
1	CA	1262	A
1	CA	1266	G
1	CA	1268	A
1	CA	1271	G
1	CA	1272	A
1	CA	1275	A
1	CA	1293	C
1	CA	1300	G
1	CA	1301	A
1	CA	1321	A
1	CA	1329	U
1	CA	1352	U
1	CA	1359	A
1	CA	1365	A
1	CA	1368	G
1	CA	1378	A
1	CA	1379	U
1	CA	1383	A
1	CA	1395	A
1	CA	1403	A
1	CA	1413	A
1	CA	1416	G
1	CA	1417	C
1	CA	1419	A
1	CA	1420	A

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Mol	Chain	Res	Type
1	CA	1428	C
1	CA	1437	C
1	CA	1451	C
1	CA	1452	G
1	CA	1453	A
1	CA	1458	U
1	CA	1478	G
1	CA	1482	G
1	CA	1490	A
1	CA	1493	C
1	CA	1509	A
1	CA	1510	G
1	CA	1515	A
1	CA	1522	A
1	CA	1532	A
1	CA	1534	U
1	CA	1535	A
1	CA	1536	C
1	CA	1537	G
1	CA	1540	G
1	CA	1558	C
1	CA	1560	G
1	CA	1566	A
1	CA	1569	A
1	CA	1578	U
1	CA	1584	U
1	CA	1585	C
1	CA	1587	G
1	CA	1607	C
1	CA	1608	A
1	CA	1610	A
1	CA	1611	C
1	CA	1634	A
1	CA	1647	U
1	CA	1648	U
1	CA	1649	G
1	CA	1674	G
1	CA	1675	C
1	CA	1715	G
1	CA	1722	A
1	CA	1723	G
1	CA	1729	U

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Mol	Chain	Res	Type
1	CA	1730	C
1	CA	1731	G
1	CA	1732	C
1	CA	1733	G
1	CA	1735	A
1	CA	1738	G
1	CA	1756	G
1	CA	1757	A
1	CA	1758	U
1	CA	1764	C
1	CA	1773	A
1	CA	1782	U
1	CA	1786	A
1	CA	1791	A
1	CA	1799	G
1	CA	1800	C
1	CA	1808	A
1	CA	1811	G
1	CA	1815	A
1	CA	1816	C
1	CA	1829	A
1	CA	1870	C
1	CA	1871	A
1	CA	1872	A
1	CA	1873	G
1	CA	1875	G
1	CA	1896	G
1	CA	1906	G
1	CA	1914	C
1	CA	1915	3TD
1	CA	1920	C
1	CA	1929	G
1	CA	1930	G
1	CA	1937	A
1	CA	1938	A
1	CA	1955	U
1	CA	1964	G
1	CA	1966	A
1	CA	1967	C
1	CA	1970	A
1	CA	1971	U
1	CA	1972	G

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Mol	Chain	Res	Type
1	CA	1982	U
1	CA	1991	U
1	CA	1993	U
1	CA	1997	C
1	CA	2020	A
1	CA	2022	U
1	CA	2023	C
1	CA	2031	A
1	CA	2033	A
1	CA	2036	C
1	CA	2043	C
1	CA	2055	C
1	CA	2056	G
1	CA	2060	A
1	CA	2061	G
1	CA	2062	A
1	CA	2069	G7M
1	CA	2072	C
1	CA	2080	A
1	CA	2093	G
1	CA	2095	A
1	CA	2101	A
1	CA	2103	C
1	CA	2104	C
1	CA	2107	G
1	CA	2111	U
1	CA	2112	G
1	CA	2113	U
1	CA	2115	G
1	CA	2116	G
1	CA	2117	A
1	CA	2118	U
1	CA	2119	A
1	CA	2121	G
1	CA	2124	G
1	CA	2125	G
1	CA	2126	A
1	CA	2127	G
1	CA	2128	G
1	CA	2131	U
1	CA	2132	U
1	CA	2133	G

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Mol	Chain	Res	Type
1	CA	2136	G
1	CA	2147	A
1	CA	2155	U
1	CA	2157	G
1	CA	2158	A
1	CA	2164	C
1	CA	2165	C
1	CA	2166	U
1	CA	2168	G
1	CA	2169	A
1	CA	2171	A
1	CA	2172	U
1	CA	2173	A
1	CA	2178	C
1	CA	2183	A
1	CA	2186	G
1	CA	2187	U
1	CA	2189	U
1	CA	2190	G
1	CA	2198	A
1	CA	2203	U
1	CA	2204	G
1	CA	2211	A
1	CA	2212	A
1	CA	2223	G
1	CA	2225	A
1	CA	2226	C
1	CA	2238	G
1	CA	2239	G
1	CA	2243	U
1	CA	2259	U
1	CA	2266	A
1	CA	2278	A
1	CA	2280	G
1	CA	2283	C
1	CA	2287	A
1	CA	2288	A
1	CA	2294	G
1	CA	2305	U
1	CA	2311	A
1	CA	2312	U
1	CA	2322	A

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Mol	Chain	Res	Type
1	CA	2325	G
1	CA	2326	C
1	CA	2327	A
1	CA	2333	A
1	CA	2334	U
1	CA	2335	A
1	CA	2345	G
1	CA	2347	C
1	CA	2350	C
1	CA	2354	C
1	CA	2357	G
1	CA	2361	G
1	CA	2383	G
1	CA	2385	C
1	CA	2396	G
1	CA	2402	U
1	CA	2406	A
1	CA	2423	U
1	CA	2424	C
1	CA	2425	A
1	CA	2426	A
1	CA	2429	G
1	CA	2430	A
1	CA	2435	A
1	CA	2441	U
1	CA	2445	2MG
1	CA	2448	A
1	CA	2449	H2U
1	CA	2470	G
1	CA	2475	C
1	CA	2476	A
1	CA	2478	A
1	CA	2491	U
1	CA	2498	OMC
1	CA	2502	G
1	CA	2505	G
1	CA	2518	A
1	CA	2554	U
1	CA	2562	U
1	CA	2566	A
1	CA	2567	G
1	CA	2573	C

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Mol	Chain	Res	Type
1	CA	2582	G
1	CA	2585	U
1	CA	2586	U
1	CA	2592	G
1	CA	2603	G
1	CA	2609	U
1	CA	2613	U
1	CA	2615	U
1	CA	2629	U
1	CA	2646	C
1	CA	2654	A
1	CA	2663	G
1	CA	2681	C
1	CA	2689	U
1	CA	2690	U
1	CA	2714	G
1	CA	2716	C
1	CA	2718	G
1	CA	2726	A
1	CA	2732	G
1	CA	2733	A
1	CA	2739	U
1	CA	2744	G
1	CA	2748	A
1	CA	2749	A
1	CA	2750	A
1	CA	2764	A
1	CA	2778	A
1	CA	2791	G
1	CA	2792	A
1	CA	2794	C
1	CA	2798	U
1	CA	2799	A
1	CA	2801	G
1	CA	2818	U
1	CA	2820	A
1	CA	2825	G
1	CA	2833	U
1	CA	2835	A
1	CA	2836	U
1	CA	2849	U
1	CA	2850	A

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Mol	Chain	Res	Type
1	CA	2861	U
1	CA	2866	U
1	CA	2867	G
1	CA	2872	A
1	CA	2873	A
1	CA	2879	A
1	CA	2880	C
1	CA	2883	A
1	CA	2884	U
1	CA	2891	U
1	CA	2895	G
1	CA	2901	C
1	CA	2903	U
2	CB	9	G
2	CB	13	G
2	CB	16	G
2	CB	24	G
2	CB	35	C
2	CB	41	G
2	CB	44	G
2	CB	45	A
2	CB	54	G
2	CB	59	A
2	CB	64	G
2	CB	67	G
2	CB	88	C
2	CB	89	U
2	CB	90	C
2	CB	99	A
2	CB	109	A
2	CB	119	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	102	U
1	CA	335	C
1	CA	404	A
1	CA	647	G
1	CA	784	G
1	CA	1078	U
1	CA	2118	U

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Mol	Chain	Res	Type
1	CA	2146	C
1	CA	2225	A
1	CA	2326	C
1	CA	2425	A
1	CA	2680	U

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

32 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	$\# Z > 2$
13	4D4	CN	81	13	9,11,12	2.05	2 (22%)	7,13,15	0.76	0
4	MEQ	CD	150	4	8,9,10	0.69	0	5,10,12	0.80	0
1	PSU	CA	2504	1	18,21,22	1.52	4 (22%)	21,30,33	1.97	4 (19%)
1	2MG	CA	2445	1	23,26,27	1.37	3 (13%)	33,38,41	2.11	6 (18%)
32	A0G	A	9	32	3,5,6	0.65	0	1,5,7	0.97	0
1	PSU	CA	1917	1	18,21,22	1.43	3 (16%)	21,30,33	2.07	4 (19%)
1	5MU	CA	1939	1	19,22,23	1.42	5 (26%)	27,32,35	2.35	6 (22%)
1	PSU	CA	2605	1	18,21,22	1.36	4 (22%)	21,30,33	2.06	4 (19%)
32	A0G	A	21	32	3,5,6	0.58	0	1,5,7	3.44	1 (100%)
32	BB9	A	6	32	2,5,6	0.51	0	1,5,7	0.96	0
32	A0G	A	18	32	3,5,6	0.61	0	1,5,7	2.16	1 (100%)
1	PSU	CA	955	1	18,21,22	1.42	3 (16%)	21,30,33	2.13	4 (19%)
1	2MA	CA	2503	1	22,25,26	1.40	4 (18%)	32,37,40	2.43	9 (28%)
1	PSU	CA	1911	1	18,21,22	1.39	3 (16%)	21,30,33	1.99	3 (14%)
32	BB9	A	3	32	2,5,6	0.31	0	1,5,7	1.86	0
1	H2U	CA	2449	1	18,21,22	1.15	3 (16%)	19,30,33	0.86	0
1	1MG	CA	745	1	23,26,27	1.15	3 (13%)	33,39,42	1.74	6 (18%)
1	6MZ	CA	2030	1	22,25,26	1.51	5 (22%)	29,36,39	2.27	11 (37%)
1	G7M	CA	2069	1	23,26,27	1.49	4 (17%)	34,39,42	1.75	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	CA	2457	1	18,21,22	1.45	4 (22%)	21,30,33	2.12	3 (14%)
1	5MU	CA	747	1	19,22,23	1.39	4 (21%)	27,32,35	2.09	7 (25%)
1	OMU	CA	2552	1	19,22,23	1.26	3 (15%)	25,31,34	1.75	5 (20%)
1	PSU	CA	2580	1	18,21,22	1.60	5 (27%)	21,30,33	2.00	5 (23%)
32	BB9	A	12	32	2,5,6	0.34	0	1,5,7	2.28	1 (100%)
1	PSU	CA	746	1	18,21,22	1.38	4 (22%)	21,30,33	1.97	4 (19%)
1	6MZ	CA	1618	1	22,25,26	1.40	4 (18%)	29,36,39	2.14	10 (34%)
1	OMG	CA	2251	1	23,26,27	1.20	3 (13%)	32,38,41	2.04	7 (21%)
1	OMC	CA	2498	1	19,22,23	0.89	0	25,31,34	1.22	2 (8%)
1	5MC	CA	1962	1	19,22,23	1.39	3 (15%)	26,32,35	1.04	2 (7%)
32	A0G	A	15	32	3,5,6	0.57	0	1,5,7	1.49	0
1	2MG	CA	1835	1	23,26,27	1.22	3 (13%)	33,38,41	2.33	7 (21%)
1	3TD	CA	1915	1	19,22,23	1.63	4 (21%)	23,32,35	2.12	4 (17%)

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
13	4D4	CN	81	13	-	1/11/12/14	-
4	MEQ	CD	150	4	-	6/8/9/11	-
1	PSU	CA	2504	1	-	2/7/25/26	0/2/2/2
1	2MG	CA	2445	1	-	2/9/27/28	0/3/3/3
32	A0G	A	9	32	-	0/0/4/6	-
1	PSU	CA	1917	1	-	1/7/25/26	0/2/2/2
1	5MU	CA	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	CA	2605	1	-	0/7/25/26	0/2/2/2
32	A0G	A	21	32	-	0/0/4/6	-
32	BB9	A	6	32	-	0/0/4/6	-
32	A0G	A	18	32	-	0/0/4/6	-
1	PSU	CA	955	1	-	0/7/25/26	0/2/2/2
1	2MA	CA	2503	1	-	1/7/25/26	0/3/3/3
1	PSU	CA	1911	1	-	0/7/25/26	0/2/2/2
32	BB9	A	3	32	-	0/0/4/6	-
1	H2U	CA	2449	1	-	2/7/38/39	0/2/2/2
1	1MG	CA	745	1	-	0/7/25/26	0/3/3/3
1	6MZ	CA	2030	1	-	2/9/27/28	0/3/3/3
1	G7M	CA	2069	1	-	1/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	CA	2457	1	-	0/7/25/26	0/2/2/2
1	5MU	CA	747	1	-	1/7/25/26	0/2/2/2
1	OMU	CA	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	CA	2580	1	-	1/7/25/26	0/2/2/2
32	BB9	A	12	32	-	0/0/4/6	-
1	PSU	CA	746	1	-	0/7/25/26	0/2/2/2
1	6MZ	CA	1618	1	-	0/9/27/28	0/3/3/3
1	OMG	CA	2251	1	-	0/9/27/28	0/3/3/3
1	OMC	CA	2498	1	-	0/9/27/28	0/2/2/2
1	5MC	CA	1962	1	-	0/7/25/26	0/2/2/2
32	A0G	A	15	32	-	0/0/4/6	-
1	2MG	CA	1835	1	-	0/9/27/28	0/3/3/3
1	3TD	CA	1915	1	-	2/7/25/26	0/2/2/2

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1962	5MC	C5-C4	4.79	1.47	1.44
1	CA	2030	6MZ	C5-C4	4.42	1.47	1.39
1	CA	2069	G7M	C5-N7	-4.30	1.34	1.39
13	CN	81	4D4	CZ-NE	4.23	1.41	1.33
1	CA	1618	6MZ	C5-C4	4.02	1.46	1.39
1	CA	2503	2MA	C5-C4	3.70	1.45	1.39
1	CA	1917	PSU	C6-C5	3.61	1.39	1.35
1	CA	1911	PSU	C6-C5	3.53	1.39	1.35
1	CA	1915	3TD	C6-C5	3.45	1.39	1.35
1	CA	2580	PSU	C6-C5	3.40	1.39	1.35
1	CA	1915	3TD	C10-N3	3.38	1.53	1.47
1	CA	2580	PSU	C4-N3	-3.34	1.32	1.38
1	CA	2504	PSU	C6-C5	3.30	1.38	1.35
1	CA	747	5MU	C4-N3	-3.17	1.32	1.38
1	CA	2069	G7M	C5-C4	3.16	1.46	1.38
1	CA	1939	5MU	C4-N3	-3.16	1.32	1.38
1	CA	745	1MG	C5-C4	3.12	1.47	1.38
1	CA	2445	2MG	C6-N1	-3.11	1.33	1.38
1	CA	1915	3TD	C4-N3	-3.05	1.34	1.40
1	CA	1835	2MG	C5-C4	3.03	1.47	1.38
1	CA	955	PSU	C6-C5	3.02	1.38	1.35
1	CA	2445	2MG	C5-N7	-2.98	1.33	1.39
1	CA	2503	2MA	C5-N7	-2.96	1.33	1.39
1	CA	2449	H2U	C2-N3	-2.95	1.32	1.38
1	CA	2251	OMG	C5-C4	2.94	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	2552	OMU	C4-N3	-2.91	1.33	1.38
1	CA	2605	PSU	C4-N3	-2.90	1.33	1.38
1	CA	2504	PSU	C4-N3	-2.90	1.33	1.38
1	CA	2457	PSU	C6-C5	2.87	1.38	1.35
1	CA	2251	OMG	C6-N1	-2.86	1.33	1.38
1	CA	2445	2MG	C5-C4	2.85	1.46	1.38
1	CA	746	PSU	C6-C5	2.84	1.38	1.35
1	CA	2457	PSU	C4-N3	-2.82	1.33	1.38
1	CA	2069	G7M	C6-N1	-2.81	1.33	1.38
1	CA	1618	6MZ	C5-N7	-2.79	1.34	1.39
1	CA	955	PSU	C4-N3	-2.76	1.33	1.38
1	CA	2030	6MZ	C5-C6	2.75	1.48	1.41
1	CA	1939	5MU	C6-C5	2.75	1.39	1.34
13	CN	81	4D4	CZ-NH2	2.73	1.42	1.32
1	CA	747	5MU	C6-N1	-2.68	1.33	1.38
1	CA	1911	PSU	C4-N3	-2.64	1.33	1.38
1	CA	746	PSU	C4-N3	-2.62	1.33	1.38
1	CA	1835	2MG	C6-N1	-2.62	1.33	1.38
1	CA	2030	6MZ	C5-N7	-2.61	1.34	1.39
1	CA	2449	H2U	C4-N3	-2.55	1.33	1.37
1	CA	1917	PSU	C4-N3	-2.53	1.34	1.38
1	CA	1939	5MU	C2-N3	-2.53	1.33	1.38
1	CA	2605	PSU	C2-N3	-2.50	1.33	1.37
1	CA	2552	OMU	C2-N3	-2.50	1.33	1.38
1	CA	2580	PSU	C2-N3	-2.48	1.33	1.37
1	CA	2504	PSU	C2-N3	-2.44	1.33	1.37
1	CA	2457	PSU	C2-N3	-2.43	1.33	1.37
1	CA	1962	5MC	C6-C5	2.42	1.38	1.34
1	CA	1939	5MU	C6-N1	-2.40	1.33	1.38
1	CA	1962	5MC	C6-N1	-2.37	1.34	1.38
1	CA	1618	6MZ	C5-C6	2.37	1.47	1.41
1	CA	2504	PSU	C2-N1	-2.36	1.33	1.36
1	CA	746	PSU	C2-N3	-2.33	1.33	1.37
1	CA	747	5MU	C6-C5	2.33	1.38	1.34
1	CA	745	1MG	C5-N7	-2.31	1.34	1.39
1	CA	2605	PSU	C2-N1	-2.28	1.33	1.36
1	CA	747	5MU	C2-N3	-2.28	1.34	1.38
1	CA	2030	6MZ	C8-N7	2.27	1.36	1.31
1	CA	955	PSU	C2-N3	-2.26	1.33	1.37
1	CA	2030	6MZ	C4-N9	-2.25	1.33	1.37
1	CA	1915	3TD	C2-N1	-2.25	1.34	1.37
1	CA	1835	2MG	C5-N7	-2.25	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	2503	2MA	C5-C6	2.24	1.47	1.41
1	CA	2580	PSU	C2-N1	-2.23	1.33	1.36
1	CA	2503	2MA	C4-N9	-2.23	1.33	1.37
1	CA	2449	H2U	C2-N1	-2.23	1.32	1.35
1	CA	2251	OMG	C5-N7	-2.21	1.34	1.39
1	CA	2580	PSU	O4'-C1'	-2.20	1.40	1.43
1	CA	2552	OMU	C5-C4	-2.19	1.38	1.43
1	CA	2457	PSU	C2-N1	-2.18	1.33	1.36
1	CA	2069	G7M	C5-C6	2.15	1.49	1.43
1	CA	1917	PSU	C2-N1	-2.09	1.33	1.36
1	CA	2605	PSU	C6-C5	2.08	1.37	1.35
1	CA	1618	6MZ	C4-N9	-2.05	1.33	1.37
1	CA	746	PSU	C2-N1	-2.04	1.34	1.36
1	CA	745	1MG	C2-N1	2.01	1.40	1.37
1	CA	1939	5MU	C4-C5	2.01	1.48	1.44
1	CA	1911	PSU	C2-N3	-2.00	1.34	1.37

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	2503	2MA	C5-C4-N3	-8.68	118.04	127.18
1	CA	1835	2MG	C2-N3-C4	7.98	121.98	112.00
1	CA	1915	3TD	N1-C2-N3	7.95	121.91	116.13
1	CA	2503	2MA	N3-C4-N9	7.35	136.32	126.99
1	CA	1835	2MG	C5-C4-N3	-6.66	117.79	128.39
1	CA	2445	2MG	C2-N3-C4	6.63	120.29	112.00
1	CA	2457	PSU	N1-C2-N3	6.57	122.10	115.17
1	CA	2580	PSU	N1-C2-N3	6.49	122.01	115.17
1	CA	2445	2MG	C5-C4-N3	-6.46	118.11	128.39
1	CA	955	PSU	N1-C2-N3	6.37	121.89	115.17
1	CA	2251	OMG	C5-C4-N3	-6.22	118.49	128.39
1	CA	1917	PSU	N1-C2-N3	6.17	121.68	115.17
1	CA	1911	PSU	N1-C2-N3	6.09	121.59	115.17
1	CA	2605	PSU	N1-C2-N3	5.97	121.47	115.17
1	CA	1939	5MU	N3-C2-N1	5.92	122.59	114.89
1	CA	2504	PSU	N1-C2-N3	5.84	121.33	115.17
1	CA	1939	5MU	C4-N3-C2	-5.81	119.72	127.34
1	CA	746	PSU	N1-C2-N3	5.73	121.22	115.17
1	CA	1618	6MZ	C5-C4-N3	-5.54	119.09	126.72
1	CA	745	1MG	C5-C4-N3	-5.38	119.83	128.39
1	CA	2069	G7M	C5-C4-N3	-5.27	118.19	128.15
1	CA	2251	OMG	C2-N3-C4	5.19	121.24	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	747	5MU	N3-C2-N1	5.13	121.56	114.89
1	CA	2069	G7M	C2-N3-C4	5.10	121.09	112.30
1	CA	2069	G7M	N9-C4-N3	5.04	136.03	125.95
1	CA	747	5MU	C4-N3-C2	-5.03	120.74	127.34
1	CA	2030	6MZ	C5-C4-N3	-4.89	119.98	126.72
1	CA	2251	OMG	N9-C4-N3	4.87	135.70	125.95
1	CA	2445	2MG	N9-C4-N3	4.84	135.64	125.95
1	CA	2030	6MZ	C6-C5-N7	4.80	137.66	132.43
1	CA	1618	6MZ	N3-C4-N9	4.71	135.17	127.17
1	CA	1835	2MG	N9-C4-N3	4.63	135.22	125.95
1	CA	1939	5MU	C5-C4-N3	4.61	119.33	115.32
1	CA	2552	OMU	C4-N3-C2	-4.55	120.97	126.61
1	CA	1939	5MU	C5-C6-N1	-4.53	118.39	123.31
1	CA	2552	OMU	N3-C2-N1	4.49	120.73	114.89
1	CA	2605	PSU	C4-N3-C2	-4.45	120.24	126.37
1	CA	2030	6MZ	C9-N6-C6	-4.42	118.75	122.85
1	CA	955	PSU	C4-N3-C2	-4.42	120.28	126.37
1	CA	745	1MG	C2-N3-C4	4.35	121.75	111.98
1	CA	2030	6MZ	C4-C5-N7	-4.28	105.69	110.58
1	CA	2457	PSU	C4-N3-C2	-4.26	120.51	126.37
1	CA	1939	5MU	O4-C4-C5	-4.11	120.22	124.92
1	CA	746	PSU	C4-N3-C2	-4.10	120.73	126.37
1	CA	1917	PSU	O2-C2-N1	-4.06	118.60	122.79
1	CA	745	1MG	N9-C4-N3	4.03	134.01	125.95
1	CA	747	5MU	C5-C4-N3	3.99	118.79	115.32
1	CA	1911	PSU	C4-N3-C2	-3.99	120.88	126.37
1	CA	1917	PSU	C4-N3-C2	-3.95	120.93	126.37
1	CA	955	PSU	O2-C2-N1	-3.93	118.73	122.79
1	CA	2504	PSU	C4-N3-C2	-3.91	120.99	126.37
1	CA	2457	PSU	O2-C2-N1	-3.86	118.81	122.79
1	CA	1939	5MU	O2-C2-N1	-3.73	117.95	122.80
1	CA	2605	PSU	O2-C2-N1	-3.72	118.95	122.79
1	CA	2498	OMC	O2-C2-N3	-3.69	116.52	122.33
1	CA	747	5MU	O4-C4-C5	-3.67	120.72	124.92
1	CA	2552	OMU	C5-C4-N3	3.64	119.90	114.80
1	CA	1618	6MZ	C2-N3-C4	3.62	120.67	111.83
1	CA	1915	3TD	C4-N3-C2	-3.61	120.79	124.61
1	CA	747	5MU	C5-C6-N1	-3.61	119.39	123.31
1	CA	2580	PSU	C4-N3-C2	-3.48	121.58	126.37
32	A	21	A0G	O-C-CA	-3.44	121.08	125.39
1	CA	1911	PSU	O2-C2-N1	-3.39	119.29	122.79
1	CA	1618	6MZ	N1-C2-N3	-3.36	123.50	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	2251	OMG	C6-C5-N7	3.33	136.34	130.29
1	CA	2504	PSU	O2-C2-N1	-3.32	119.37	122.79
1	CA	2030	6MZ	N3-C4-N9	3.30	132.78	127.17
1	CA	1962	5MC	C5-C6-N1	-3.28	119.75	123.31
1	CA	1835	2MG	C6-C5-N7	3.28	136.26	130.29
1	CA	2030	6MZ	C2-N3-C4	3.22	119.70	111.83
1	CA	746	PSU	O2-C2-N1	-3.22	119.47	122.79
1	CA	1618	6MZ	C9-N6-C6	-3.01	120.05	122.85
1	CA	746	PSU	C6-C5-C4	-2.98	116.16	118.17
1	CA	2030	6MZ	N1-C2-N3	-2.98	124.07	128.58
1	CA	1618	6MZ	C4-C5-N7	-2.97	107.19	110.58
1	CA	1618	6MZ	C4-N9-C8	2.96	108.85	105.74
1	CA	1618	6MZ	C6-C5-N7	2.92	135.61	132.43
1	CA	745	1MG	C6-C5-N7	2.88	135.77	129.36
1	CA	2030	6MZ	C5-N7-C8	2.84	107.92	103.45
1	CA	745	1MG	C4-C5-N7	-2.79	106.25	110.67
1	CA	2504	PSU	C6-C5-C4	-2.77	116.30	118.17
1	CA	2580	PSU	O2-C2-N1	-2.77	119.93	122.79
1	CA	1835	2MG	C4-C5-N7	-2.69	106.41	110.67
1	CA	2552	OMU	O4-C4-C5	-2.68	120.53	125.16
1	CA	2503	2MA	C4-N9-C8	2.66	108.54	105.74
1	CA	2503	2MA	N6-C6-N1	2.61	120.55	117.03
1	CA	1915	3TD	C1'-C5-C4	2.58	121.52	117.61
1	CA	2445	2MG	C6-C5-N7	2.49	134.82	130.29
1	CA	2069	G7M	C5-C6-N1	2.48	116.98	111.84
1	CA	2503	2MA	N3-C2-N1	-2.47	121.41	125.77
1	CA	2251	OMG	C4-C5-N7	-2.46	106.77	110.67
1	CA	1917	PSU	C6-C5-C4	-2.46	116.52	118.17
1	CA	2445	2MG	C4-C5-N7	-2.45	106.78	110.67
1	CA	2580	PSU	O4'-C1'-C2'	2.44	108.52	105.15
1	CA	1618	6MZ	C5-N7-C8	2.42	107.26	103.45
1	CA	1835	2MG	N1-C2-N2	2.39	119.00	116.56
1	CA	2503	2MA	C4-C5-N7	-2.37	107.87	110.58
1	CA	1962	5MC	C5-C4-N3	-2.36	119.34	121.75
1	CA	2030	6MZ	C2-N1-C6	2.35	123.04	115.24
1	CA	2503	2MA	CM2-C2-N1	2.34	120.63	117.13
1	CA	2503	2MA	C2-N1-C6	2.33	121.69	118.10
1	CA	2251	OMG	O6-C6-C5	-2.28	120.50	126.53
32	A	12	BB9	O-C-CA	-2.28	122.53	125.39
1	CA	2503	2MA	C2-N3-C4	2.26	122.77	115.02
1	CA	2030	6MZ	C4-N9-C8	2.24	108.09	105.74
1	CA	955	PSU	C6-C5-C4	-2.24	116.67	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	2552	OMU	O2-C2-N1	-2.17	119.97	122.80
32	A	18	A0G	O-C-CA	-2.16	122.68	125.39
1	CA	2580	PSU	O2-C2-N3	-2.15	118.05	121.86
1	CA	2605	PSU	C5-C6-N1	-2.14	119.17	122.14
1	CA	1915	3TD	O4'-C1'-C2'	2.13	108.10	105.15
1	CA	747	5MU	O2-C2-N1	-2.12	120.04	122.80
1	CA	1618	6MZ	N9-C8-N7	-2.09	110.97	113.94
1	CA	2445	2MG	C2-N1-C6	-2.07	122.05	124.55
1	CA	1835	2MG	O6-C6-C5	-2.06	121.10	126.53
1	CA	2251	OMG	C5-C6-N1	2.05	118.48	113.25
1	CA	2069	G7M	O6-C6-C5	-2.05	123.44	128.01
1	CA	2030	6MZ	N9-C8-N7	-2.03	111.05	113.94
1	CA	745	1MG	C8-N7-C5	2.02	107.86	104.26
1	CA	747	5MU	C1'-N1-C2	2.02	121.22	117.59
1	CA	2498	OMC	O2-C2-N1	2.01	122.85	118.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	CD	150	MEQ	O-C-CA-CB
4	CD	150	MEQ	CG-CD-NE2-CE
1	CA	1915	3TD	O4'-C4'-C5'-O5'
1	CA	2445	2MG	C3'-C4'-C5'-O5'
1	CA	2449	H2U	O4'-C4'-C5'-O5'
1	CA	2504	PSU	O4'-C4'-C5'-O5'
1	CA	2445	2MG	O4'-C4'-C5'-O5'
1	CA	1915	3TD	C3'-C4'-C5'-O5'
1	CA	2030	6MZ	O4'-C4'-C5'-O5'
1	CA	2449	H2U	C3'-C4'-C5'-O5'
4	CD	150	MEQ	OE1-CD-NE2-CE
1	CA	2030	6MZ	C3'-C4'-C5'-O5'
4	CD	150	MEQ	NE2-CD-CG-CB
4	CD	150	MEQ	OE1-CD-CG-CB
1	CA	2504	PSU	C3'-C4'-C5'-O5'
4	CD	150	MEQ	N-CA-CB-CG
1	CA	1917	PSU	O4'-C1'-C5-C4
1	CA	2503	2MA	C4'-C5'-O5'-P
13	CN	81	4D4	O-C-CA-CB
1	CA	2580	PSU	O4'-C4'-C5'-O5'
1	CA	747	5MU	C4'-C5'-O5'-P
1	CA	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	CA	1939	5MU	1	0
1	CA	1915	3TD	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

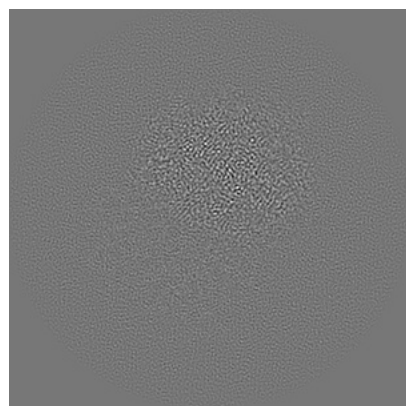
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20638. These allow visual inspection of the internal detail of the map and identification of artifacts.

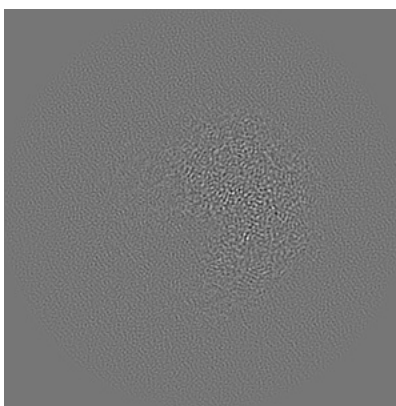
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

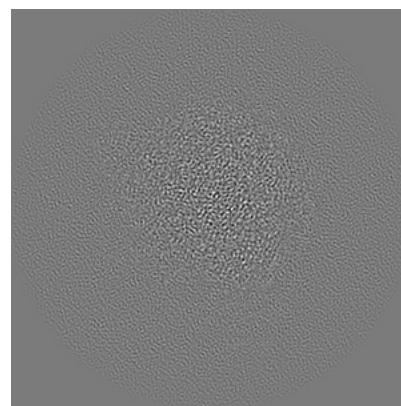
6.1.1 Primary map



X

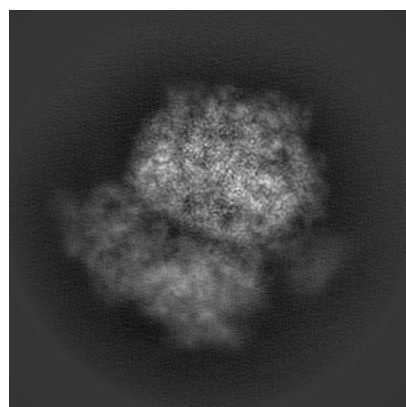


Y

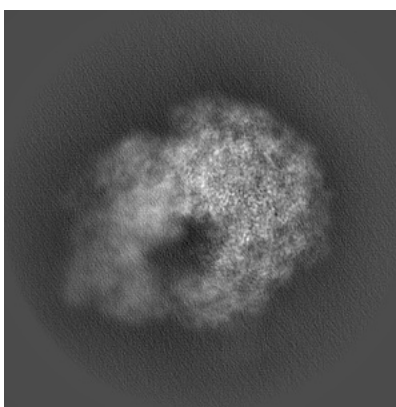


Z

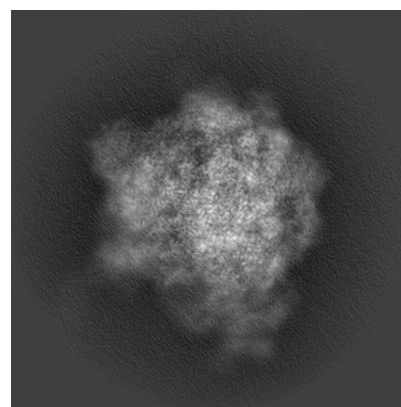
6.1.2 Raw map



X



Y

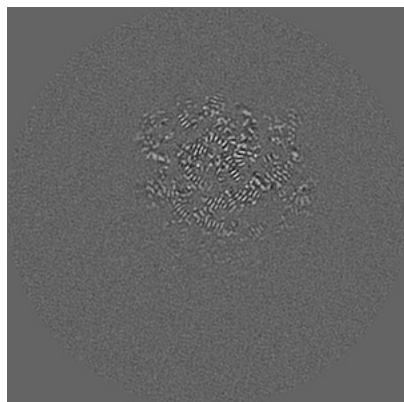


Z

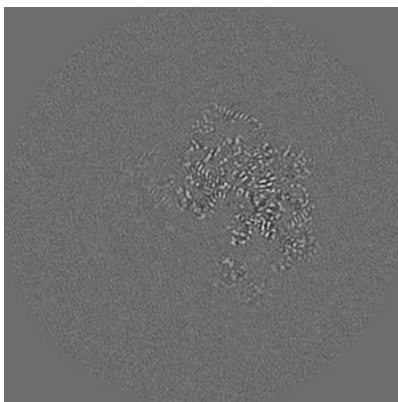
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

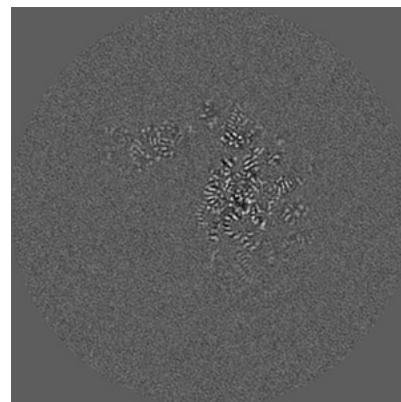
6.2.1 Primary map



X Index: 160

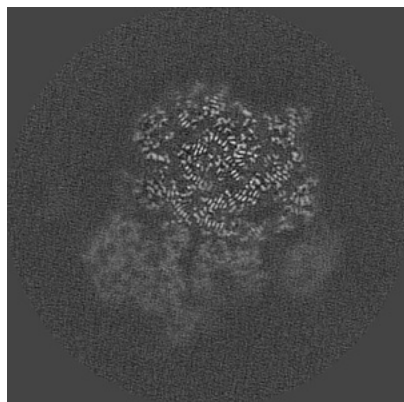


Y Index: 160

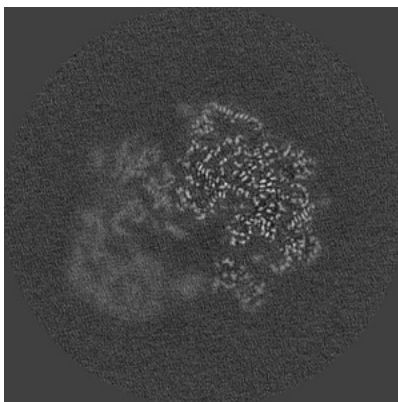


Z Index: 160

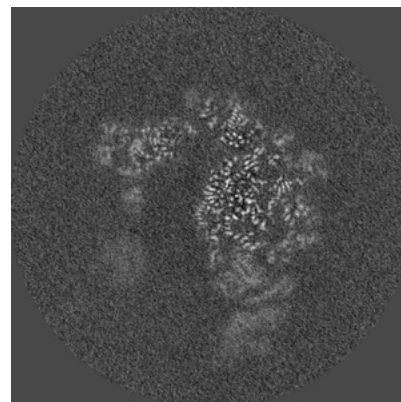
6.2.2 Raw map



X Index: 160



Y Index: 160

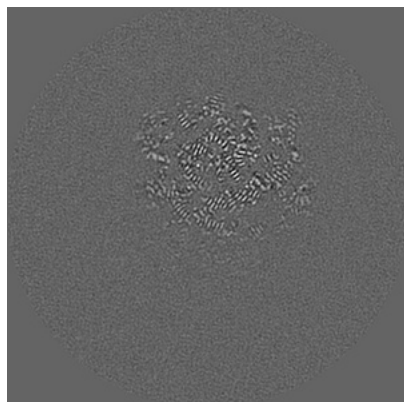


Z Index: 160

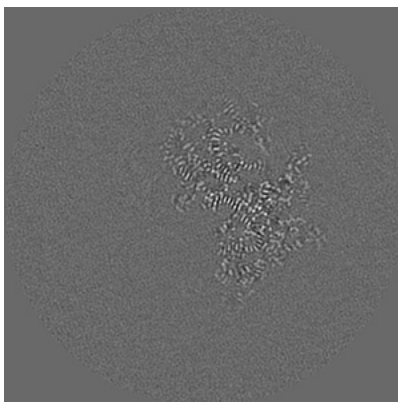
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

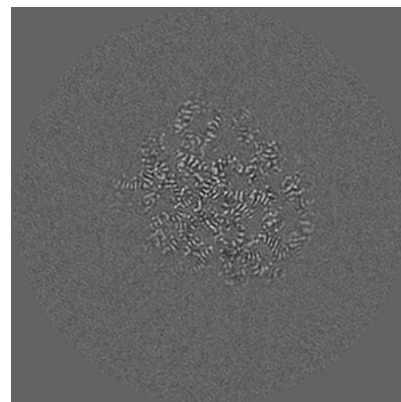
6.3.1 Primary map



X Index: 160

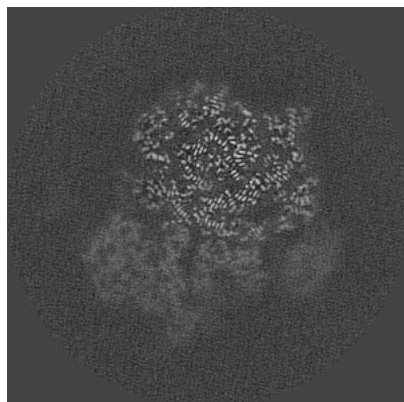


Y Index: 182

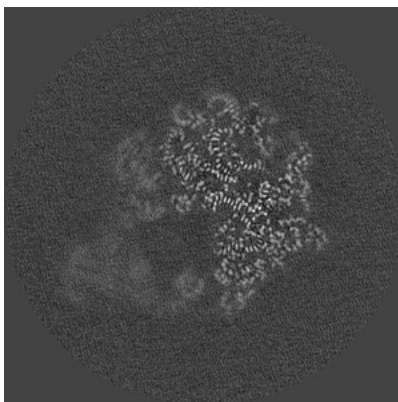


Z Index: 191

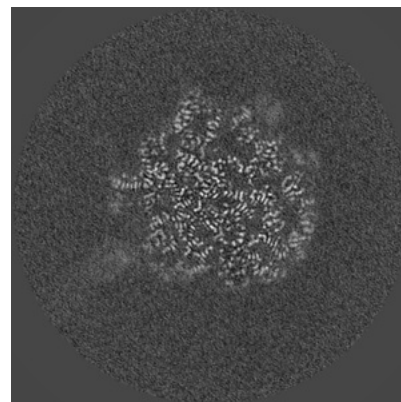
6.3.2 Raw map



X Index: 160



Y Index: 182

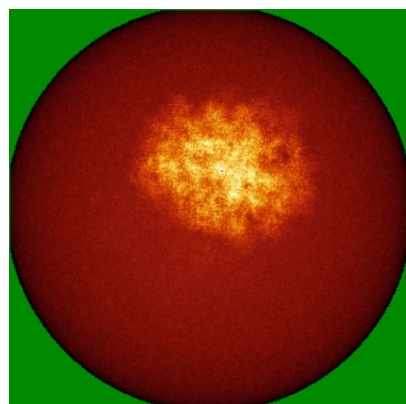


Z Index: 191

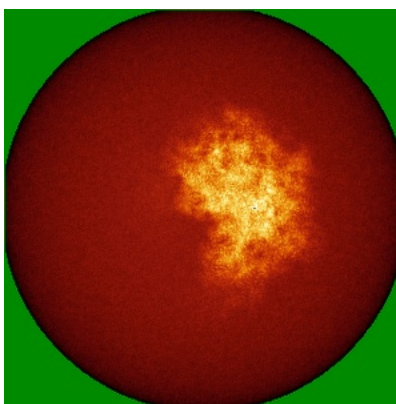
The images above show the largest variance slices of the map in three orthogonal directions.

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

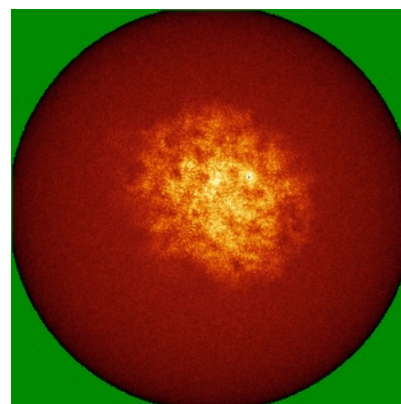
6.4.1 Primary map



X

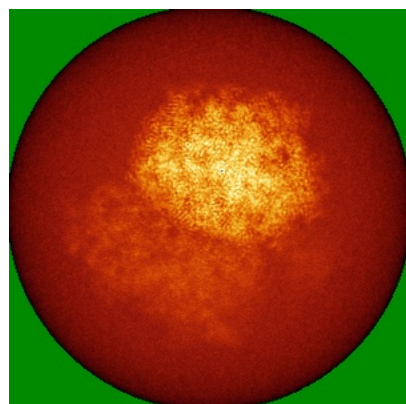


Y

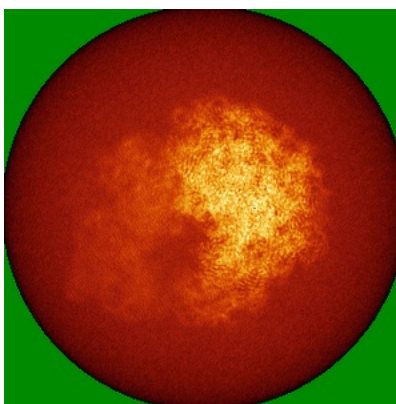


Z

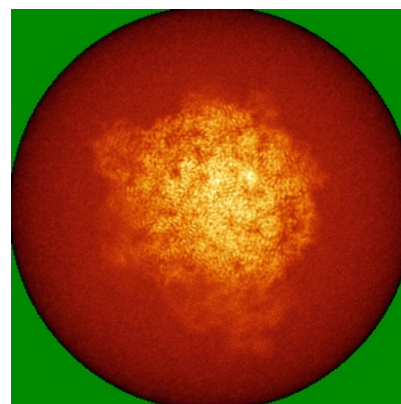
6.4.2 Raw map



X



Y

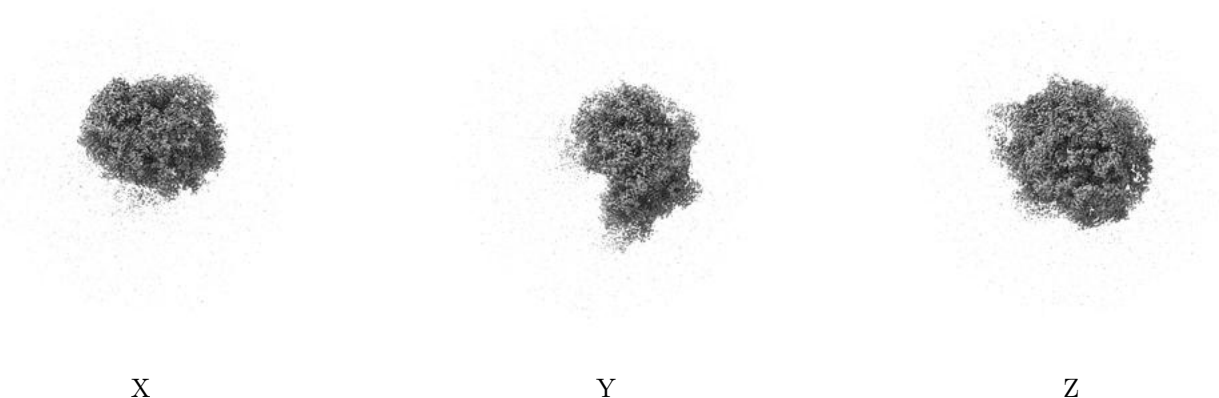


Z

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

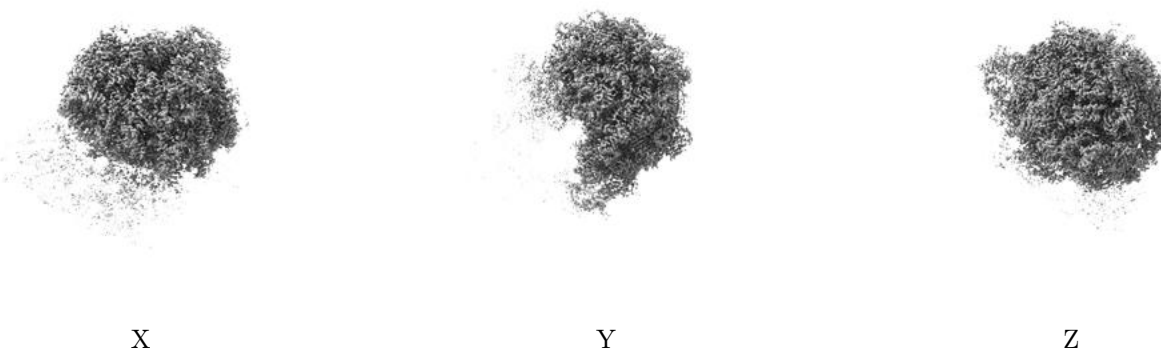
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

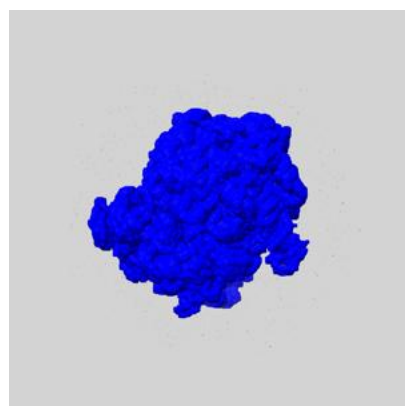
6.6 Mask visualisation [i](#)

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

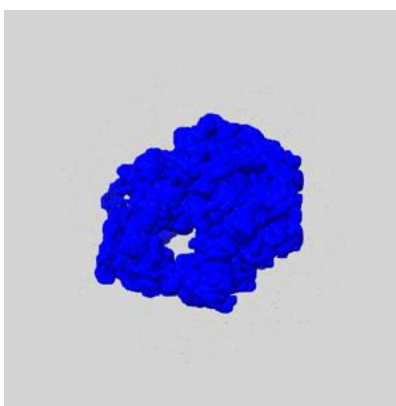
A mask typically either:

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

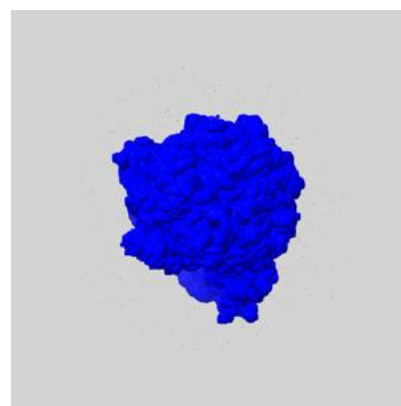
6.6.1 emd_20638_msk_1.map [i](#)



X



Y

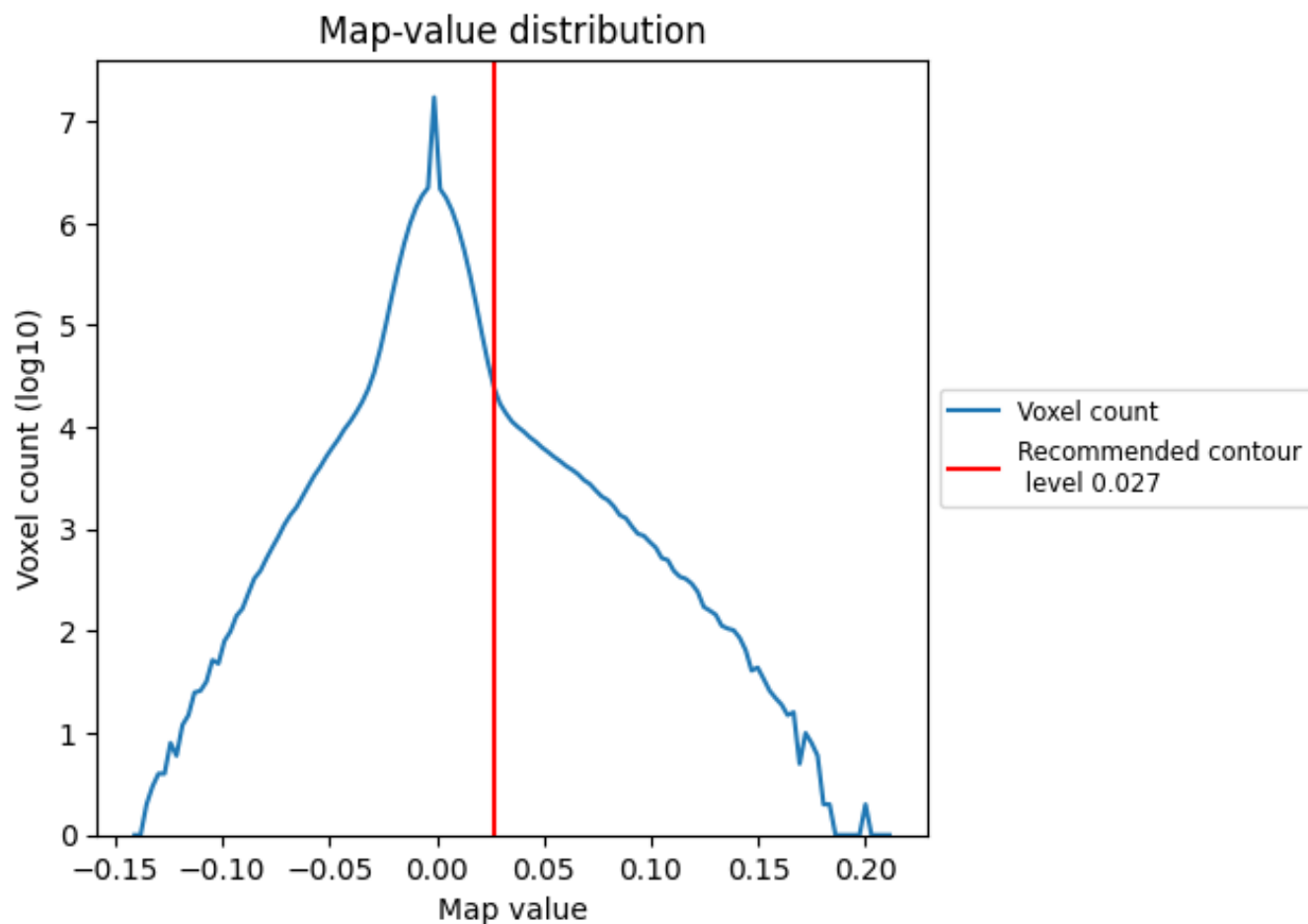


Z

7 Map analysis [i](#)

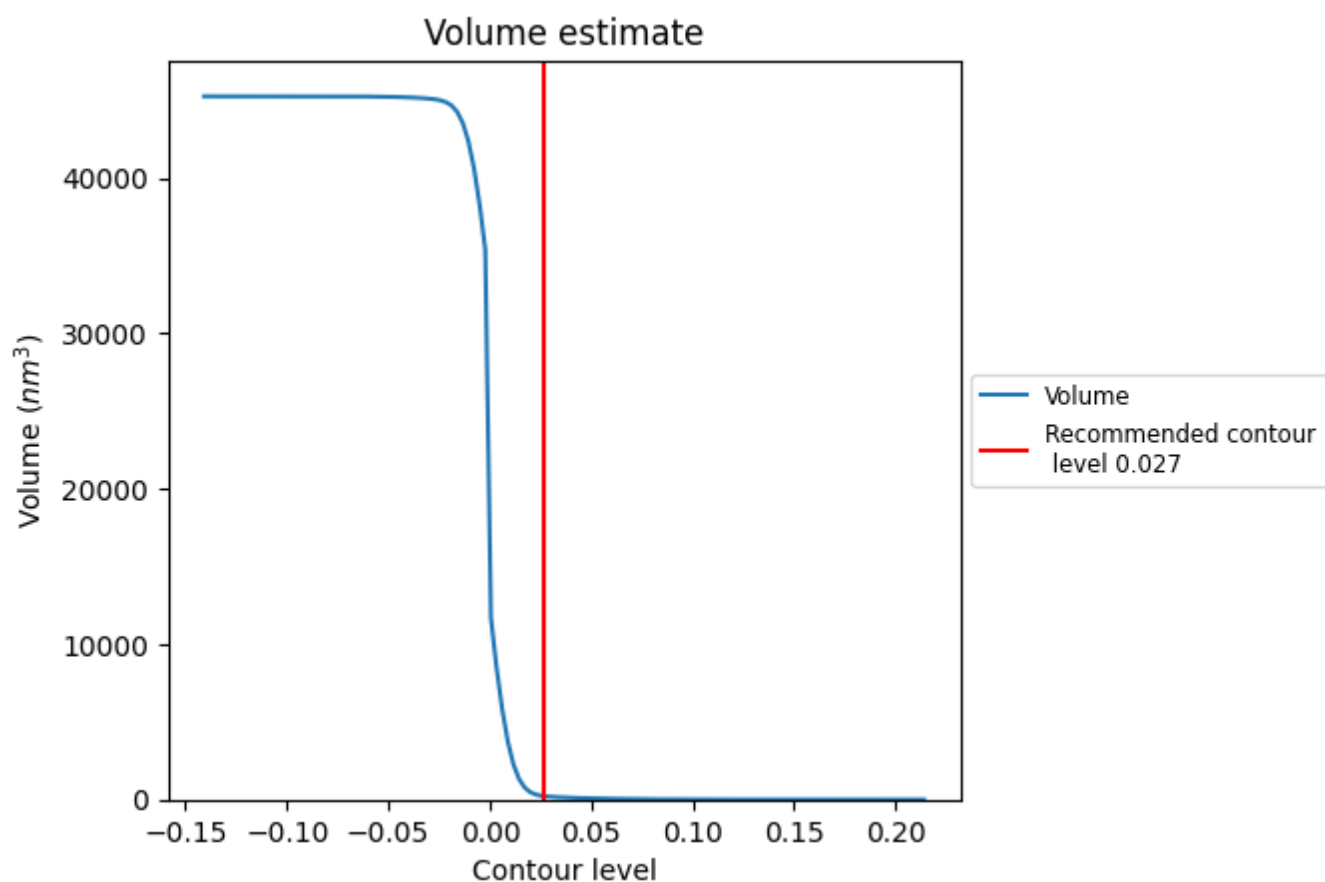
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

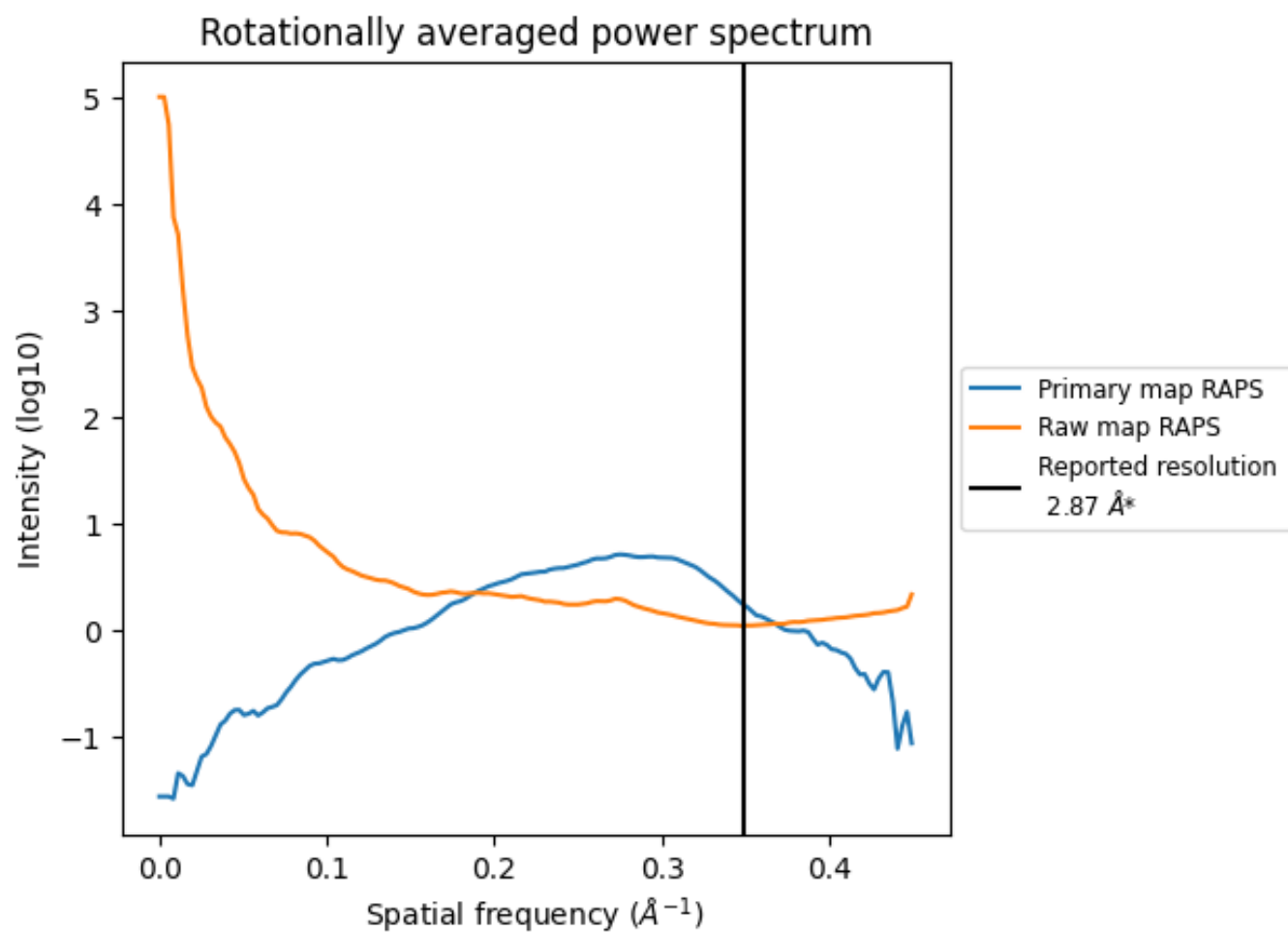
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm^3 ; this corresponds to an approximate mass of 198 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 ⓘ

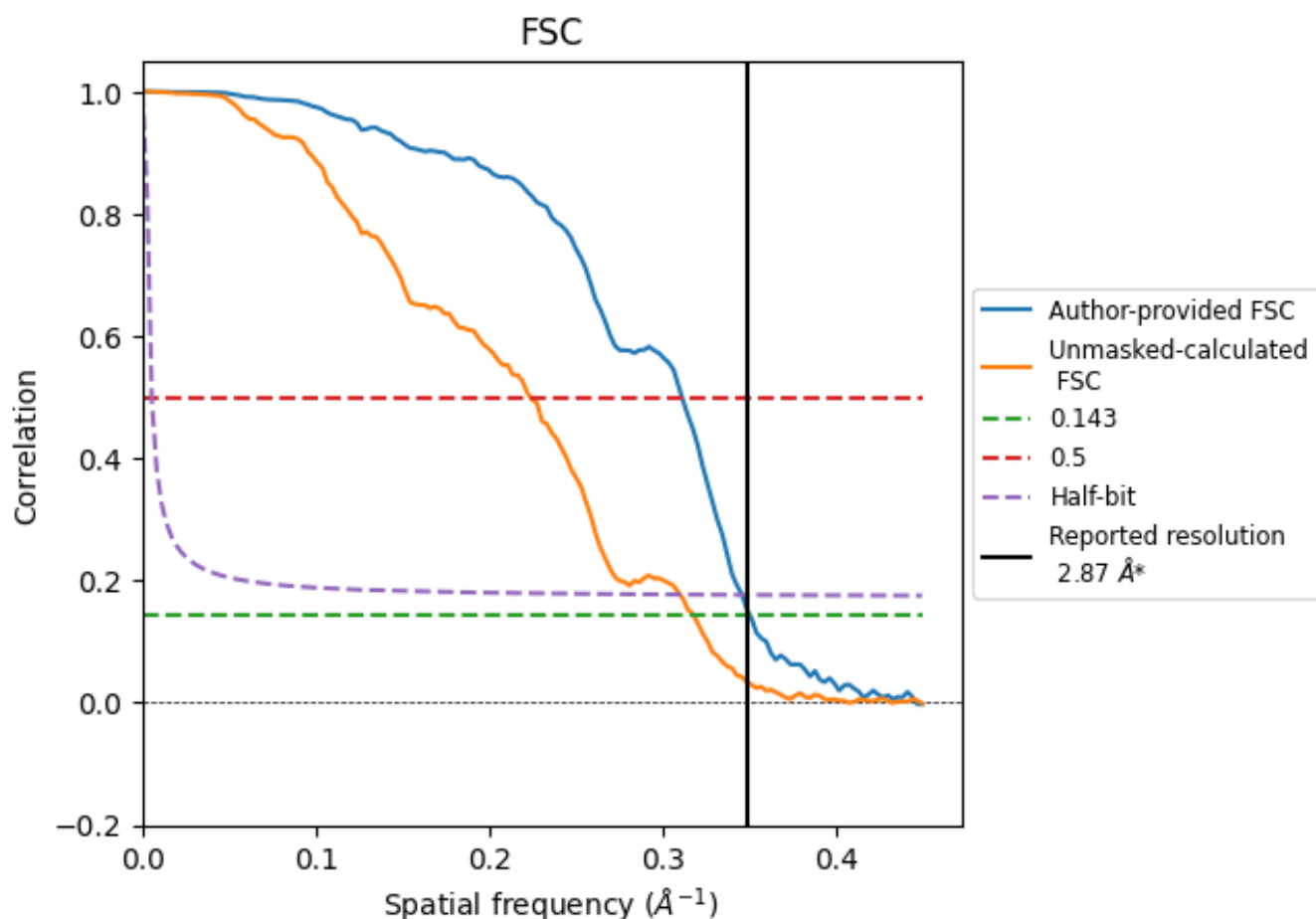


*Reported resolution corresponds to spatial frequency of 0.348 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.348 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

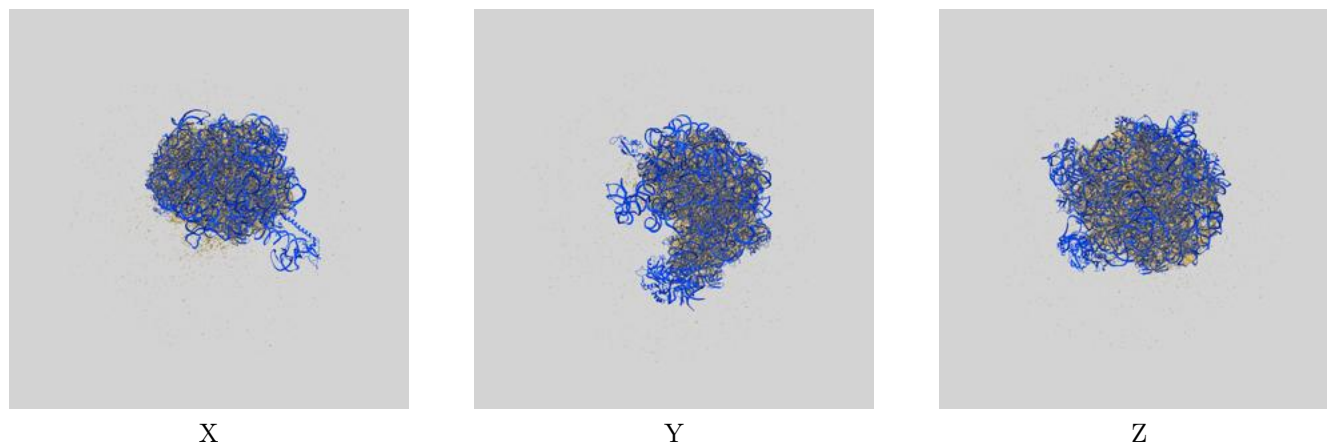
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.86	3.22	2.90
Unmasked-calculated*	3.15	4.47	3.23

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

9 Map-model fit [i](#)

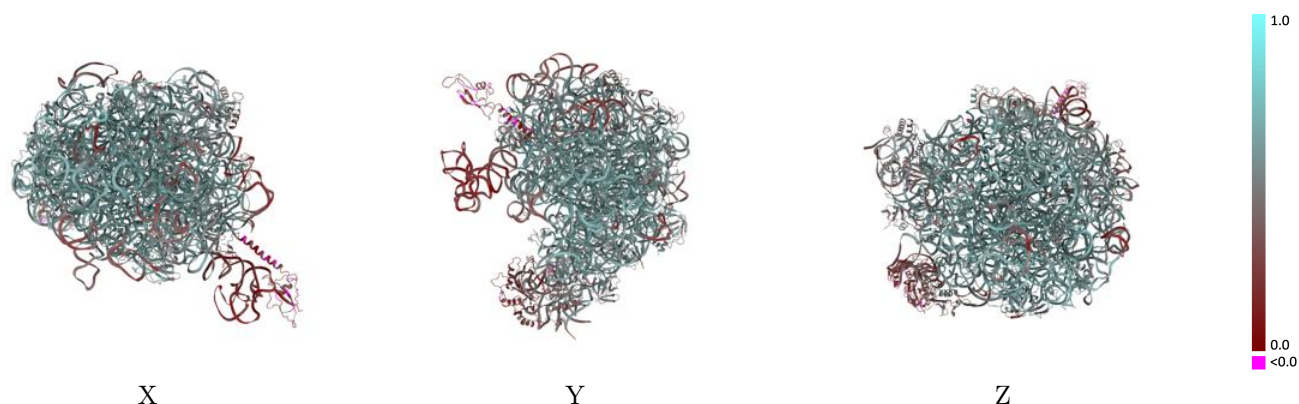
This section contains information regarding the fit between EMDB map EMD-20638 and PDB model 6U48. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



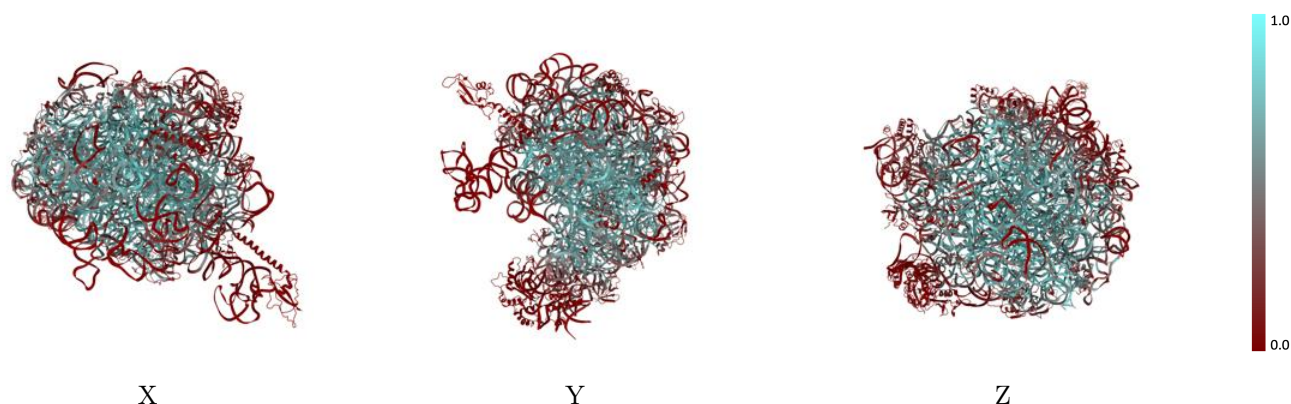
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



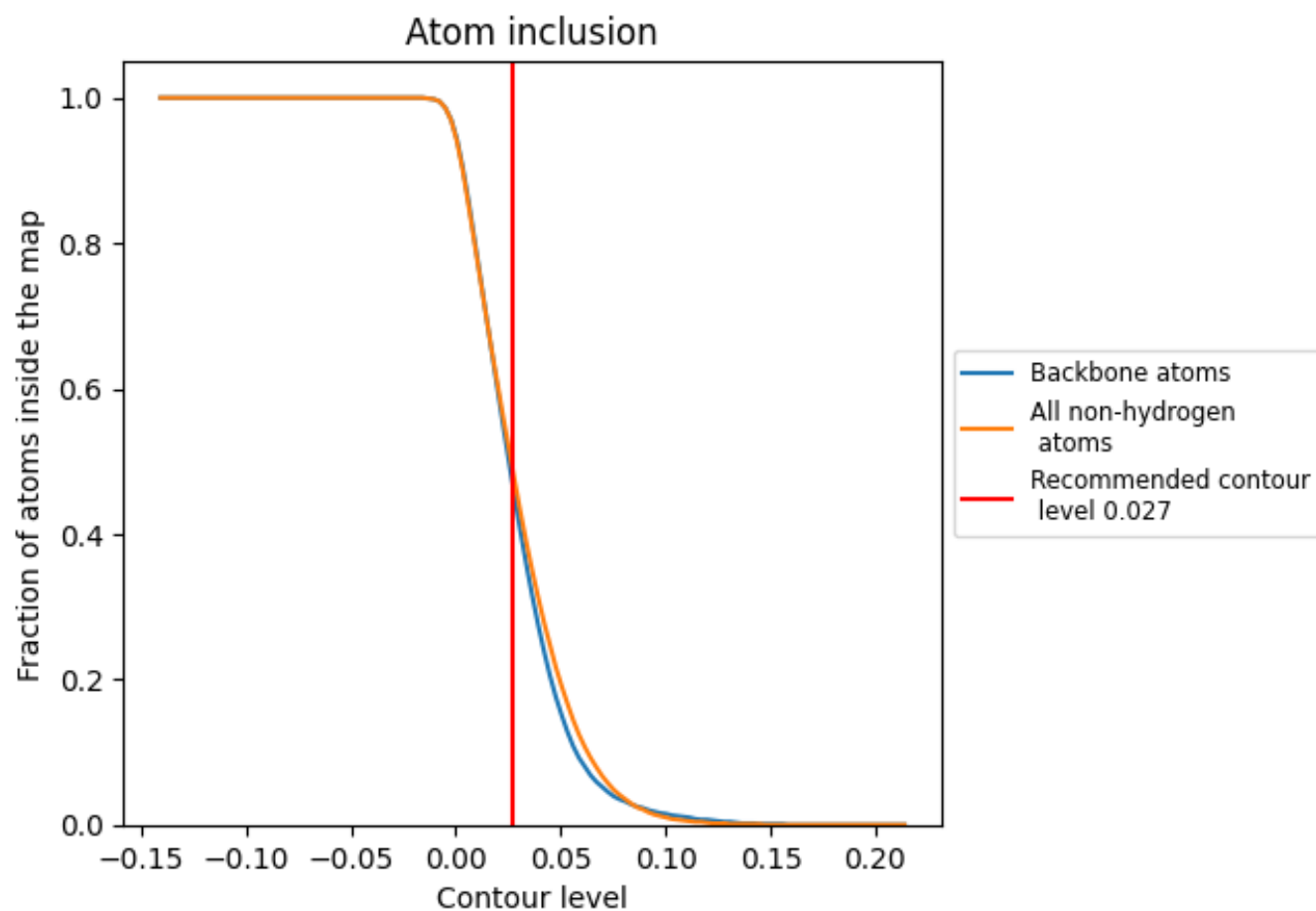
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 49% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4900	0.5490
A	0.8360	0.6630
C0	0.4440	0.5520
C1	0.4860	0.5580
C2	0.2470	0.5150
C3	0.7010	0.6180
C4	0.6900	0.6200
C5	0.3770	0.5490
CA	0.5560	0.5680
CB	0.2110	0.5010
CC	0.5350	0.5950
CD	0.5300	0.5850
CE	0.3490	0.5270
CF	0.0010	0.2810
CG	0.0250	0.3930
CH	0.0190	0.2610
CJ	0.0000	0.1940
CK	0.5300	0.5870
CL	0.4470	0.5610
CM	0.4520	0.5610
CN	0.4570	0.5690
CO	0.6070	0.6050
CP	0.0760	0.4580
CQ	0.3910	0.5560
CR	0.6290	0.6030
CS	0.3680	0.5450
CT	0.5210	0.5770
CU	0.3650	0.5250
CV	0.0960	0.4640
CW	0.1830	0.4930
CX	0.5770	0.5950
CY	0.4430	0.5650
CZ	0.0980	0.4650

