



Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 05:04 pm BST

PDB ID : 9H91 / pdb_00009h91
EMDB ID : EMD-51947
Title : Cryo-EM structure of the *Vibrio natrigens* 50S ribosomal subunit in complex with the proline-rich antimicrobial peptide Bac5(1-17).
Authors : Raulf, K.F.; Koller, T.O.; Beckert, B.; Morici, M.; Lepak, A.; Bange, G.; Wilson, D.N.
Deposited on : 2024-10-29
Resolution : 2.70 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:

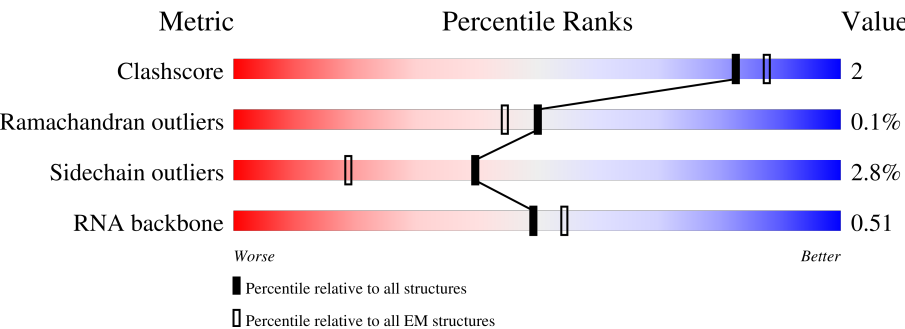
EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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.















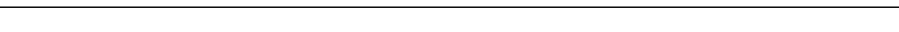

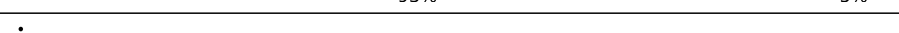

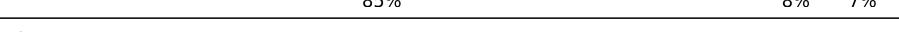

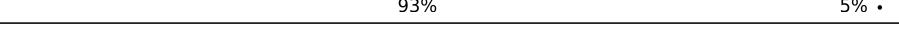




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. 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	0	56	
2	1	56	
3	2	44	
4	3	64	
5	4	37	
6	9	17	
7	B	121	

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Mol	Chain	Length	Quality of chain
8	C	274	 86% 13%
9	D	209	 89% 11%
10	E	200	 89% 10%
11	G	177	 8% 89% 10%
12	H	150	 26% 73%
13	J	142	 80% 19%
14	K	123	 85% 15%
15	L	144	 88% 12%
16	M	136	 85% 13%
17	N	126	 83% 10% 5%
18	O	117	 90% 9%
19	P	117	 81% 15%
20	Q	117	 89% 9%
21	R	103	 93% 5%
22	S	110	 90% 9%
23	T	100	 5% 85% 8% 7%
24	U	105	 74% 16% 9%
25	V	92	 93% 5%
26	W	85	 82% 9% 8%
27	X	78	 83% 15%
28	Y	63	 8% 79% 19%
29	Z	58	 79% 21%
30	A	2721	 66% 29% 5%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83760 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 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	53	Total	C	N	O	S	0	0
			415	250	88	76	1		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	54	Total	C	N	O	S	0	0
			440	281	83	74	2		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			362	222	86	52	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	63	Total	C	N	O	S	0	0
			502	320	102	77	3		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			296	181	65	46	4		

- Molecule 6 is a protein called Cathelicidin-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	9	17	Total	C	N	O	0	0
			154	104	32	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	121	Total	C	N	O	P	0	0
			2583	1153	464	845	121		

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	272	Total	C	N	O	S	0	0
			2093	1294	426	367	6		

- Molecule 9 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	209	Total	C	N	O	S	0	0
			1570	978	292	294	6		

- Molecule 10 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	200	Total	C	N	O	S	0	0
			1535	963	277	289	6		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	176	Total	C	N	O	S	0	0
			1312	825	238	247	2		

- Molecule 12 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	40	Total	C	N	O	S	0	0
			293	187	51	53	2		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	142	Total	C	N	O	S	0	0
			1124	719	202	199	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	123	Total	C	N	O	S	0	0
			947	591	183	166	7		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	143	Total	C	N	O	S	0	0
			1034	644	200	189	1		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	135	Total	C	N	O	S	0	0
			1084	689	212	179	4		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	120	Total	C	N	O	S	0	0
			955	594	194	163	4		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	O	116	Total	C	N	O	0	0
			880	545	178	157		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	114	Total	C	N	O	S	0	0
			907	566	175	165	1		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Q	116	Total	C	N	O	0	0
			938	597	191	150		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	103	Total	C	N	O	S	0	0
			812	510	156	145	1		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	110	Total	C	N	O	S	0	0
			852	530	162	157	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	93	Total	C	N	O	S	0	0
			732	462	134	134	2		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	U	96	Total	C	N	O		
			725	456	136	133	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	92	Total	C	N	O	S	0	0
			730	466	131	130	3		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	78	Total	C	N	O		
			598	371	118	109	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	77	Total	C	N	O	S	0	0
			624	384	132	105	3		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	62	Total	C	N	O	S	0	0
			493	302	96	93	2		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	58	Total	C	N	O	S	0	0
			458	289	84	81	4		

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A	2718	Total	C	N	O	P	0	0
			58293	26012	10670	18893	2718		

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	4	1	Total	Zn	0
			1	1	


- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	9	13	Total	O	0
			13	13	
32	A	5	Total	O	0
			5	5	

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: 50S ribosomal protein L32

Chain 0: 




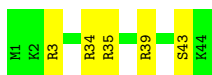
- Molecule 2: 50S ribosomal protein L33

Chain 1: 




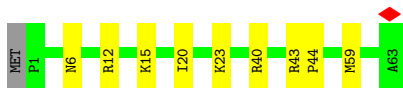
- Molecule 3: 50S ribosomal protein L34

Chain 2: 




- Molecule 4: 50S ribosomal protein L35

Chain 3: 

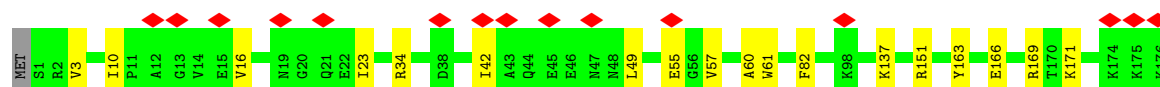
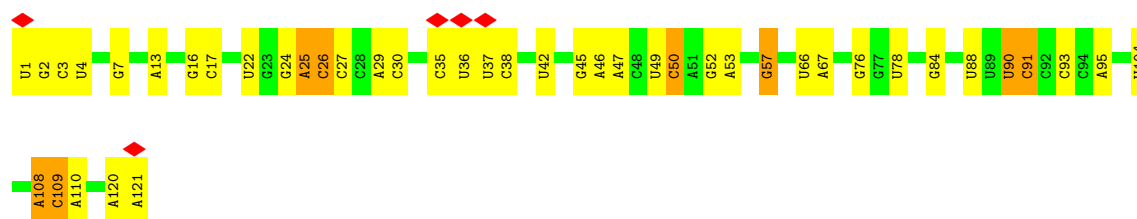
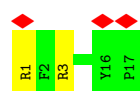


- Molecule 5: 50S ribosomal protein L36

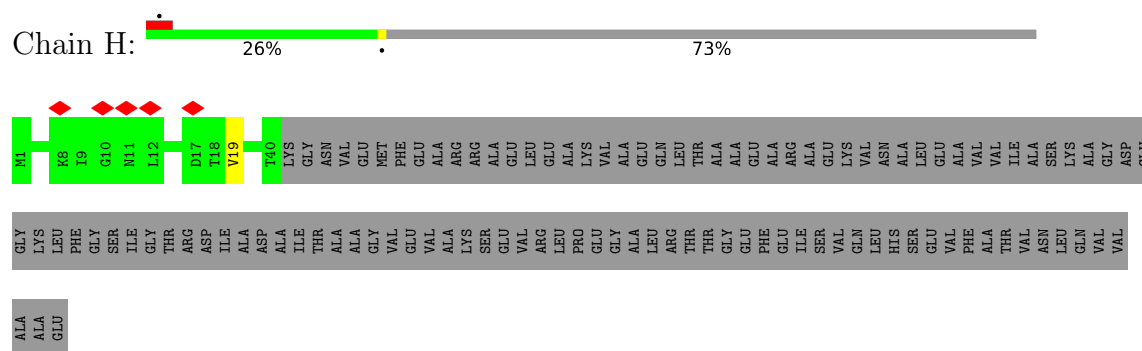
Chain 4: 



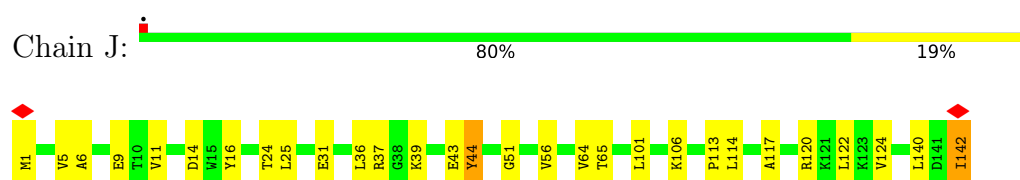
- Molecule 6: Cathelicidin-2



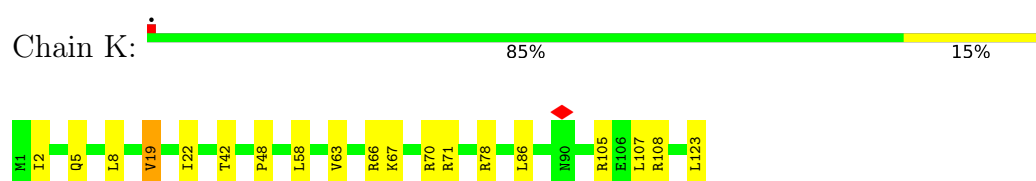
- Molecule 12: Large ribosomal subunit protein bL9



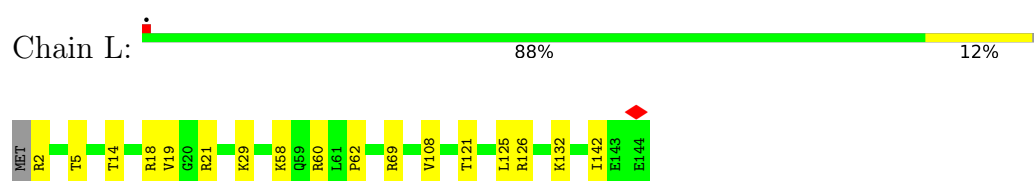
- Molecule 13: 50S ribosomal protein L13



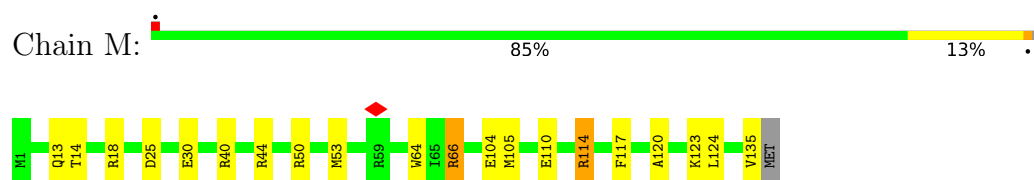
- Molecule 14: 50S ribosomal protein L14



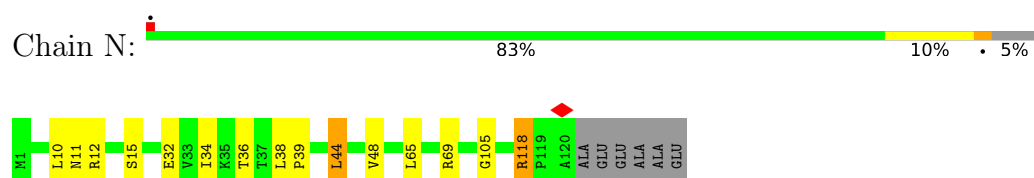
- Molecule 15: 50S ribosomal protein L15



- Molecule 16: 50S ribosomal protein L16



- Molecule 17: 50S ribosomal protein L17




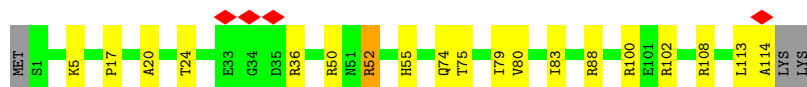
- Molecule 18: 50S ribosomal protein L18

Chain O:  90% 9%




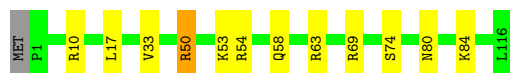
- Molecule 19: 50S ribosomal protein L19

Chain P:  81% 15%



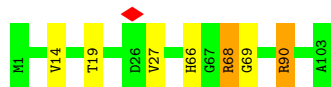
- Molecule 20: 50S ribosomal protein L20

Chain Q:  89% 9%




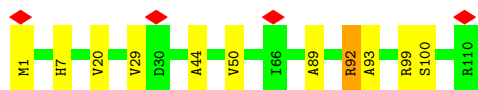
- Molecule 21: 50S ribosomal protein L21

Chain R:  93% 5%




- Molecule 22: 50S ribosomal protein L22

Chain S:  90% 9%



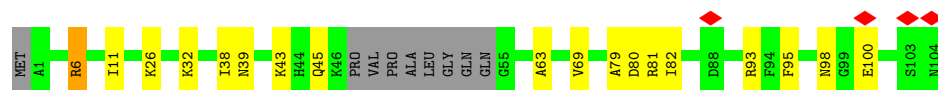
- Molecule 23: 50S ribosomal protein L23

Chain T:  5% 85% 8% 7%

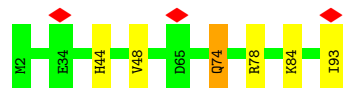


- Molecule 24: 50S ribosomal protein L24

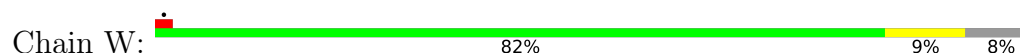
Chain U:  74% 16% 9%



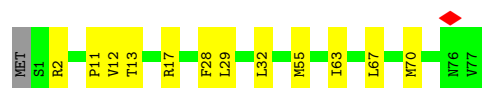
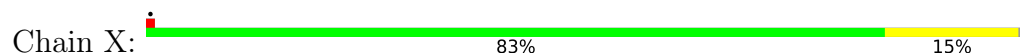
- Molecule 25: 50S ribosomal protein L25



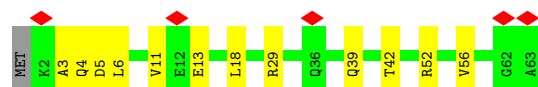
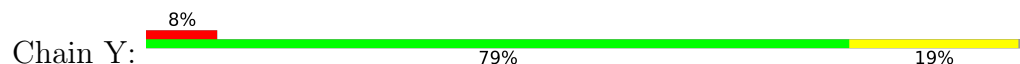
- Molecule 26: 50S ribosomal protein L27



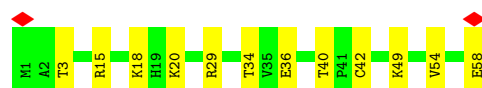
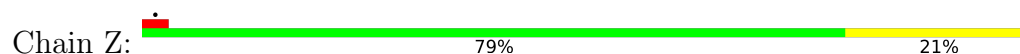
- Molecule 27: 50S ribosomal protein L28



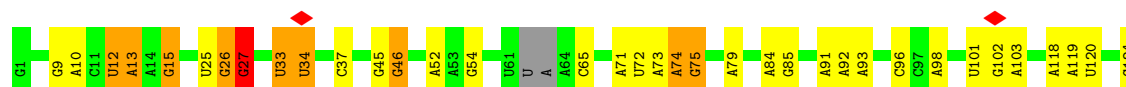
- Molecule 28: 50S ribosomal protein L29

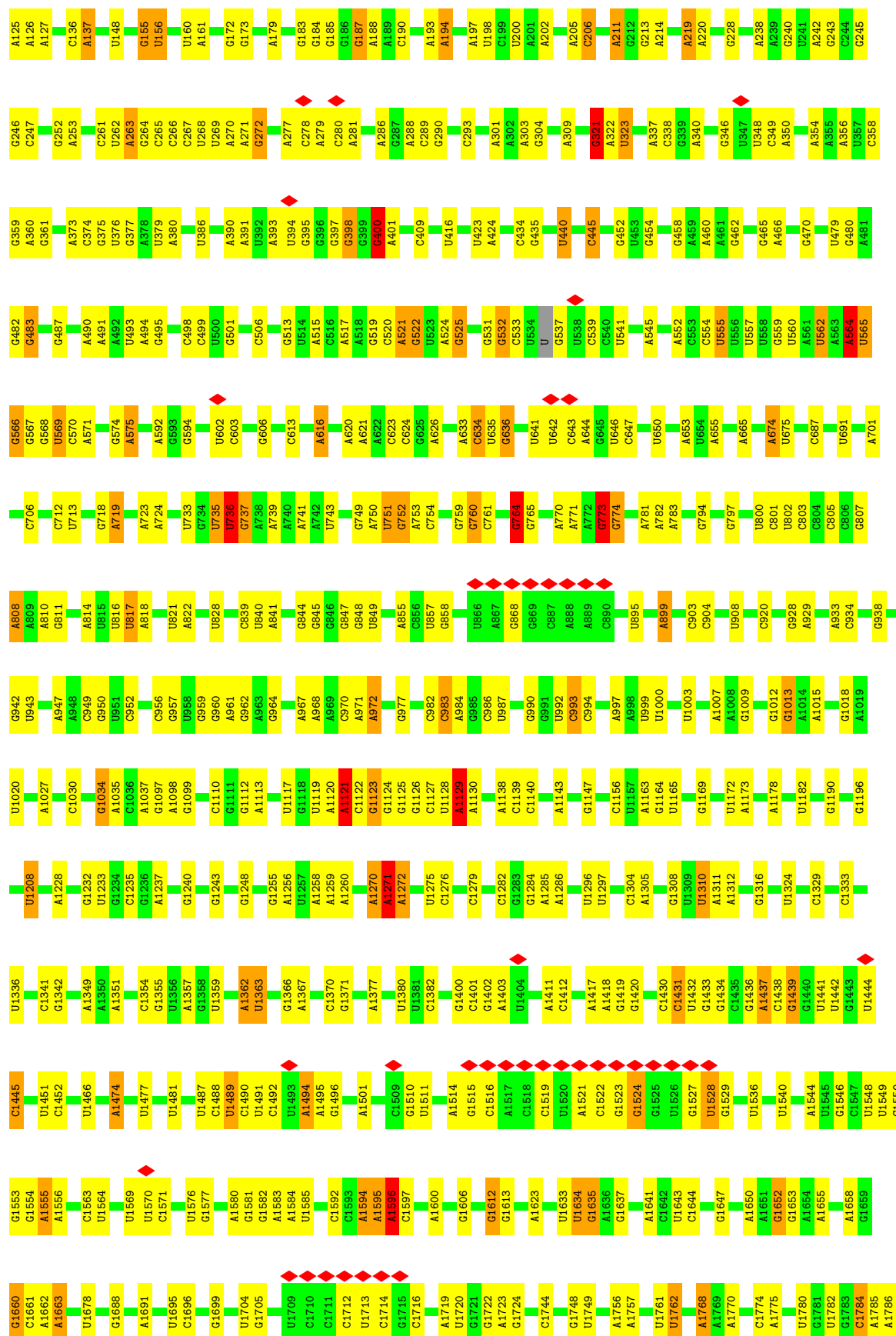


- Molecule 29: 50S ribosomal protein L30



- Molecule 30: 23S ribosomal RNA







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	294068	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.600	Depositor
Minimum map value	-0.304	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.055	Depositor
Map size (\AA)	441.376, 441.376, 441.376	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

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

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	0	0.78	0/419	1.04	1/559 (0.2%)
2	1	0.71	0/448	1.03	0/594
3	2	0.83	0/365	0.96	0/478
4	3	0.88	0/510	1.01	0/677
5	4	0.84	0/297	0.98	0/389
6	9	0.73	0/163	1.03	0/223
7	B	0.58	0/2888	1.08	18/4498 (0.4%)
8	C	0.83	1/2134 (0.0%)	0.99	2/2874 (0.1%)
9	D	0.75	0/1591	0.99	1/2139 (0.0%)
10	E	0.70	0/1554	1.01	2/2093 (0.1%)
11	G	0.62	0/1330	0.95	0/1798
12	H	0.60	0/295	0.95	0/396
13	J	0.78	0/1147	0.98	0/1544
14	K	0.73	0/957	1.02	1/1283 (0.1%)
15	L	0.81	0/1042	1.01	1/1389 (0.1%)
16	M	0.75	0/1104	0.99	1/1475 (0.1%)
17	N	0.80	0/969	0.99	0/1297
18	O	0.71	0/889	1.03	1/1193 (0.1%)
19	P	0.80	2/917 (0.2%)	0.93	1/1225 (0.1%)
20	Q	0.83	0/952	1.06	1/1268 (0.1%)
21	R	0.71	0/823	0.93	0/1100
22	S	0.77	0/860	0.94	0/1153
23	T	0.62	0/736	0.91	0/980
24	U	0.63	0/729	1.00	0/968
25	V	0.69	0/744	0.95	0/1000
26	W	0.82	0/605	0.97	0/803
27	X	0.69	0/632	1.00	0/843
28	Y	0.58	0/494	1.06	0/660
29	Z	0.73	0/463	0.95	1/620 (0.2%)
30	A	0.65	0/65271	1.12	388/101794 (0.4%)
All	All	0.67	3/91328 (0.0%)	1.09	419/137313 (0.3%)

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
1	0	0	3
2	1	0	1
3	2	0	1
4	3	0	2
5	4	0	1
6	9	0	1
8	C	0	9
9	D	0	1
10	E	0	2
11	G	0	3
13	J	0	2
14	K	0	4
15	L	0	3
16	M	0	5
17	N	0	1
18	O	0	2
19	P	0	5
20	Q	0	4
21	R	0	2
22	S	0	2
24	U	0	1
25	V	0	1
26	W	0	1
27	X	0	1
28	Y	0	2
29	Z	0	1
30	A	0	13
All	All	0	74

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	55	HIS	CG-CD2	-6.94	1.28	1.35
19	P	20	ALA	CA-CB	-6.46	1.46	1.53
8	C	52	HIS	CG-CD2	-5.91	1.29	1.35

All (419) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1784	C	O3'-P-O5'	-13.19	84.22	104.00
30	A	2873	C	O3'-P-O5'	-12.00	85.99	104.00
30	A	674	A	O3'-P-O5'	-10.55	88.17	104.00
30	A	2483	A	O3'-P-O5'	10.23	119.35	104.00
30	A	751	U	O3'-P-O5'	-10.05	88.93	104.00
30	A	759	G	O3'-P-O5'	-10.01	88.98	104.00
30	A	2184	A	O3'-P-O5'	-9.63	89.55	104.00
30	A	321	G	O3'-P-O5'	-9.26	90.11	104.00
7	B	16	G	O3'-P-O5'	-9.22	90.17	104.00
30	A	1123	G	O3'-P-O5'	-9.07	90.40	104.00
30	A	2486	U	O3'-P-O5'	-9.01	90.49	104.00
30	A	202	A	O3'-P-O5'	-8.74	90.88	104.00
30	A	797	G	O3'-P-O5'	-8.64	91.03	104.00
30	A	1584	A	O3'-P-O5'	-8.62	91.07	104.00
30	A	2484	C	C3'-C2'-O2'	8.59	123.59	110.70
30	A	2764	A	O3'-P-O5'	-8.49	91.26	104.00
30	A	397	G	O3'-P-O5'	-8.49	91.27	104.00
30	A	1926	U	C2'-C3'-O3'	8.45	122.18	109.50
30	A	2438	C	O3'-P-O5'	-8.33	91.51	104.00
30	A	566	G	O3'-P-O5'	-8.32	91.52	104.00
30	A	1818	U	C4'-C3'-O3'	-8.27	100.59	113.00
30	A	2020	U	O3'-P-O5'	-8.25	91.63	104.00
30	A	2747	G	O3'-P-O5'	-8.17	91.75	104.00
30	A	1658	A	O3'-P-O5'	-8.11	91.83	104.00
30	A	1662	A	O3'-P-O5'	-8.10	91.85	104.00
30	A	493	U	O3'-P-O5'	-8.08	91.88	104.00
30	A	2622	U	O3'-P-O5'	-8.08	91.88	104.00
30	A	1312	A	O3'-P-O5'	-7.96	92.05	104.00
30	A	814	A	O3'-P-O5'	-7.93	92.11	104.00
30	A	665	A	O3'-P-O5'	-7.92	92.13	104.00
30	A	541	U	O3'-P-O5'	-7.88	92.19	104.00
30	A	1377	A	O3'-P-O5'	-7.87	92.20	104.00
30	A	379	U	O3'-P-O5'	-7.86	92.22	104.00
30	A	2510	G	O3'-P-O5'	-7.77	92.34	104.00
30	A	2014	U	O3'-P-O5'	-7.76	92.36	104.00
30	A	568	G	O3'-P-O5'	-7.74	92.39	104.00
30	A	574	G	O3'-P-O5'	-7.67	92.49	104.00
30	A	2614	U	O3'-P-O5'	-7.67	92.50	104.00
30	A	750	A	C4'-C3'-O3'	-7.55	101.68	113.00
30	A	513	G	O3'-P-O5'	-7.54	92.69	104.00
30	A	2750	A	O3'-P-O5'	-7.52	92.71	104.00
8	C	10	PRO	N-CA-C	-7.50	99.42	111.19
30	A	2023	A	O3'-P-O5'	-7.47	92.79	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1634	U	O3'-P-O5'	-7.42	92.87	104.00
30	A	805	C	O3'-P-O5'	-7.40	92.90	104.00
30	A	2248	U	O3'-P-O5'	-7.40	92.90	104.00
30	A	2258	U	C2'-C3'-O3'	-7.40	102.60	113.70
30	A	749	G	O3'-P-O5'	-7.40	92.90	104.00
30	A	13	A	O3'-P-O5'	-7.38	92.92	104.00
30	A	2076	A	O3'-P-O5'	-7.38	92.93	104.00
30	A	1967	A	C2'-C3'-O3'	-7.38	102.64	113.70
30	A	1653	G	O3'-P-O5'	-7.37	92.94	104.00
30	A	895	U	O3'-P-O5'	-7.33	93.00	104.00
30	A	1980	C	O3'-P-O5'	-7.33	93.01	104.00
30	A	1650	A	C4'-C3'-O3'	-7.33	102.01	113.00
30	A	124	G	O3'-P-O5'	-7.32	93.03	104.00
30	A	2369	G	O3'-P-O5'	-7.29	93.06	104.00
30	A	2237	G	C3'-C2'-O2'	7.29	121.63	110.70
30	A	2415	G	O3'-P-O5'	-7.28	93.08	104.00
30	A	999	U	O3'-P-O5'	-7.28	93.09	104.00
30	A	1585	U	O3'-P-O5'	-7.27	93.10	104.00
30	A	1282	C	O3'-P-O5'	-7.26	93.10	104.00
30	A	560	U	O3'-P-O5'	-7.25	93.12	104.00
30	A	1643	U	O3'-P-O5'	-7.20	93.20	104.00
30	A	1351	A	O3'-P-O5'	-7.19	93.22	104.00
30	A	848	G	O3'-P-O5'	-7.18	93.23	104.00
30	A	2246	C	O3'-P-O5'	-7.17	93.25	104.00
30	A	193	A	C4'-C3'-O3'	-7.16	102.26	113.00
30	A	960	G	O3'-P-O5'	-7.16	93.26	104.00
30	A	72	U	O3'-P-O5'	-7.13	93.30	104.00
30	A	398	G	O3'-P-O5'	-7.13	93.30	104.00
30	A	770	A	O3'-P-O5'	-7.12	93.32	104.00
30	A	173	G	O3'-P-O5'	-7.11	93.34	104.00
30	A	621	A	O3'-P-O5'	-7.10	93.34	104.00
30	A	1140	C	O3'-P-O5'	-7.08	93.37	104.00
30	A	2483	A	C2'-C3'-O3'	7.08	120.12	109.50
30	A	1434	G	O3'-P-O5'	-7.04	93.44	104.00
30	A	2007	A	O3'-P-O5'	-7.03	93.45	104.00
30	A	957	G	O3'-P-O5'	-7.02	93.47	104.00
30	A	1169	G	O3'-P-O5'	-7.02	93.48	104.00
30	A	982	C	O3'-P-O5'	-6.98	93.53	104.00
30	A	73	A	O3'-P-O5'	-6.98	93.53	104.00
30	A	187	G	O3'-P-O5'	-6.98	93.53	104.00
30	A	2054	U	O3'-P-O5'	-6.98	93.53	104.00
30	A	2453	C	O3'-P-O5'	-6.97	93.54	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	54	G	O3'-P-O5'	-6.95	93.58	104.00
7	B	50	C	O3'-P-O5'	-6.94	93.59	104.00
30	A	9	G	O3'-P-O5'	-6.93	93.61	104.00
30	A	2081	A	O3'-P-O5'	-6.89	93.66	104.00
30	A	1439	G	O3'-P-O5'	-6.86	93.71	104.00
30	A	1655	A	C2'-C3'-O3'	-6.86	103.41	113.70
30	A	1842	A	O3'-P-O5'	-6.86	93.72	104.00
30	A	386	U	O3'-P-O5'	-6.85	93.72	104.00
30	A	2571	U	O3'-P-O5'	-6.85	93.73	104.00
30	A	2750	A	C2'-C3'-O3'	-6.85	103.43	113.70
30	A	2009	C	C4'-C3'-O3'	-6.84	102.73	113.00
30	A	2767	A	O3'-P-O5'	-6.83	93.76	104.00
30	A	2763	G	O3'-P-O5'	-6.80	93.80	104.00
30	A	928	G	C2'-C3'-O3'	-6.79	103.51	113.70
30	A	1660	G	O3'-P-O5'	-6.78	93.83	104.00
30	A	2523	U	O3'-P-O5'	-6.77	93.84	104.00
30	A	992	U	C4'-C3'-O3'	-6.77	102.85	113.00
30	A	493	U	C4'-C3'-O3'	-6.76	102.85	113.00
30	A	2817	G	O3'-P-O5'	-6.73	93.91	104.00
7	B	78	U	O3'-P-O5'	-6.70	93.95	104.00
30	A	990	G	O3'-P-O5'	-6.68	93.98	104.00
30	A	2282	U	O3'-P-O5'	-6.68	93.97	104.00
30	A	499	C	O3'-P-O5'	-6.66	94.00	104.00
30	A	810	A	O3'-P-O5'	-6.66	94.01	104.00
30	A	1551	C	O3'-P-O5'	-6.64	94.04	104.00
30	A	1012	G	C3'-C2'-O2'	-6.62	104.67	114.60
30	A	483	G	O3'-P-O5'	-6.62	94.07	104.00
30	A	1441	U	C2'-C3'-O3'	-6.61	103.79	113.70
30	A	1431	C	O3'-P-O5'	-6.60	94.10	104.00
30	A	1550	C	O3'-P-O5'	-6.59	94.11	104.00
30	A	1749	U	O3'-P-O5'	-6.59	94.11	104.00
30	A	1018	G	O3'-P-O5'	-6.57	94.14	104.00
30	A	2236	G	O3'-P-O5'	-6.57	94.14	104.00
30	A	266	C	O3'-P-O5'	-6.57	94.15	104.00
30	A	1637	G	O3'-P-O5'	-6.55	94.18	104.00
30	A	2536	G	C4'-C3'-O3'	-6.55	103.18	113.00
7	B	84	G	O3'-P-O5'	-6.54	94.19	104.00
30	A	2044	A	O3'-P-O5'	-6.53	94.21	104.00
16	M	14	THR	CA-CB-OG1	-6.52	99.82	109.60
30	A	2497	U	O3'-P-O5'	-6.49	94.27	104.00
30	A	952	C	O3'-P-O5'	-6.47	94.29	104.00
30	A	1596	A	O3'-P-O5'	-6.46	94.31	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1182	U	O3'-P-O5'	-6.45	94.33	104.00
7	B	76	G	O3'-P-O5'	-6.43	94.35	104.00
30	A	993	C	C4'-C3'-O3'	-6.41	103.39	113.00
30	A	2804	C	O3'-P-O5'	-6.41	94.39	104.00
30	A	2600	A	O3'-P-O5'	-6.39	94.41	104.00
30	A	2521	G	O3'-P-O5'	-6.39	94.42	104.00
30	A	1233	U	C4'-C3'-O3'	-6.37	103.44	113.00
30	A	2609	G	O3'-P-O5'	-6.36	94.46	104.00
30	A	606	G	O3'-P-O5'	-6.35	94.47	104.00
30	A	2586	A	O3'-P-O5'	-6.35	94.48	104.00
30	A	265	C	O3'-P-O5'	-6.34	94.49	104.00
30	A	1869	U	O3'-P-O5'	-6.33	94.50	104.00
30	A	359	G	O3'-P-O5'	-6.33	94.50	104.00
30	A	733	U	O3'-P-O5'	-6.33	94.51	104.00
30	A	2209	G	O3'-P-O5'	-6.31	94.54	104.00
7	B	91	C	O3'-P-O5'	-6.30	94.54	104.00
30	A	1583	A	C4'-C3'-O3'	-6.30	103.54	113.00
30	A	904	C	C4'-C3'-O3'	-6.30	103.55	113.00
30	A	1606	G	O3'-P-O5'	-6.30	94.55	104.00
30	A	2335	G	O3'-P-O5'	-6.29	94.56	104.00
30	A	515	A	C4'-C3'-O3'	-6.29	103.57	113.00
30	A	2505	U	O3'-P-O5'	-6.29	94.57	104.00
30	A	1987	C	O3'-P-O5'	-6.28	94.58	104.00
30	A	2741	C	O3'-P-O5'	-6.28	94.59	104.00
30	A	532	G	O3'-P-O5'	-6.27	94.60	104.00
30	A	374	C	C4'-C3'-O3'	-6.25	103.62	113.00
30	A	2040	A	O3'-P-O5'	-6.25	94.62	104.00
30	A	2482	C	C4'-C3'-O3'	-6.24	103.63	113.00
30	A	781	A	O3'-P-O5'	-6.23	94.65	104.00
30	A	994	C	O3'-P-O5'	-6.23	94.66	104.00
30	A	1110	C	O3'-P-O5'	-6.23	94.66	104.00
7	B	25	A	O3'-P-O5'	-6.22	94.67	104.00
30	A	1641	A	O3'-P-O5'	-6.20	94.69	104.00
30	A	2699	U	O3'-P-O5'	-6.19	94.72	104.00
30	A	736	U	O3'-P-O5'	-6.16	94.76	104.00
30	A	1761	U	O3'-P-O5'	-6.16	94.76	104.00
30	A	2257	G	O3'-P-O5'	-6.14	94.79	104.00
9	D	148	GLN	CB-CA-C	-6.13	102.63	112.07
30	A	340	A	O3'-P-O5'	-6.13	94.80	104.00
30	A	288	A	O3'-P-O5'	-6.13	94.81	104.00
30	A	1359	U	O3'-P-O5'	-6.09	94.86	104.00
30	A	943	U	O3'-P-O5'	-6.07	94.90	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1843	U	O3'-P-O5'	-6.07	94.90	104.00
30	A	1762	U	C4'-C3'-O3'	-6.07	103.90	113.00
30	A	564	A	O3'-P-O5'	-6.06	94.91	104.00
10	E	82	VAL	N-CA-CB	-6.05	104.11	111.00
30	A	2673	U	C4'-C3'-O3'	-6.04	103.93	113.00
30	A	959	G	O3'-P-O5'	-6.04	94.95	104.00
30	A	2566	U	C4'-C3'-O3'	-6.03	103.96	113.00
30	A	25	U	O3'-P-O5'	-6.02	94.97	104.00
30	A	2502	A	O3'-P-O5'	-6.00	95.00	104.00
30	A	1310	U	C4'-C3'-O3'	-5.99	104.02	113.00
30	A	1138	A	O3'-P-O5'	-5.98	95.03	104.00
30	A	434	C	C4'-C3'-O3'	-5.97	104.04	113.00
30	A	857	U	O3'-P-O5'	-5.97	95.04	104.00
30	A	2057	A	C2'-C3'-O3'	-5.96	104.75	113.70
30	A	2556	G	O3'-P-O5'	-5.95	95.08	104.00
30	A	1030	C	O3'-P-O5'	-5.95	95.08	104.00
30	A	2831	U	O3'-P-O5'	-5.92	95.12	104.00
30	A	2865	A	O3'-P-O5'	-5.91	95.13	104.00
30	A	849	U	O3'-P-O5'	-5.91	95.14	104.00
30	A	1208	U	O3'-P-O5'	-5.90	95.15	104.00
30	A	2065	U	O3'-P-O5'	-5.89	95.16	104.00
30	A	238	A	O3'-P-O5'	-5.89	95.17	104.00
30	A	2572	U	O3'-P-O5'	-5.89	95.17	104.00
30	A	2285	U	O3'-P-O5'	-5.88	95.18	104.00
30	A	458	G	O3'-P-O5'	-5.87	95.19	104.00
30	A	724	A	C2'-C3'-O3'	-5.87	104.90	113.70
30	A	562	U	O3'-P-O5'	-5.87	95.20	104.00
30	A	773	G	O3'-P-O5'	-5.87	95.20	104.00
30	A	1228	A	C1'-C2'-O2'	5.86	117.18	108.40
30	A	2752	G	O3'-P-O5'	-5.85	95.22	104.00
7	B	47	A	O3'-P-O5'	-5.85	95.22	104.00
30	A	1363	U	O3'-P-O5'	-5.84	95.23	104.00
30	A	2066	A	O3'-P-O5'	-5.84	95.24	104.00
30	A	517	A	O3'-P-O5'	-5.83	95.25	104.00
30	A	739	A	O3'-P-O5'	-5.83	95.25	104.00
30	A	1129	A	O3'-P-O5'	-5.83	95.26	104.00
30	A	2343	G	C2'-C3'-O3'	-5.82	104.97	113.70
30	A	977	G	O3'-P-O5'	-5.82	95.27	104.00
30	A	1271	A	O3'-P-O5'	-5.82	95.28	104.00
30	A	2708	G	C4'-C3'-O3'	-5.81	104.28	113.00
30	A	1333	C	O3'-P-O5'	-5.81	95.29	104.00
30	A	760	G	O3'-P-O5'	-5.80	95.30	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1800	C	O3'-P-O5'	-5.80	95.30	104.00
30	A	2360	C	O3'-P-O5'	-5.79	95.31	104.00
14	K	48	PRO	N-CA-C	5.79	121.58	113.53
30	A	1437	A	O3'-P-O5'	-5.79	95.31	104.00
30	A	2806	U	C4'-C3'-O3'	-5.79	104.32	113.00
30	A	2832	G	C2'-C3'-O3'	-5.79	105.02	113.70
30	A	1991	A	C2'-C3'-O3'	-5.78	105.02	113.70
30	A	655	A	O3'-P-O5'	-5.78	95.33	104.00
30	A	2234	C	O3'-P-O5'	-5.78	95.34	104.00
7	B	4	U	O3'-P-O5'	-5.77	95.34	104.00
30	A	594	G	O3'-P-O5'	-5.74	95.39	104.00
30	A	2393	A	C4'-C3'-O3'	-5.72	104.42	113.00
30	A	1597	C	C4'-C3'-O3'	-5.72	104.42	113.00
30	A	1613	G	O3'-P-O5'	-5.72	95.42	104.00
30	A	1990	G	O3'-P-O5'	-5.72	95.42	104.00
30	A	2558	A	O3'-P-O5'	-5.71	95.44	104.00
30	A	148	U	O3'-P-O5'	-5.70	95.45	104.00
30	A	1489	U	O3'-P-O5'	-5.70	95.45	104.00
30	A	2439	A	O3'-P-O5'	-5.69	95.46	104.00
7	B	95	A	O3'-P-O5'	-5.69	95.47	104.00
30	A	1357	A	O3'-P-O5'	-5.68	95.47	104.00
30	A	495	G	O3'-P-O5'	-5.68	95.48	104.00
30	A	1688	G	O3'-P-O5'	-5.68	95.48	104.00
30	A	2547	U	O3'-P-O5'	-5.68	95.48	104.00
30	A	228	G	O3'-P-O5'	-5.67	95.50	104.00
30	A	2047	G	O3'-P-O5'	-5.67	95.50	104.00
30	A	2403	C	O3'-P-O5'	-5.66	95.50	104.00
30	A	908	U	O3'-P-O5'	-5.66	95.51	104.00
30	A	1366	G	O3'-P-O5'	-5.66	95.51	104.00
30	A	1955	A	O3'-P-O5'	-5.66	95.51	104.00
30	A	555	U	C4'-C3'-O3'	-5.66	104.51	113.00
30	A	2716	C	O3'-P-O5'	-5.66	95.52	104.00
30	A	400	G	C3'-C2'-O2'	-5.66	106.12	114.60
30	A	811	G	O3'-P-O5'	-5.66	95.52	104.00
8	C	128	THR	CA-CB-OG1	-5.65	101.12	109.60
15	L	5	THR	CA-CB-OG1	-5.65	101.13	109.60
30	A	1003	U	O3'-P-O5'	-5.64	95.53	104.00
30	A	1663	A	C4'-C3'-O3'	-5.63	104.55	113.00
30	A	1511	U	O3'-P-O5'	-5.63	95.56	104.00
30	A	2402	C	O3'-P-O5'	-5.62	95.56	104.00
30	A	938	G	O3'-P-O5'	-5.62	95.57	104.00
30	A	462	G	O3'-P-O5'	-5.62	95.57	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	737	G	C1'-O4'-C4'	-5.62	104.28	109.90
30	A	185	G	O3'-P-O5'	-5.61	95.59	104.00
30	A	743	U	O3'-P-O5'	-5.61	95.59	104.00
30	A	2044	A	C2'-C3'-O3'	-5.61	105.29	113.70
30	A	400	G	O3'-P-O5'	-5.60	95.60	104.00
30	A	1165	U	O3'-P-O5'	-5.59	95.62	104.00
30	A	749	G	OP1-P-O3'	5.57	124.70	108.00
30	A	2272	G	O3'-P-O5'	-5.56	95.66	104.00
30	A	1756	A	O3'-P-O5'	5.56	112.34	104.00
30	A	1635	G	O3'-P-O5'	-5.55	95.67	104.00
30	A	1366	G	C4'-C3'-O3'	-5.55	104.68	113.00
30	A	1563	C	O3'-P-O5'	-5.54	95.69	104.00
30	A	1612	G	O3'-P-O5'	-5.54	95.69	104.00
30	A	252	G	C2'-C3'-O3'	-5.53	105.40	113.70
30	A	2508	U	O3'-P-O5'	-5.53	95.70	104.00
30	A	1678	U	C4'-C3'-O3'	-5.53	104.71	113.00
30	A	653	A	C1'-C2'-O2'	5.52	116.68	108.40
30	A	1954	G	O3'-P-O5'	-5.52	95.72	104.00
30	A	15	G	O3'-P-O5'	-5.51	95.73	104.00
30	A	2365	G	O3'-P-O5'	-5.50	95.75	104.00
30	A	569	U	O3'-P-O5'	-5.50	95.75	104.00
30	A	1956	A	C2'-C3'-O3'	5.49	117.73	109.50
30	A	466	A	O3'-P-O5'	-5.49	95.77	104.00
30	A	1661	C	C4'-C3'-O3'	-5.47	104.79	113.00
7	B	90	U	O3'-P-O5'	-5.47	95.80	104.00
30	A	1235	C	O3'-P-O5'	-5.47	95.80	104.00
30	A	1592	C	C4'-C3'-O3'	-5.46	104.80	113.00
30	A	1977	U	O3'-P-O5'	5.46	112.20	104.00
30	A	172	G	O3'-P-O5'	-5.46	95.81	104.00
30	A	858	G	O3'-P-O5'	-5.45	95.82	104.00
7	B	66	U	O3'-P-O5'	-5.45	95.82	104.00
30	A	2037	U	O3'-P-O5'	-5.44	95.84	104.00
30	A	1139	C	O3'-P-O5'	-5.44	95.85	104.00
30	A	1271	A	C2'-C3'-O3'	-5.44	105.55	113.70
30	A	650	U	C2'-C3'-O3'	-5.43	105.55	113.70
30	A	2731	C	O3'-P-O5'	-5.43	95.85	104.00
30	A	2805	G	O3'-P-O5'	-5.43	95.85	104.00
30	A	1035	A	O3'-P-O5'	-5.43	95.85	104.00
30	A	2627	A	C4'-C3'-C2'	-5.43	97.17	102.60
30	A	2468	A	O3'-P-O5'	-5.43	95.85	104.00
30	A	206	C	O3'-P-O5'	-5.43	95.86	104.00
30	A	525	G	C4'-C3'-C2'	-5.43	97.17	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	506	C	O3'-P-O5'	-5.42	95.86	104.00
30	A	1380	U	C1'-C2'-O2'	-5.42	103.66	111.80
30	A	1935	G	O3'-P-O5'	-5.42	95.88	104.00
30	A	27	G	O3'-P-O5'	-5.41	95.88	104.00
30	A	137	A	O3'-P-O5'	-5.41	95.88	104.00
30	A	1172	U	C4'-C3'-O3'	-5.41	104.88	113.00
30	A	752	G	O3'-P-O5'	-5.41	95.89	104.00
30	A	1780	U	O3'-P-O5'	-5.40	95.90	104.00
30	A	1980	C	C2'-C3'-O3'	-5.39	105.62	113.70
30	A	845	G	O3'-P-O5'	-5.39	95.92	104.00
30	A	2630	G	O3'-P-O5'	-5.38	95.92	104.00
30	A	2753	C	O3'-P-O5'	-5.38	95.92	104.00
30	A	26	G	C4'-C3'-O3'	-5.38	104.92	113.00
30	A	1555	A	C2'-C3'-O3'	-5.38	105.63	113.70
30	A	928	G	C4'-C3'-C2'	-5.38	97.22	102.60
30	A	288	A	C4'-C3'-O3'	-5.38	104.93	113.00
30	A	1846	G	O3'-P-O5'	-5.38	95.94	104.00
30	A	2008	U	C2'-C3'-O3'	5.37	117.55	109.50
30	A	211	A	O3'-P-O5'	-5.35	95.97	104.00
30	A	719	A	O3'-P-O5'	-5.34	95.99	104.00
30	A	817	U	C4'-C3'-O3'	-5.34	104.99	113.00
30	A	2515	G	O3'-P-O5'	-5.34	95.99	104.00
30	A	2511	G	O3'-P-O5'	-5.34	95.99	104.00
30	A	531	G	O3'-P-O5'	-5.33	96.00	104.00
30	A	844	G	O3'-P-O5'	-5.33	96.00	104.00
30	A	997	A	C4'-C3'-O3'	-5.33	105.00	113.00
30	A	2236	G	C2'-C3'-O3'	5.33	117.50	109.50
30	A	1774	C	C2'-C3'-O3'	-5.33	105.71	113.70
30	A	2056	A	C4'-C3'-C2'	-5.33	97.27	102.60
30	A	1272	A	O3'-P-O5'	-5.33	96.01	104.00
30	A	2010	G	C4'-C3'-O3'	-5.31	105.03	113.00
30	A	2582	U	C2'-C3'-O3'	-5.31	105.73	113.70
30	A	490	A	O3'-P-O5'	-5.31	96.04	104.00
30	A	2034	G	O3'-P-O5'	-5.31	96.04	104.00
30	A	1258	A	O3'-P-O5'	-5.31	96.04	104.00
30	A	616	A	O3'-P-O5'	-5.30	96.05	104.00
30	A	1125	G	C2'-C3'-O3'	-5.30	105.75	113.70
30	A	245	G	C4'-C3'-O3'	-5.30	105.05	113.00
30	A	435	G	O3'-P-O5'	-5.29	96.06	104.00
30	A	1124	G	O3'-P-O5'	-5.29	96.07	104.00
30	A	2417	U	O3'-P-O5'	-5.29	96.07	104.00
30	A	2819	U	O3'-P-O5'	-5.29	96.07	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	2519	U	O3'-P-O5'	-5.29	96.07	104.00
19	P	24	THR	CA-CB-OG1	-5.28	101.67	109.60
30	A	1536	U	O3'-P-O5'	-5.28	96.08	104.00
7	B	7	G	O3'-P-O5'	-5.28	96.08	104.00
30	A	1997	U	C2'-C3'-O3'	-5.28	105.78	113.70
30	A	545	A	C2'-C3'-O3'	-5.28	105.79	113.70
30	A	1121	A	O3'-P-O5'	-5.27	96.09	104.00
30	A	2306	U	O3'-P-O5'	-5.26	96.10	104.00
7	B	13	A	O3'-P-O5'	-5.26	96.11	104.00
30	A	570	C	O3'-P-O5'	-5.26	96.11	104.00
30	A	999	U	C2'-C3'-O3'	5.26	117.39	109.50
30	A	1127	C	C4'-C3'-O3'	-5.26	105.11	113.00
30	A	967	A	C4'-C3'-C2'	-5.25	97.35	102.60
30	A	1362	A	O3'-P-O5'	-5.25	96.12	104.00
30	A	200	U	C4'-C3'-O3'	-5.24	105.14	113.00
30	A	1196	G	O3'-P-O5'	-5.23	96.15	104.00
30	A	2399	G	O3'-P-O5'	-5.23	96.16	104.00
30	A	986	C	O3'-P-O5'	-5.22	96.17	104.00
30	A	1420	G	O3'-P-O5'	-5.22	96.17	104.00
30	A	2006	A	C4'-C3'-O3'	-5.22	105.17	113.00
30	A	26	G	O3'-P-O5'	-5.21	96.18	104.00
30	A	2476	G	O3'-P-O5'	-5.21	96.18	104.00
30	A	188	A	O3'-P-O5'	-5.21	96.18	104.00
30	A	2223	G	C2'-C3'-O3'	-5.21	105.89	113.70
30	A	2412	A	O3'-P-O5'	-5.20	96.19	104.00
30	A	79	A	O3'-P-O5'	-5.20	96.20	104.00
30	A	1866	U	O3'-P-O5'	-5.19	96.22	104.00
30	A	2054	U	C2'-C3'-O3'	-5.18	105.93	113.70
7	B	93	C	O3'-P-O5'	-5.17	96.24	104.00
30	A	1652	G	O3'-P-O5'	-5.17	96.25	104.00
30	A	1553	G	O3'-P-O5'	-5.16	96.25	104.00
30	A	1644	C	C4'-C3'-O3'	-5.16	105.26	113.00
30	A	1248	G	O3'-P-O5'	-5.14	96.29	104.00
30	A	2836	A	O3'-P-O5'	-5.14	96.29	104.00
30	A	691	U	O3'-P-O5'	-5.14	96.29	104.00
1	0	19	ASP	CA-CB-CG	5.14	117.74	112.60
30	A	1445	C	O3'-P-O5'	-5.14	96.29	104.00
30	A	2854	A	O3'-P-O5'	-5.14	96.30	104.00
30	A	267	C	P-O5'-C5'	-5.13	113.20	120.90
30	A	2456	G	O3'-P-O5'	-5.13	96.30	104.00
30	A	2231	U	C4'-C3'-O3'	-5.13	105.30	113.00
30	A	964	G	C4'-C3'-O3'	-5.13	105.31	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	557	U	C4'-C3'-O3'	-5.13	105.31	113.00
30	A	52	A	O3'-P-O5'	-5.13	96.31	104.00
30	A	565	U	O3'-P-O5'	-5.12	96.33	104.00
30	A	1956	A	C4'-C3'-O3'	-5.12	101.73	109.40
30	A	358	C	O3'-P-O5'	-5.11	96.33	104.00
7	B	52	G	O3'-P-O5'	-5.11	96.34	104.00
30	A	454	G	O3'-P-O5'	-5.11	96.34	104.00
30	A	761	C	O3'-P-O5'	-5.11	96.34	104.00
7	B	108	A	C4'-C3'-O3'	-5.10	105.35	113.00
30	A	1178	A	O3'-P-O5'	-5.10	96.35	104.00
30	A	2869	A	C4'-C3'-O3'	-5.09	105.36	113.00
30	A	1528	U	O3'-P-O5'	-5.09	96.36	104.00
30	A	2432	G	O3'-P-O5'	-5.09	96.36	104.00
30	A	764	G	O3'-P-O5'	-5.09	96.37	104.00
30	A	567	G	O3'-P-O5'	-5.08	96.38	104.00
30	A	620	A	C2'-C3'-O3'	-5.08	106.08	113.70
30	A	1976	C	O3'-P-O5'	-5.08	96.37	104.00
10	E	144	ASP	CA-CB-CG	5.08	117.68	112.60
30	A	2509	G	O3'-P-O5'	-5.08	96.38	104.00
7	B	22	U	O3'-P-O5'	-5.07	96.39	104.00
30	A	1691	A	O3'-P-O5'	-5.07	96.40	104.00
30	A	1884	U	O3'-P-O5'	-5.06	96.41	104.00
29	Z	34	THR	CA-CB-OG1	-5.05	102.02	109.60
30	A	522	G	O3'-P-O5'	-5.05	96.43	104.00
18	O	12	THR	CA-CB-OG1	-5.05	102.03	109.60
30	A	487	G	O3'-P-O5'	-5.05	96.43	104.00
20	Q	58	GLN	N-CA-CB	5.04	117.53	110.12
30	A	1930	U	O3'-P-O5'	-5.04	96.44	104.00
30	A	1556	A	C4'-C3'-O3'	-5.04	105.45	113.00
30	A	1147	G	O3'-P-O5'	-5.03	96.45	104.00
30	A	1647	G	O3'-P-O5'	-5.03	96.45	104.00
30	A	2833	U	C2'-C3'-O3'	-5.03	106.15	113.70
30	A	2197	U	O3'-P-O5'	-5.03	96.46	104.00
30	A	641	U	C2'-C3'-O3'	-5.01	106.18	113.70
30	A	127	A	C4'-C3'-O3'	-5.01	105.48	113.00
30	A	814	A	OP1-P-O3'	5.01	123.03	108.00
30	A	1382	C	C4'-C3'-O3'	-5.01	105.48	113.00
30	A	1528	U	C2'-C3'-O3'	5.01	117.01	109.50
30	A	2561	C	C2'-C3'-O3'	-5.00	106.19	113.70
30	A	240	G	C3'-C2'-C1'	-5.00	96.50	101.50

There are no chirality outliers.

All (74) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	12	ARG	Sidechain
1	0	48	ARG	Sidechain
1	0	9	ARG	Sidechain
2	1	6	ARG	Sidechain
3	2	35	ARG	Sidechain
4	3	12	ARG	Sidechain
4	3	40	ARG	Sidechain
5	4	19	ARG	Sidechain
6	9	3	ARG	Sidechain
30	A	1129	A	Sidechain
30	A	1308	G	Sidechain
30	A	1791	G	Sidechain
30	A	2550	A	Sidechain
30	A	27	G	Sidechain
30	A	2843	G	Sidechain
30	A	452	G	Sidechain
30	A	501	G	Sidechain
30	A	564	A	Sidechain
30	A	947	A	Sidechain
30	A	968	A	Sidechain
30	A	970	C	Sidechain
30	A	972	A	Sidechain
8	C	100	ARG	Sidechain
8	C	12	ARG	Sidechain
8	C	166	ARG	Sidechain
8	C	176	ARG	Sidechain
8	C	242	ARG	Sidechain
8	C	269	ARG	Sidechain
8	C	270	ARG	Sidechain
8	C	42	ARG	Sidechain
8	C	51	ARG	Sidechain
9	D	83	ARG	Sidechain
10	E	66	ARG	Sidechain
10	E	78	ARG	Sidechain
11	G	151	ARG	Sidechain
11	G	169	ARG	Sidechain
11	G	34	ARG	Sidechain
13	J	120	ARG	Sidechain
13	J	37	ARG	Sidechain
14	K	105	ARG	Sidechain
14	K	108	ARG	Sidechain
14	K	70	ARG	Sidechain

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Mol	Chain	Res	Type	Group
14	K	78	ARG	Sidechain
15	L	126	ARG	Sidechain
15	L	18	ARG	Sidechain
15	L	69	ARG	Sidechain
16	M	114	ARG	Sidechain
16	M	18	ARG	Sidechain
16	M	40	ARG	Sidechain
16	M	44	ARG	Sidechain
16	M	66	ARG	Sidechain
17	N	118	ARG	Sidechain
18	O	81	ARG	Sidechain
18	O	94	ARG	Sidechain
19	P	100	ARG	Sidechain
19	P	108	ARG	Sidechain
19	P	36	ARG	Sidechain
19	P	52	ARG	Sidechain
19	P	88	ARG	Sidechain
20	Q	10	ARG	Sidechain
20	Q	50	ARG	Sidechain
20	Q	54	ARG	Sidechain
20	Q	63	ARG	Sidechain
21	R	68	ARG	Sidechain
21	R	90	ARG	Sidechain
22	S	92	ARG	Sidechain
22	S	99	ARG	Sidechain
24	U	6	ARG	Sidechain
25	V	78	ARG	Sidechain
26	W	21	ARG	Sidechain
27	X	17	ARG	Sidechain
28	Y	29	ARG	Sidechain
28	Y	52	ARG	Sidechain
29	Z	29	ARG	Sidechain

5.2 Too-close contacts

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	0	415	0	430	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	440	0	468	2	0
3	2	362	0	411	3	0
4	3	502	0	570	4	0
5	4	296	0	335	3	0
6	9	154	0	165	1	0
7	B	2583	0	1305	9	0
8	C	2093	0	2161	16	0
9	D	1570	0	1606	15	0
10	E	1535	0	1588	9	0
11	G	1312	0	1365	8	0
12	H	293	0	315	0	0
13	J	1124	0	1166	11	0
14	K	947	0	1014	10	0
15	L	1034	0	1116	6	0
16	M	1084	0	1152	9	0
17	N	955	0	1006	8	0
18	O	880	0	919	4	0
19	P	907	0	954	5	0
20	Q	938	0	1007	5	0
21	R	812	0	843	3	0
22	S	852	0	897	6	0
23	T	732	0	806	3	0
24	U	725	0	772	9	0
25	V	730	0	740	3	0
26	W	598	0	615	2	0
27	X	624	0	659	7	0
28	Y	493	0	518	2	0
29	Z	458	0	498	5	0
30	A	58293	0	29320	188	0
31	4	1	0	0	0	0
32	9	13	0	0	0	0
32	A	5	0	0	0	0
All	All	83760	0	54721	308	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 2.

All (308) 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)
8:C:210:THR:HG22	8:C:215:VAL:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:28:PRO:HG2	8:C:33:LEU:HD11	1.79	0.63
30:A:764:G:O2'	30:A:783:A:N7	2.30	0.62
30:A:1007:A:N1	30:A:1128:U:O2'	2.30	0.60
13:J:65:THR:HG21	30:A:1128:U:H2'	1.84	0.60
30:A:1270:A:O2'	30:A:1272:A:OP2	2.17	0.60
1:O:8:THR:CG2	30:A:2006:A:H5'	2.34	0.58
30:A:12:U:H2'	30:A:12:U:O2	2.05	0.57
15:L:21:ARG:HA	30:A:800:U:H2'	1.88	0.56
24:U:32:LYS:HB3	24:U:63:ALA:HB1	1.86	0.56
30:A:773:G:H5'	30:A:774:G:OP1	2.06	0.56
30:A:1594:A:O2'	30:A:1596:A:OP2	2.20	0.55
4:3:59:MET:SD	15:L:58:LYS:HD2	2.47	0.55
20:Q:50:ARG:HD3	30:A:1143:A:C5	2.43	0.54
30:A:1418:A:H2'	30:A:1419:G:O4'	2.09	0.53
16:M:53:MET:HG3	16:M:120:ALA:HB2	1.89	0.52
17:N:12:ARG:NH1	30:A:1260:A:O2'	2.42	0.52
7:B:104:U:O2'	25:V:74:GLN:NE2	2.42	0.52
30:A:1007:A:C2	30:A:1128:U:C2	2.96	0.52
21:R:68:ARG:NH2	30:A:1208:U:OP2	2.43	0.52
14:K:67:LYS:NZ	30:A:2712:A:N3	2.56	0.52
14:K:66:ARG:HD3	30:A:1652:G:OP1	2.08	0.52
30:A:45:G:H5'	30:A:46:G:OP1	2.09	0.52
7:B:49:U:H2'	7:B:50:C:C6	2.45	0.52
4:3:23:LYS:HB3	15:L:62:PRO:HG2	1.92	0.51
8:C:226:PRO:HG3	8:C:233:GLY:HA3	1.93	0.51
13:J:140:LEU:HD21	13:J:142:ILE:HD12	1.92	0.51
22:S:93:ALA:HB2	30:A:1600:A:C2	2.45	0.51
30:A:304:G:H5'	30:A:323:U:O2'	2.09	0.51
30:A:482:G:H2'	30:A:483:G:O4'	2.10	0.51
30:A:1417:A:H2'	30:A:1418:A:C8	2.45	0.51
30:A:2646:A:H2'	30:A:2647:G:O4'	2.11	0.51
27:X:11:PRO:HB3	27:X:29:LEU:HD23	1.93	0.51
6:9:1:ARG:N	30:A:2480:G:OP2	2.35	0.50
30:A:1112:G:C6	30:A:1113:A:N6	2.79	0.50
24:U:43:LYS:HG3	24:U:45:GLN:HG3	1.93	0.50
30:A:1890:G:O2'	30:A:1914:A:N1	2.40	0.50
30:A:1316:G:N7	30:A:1595:A:H2'	2.27	0.50
9:D:8:LYS:NZ	9:D:195:GLY:O	2.41	0.50
24:U:81:ARG:NH2	30:A:293:C:OP2	2.45	0.50
30:A:1401:C:H2'	30:A:1402:G:O4'	2.11	0.50
16:M:25:ASP:O	16:M:66:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:565:U:H2'	30:A:566:G:C8	2.47	0.50
16:M:13:GLN:HG3	30:A:899:A:C5	2.47	0.50
20:Q:53:LYS:NZ	30:A:983:C:OP2	2.45	0.50
30:A:2807:A:O2'	30:A:2812:A:N1	2.42	0.50
30:A:2259:A:H2'	30:A:2260:A:C8	2.47	0.49
7:B:1:U:H3	7:B:120:A:H2	1.61	0.49
17:N:38:LEU:N	17:N:39:PRO:HD2	2.27	0.49
30:A:301:A:N3	30:A:321:G:O2'	2.44	0.49
30:A:840:U:H2'	30:A:841:A:C8	2.47	0.49
30:A:2642:U:C5	30:A:2650:G:N2	2.81	0.49
30:A:735:U:H2'	30:A:735:U:O2	2.13	0.49
30:A:1013:G:H1'	30:A:1121:A:C2	2.46	0.49
30:A:807:G:H5'	30:A:828:U:OP1	2.12	0.49
30:A:1966:G:O2'	30:A:1968:U:OP2	2.29	0.49
8:C:97:ASP:HB3	30:A:1474:A:H2'	1.94	0.49
7:B:24:G:N7	7:B:57:G:H2'	2.27	0.49
30:A:1867:C:H2'	30:A:1868:U:O4'	2.13	0.49
9:D:5:ILE:CD1	9:D:202:ILE:HG12	2.43	0.49
30:A:2533:A:H2'	30:A:2534:U:C6	2.47	0.48
10:E:78:ARG:NH2	30:A:460:A:OP1	2.46	0.48
30:A:1762:U:H2'	30:A:1768:A:N6	2.29	0.48
29:Z:3:THR:HB	29:Z:36:GLU:HG2	1.95	0.48
30:A:465:G:H4'	30:A:491:A:N1	2.28	0.48
30:A:521:A:N7	30:A:2007:A:O2'	2.41	0.48
30:A:2811:U:O2	30:A:2811:U:O4'	2.32	0.48
25:V:44:HIS:CE1	25:V:48:VAL:HG21	2.49	0.48
30:A:633:A:H2'	30:A:634:C:O4'	2.14	0.48
30:A:899:A:N1	30:A:2263:G:H1'	2.28	0.48
9:D:150:GLN:HB2	30:A:2558:A:N7	2.29	0.48
30:A:821:U:H2'	30:A:822:A:C8	2.48	0.48
30:A:2048:A:N3	30:A:2048:A:H2'	2.29	0.48
2:1:22:THR:HG21	30:A:2405:U:H4'	1.94	0.48
11:G:3:VAL:HG21	30:A:2734:A:H4'	1.95	0.48
27:X:13:THR:HG21	30:A:187:G:OP2	2.14	0.48
30:A:1034:G:HO2'	30:A:1097:G:H1	1.61	0.48
14:K:2:ILE:HG12	14:K:8:LEU:HD21	1.96	0.48
29:Z:49:LYS:HE3	30:A:840:U:H5''	1.96	0.48
30:A:623:C:H2'	30:A:624:C:C6	2.49	0.48
30:A:736:U:O2	30:A:2000:A:H1'	2.14	0.48
22:S:93:ALA:HB2	30:A:1600:A:N1	2.29	0.47
30:A:33:U:H4'	30:A:34:U:OP1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:271:ARG:NH2	30:A:1782:U:OP2	2.39	0.47
9:D:121:ALA:HB1	9:D:127:PHE:CD2	2.48	0.47
14:K:22:ILE:HD11	14:K:42:THR:HG22	1.95	0.47
30:A:183:G:H2'	30:A:184:G:O4'	2.14	0.47
7:B:53:A:N7	18:O:64:TYR:OH	2.39	0.47
8:C:61:TYR:CE1	30:A:1800:C:H3'	2.50	0.47
18:O:111:ARG:NH2	30:A:2362:A:N3	2.62	0.47
30:A:2665:A:H2'	30:A:2666:C:O4'	2.14	0.47
30:A:2492:U:H5	30:A:2571:U:O4	1.98	0.47
30:A:1918:A:H2'	30:A:1919:G:O4'	2.15	0.47
8:C:2:ILE:HD11	8:C:201:LEU:HB2	1.96	0.47
13:J:6:ALA:HB1	13:J:11:VAL:CG1	2.45	0.47
19:P:113:LEU:O	19:P:114:ALA:C	2.58	0.46
30:A:554:C:H2'	30:A:555:U:O4'	2.15	0.46
30:A:1015:A:N6	30:A:1112:G:H2'	2.30	0.46
30:A:1492:C:H4'	30:A:1494:A:C5	2.49	0.46
30:A:2381:C:H2'	30:A:2382:G:O4'	2.14	0.46
30:A:524:A:H2'	30:A:525:G:O4'	2.15	0.46
10:E:82:VAL:O	10:E:83:THR:C	2.58	0.46
30:A:2222:U:H2'	30:A:2223:G:O4'	2.15	0.46
30:A:261:C:H2'	30:A:262:U:O4'	2.16	0.46
8:C:59:HIS:HA	30:A:1554:G:H5'	1.97	0.46
9:D:19:GLY:HA3	19:P:79:ILE:HG13	1.97	0.46
9:D:81:GLU:OE1	30:A:2621:A:O2'	2.33	0.46
13:J:122:LEU:HG	13:J:124:VAL:HG23	1.97	0.46
14:K:58:LEU:HD11	14:K:86:LEU:HD13	1.97	0.46
30:A:736:U:C5	30:A:2599:U:C5	3.03	0.46
11:G:10:ILE:HD11	11:G:49:LEU:HG	1.98	0.46
30:A:91:A:H1'	30:A:92:A:C8	2.50	0.46
4:3:43:ARG:N	4:3:44:PRO:CD	2.78	0.46
10:E:1:MET:HE1	10:E:112:VAL:HG11	1.98	0.46
8:C:30:ALA:N	8:C:31:PRO:CD	2.79	0.46
11:G:163:TYR:HB2	11:G:166:GLU:HB2	1.98	0.45
30:A:634:C:H2'	30:A:636:G:C8	2.50	0.45
30:A:2219:U:H2'	30:A:2220:G:C8	2.52	0.45
8:C:75:ALA:HB2	8:C:95:TYR:CD2	2.51	0.45
10:E:180:ILE:HG23	15:L:2:ARG:HB3	1.99	0.45
30:A:1514:A:H2'	30:A:1515:G:O4'	2.17	0.45
10:E:148:VAL:HA	10:E:169:ARG:O	2.16	0.45
16:M:105:MET:HE3	16:M:117:PHE:CE2	2.51	0.45
30:A:26:G:C6	30:A:27:G:N1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:155:G:H3'	30:A:156:U:H6	1.82	0.45
30:A:571:A:C2	30:A:1243:G:C2	3.05	0.45
4:3:15:LYS:HD2	4:3:20:ILE:HD13	1.97	0.45
17:N:10:LEU:O	17:N:11:ASN:C	2.60	0.45
28:Y:6:LEU:HB2	28:Y:56:VAL:HG21	1.99	0.45
30:A:289:C:H2'	30:A:290:G:O4'	2.17	0.45
30:A:646:U:H2'	30:A:647:C:C6	2.51	0.45
13:J:43:GLU:O	13:J:44:TYR:C	2.60	0.44
23:T:7:ILE:HG23	23:T:46:ALA:HA	1.99	0.44
30:A:1296:U:H4'	30:A:1297:U:O5'	2.17	0.44
30:A:2279:G:H2'	30:A:2280:G:O4'	2.18	0.44
30:A:2313:A:H2'	30:A:2314:A:C8	2.51	0.44
8:C:49:THR:HB	30:A:1789:U:O2	2.17	0.44
13:J:14:ASP:HB2	13:J:16:TYR:CE1	2.52	0.44
14:K:19:VAL:HG11	14:K:86:LEU:HD21	1.99	0.44
30:A:2024:G:H2'	30:A:2025:U:O4'	2.17	0.44
9:D:25:THR:HG21	9:D:193:VAL:HB	2.00	0.44
22:S:20:VAL:HG11	22:S:44:ALA:HA	1.97	0.44
30:A:1370:C:H2'	30:A:1371:G:C8	2.52	0.44
30:A:1981:U:H3'	30:A:1982:C:H2'	1.99	0.44
30:A:2678:G:H2'	30:A:2679:G:O4'	2.18	0.44
9:D:150:GLN:NE2	30:A:2018:G:H1'	2.33	0.44
9:D:12:THR:OG1	9:D:13:ARG:N	2.50	0.44
30:A:2775:C:H2'	30:A:2879:A:C2	2.52	0.44
5:4:7:VAL:HG21	5:4:23:VAL:HG12	1.99	0.44
8:C:5:CYS:SG	8:C:12:ARG:NH1	2.91	0.44
13:J:56:VAL:HG11	13:J:101:LEU:CD2	2.48	0.44
17:N:34:ILE:HG22	17:N:36:THR:HG23	1.99	0.44
19:P:50:ARG:CZ	19:P:52:ARG:HG3	2.48	0.44
30:A:380:A:H1'	30:A:400:G:O4'	2.17	0.44
30:A:1259:A:N1	30:A:1279:C:O2'	2.42	0.44
30:A:2448:C:O2	30:A:2477:U:H5	2.01	0.44
16:M:123:LYS:NZ	30:A:2469:C:N3	2.55	0.44
30:A:2412:A:H4'	30:A:2413:C:OP2	2.17	0.44
20:Q:69:ARG:NH2	20:Q:74:SER:OG	2.51	0.43
8:C:2:ILE:HG23	8:C:16:VAL:CG1	2.48	0.43
30:A:1580:A:H2'	30:A:1581:G:O4'	2.18	0.43
7:B:67:A:N6	7:B:108:A:H2'	2.33	0.43
10:E:83:THR:HG21	30:A:575:A:H5'	1.99	0.43
24:U:11:ILE:HG21	24:U:79:ALA:HB2	2.00	0.43
30:A:37:C:H4'	30:A:440:U:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:67:A:C6	7:B:109:C:C6	3.06	0.43
21:R:27:VAL:O	21:R:66:HIS:NE2	2.49	0.43
30:A:1354:C:H2'	30:A:1355:G:O4'	2.18	0.43
30:A:2855:G:H2'	30:A:2856:C:O4'	2.18	0.43
27:X:12:VAL:HG22	27:X:28:PHE:HB2	1.99	0.43
18:O:34:HIS:O	18:O:102:ARG:NH2	2.52	0.43
21:R:69:GLY:O	21:R:90:ARG:HD2	2.19	0.43
30:A:2632:C:H2'	30:A:2633:U:O4'	2.18	0.43
3:2:34:ARG:CZ	3:2:39:ARG:HD3	2.48	0.43
13:J:39:LYS:HD2	13:J:44:TYR:CE1	2.54	0.43
16:M:50:ARG:HA	16:M:53:MET:HE2	1.99	0.43
29:Z:40:THR:HG22	29:Z:42:CYS:H	1.83	0.43
30:A:242:A:H2'	30:A:243:G:O4'	2.17	0.43
30:A:1544:A:O4'	30:A:1546:G:C8	2.71	0.43
5:4:7:VAL:HG13	5:4:37:GLY:HA2	2.01	0.43
14:K:71:ARG:HH22	14:K:123:LEU:C	2.27	0.43
30:A:1275:U:H2'	30:A:1276:C:C6	2.53	0.43
15:L:108:VAL:HB	15:L:125:LEU:HD22	2.00	0.43
17:N:65:LEU:O	17:N:69:ARG:HG2	2.19	0.43
30:A:13:A:O2'	30:A:15:G:N7	2.45	0.43
30:A:559:G:H2'	30:A:2016:A:N7	2.34	0.43
30:A:818:A:N7	30:A:2233:A:O2'	2.47	0.43
30:A:1945:G:H2'	30:A:1946:A:O4'	2.18	0.43
30:A:2277:U:H2'	30:A:2278:G:C8	2.54	0.43
9:D:155:VAL:O	30:A:2605:C:H5'	2.18	0.43
30:A:1922:A:H2	30:A:1929:U:H3	1.65	0.43
2:1:23:THR:OG1	2:1:24:ASP:N	2.51	0.42
11:G:57:VAL:HB	11:G:60:ALA:HB2	2.00	0.42
13:J:36:LEU:O	13:J:51:GLY:HA3	2.19	0.42
18:O:35:VAL:HG13	18:O:74:VAL:HG21	1.99	0.42
29:Z:15:ARG:O	29:Z:20:LYS:NZ	2.52	0.42
30:A:1612:G:H2'	30:A:1612:G:N3	2.34	0.42
30:A:2253:A:H5''	30:A:2254:A:H5'	2.01	0.42
9:D:68:PHE:CE1	9:D:79:LEU:HD21	2.54	0.42
14:K:58:LEU:HD11	14:K:86:LEU:HB3	1.99	0.42
30:A:85:G:C5	30:A:98:A:C2	3.08	0.42
30:A:190:C:H6	30:A:190:C:O5'	2.02	0.42
30:A:613:C:O2	30:A:646:U:H4'	2.19	0.42
30:A:1623:A:H5'	30:A:1744:C:O2'	2.19	0.42
30:A:2357:G:C6	30:A:2358:U:C5	3.07	0.42
30:A:2673:U:H2'	30:A:2674:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:44:LEU:HD22	17:N:48:VAL:HG23	2.02	0.42
20:Q:33:VAL:HG21	30:A:2005:A:H4'	2.01	0.42
3:2:3:ARG:HH22	30:A:741:A:P	2.41	0.42
5:4:7:VAL:HG22	5:4:37:GLY:HA3	2.02	0.42
8:C:145:LEU:HD11	8:C:153:LEU:HD21	2.01	0.42
17:N:32:GLU:HB3	17:N:118:ARG:HD2	2.02	0.42
20:Q:80:ASN:ND2	20:Q:84:LYS:HE2	2.35	0.42
7:B:26:C:H2'	7:B:27:C:O4'	2.19	0.42
24:U:11:ILE:CG2	24:U:79:ALA:HB2	2.49	0.42
30:A:1837:A:N1	30:A:2073:G:H1'	2.35	0.42
30:A:2300:G:H2'	30:A:2301:U:C6	2.54	0.42
1:0:3:GLN:HA	30:A:2601:U:C2	2.55	0.42
28:Y:39:GLN:O	28:Y:42:THR:HG22	2.19	0.42
30:A:2835:U:C6	30:A:2853:G:N2	2.88	0.42
30:A:2838:G:H2'	30:A:2839:C:O4'	2.19	0.42
13:J:24:THR:O	13:J:25:LEU:C	2.63	0.42
30:A:712:C:H2'	30:A:713:U:O4'	2.20	0.42
17:N:105:GLY:HA3	30:A:1271:A:N7	2.35	0.42
27:X:67:LEU:HD12	27:X:70:MET:CE	2.50	0.42
30:A:2828:G:H2'	30:A:2829:G:O4'	2.20	0.42
11:G:23:ILE:HG12	11:G:42:ILE:HD13	2.01	0.42
26:W:52:ASP:CG	26:W:54:THR:HG1	2.28	0.42
30:A:1576:U:H2'	30:A:1577:G:O4'	2.20	0.41
30:A:2273:A:N3	30:A:2273:A:H2'	2.35	0.41
16:M:13:GLN:HB3	30:A:942:G:H5''	2.02	0.41
22:S:7:HIS:HB2	22:S:50:VAL:HG22	2.02	0.41
30:A:751:U:H4'	30:A:752:G:O5'	2.19	0.41
30:A:1341:C:H2'	30:A:1342:G:O4'	2.20	0.41
30:A:1864:G:H2'	30:A:1865:C:O4'	2.19	0.41
30:A:263:A:N1	30:A:416:U:O2'	2.51	0.41
30:A:1770:A:H1'	30:A:1924:A:N6	2.36	0.41
30:A:2314:A:H2'	30:A:2315:U:C6	2.55	0.41
7:B:29:A:H2'	7:B:30:C:O4'	2.21	0.41
22:S:89:ALA:HB1	30:A:737:G:C8	2.55	0.41
30:A:219:A:N1	30:A:263:A:O2'	2.49	0.41
30:A:1842:A:H61	30:A:1870:G:H1'	1.85	0.41
8:C:164:VAL:HG11	8:C:180:MET:HE1	2.01	0.41
24:U:82:ILE:CG2	24:U:93:ARG:HB3	2.50	0.41
30:A:950:G:H21	30:A:2236:G:H1	1.67	0.41
30:A:1875:A:H2'	30:A:1876:A:O4'	2.20	0.41
30:A:2805:G:H2'	30:A:2807:A:N7	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:74:GLN:O	19:P:75:THR:C	2.64	0.41
30:A:1037:A:C2	30:A:2737:G:C4	3.08	0.41
30:A:1982:C:H4'	30:A:1983:C:OP1	2.20	0.41
30:A:2632:C:OP2	30:A:2718:G:O2'	2.36	0.41
16:M:110:GLU:OE2	16:M:114:ARG:NH1	2.53	0.41
19:P:17:PRO:HG3	19:P:83:ILE:O	2.21	0.41
23:T:61:LEU:HD12	23:T:61:LEU:C	2.45	0.41
30:A:1548:U:H2'	30:A:1549:U:O4'	2.21	0.41
9:D:148:GLN:HE21	9:D:148:GLN:HB2	1.71	0.41
25:V:44:HIS:NE2	25:V:48:VAL:HG21	2.35	0.41
30:A:65:C:O2'	30:A:445:C:N3	2.51	0.41
30:A:802:U:H2'	30:A:803:C:C6	2.56	0.41
30:A:808:A:C4	30:A:1173:A:C2	3.09	0.41
30:A:2733:G:C2	30:A:2742:U:C5	3.09	0.41
9:D:155:VAL:HG21	30:A:2604:G:H21	1.86	0.41
10:E:100:TYR:CZ	10:E:104:MET:HE3	2.56	0.41
16:M:64:TRP:HB2	16:M:104:GLU:HB2	2.03	0.41
27:X:2:ARG:C	27:X:32:LEU:HD11	2.46	0.41
30:A:243:G:O2'	30:A:373:A:N1	2.49	0.41
30:A:818:A:N7	30:A:2234:C:H5'	2.36	0.41
30:A:1519:C:C2	30:A:1524:G:C6	3.09	0.41
30:A:1723:A:H2'	30:A:1724:G:O4'	2.21	0.41
30:A:2450:G:H2'	30:A:2451:C:O4'	2.21	0.41
3:2:3:ARG:HA	3:2:3:ARG:HD3	1.93	0.41
8:C:27:LYS:NZ	30:A:1554:G:N7	2.63	0.41
26:W:33:ILE:HG21	26:W:76:VAL:HG11	2.03	0.41
27:X:29:LEU:HD12	30:A:2216:G:H5''	2.03	0.41
30:A:194:A:H2'	30:A:194:A:N3	2.35	0.41
30:A:687:C:O2'	30:A:723:A:N6	2.54	0.41
30:A:1704:U:H2'	30:A:1705:G:O4'	2.21	0.41
11:G:82:PHE:CE2	11:G:137:LYS:HB2	2.56	0.40
13:J:114:LEU:O	13:J:117:ALA:HB3	2.20	0.40
24:U:98:ASN:HB3	24:U:100:GLU:HG2	2.02	0.40
30:A:933:A:C4	30:A:2434:A:C2	3.10	0.40
11:G:16:VAL:HG11	11:G:49:LEU:HD11	2.04	0.40
24:U:80:ASP:OD2	24:U:95:PHE:HB3	2.21	0.40
27:X:63:ILE:HG13	27:X:67:LEU:HD13	2.03	0.40
30:A:1430:C:H2'	30:A:1431:C:C6	2.56	0.40
30:A:1432:U:H2'	30:A:1433:G:O4'	2.22	0.40
30:A:2377:G:N2	30:A:2415:G:O4'	2.55	0.40
10:E:47:THR:HG22	10:E:85:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:38:ILE:HG22	24:U:39:ASN:N	2.36	0.40
30:A:74:A:H4'	30:A:75:G:O5'	2.21	0.40
30:A:271:A:H2'	30:A:272:G:O4'	2.21	0.40
30:A:2072:U:H2'	30:A:2073:G:C8	2.57	0.40
9:D:56:LYS:HD2	9:D:59:ARG:HG3	2.04	0.40
9:D:109:VAL:O	9:D:171:THR:HA	2.22	0.40
11:G:171:LYS:NZ	30:A:2516:A:N7	2.64	0.40
14:K:22:ILE:HD12	30:A:1938:A:C5	2.56	0.40
15:L:132:LYS:HG3	15:L:142:ILE:HD13	2.02	0.40
22:S:1:MET:SD	22:S:1:MET:C	3.04	0.40
23:T:19:LYS:NZ	30:A:1324:U:OP1	2.48	0.40
30:A:1695:U:H2'	30:A:1696:C:O4'	2.22	0.40
30:A:2248:U:OP1	30:A:2373:U:O2'	2.32	0.40
30:A:2836:A:N7	30:A:2854:A:O2'	2.52	0.40
10:E:148:VAL:HB	10:E:187:MET:HG2	2.03	0.40
14:K:63:VAL:HG12	14:K:107:LEU:HD11	2.04	0.40
29:Z:18:LYS:HG2	30:A:839:C:H5''	2.03	0.40
30:A:205:A:H2'	30:A:206:C:O4'	2.22	0.40
30:A:390:A:C2	30:A:391:A:C4	3.09	0.40
30:A:1900:C:O2	30:A:1900:C:O4'	2.39	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	0	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
2	1	52/56 (93%)	50 (96%)	2 (4%)	0	100	100
3	2	42/44 (96%)	42 (100%)	0	0	100	100
4	3	61/64 (95%)	59 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
6	9	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
8	C	270/274 (98%)	255 (94%)	15 (6%)	0	100	100
9	D	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
10	E	198/200 (99%)	197 (100%)	1 (0%)	0	100	100
11	G	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
12	H	38/150 (25%)	36 (95%)	2 (5%)	0	100	100
13	J	140/142 (99%)	134 (96%)	5 (4%)	1 (1%)	19	42
14	K	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	16	38
15	L	141/144 (98%)	135 (96%)	5 (4%)	1 (1%)	19	42
16	M	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
17	N	118/126 (94%)	113 (96%)	5 (4%)	0	100	100
18	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
19	P	112/117 (96%)	109 (97%)	3 (3%)	0	100	100
20	Q	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
21	R	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
23	T	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
24	U	92/105 (88%)	87 (95%)	5 (5%)	0	100	100
25	V	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
26	W	76/85 (89%)	72 (95%)	4 (5%)	0	100	100
27	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Y	60/63 (95%)	57 (95%)	2 (3%)	1 (2%)	7	20
29	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
All	All	2885/3100 (93%)	2780 (96%)	101 (4%)	4 (0%)	50	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	Y	3	ALA
13	J	44	TYR
14	K	5	GLN
15	L	29	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	43/46 (94%)	41 (95%)	2 (5%)	22	49
2	1	47/49 (96%)	47 (100%)	0	100	100
3	2	36/36 (100%)	35 (97%)	1 (3%)	38	68
4	3	52/53 (98%)	51 (98%)	1 (2%)	52	79
5	4	34/34 (100%)	34 (100%)	0	100	100
6	9	17/17 (100%)	17 (100%)	0	100	100
8	C	218/220 (99%)	217 (100%)	1 (0%)	86	95
9	D	162/162 (100%)	160 (99%)	2 (1%)	67	86
10	E	161/161 (100%)	154 (96%)	7 (4%)	25	52
11	G	135/136 (99%)	133 (98%)	2 (2%)	60	83
12	H	31/112 (28%)	30 (97%)	1 (3%)	34	63
13	J	117/117 (100%)	109 (93%)	8 (7%)	13	32
14	K	104/104 (100%)	103 (99%)	1 (1%)	73	89
15	L	105/106 (99%)	101 (96%)	4 (4%)	28	56
16	M	110/111 (99%)	107 (97%)	3 (3%)	40	69
17	N	99/102 (97%)	97 (98%)	2 (2%)	50	78
18	O	83/84 (99%)	81 (98%)	2 (2%)	44	73
19	P	97/100 (97%)	94 (97%)	3 (3%)	35	64
20	Q	89/90 (99%)	88 (99%)	1 (1%)	70	87
21	R	85/85 (100%)	83 (98%)	2 (2%)	44	73
22	S	90/90 (100%)	87 (97%)	3 (3%)	33	62
23	T	79/83 (95%)	75 (95%)	4 (5%)	20	45
24	U	74/81 (91%)	71 (96%)	3 (4%)	26	54
25	V	77/77 (100%)	74 (96%)	3 (4%)	27	56
26	W	62/66 (94%)	59 (95%)	3 (5%)	21	48
27	X	67/68 (98%)	66 (98%)	1 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	Y	52/53 (98%)	47 (90%)	5 (10%)	7	17
29	Z	52/52 (100%)	50 (96%)	2 (4%)	28	56
All	All	2378/2495 (95%)	2311 (97%)	67 (3%)	40	68

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	40	ASN
1	0	53	ILE
3	2	43	SER
4	3	6	ASN
8	C	218	THR
9	D	110	THR
9	D	148	GLN
10	E	79	SER
10	E	116	ARG
10	E	125	VAL
10	E	137	LEU
10	E	142	LEU
10	E	175	ASP
10	E	195	VAL
11	G	55	GLU
11	G	61	TRP
12	H	19	VAL
13	J	1	MET
13	J	5	VAL
13	J	9	GLU
13	J	31	GLU
13	J	64	VAL
13	J	106	LYS
13	J	113	PRO
13	J	142	ILE
14	K	19	VAL
15	L	14	THR
15	L	19	VAL
15	L	60	ARG
15	L	121	THR
16	M	30	GLU
16	M	124	LEU
16	M	135	VAL
17	N	15	SER

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Mol	Chain	Res	Type
17	N	44	LEU
18	O	47	VAL
18	O	112	GLU
19	P	5	LYS
19	P	80	VAL
19	P	102	ARG
20	Q	17	LEU
21	R	14	VAL
21	R	19	THR
22	S	29	VAL
22	S	92	ARG
22	S	100	SER
23	T	10	VAL
23	T	18	GLU
23	T	25	GLU
23	T	37	ASP
24	U	6	ARG
24	U	26	LYS
24	U	69	VAL
25	V	74	GLN
25	V	84	LYS
25	V	93	ILE
26	W	14	SER
26	W	37	ARG
26	W	51	LYS
27	X	55	MET
28	Y	4	GLN
28	Y	5	ASP
28	Y	11	VAL
28	Y	13	GLU
28	Y	18	LEU
29	Z	54	VAL
29	Z	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	6	ASN
8	C	36	ASN
8	C	39	ASN
8	C	272	ASN
9	D	102	ASN

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Mol	Chain	Res	Type
9	D	148	GLN
9	D	150	GLN
9	D	173	GLN
10	E	93	GLN
10	E	162	ASN
11	G	37	ASN
11	G	138	GLN
14	K	34	HIS
19	P	40	GLN
19	P	65	ASN
22	S	31	GLN
22	S	70	ASN
23	T	59	ASN
25	V	74	GLN
27	X	35	HIS
28	Y	15	ASN
28	Y	25	GLN
28	Y	31	GLN
28	Y	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	A	2712/2721 (99%)	383 (14%)	54 (1%)
7	B	120/121 (99%)	18 (15%)	3 (2%)
All	All	2832/2842 (99%)	401 (14%)	57 (2%)

All (401) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	B	2	G
7	B	3	C
7	B	17	C
7	B	25	A
7	B	26	C
7	B	35	C
7	B	36	U
7	B	37	U
7	B	38	C
7	B	45	G
7	B	46	A

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Mol	Chain	Res	Type
7	B	57	G
7	B	88	U
7	B	90	U
7	B	91	C
7	B	109	C
7	B	110	A
7	B	121	A
30	A	10	A
30	A	12	U
30	A	34	U
30	A	46	G
30	A	71	A
30	A	74	A
30	A	75	G
30	A	84	A
30	A	93	A
30	A	96	C
30	A	101	U
30	A	102	G
30	A	103	A
30	A	118	A
30	A	119	A
30	A	120	U
30	A	125	A
30	A	126	A
30	A	136	C
30	A	137	A
30	A	155	G
30	A	156	U
30	A	160	U
30	A	161	A
30	A	179	A
30	A	194	A
30	A	197	A
30	A	198	U
30	A	211	A
30	A	213	G
30	A	214	A
30	A	219	A
30	A	220	A
30	A	246	G
30	A	247	C

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Mol	Chain	Res	Type
30	A	253	A
30	A	263	A
30	A	264	G
30	A	268	U
30	A	269	U
30	A	270	A
30	A	272	G
30	A	277	A
30	A	278	C
30	A	279	A
30	A	280	C
30	A	281	A
30	A	286	A
30	A	303	A
30	A	309	A
30	A	321	G
30	A	322	A
30	A	323	U
30	A	337	A
30	A	338	C
30	A	346	G
30	A	348	U
30	A	349	C
30	A	350	A
30	A	354	A
30	A	356	A
30	A	360	A
30	A	361	G
30	A	375	G
30	A	376	U
30	A	377	G
30	A	393	A
30	A	394	U
30	A	395	G
30	A	398	G
30	A	400	G
30	A	401	A
30	A	409	C
30	A	423	U
30	A	424	A
30	A	440	U
30	A	445	C

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Mol	Chain	Res	Type
30	A	470	G
30	A	479	U
30	A	480	G
30	A	494	A
30	A	498	C
30	A	519	G
30	A	520	C
30	A	521	A
30	A	522	G
30	A	532	G
30	A	533	C
30	A	539	C
30	A	552	A
30	A	562	U
30	A	564	A
30	A	569	U
30	A	575	A
30	A	592	A
30	A	602	U
30	A	603	C
30	A	616	A
30	A	626	A
30	A	634	C
30	A	635	U
30	A	636	G
30	A	642	U
30	A	643	C
30	A	644	A
30	A	674	A
30	A	675	U
30	A	701	A
30	A	706	C
30	A	718	G
30	A	719	A
30	A	736	U
30	A	753	A
30	A	754	C
30	A	760	G
30	A	764	G
30	A	765	G
30	A	771	A
30	A	773	G

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Mol	Chain	Res	Type
30	A	774	G
30	A	782	A
30	A	794	G
30	A	801	C
30	A	808	A
30	A	816	U
30	A	817	U
30	A	847	G
30	A	855	A
30	A	868	G
30	A	899	A
30	A	903	C
30	A	920	C
30	A	929	A
30	A	934	C
30	A	949	C
30	A	956	C
30	A	962	G
30	A	971	A
30	A	983	C
30	A	984	A
30	A	987	U
30	A	993	C
30	A	1000	U
30	A	1009	G
30	A	1013	G
30	A	1020	U
30	A	1027	A
30	A	1034	G
30	A	1098	A
30	A	1099	G
30	A	1117	U
30	A	1119	U
30	A	1120	A
30	A	1121	A
30	A	1122	C
30	A	1123	G
30	A	1126	G
30	A	1129	A
30	A	1130	A
30	A	1156	C
30	A	1164	G

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Mol	Chain	Res	Type
30	A	1190	G
30	A	1232	G
30	A	1237	A
30	A	1240	G
30	A	1255	G
30	A	1256	A
30	A	1270	A
30	A	1271	A
30	A	1284	G
30	A	1285	A
30	A	1286	A
30	A	1305	A
30	A	1310	U
30	A	1311	A
30	A	1329	C
30	A	1336	U
30	A	1349	A
30	A	1362	A
30	A	1363	U
30	A	1367	A
30	A	1400	G
30	A	1403	A
30	A	1411	A
30	A	1412	C
30	A	1436	G
30	A	1437	A
30	A	1438	C
30	A	1439	G
30	A	1442	U
30	A	1444	U
30	A	1445	C
30	A	1451	U
30	A	1452	C
30	A	1466	U
30	A	1477	U
30	A	1488	C
30	A	1489	U
30	A	1490	C
30	A	1491	U
30	A	1494	A
30	A	1495	A
30	A	1496	G

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Mol	Chain	Res	Type
30	A	1501	A
30	A	1510	G
30	A	1516	C
30	A	1521	A
30	A	1522	C
30	A	1523	G
30	A	1524	G
30	A	1527	G
30	A	1528	U
30	A	1529	G
30	A	1540	U
30	A	1552	A
30	A	1555	A
30	A	1564	U
30	A	1569	U
30	A	1570	U
30	A	1571	C
30	A	1582	G
30	A	1594	A
30	A	1595	A
30	A	1596	A
30	A	1633	U
30	A	1634	U
30	A	1635	G
30	A	1660	G
30	A	1663	A
30	A	1699	G
30	A	1712	C
30	A	1713	U
30	A	1714	C
30	A	1716	C
30	A	1719	A
30	A	1720	U
30	A	1722	G
30	A	1748	G
30	A	1757	A
30	A	1768	A
30	A	1775	A
30	A	1784	C
30	A	1785	A
30	A	1786	A
30	A	1800	C

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Mol	Chain	Res	Type
30	A	1813	A
30	A	1817	C
30	A	1831	A
30	A	1841	G
30	A	1855	U
30	A	1856	C
30	A	1857	G
30	A	1858	G
30	A	1870	G
30	A	1892	G
30	A	1893	G
30	A	1899	A
30	A	1900	C
30	A	1905	A
30	A	1915	G
30	A	1916	G
30	A	1917	U
30	A	1923	A
30	A	1924	A
30	A	1926	U
30	A	1927	C
30	A	1941	U
30	A	1951	C
30	A	1953	C
30	A	1956	A
30	A	1957	U
30	A	1958	G
30	A	1968	U
30	A	1977	U
30	A	1978	G
30	A	1979	U
30	A	1983	C
30	A	2006	A
30	A	2008	U
30	A	2009	C
30	A	2017	A
30	A	2019	A
30	A	2029	C
30	A	2035	G
30	A	2037	U
30	A	2041	C
30	A	2042	G

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Mol	Chain	Res	Type
30	A	2046	A
30	A	2047	G
30	A	2055	G
30	A	2082	C
30	A	2090	C
30	A	2173	G
30	A	2177	A
30	A	2184	A
30	A	2189	U
30	A	2190	G
30	A	2197	U
30	A	2198	A
30	A	2211	A
30	A	2224	G
30	A	2237	G
30	A	2254	A
30	A	2259	A
30	A	2264	A
30	A	2268	G
30	A	2269	C
30	A	2273	A
30	A	2283	A
30	A	2291	U
30	A	2311	G
30	A	2319	A
30	A	2321	A
30	A	2333	C
30	A	2340	A
30	A	2347	A
30	A	2369	G
30	A	2371	C
30	A	2392	A
30	A	2410	C
30	A	2411	A
30	A	2415	G
30	A	2416	A
30	A	2421	A
30	A	2427	U
30	A	2434	A
30	A	2456	G
30	A	2462	A
30	A	2467	G

Continued on next page...

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Mol	Chain	Res	Type
30	A	2468	A
30	A	2477	U
30	A	2484	C
30	A	2488	G
30	A	2489	A
30	A	2491	G
30	A	2504	A
30	A	2515	G
30	A	2533	A
30	A	2540	U
30	A	2552	A
30	A	2553	G
30	A	2559	C
30	A	2568	G
30	A	2571	U
30	A	2595	U
30	A	2599	U
30	A	2615	U
30	A	2640	A
30	A	2675	U
30	A	2676	U
30	A	2700	G
30	A	2730	G
30	A	2734	A
30	A	2736	A
30	A	2743	A
30	A	2744	A
30	A	2747	G
30	A	2751	A
30	A	2764	A
30	A	2765	U
30	A	2776	U
30	A	2777	G
30	A	2779	U
30	A	2780	A
30	A	2784	U
30	A	2785	A
30	A	2786	A
30	A	2793	U
30	A	2797	G
30	A	2799	G
30	A	2806	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	A	2807	A
30	A	2821	A
30	A	2853	G
30	A	2859	A
30	A	2860	C
30	A	2869	A
30	A	2870	U
30	A	2871	U
30	A	2872	G
30	A	2873	C
30	A	2874	C
30	A	2888	C

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	B	42	U
7	B	45	G
7	B	109	C
30	A	33	U
30	A	125	A
30	A	197	A
30	A	219	A
30	A	269	U
30	A	277	A
30	A	375	G
30	A	376	U
30	A	423	U
30	A	479	U
30	A	537	G
30	A	674	A
30	A	735	U
30	A	753	A
30	A	765	G
30	A	773	G
30	A	961	A
30	A	972	A
30	A	983	C
30	A	1120	A
30	A	1122	C
30	A	1129	A
30	A	1163	A

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Mol	Chain	Res	Type
30	A	1270	A
30	A	1284	G
30	A	1285	A
30	A	1304	C
30	A	1474	A
30	A	1481	U
30	A	1487	U
30	A	1521	A
30	A	1527	G
30	A	1569	U
30	A	1594	A
30	A	1595	A
30	A	1596	A
30	A	1633	U
30	A	1886	A
30	A	1899	A
30	A	1926	U
30	A	1949	U
30	A	2197	U
30	A	2268	G
30	A	2416	A
30	A	2433	G
30	A	2467	G
30	A	2504	A
30	A	2567	G
30	A	2742	U
30	A	2776	U
30	A	2784	U
30	A	2785	A
30	A	2821	A
30	A	2859	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
30	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2291:U	O3'	2298:U	P	16.53
1	A	1157:U	O3'	1163:A	P	16.04
1	A	2091:U	O3'	2171:G	P	14.86
1	A	1037:A	O3'	1097:G	P	14.40
1	A	869:G	O3'	887:C	P	14.30

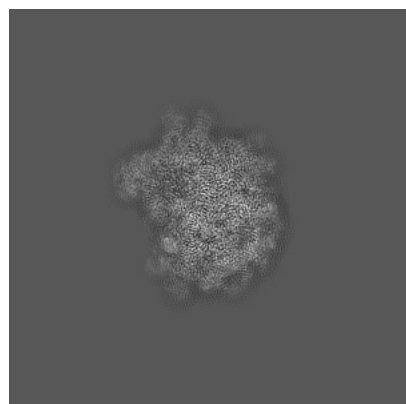
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51947. These allow visual inspection of the internal detail of the map and identification of artifacts.

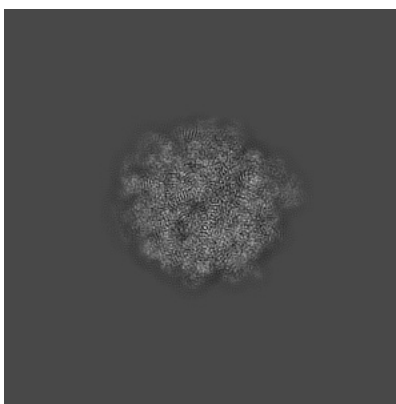
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

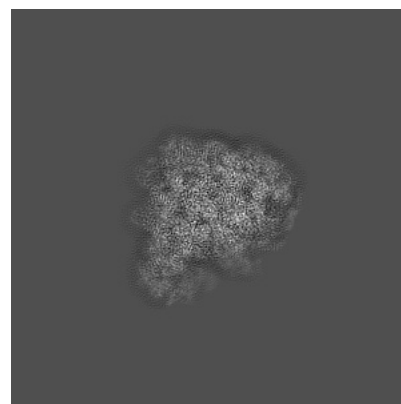
6.1.1 Primary map



X

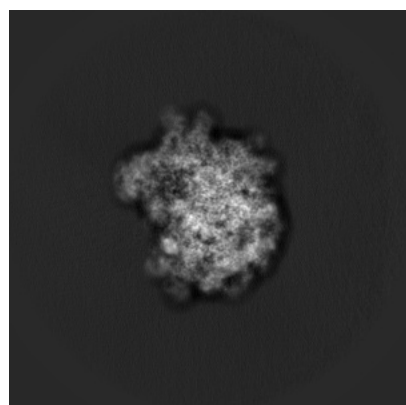


Y

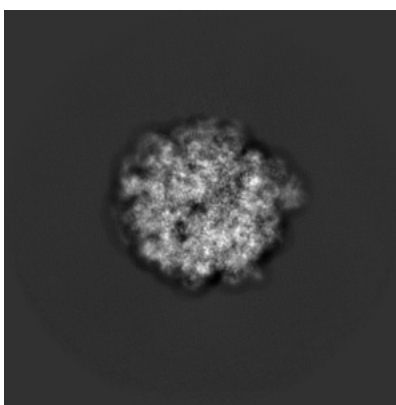


Z

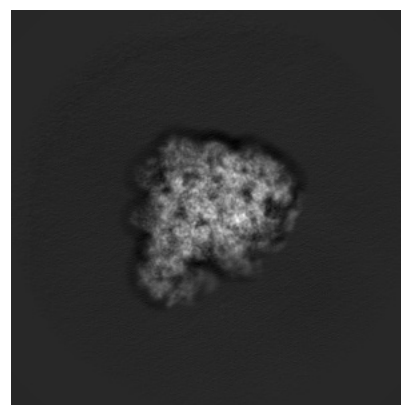
6.1.2 Raw map



X



Y

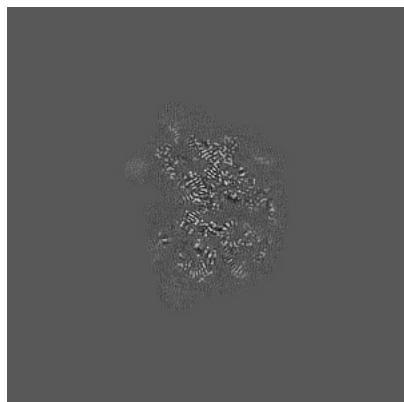


Z

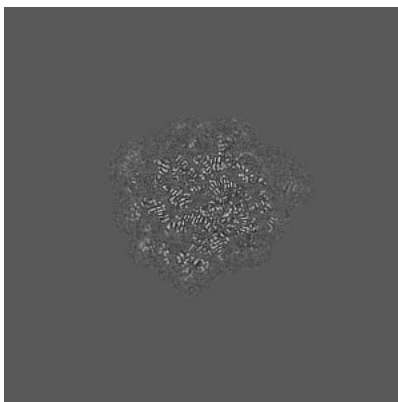
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 208

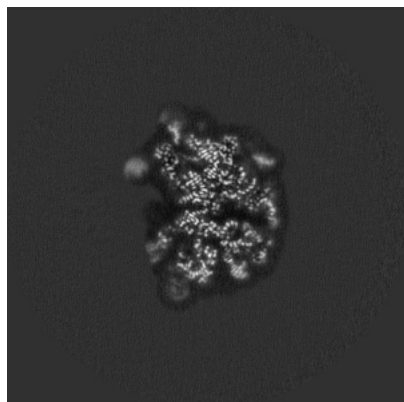


Y Index: 208

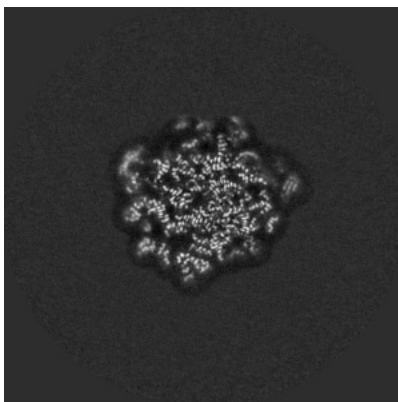


Z Index: 208

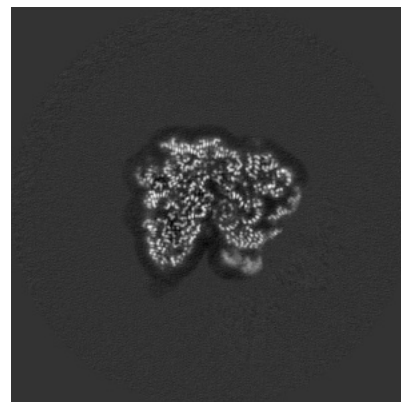
6.2.2 Raw map



X Index: 208



Y Index: 208

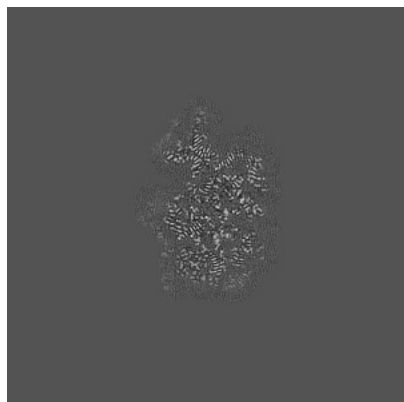


Z Index: 208

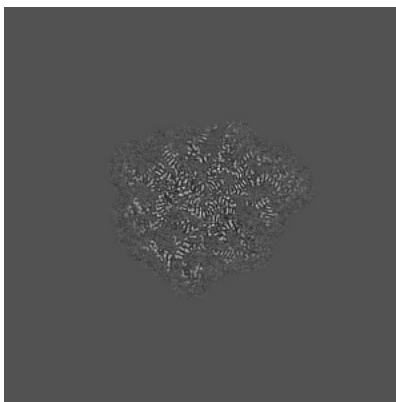
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

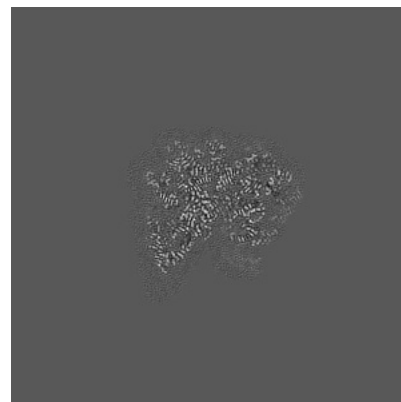
6.3.1 Primary map



X Index: 235

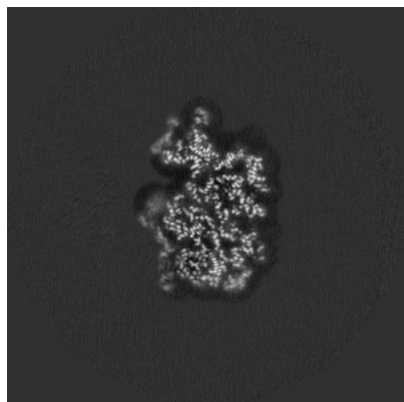


Y Index: 200

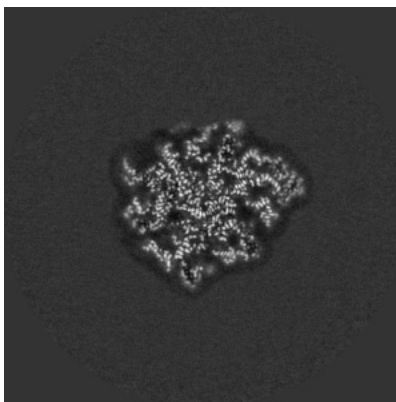


Z Index: 213

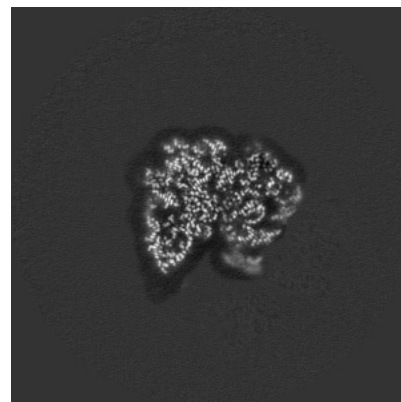
6.3.2 Raw map



X Index: 235



Y Index: 200

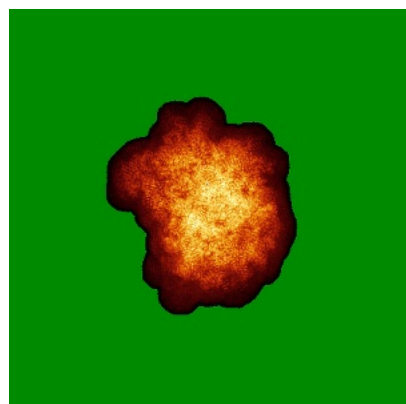


Z Index: 212

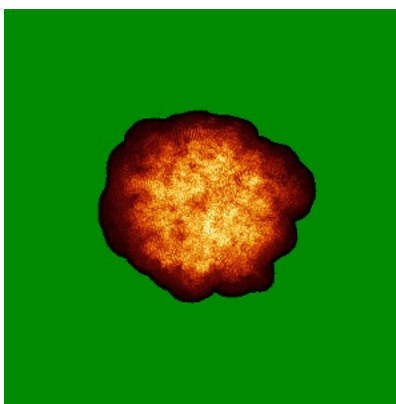
The images above show the largest variance slices of the map in three orthogonal directions.

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

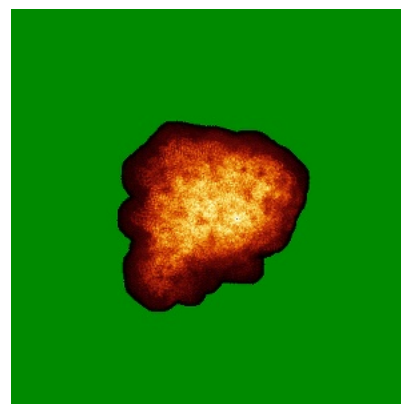
6.4.1 Primary map



X



Y

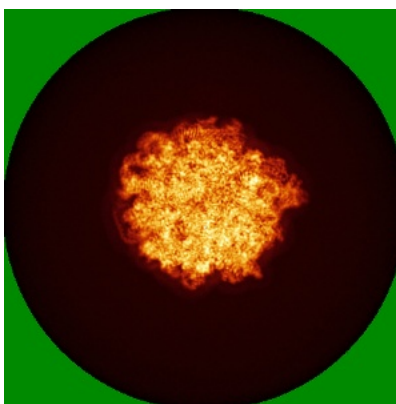


Z

6.4.2 Raw map



X



Y

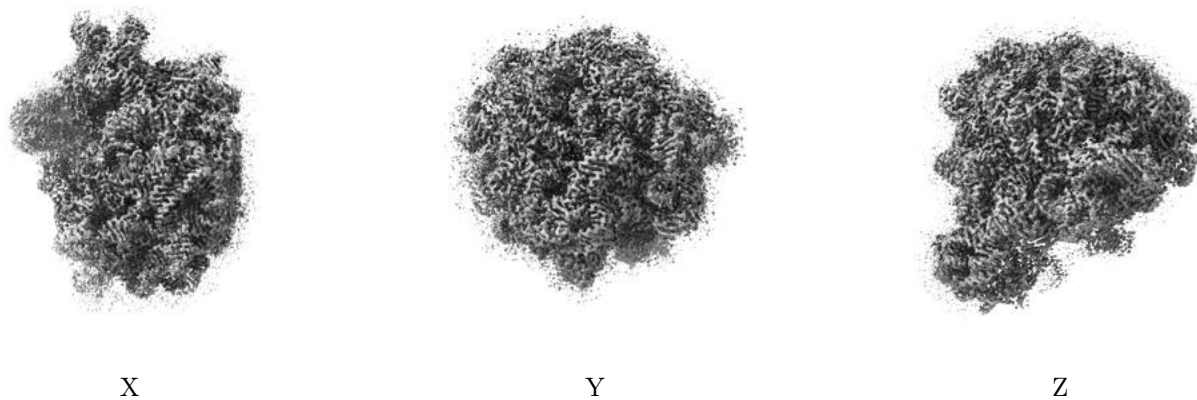


Z

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.

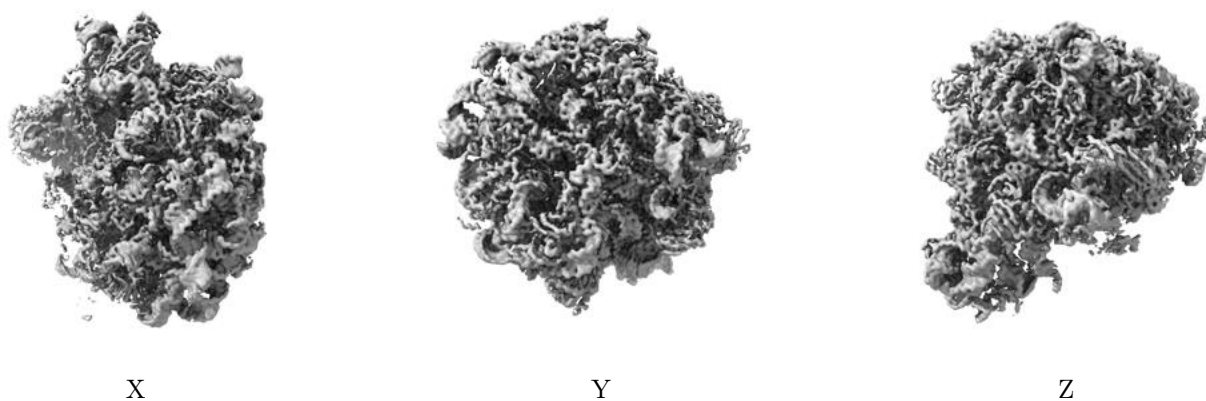
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. 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.

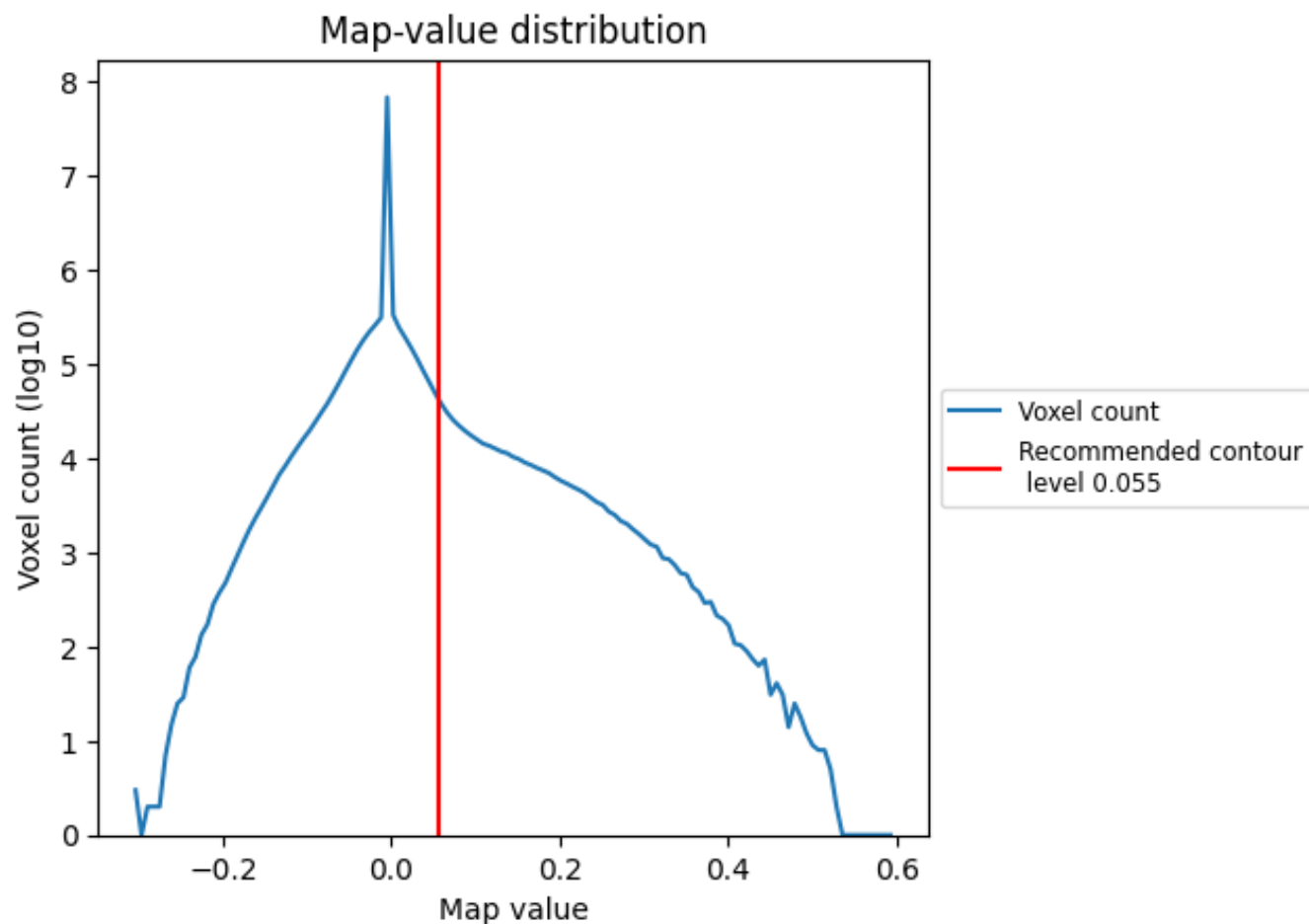
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

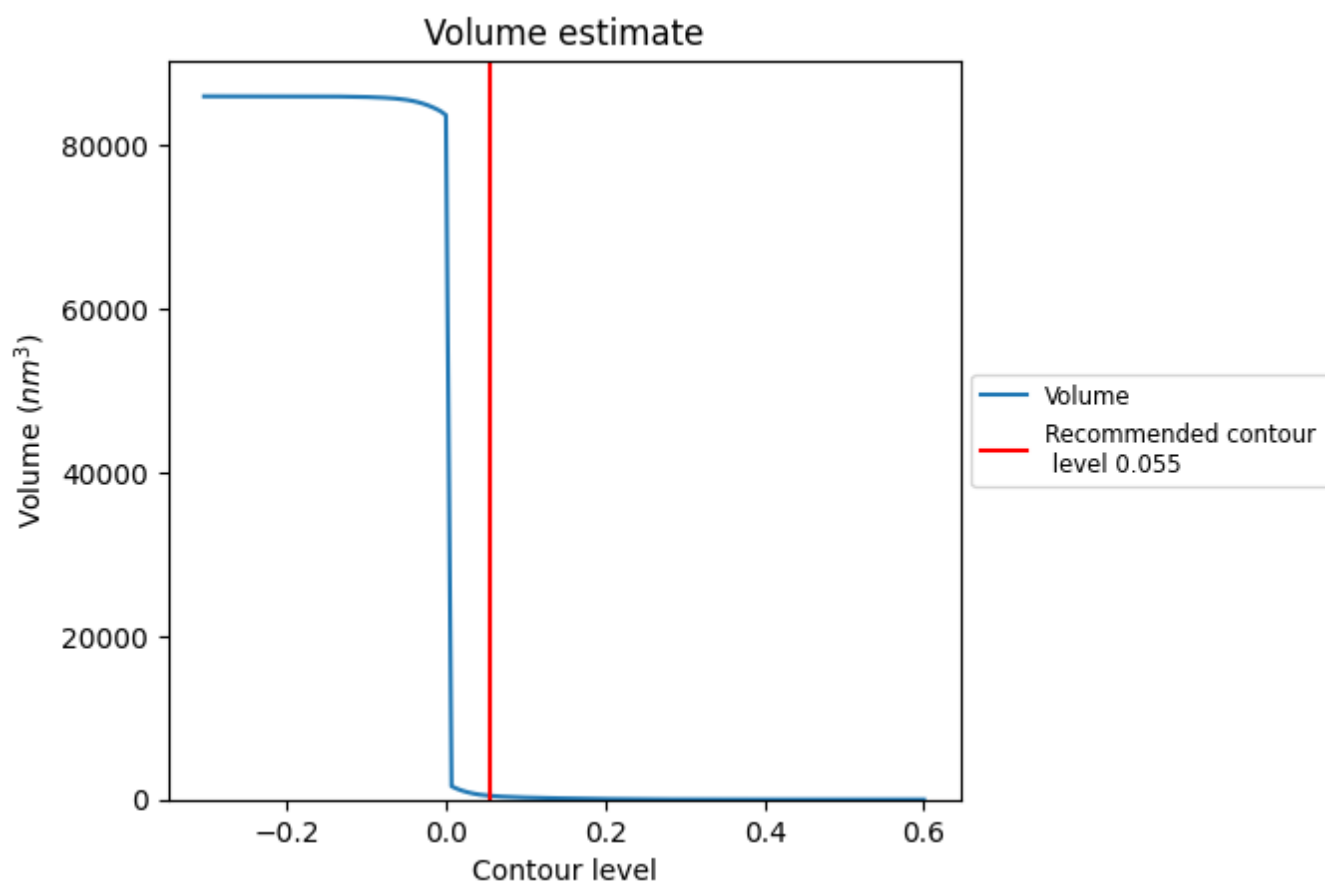
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

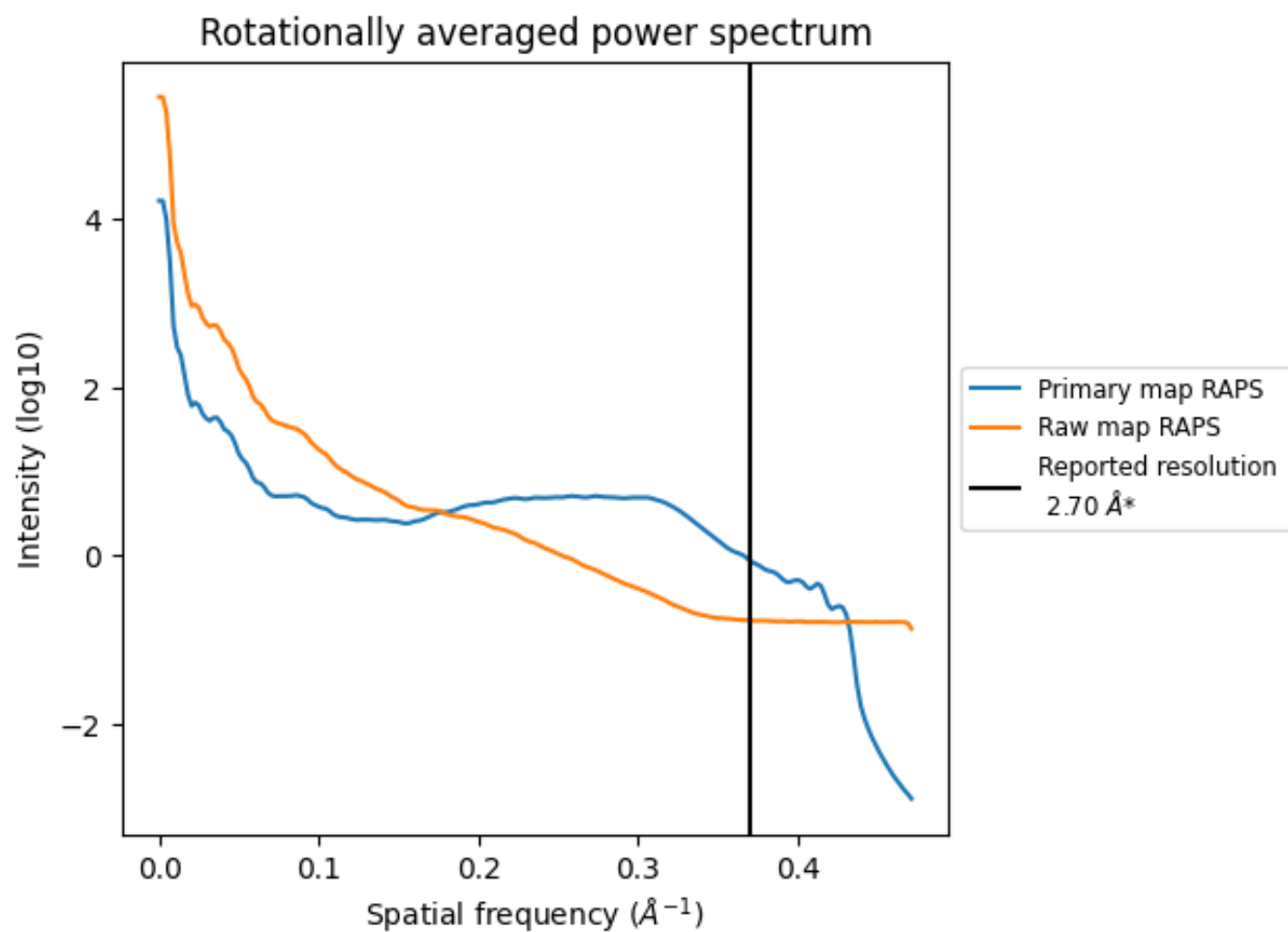
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 462 nm^3 ; this corresponds to an approximate mass of 417 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 ⓘ

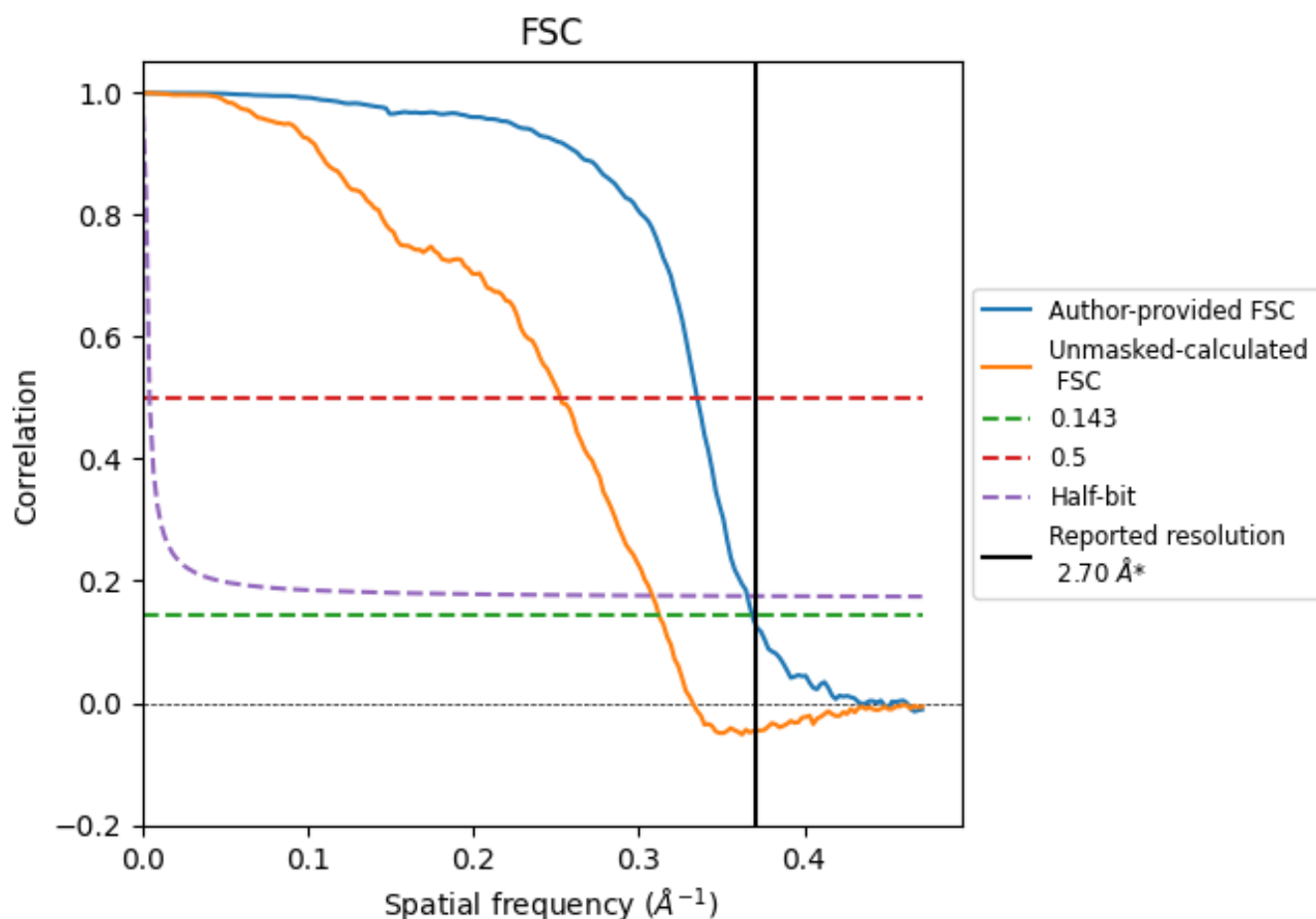


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

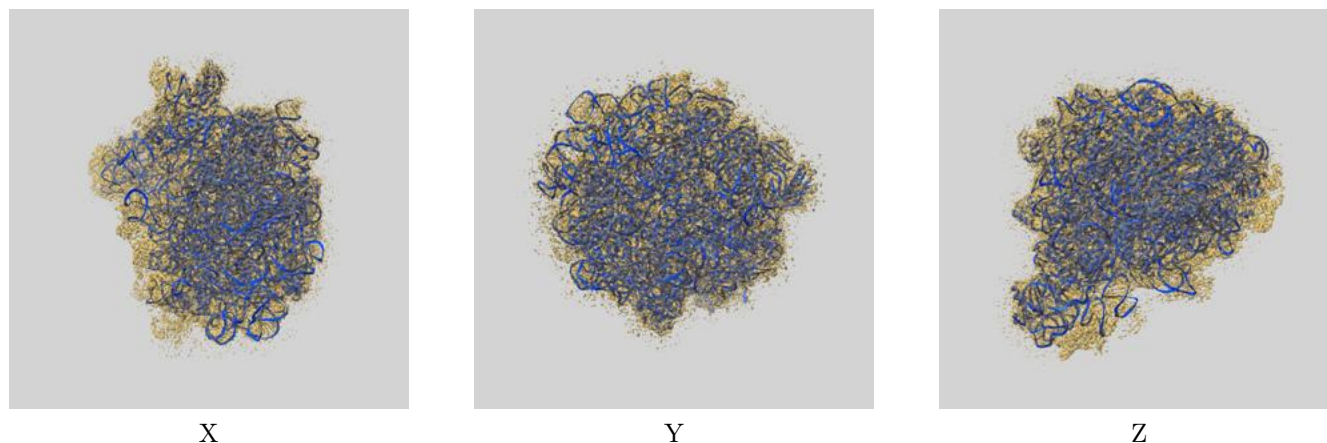
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	2.98	2.73
Unmasked-calculated*	3.20	3.96	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

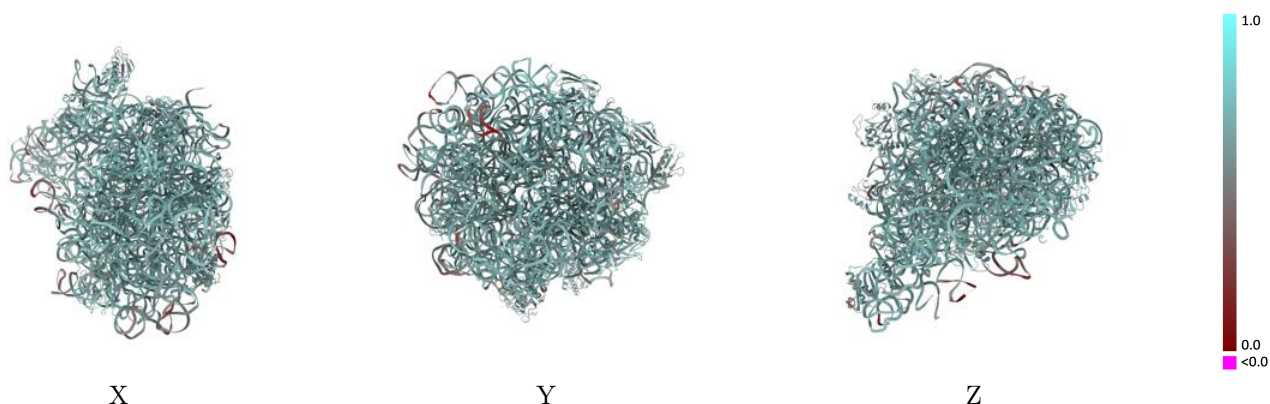
This section contains information regarding the fit between EMDB map EMD-51947 and PDB model 9H91. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



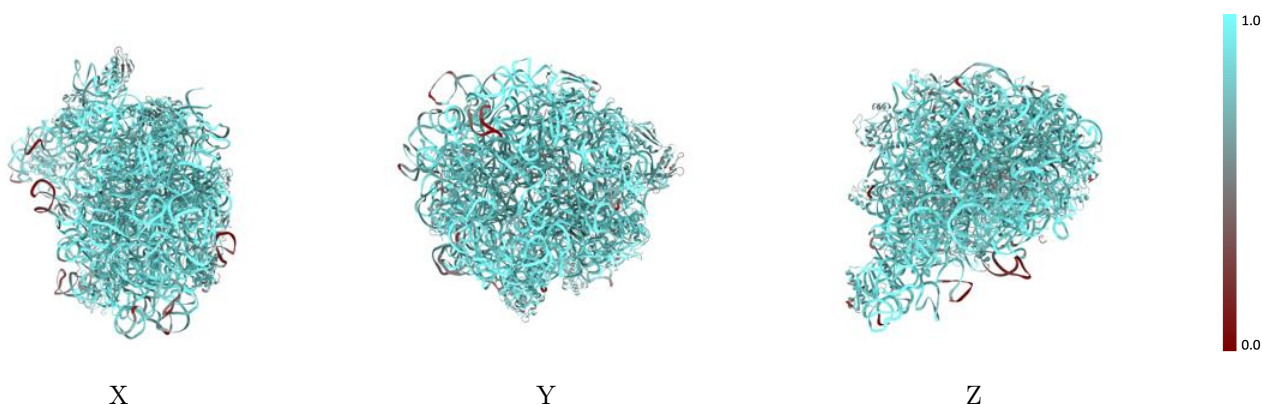
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



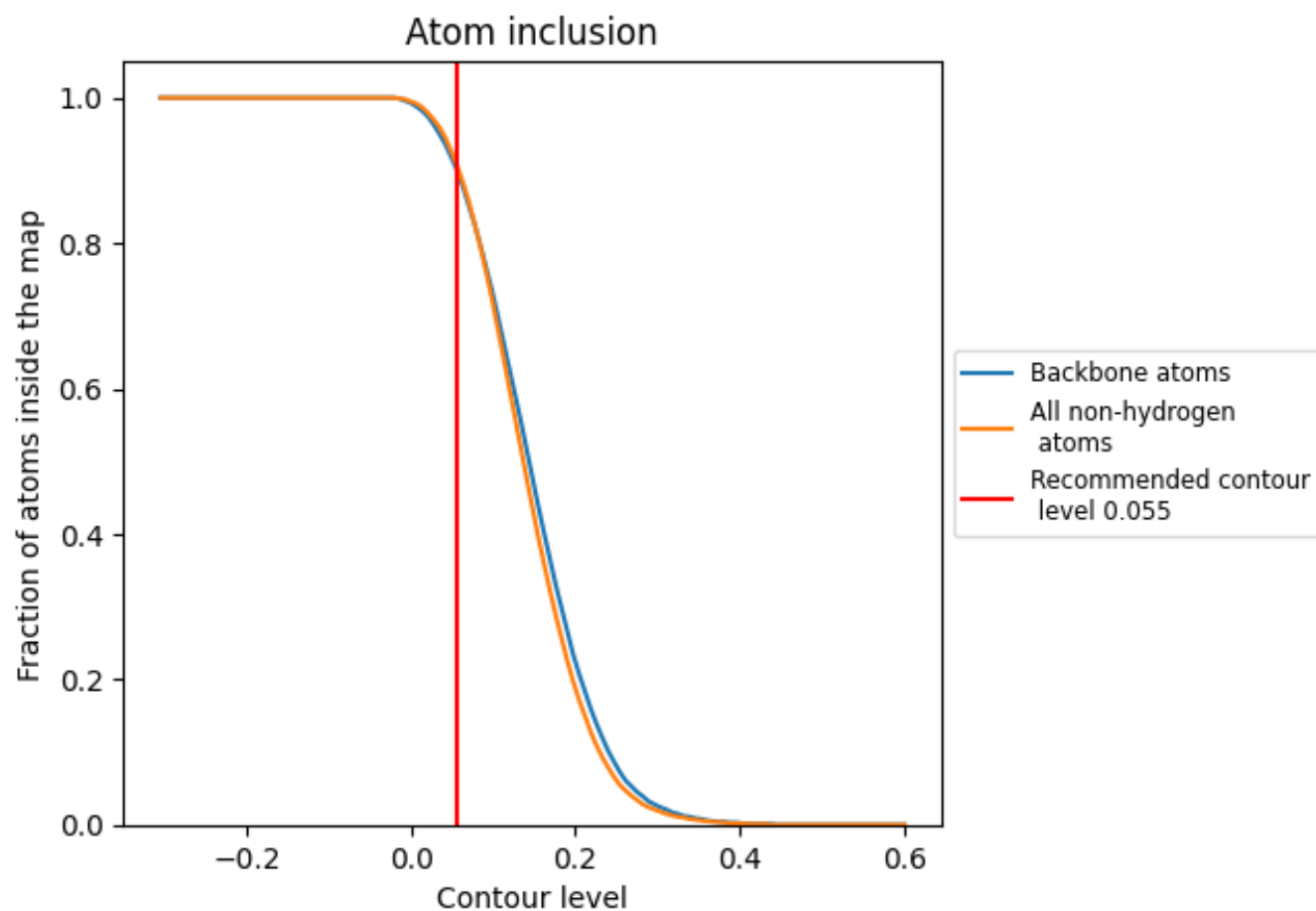
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9110	 0.6400
0	 0.9170	 0.6620
1	 0.8300	 0.6380
2	 0.9420	 0.6720
3	 0.9470	 0.6820
4	 0.9300	 0.6620
9	 0.7550	 0.6090
A	 0.9330	 0.6410
B	 0.8950	 0.6140
C	 0.9170	 0.6660
D	 0.8890	 0.6510
E	 0.8300	 0.6180
G	 0.7060	 0.5830
H	 0.7070	 0.5790
J	 0.8920	 0.6560
K	 0.8930	 0.6500
L	 0.8760	 0.6470
M	 0.8950	 0.6620
N	 0.9210	 0.6640
O	 0.8490	 0.6250
P	 0.8500	 0.6370
Q	 0.9270	 0.6660
R	 0.8580	 0.6310
S	 0.8620	 0.6390
T	 0.7820	 0.6130
U	 0.7800	 0.6060
V	 0.8380	 0.6370
W	 0.8970	 0.6640
X	 0.8810	 0.6510
Y	 0.7500	 0.5840
Z	 0.8620	 0.6340

