



Full wwPDB EM Validation Report ⓘ

May 6, 2026 – 04:56 pm BST

PDB ID : 9TEW / pdb_00009tew
EMDB ID : EMD-55844
Title : DalDro bound to the initiating Escherichia coli 70S ribosome
Authors : Berger, M.J.; Safdari, H.A.; Wilson, D.N.
Deposited on : 2025-11-26
Resolution : 2.90 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:

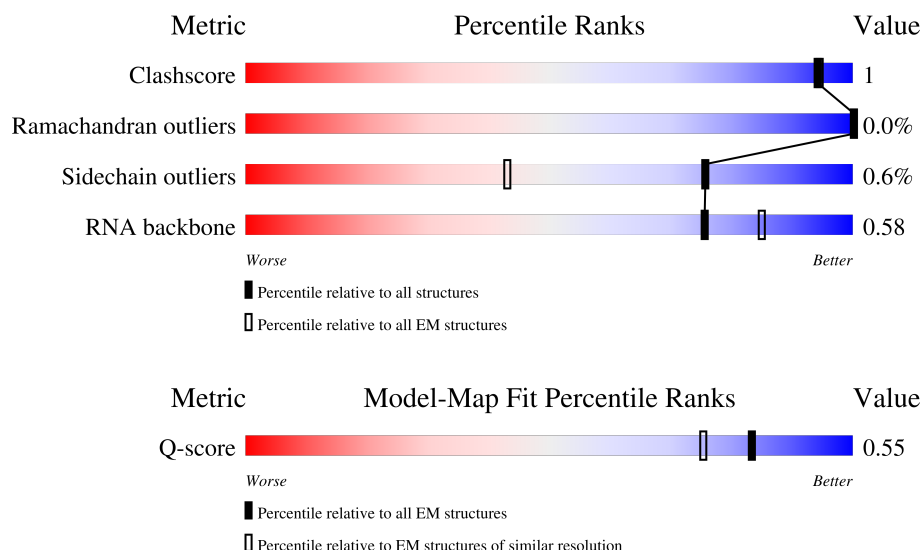
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	K	129	
2	L	124	
3	d	209	

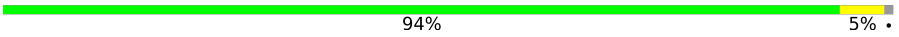
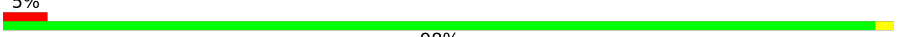

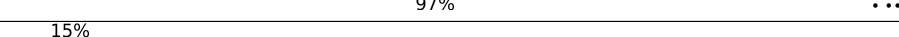


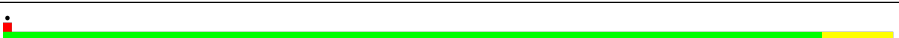
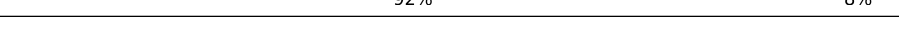
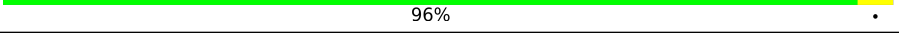
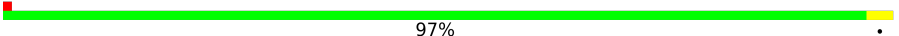

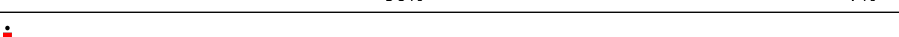
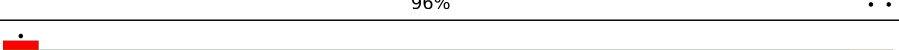
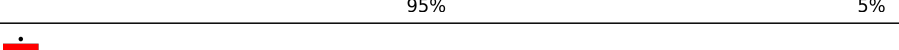
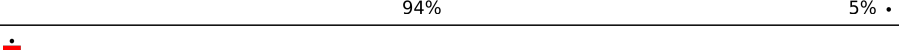

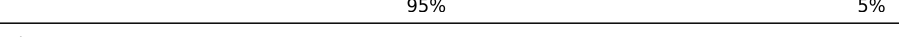
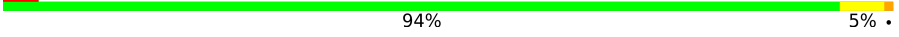






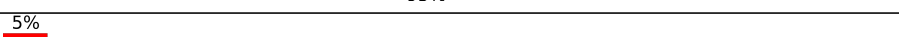
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Mol	Chain	Length	Quality of chain
4	4	70	
5	3	38	
6	a	2904	
7	A	1542	
8	0	55	
9	1	46	
10	2	65	
11	B	241	
12	C	233	
13	D	206	
14	E	167	
15	F	135	
16	H	130	
17	I	130	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	X	3	
27	Z	77	
28	b	120	

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Mol	Chain	Length	Quality of chain
29	c	273	
30	e	201	
31	f	179	
32	g	177	
33	h	149	
34	i	142	
35	j	123	
36	k	144	
37	m	127	
38	n	117	
39	o	115	
40	p	118	
41	q	103	
42	r	110	
43	s	100	
44	t	104	
45	u	94	
46	v	85	
47	w	78	
48	x	63	
49	y	59	
50	z	57	
51	l	136	
52	G	179	
53	J	103	

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Mol	Chain	Length	Quality of chain
54	U	71	<div><div></div><div>28%</div><div></div><div>97%</div><div></div><div>..</div></div>
55	8	20	<div><div></div><div>10%</div><div></div><div>65%</div><div></div><div>15%</div><div></div><div>20%</div></div>

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 139703 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 Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 2 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 3 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 4 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	59	Total	C	N	O	S	0	0
			472	293	89	84	6		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 7 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 8 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	0	49	Total	C	N	O	0	0
			405	261	74	70		

- Molecule 9 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 10 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 11 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 12 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 15 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 16 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 17 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	77	Total	C	N	O	S	0	0
			624	394	117	110	3		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 26 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 27 is a RNA chain called fMet-Initiator P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

- Molecule 28 is a RNA chain called 5s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 29 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 30 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 32 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 33 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 38 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 39 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 44 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	57	Total	C	N	O	S	0	0
			444	278	86	78	2		

- Molecule 50 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	variant	UNP P0ADY7

- Molecule 52 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	G	147	Total	C	N	O	S	0	0
			1164	728	222	210	4		

- Molecule 53 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 54 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 55 is a protein called DalDro.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	8	16	Total	C	N	O	0	0
			131	83	27	21		

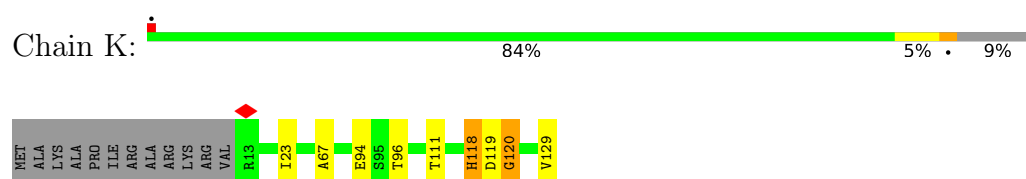
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	4	1	Total	Zn	0
			1	1	
56	3	1	Total	Zn	0
			1	1	

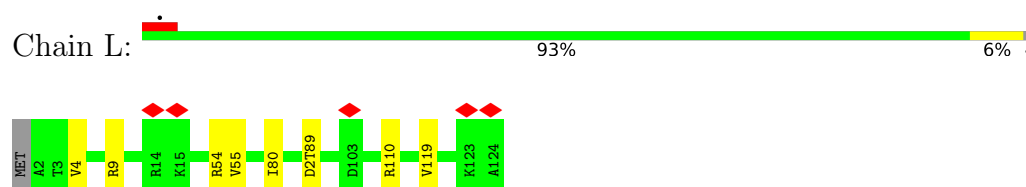
3 Residue-property plots [i](#)

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.

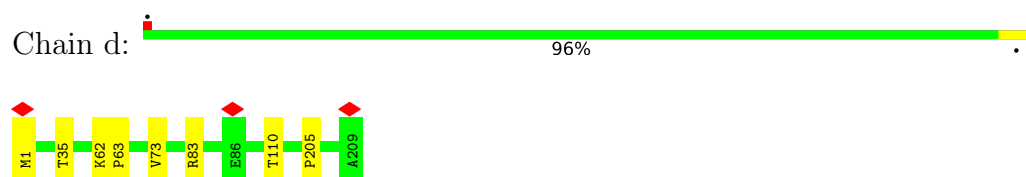
- Molecule 1: Small ribosomal subunit protein uS11



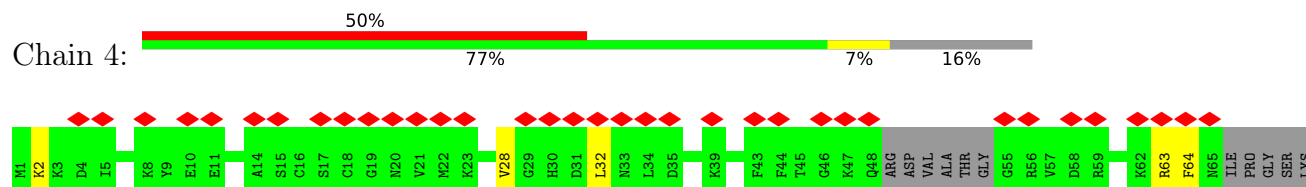
- Molecule 2: Small ribosomal subunit protein uS12



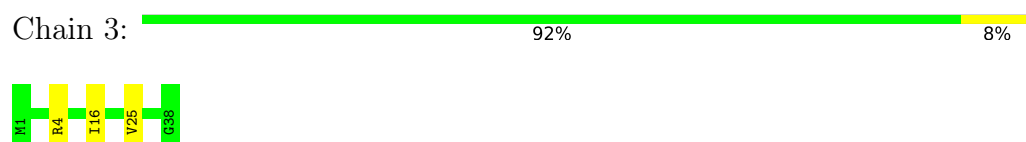
- Molecule 3: Large ribosomal subunit protein uL3



- Molecule 4: Large ribosomal subunit protein bL31A

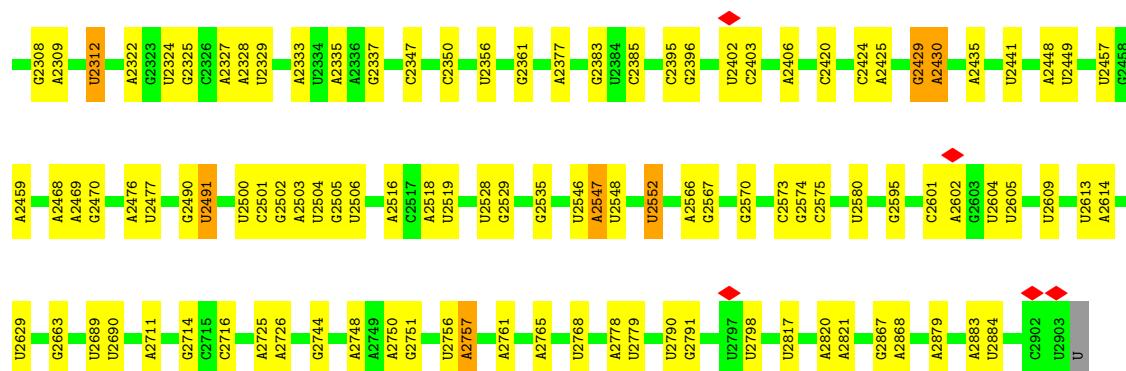


- Molecule 5: Large ribosomal subunit protein bL36A

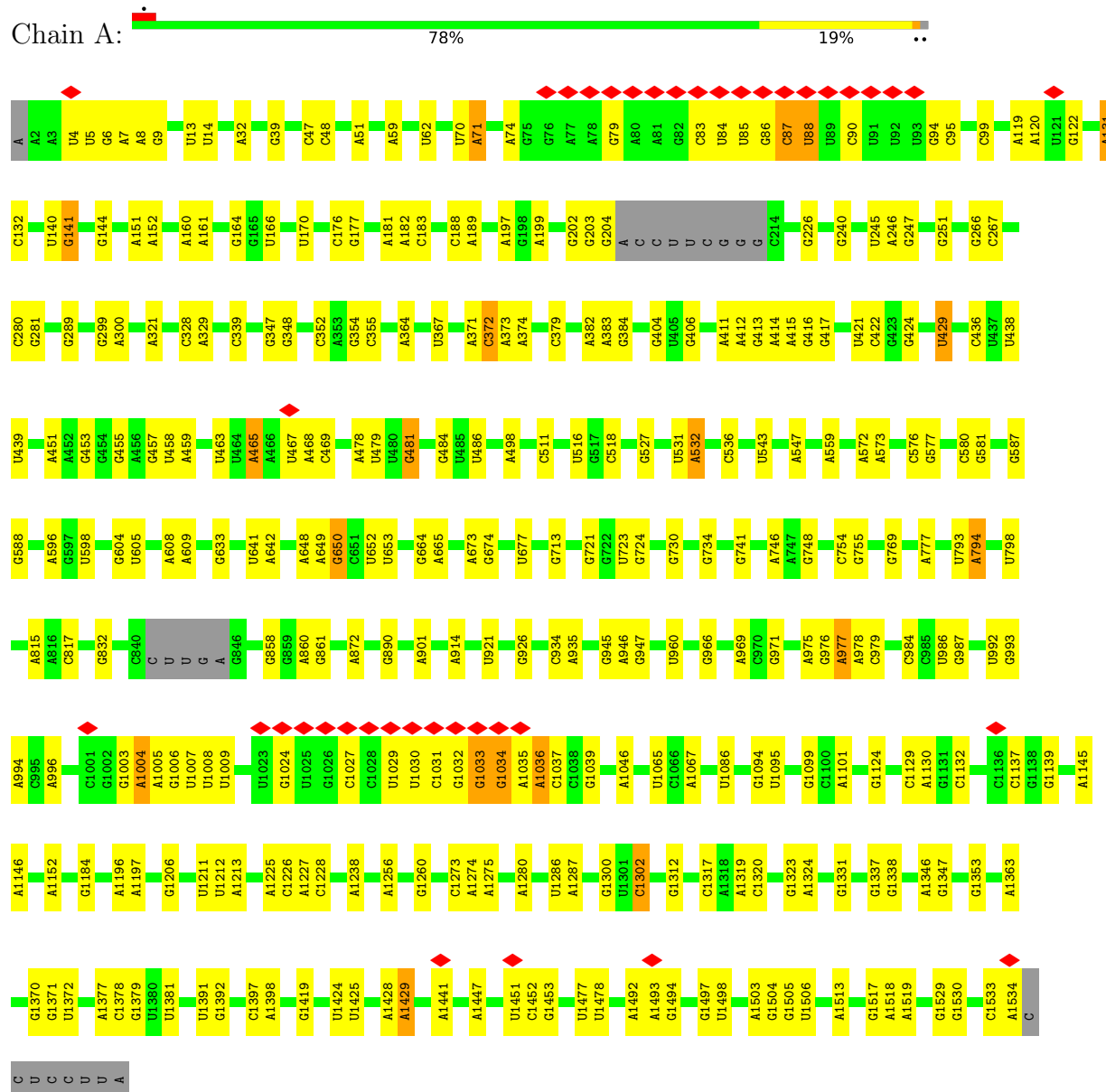


Chain a: 78% 15% 5%

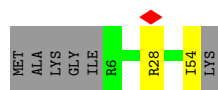
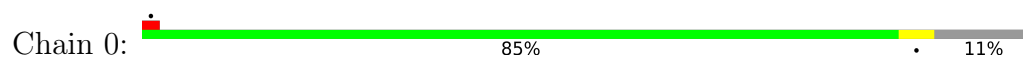




• Molecule 7: 16S rRNA



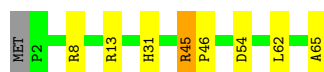
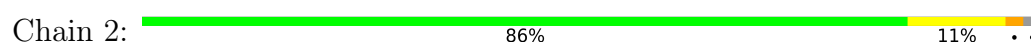
• Molecule 8: Large ribosomal subunit protein bL33



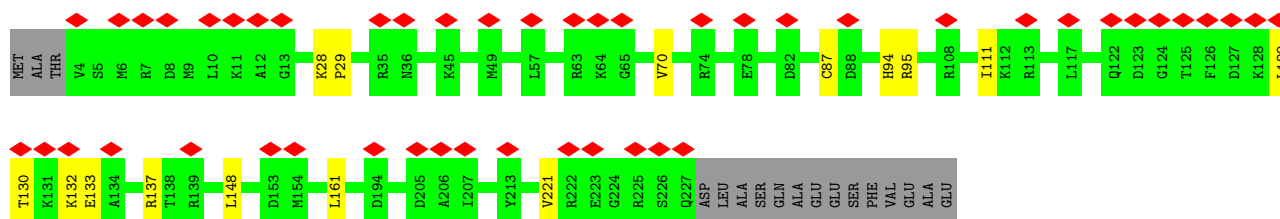
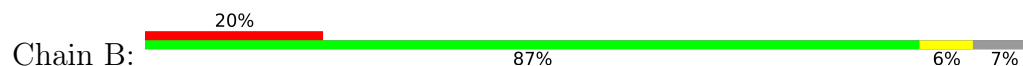
- Molecule 9: Large ribosomal subunit protein bL34



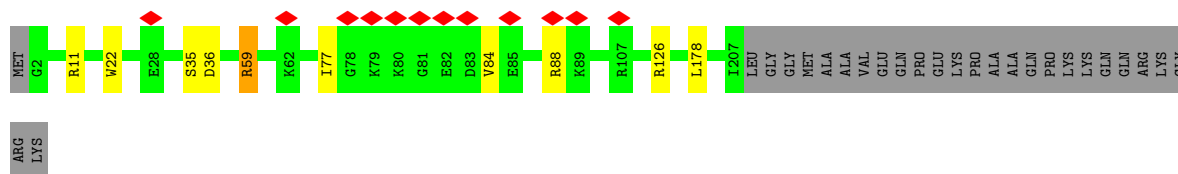
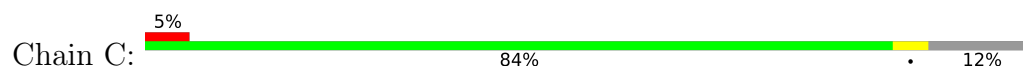
- Molecule 10: Large ribosomal subunit protein bL35



- Molecule 11: 30S ribosomal protein S2

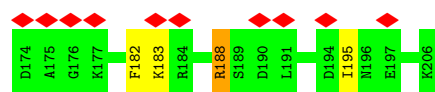


- Molecule 12: Small ribosomal subunit protein uS3

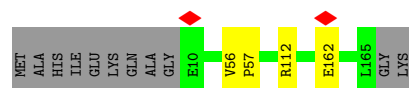


- Molecule 13: Small ribosomal subunit protein uS4

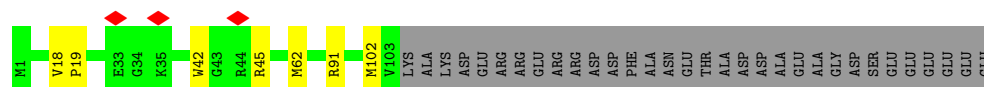




- Molecule 14: Small ribosomal subunit protein uS5



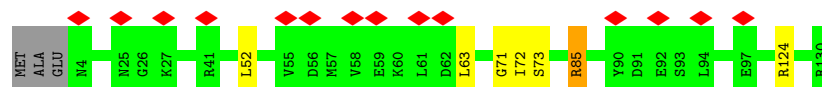
- Molecule 15: 30S ribosomal protein S6, fully modified isoform



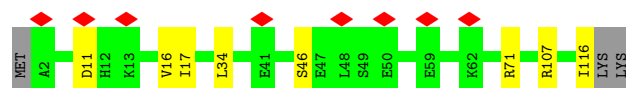
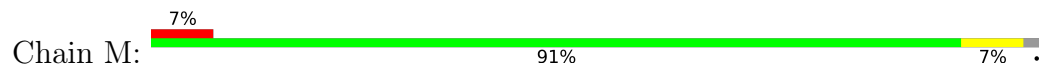
- Molecule 16: Small ribosomal subunit protein uS8



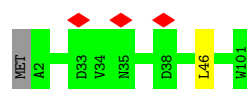
- Molecule 17: Small ribosomal subunit protein uS9



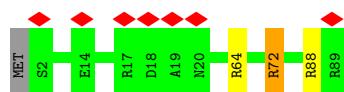
- Molecule 18: Small ribosomal subunit protein uS13



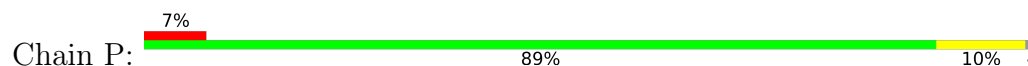
- Molecule 19: Small ribosomal subunit protein uS14



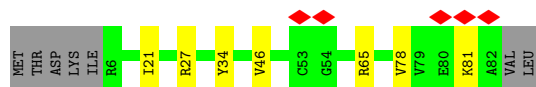
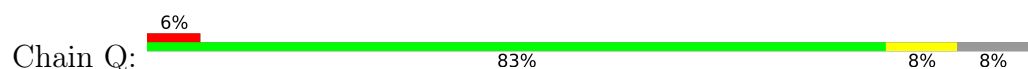
- Molecule 20: Small ribosomal subunit protein uS15



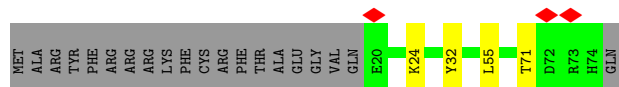
- Molecule 21: 30S ribosomal protein S16



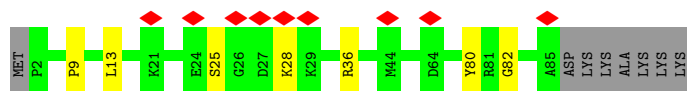
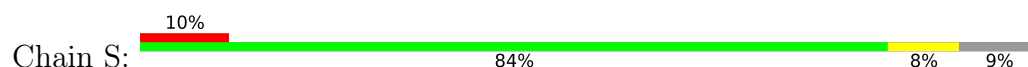
- Molecule 22: Small ribosomal subunit protein uS17



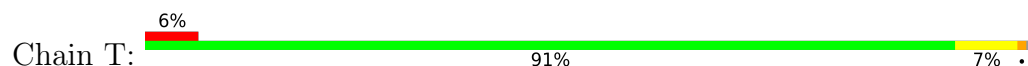
- Molecule 23: Small ribosomal subunit protein bS18



- Molecule 24: Small ribosomal subunit protein uS19



- Molecule 25: 30S ribosomal protein S20

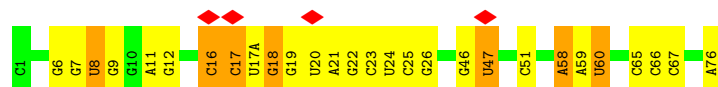


- Molecule 26: mRNA

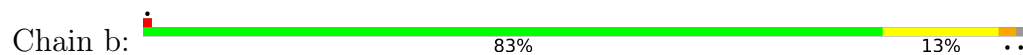


There are no outlier residues recorded for this chain.

- Molecule 27: fMet-Initiator P-site tRNA



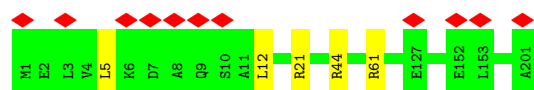
- Molecule 28: 5s rRNA



- Molecule 29: Large ribosomal subunit protein uL2



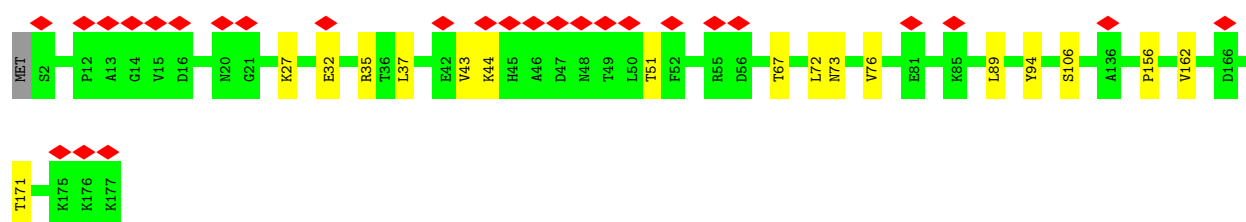
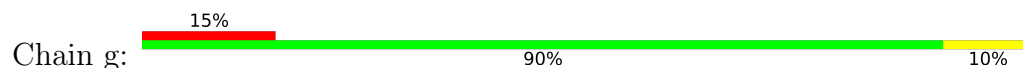
- Molecule 30: Large ribosomal subunit protein uL4



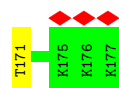
- Molecule 31: Large ribosomal subunit protein uL5

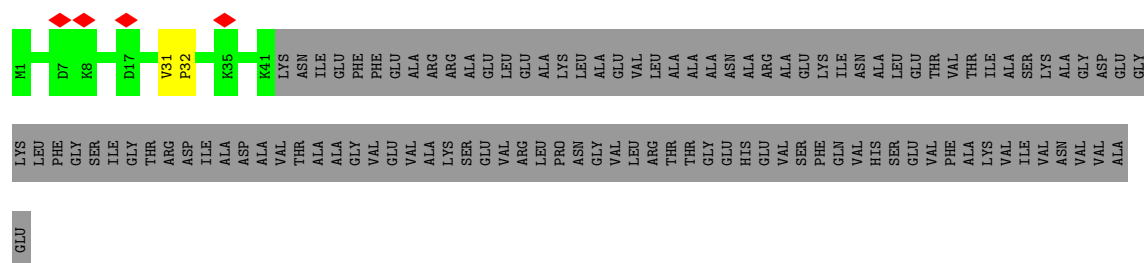


- Molecule 32: Large ribosomal subunit protein uL6



- Molecule 33: Large ribosomal subunit protein bL9





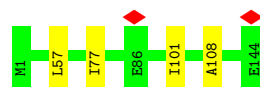
- Molecule 34: Large ribosomal subunit protein uL13



- Molecule 35: Large ribosomal subunit protein uL14



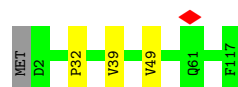
- Molecule 36: 50S ribosomal protein L15



- Molecule 37: Large ribosomal subunit protein bL17



- Molecule 38: Large ribosomal subunit protein uL18



- Molecule 39: Large ribosomal subunit protein bL19

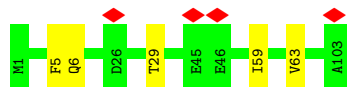




- Molecule 40: Large ribosomal subunit protein bL20



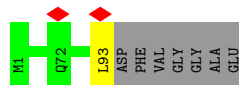
- Molecule 41: Large ribosomal subunit protein bL21



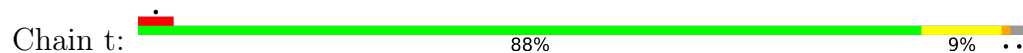
- Molecule 42: Large ribosomal subunit protein uL22



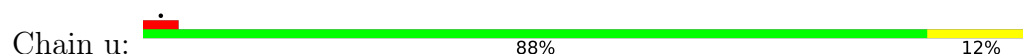
- Molecule 43: Large ribosomal subunit protein uL23



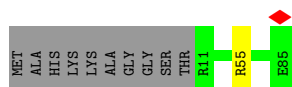
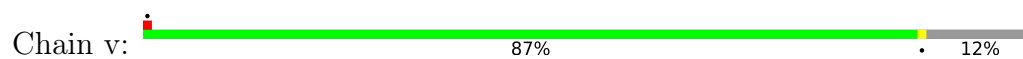
- Molecule 44: Large ribosomal subunit protein uL24



- Molecule 45: 50S ribosomal protein L25



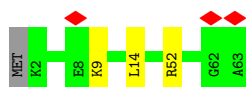
- Molecule 46: Large ribosomal subunit protein bL27



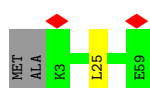
- Molecule 47: Large ribosomal subunit protein bL28



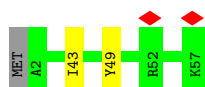
- Molecule 48: Large ribosomal subunit protein uL29



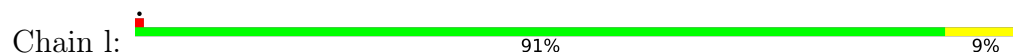
- Molecule 49: Large ribosomal subunit protein uL30



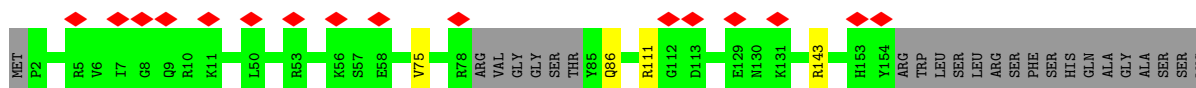
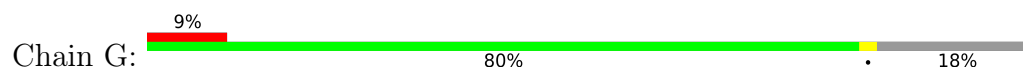
- Molecule 50: Large ribosomal subunit protein bL32



- Molecule 51: Large ribosomal subunit protein uL16

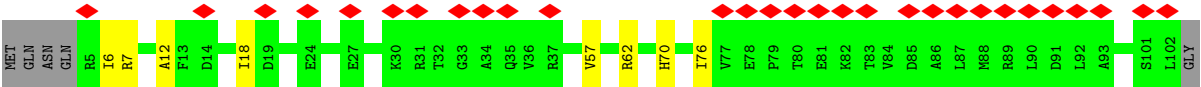
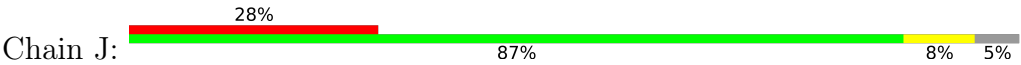


- Molecule 52: 30S ribosomal protein S7



GLN
PRO
ALA
LEU
GLY
TYR
LEU
ASN

- Molecule 53: Small ribosomal subunit protein uS10



- Molecule 54: Small ribosomal subunit protein bS21



- Molecule 55: DalDro



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228395	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 ($e^-/\text{\AA}^2$)	1.14	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 6MZ, 3TD, IAS, ZN, 5MC, 1MG, OMC, D2T, 4OC, OMU, 4D4, G7M, 5MU, MEQ, PSU, MS6, UR3, OMG, MA6, 2MG, 2MA

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	K	0.71	1/884 (0.1%)	0.97	3/1191 (0.3%)
2	L	0.57	0/960	0.83	0/1286
3	d	0.61	0/1576	0.85	0/2119
4	4	0.59	0/480	0.92	0/638
5	3	0.60	0/303	0.80	0/397
6	a	0.57	2/65651 (0.0%)	0.93	79/102413 (0.1%)
7	A	0.55	1/36236 (0.0%)	0.88	22/56520 (0.0%)
8	0	0.57	0/412	0.89	0/549
9	1	0.70	0/370	0.93	0/487
10	2	0.69	0/513	0.93	0/676
11	B	0.54	0/1784	0.95	0/2403
12	C	0.55	0/1651	0.88	0/2225
13	D	0.54	0/1665	0.94	0/2227
14	E	0.59	0/1165	0.89	0/1568
15	F	0.55	0/858	0.88	0/1160
16	H	0.58	0/989	0.87	0/1326
17	I	0.57	0/1034	0.96	1/1375 (0.1%)
18	M	0.57	0/900	0.97	0/1204
19	N	0.56	0/817	0.93	0/1088
20	O	0.57	0/722	0.97	0/964
21	P	0.55	0/653	0.86	0/877
22	Q	0.52	0/633	0.83	0/849
23	R	0.56	0/462	0.95	0/621
24	S	0.59	0/685	0.90	0/922
25	T	0.55	0/676	0.98	0/895
26	X	0.64	0/72	1.02	0/110
27	Z	0.61	0/1835	0.80	0/2859
28	b	0.55	0/2850	0.86	1/4444 (0.0%)
29	c	0.65	0/2121	0.89	0/2852
30	e	0.60	0/1571	0.91	0/2113
31	f	0.54	0/1434	0.96	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.58	0/1343	0.90	0/1816
33	h	0.58	0/306	0.95	0/413
34	i	0.61	0/1152	0.86	0/1551
35	j	0.60	0/955	0.90	0/1279
36	k	0.65	0/1062	0.89	0/1413
37	m	0.66	0/958	0.92	0/1281
38	n	0.59	0/902	0.92	0/1209
39	o	0.61	0/929	0.82	0/1242
40	p	0.66	0/960	0.91	1/1278 (0.1%)
41	q	0.57	0/829	0.84	1/1107 (0.1%)
42	r	0.64	0/864	0.90	0/1156
43	s	0.57	0/744	0.83	0/994
44	t	0.57	0/787	0.88	0/1051
45	u	0.56	0/766	0.85	0/1025
46	v	0.62	0/576	0.86	0/762
47	w	0.62	0/635	0.90	0/848
48	x	0.51	0/502	0.97	0/667
49	y	0.59	0/448	0.91	0/598
50	z	0.66	0/450	0.91	0/599
51	l	0.64	1/1073 (0.1%)	0.90	0/1433
52	G	0.56	0/1179	0.94	0/1580
53	J	0.58	0/796	0.88	0/1077
54	U	0.57	0/597	0.98	0/792
55	8	0.72	0/138	1.05	0/189
All	All	0.57	5/150913 (0.0%)	0.91	108/225644 (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
1	K	0	2
2	L	0	2
3	d	0	1
5	3	0	1
6	a	0	5
8	0	0	1
9	1	0	1
10	2	0	3
11	B	0	1
12	C	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	D	0	4
14	E	0	1
15	F	0	1
17	I	0	2
18	M	0	2
20	O	0	2
22	Q	0	2
24	S	0	1
25	T	0	2
29	c	0	3
30	e	0	2
31	f	0	2
32	g	0	1
34	i	0	2
35	j	0	1
39	o	0	2
40	p	0	2
46	v	0	1
47	w	0	3
48	x	0	1
52	G	0	2
53	J	0	2
All	All	0	62

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	120	GLY	C-N	10.27	1.47	1.33
51	l	83	GLY	C-N	7.82	1.44	1.33
6	a	2069	G7M	O3'-P	5.42	1.61	1.56
7	A	527	G7M	O3'-P	5.37	1.61	1.56
6	a	2552	OMU	O3'-P	5.27	1.61	1.56

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	120	GLY	O-C-N	-10.80	105.71	123.00
1	K	120	GLY	CA-C-N	8.91	137.21	122.87
1	K	120	GLY	C-N-CA	8.91	137.21	122.87
6	a	2601	C	C4'-C3'-O3'	8.63	125.94	113.00
6	a	2546	U	O3'-P-O5'	-7.40	92.90	104.00
6	a	204	A	O3'-P-O5'	-7.25	93.13	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	329	G	O3'-P-O5'	-7.14	93.30	104.00
6	a	781	A	O3'-P-O5'	-7.05	93.42	104.00
6	a	1969	A	O3'-P-O5'	-6.96	93.56	104.00
6	a	2049	G	O3'-P-O5'	-6.84	93.74	104.00
7	A	1377	A	O3'-P-O5'	-6.84	93.75	104.00
6	a	2094	A	O3'-P-O5'	-6.74	93.89	104.00
6	a	818	G	O3'-P-O5'	-6.65	94.03	104.00
6	a	1944	U	O3'-P-O5'	-6.64	94.03	104.00
7	A	652	U	O3'-P-O5'	-6.62	94.07	104.00
7	A	730	G	O3'-P-O5'	-6.58	94.12	104.00
6	a	2001	C	O3'-P-O5'	-6.56	94.16	104.00
6	a	1757	A	C4'-C3'-O3'	-6.40	103.40	113.00
6	a	1971	U	C4'-C3'-O3'	-6.39	103.42	113.00
7	A	1347	G	O3'-P-O5'	-6.37	94.44	104.00
6	a	525	U	O3'-P-O5'	-6.31	94.54	104.00
6	a	2879	A	O3'-P-O5'	-6.23	94.65	104.00
6	a	404	A	C2'-C3'-O3'	6.22	118.83	109.50
6	a	1565	C	O3'-P-O5'	-6.17	94.75	104.00
7	A	455	G	O3'-P-O5'	-6.06	94.91	104.00
6	a	2501	C	C4'-C3'-O3'	-6.04	103.94	113.00
6	a	1293	C	O3'-P-O5'	-6.00	94.99	104.00
6	a	1025	G	C2'-C3'-O3'	5.99	118.48	109.50
7	A	901	A	O3'-P-O5'	-5.99	95.02	104.00
6	a	2519	U	O3'-P-O5'	-5.98	95.04	104.00
6	a	1025	G	O3'-P-O5'	5.91	112.86	104.00
7	A	181	A	O3'-P-O5'	-5.83	95.26	104.00
6	a	2050	C	C4'-C3'-O3'	-5.81	104.28	113.00
6	a	571	U	O3'-P-O5'	-5.80	95.30	104.00
6	a	1775	U	O3'-P-O5'	-5.79	95.31	104.00
6	a	2337	G	O3'-P-O5'	-5.78	95.33	104.00
6	a	1328	A	O3'-P-O5'	-5.77	95.34	104.00
6	a	2768	U	O3'-P-O5'	-5.70	95.45	104.00
7	A	348	G	O3'-P-O5'	-5.67	95.49	104.00
6	a	1122	G	O3'-P-O5'	-5.66	95.51	104.00
7	A	872	A	O3'-P-O5'	-5.66	95.51	104.00
6	a	2614	A	O3'-P-O5'	-5.64	95.54	104.00
7	A	598	U	O3'-P-O5'	-5.62	95.56	104.00
6	a	2449	H2U	O3'-P-O5'	-5.61	95.58	104.00
6	a	60	G	O3'-P-O5'	-5.60	95.60	104.00
6	a	727	A	O3'-P-O5'	-5.55	95.67	104.00
28	b	90	C	O3'-P-O5'	-5.54	95.68	104.00
7	A	1504	G	O3'-P-O5'	-5.53	95.71	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	798	U	O3'-P-O5'	-5.53	95.71	104.00
6	a	1565	C	C2'-C3'-O3'	5.51	117.77	109.50
6	a	1359	A	O3'-P-O5'	-5.46	95.81	104.00
7	A	978	A	O3'-P-O5'	-5.44	95.84	104.00
7	A	246	A	O3'-P-O5'	-5.43	95.85	104.00
7	A	59	A	O3'-P-O5'	-5.43	95.85	104.00
6	a	27	G	O3'-P-O5'	-5.42	95.87	104.00
6	a	2490	G	O3'-P-O5'	-5.41	95.89	104.00
6	a	2516	A	O3'-P-O5'	-5.41	95.89	104.00
6	a	2711	A	C4'-C3'-O3'	-5.40	104.89	113.00
6	a	134	G	O3'-P-O5'	-5.40	95.90	104.00
6	a	2429	G	O3'-P-O5'	-5.40	95.90	104.00
6	a	2575	C	C2'-C3'-O3'	-5.40	105.60	113.70
6	a	2817	U	O3'-P-O5'	-5.39	95.91	104.00
6	a	2500	U	C2'-C3'-O3'	-5.39	105.62	113.70
7	A	1067	A	O3'-P-O5'	-5.39	95.92	104.00
6	a	1664	A	O3'-P-O5'	-5.38	95.93	104.00
6	a	2222	C	O3'-P-O5'	-5.38	95.93	104.00
6	a	846	U	O3'-P-O5'	-5.36	95.96	104.00
7	A	364	A	O3'-P-O5'	-5.35	95.98	104.00
6	a	505	A	O3'-P-O5'	-5.33	96.00	104.00
6	a	1378	A	O3'-P-O5'	-5.32	96.02	104.00
6	a	2761	A	O3'-P-O5'	-5.31	96.04	104.00
6	a	1410	G	O3'-P-O5'	-5.23	96.15	104.00
17	I	72	ILE	N-CA-C	5.22	115.66	110.23
6	a	528	A	O3'-P-O5'	-5.21	96.18	104.00
6	a	655	A	O3'-P-O5'	-5.21	96.19	104.00
6	a	2477	U	O3'-P-O5'	-5.20	96.20	104.00
6	a	226	A	O3'-P-O5'	-5.19	96.21	104.00
6	a	2430	A	C1'-O4'-C4'	-5.16	104.54	109.70
6	a	1857	G	O3'-P-O5'	-5.16	96.26	104.00
6	a	1974	C	O3'-P-O5'	-5.16	96.26	104.00
40	p	31	VAL	N-CA-CB	-5.13	104.27	111.25
6	a	2051	A	O3'-P-O5'	-5.13	96.31	104.00
7	A	971	G	O3'-P-O5'	-5.12	96.32	104.00
6	a	1452	G	C2'-C3'-O3'	5.11	117.17	109.50
6	a	2356	U	O3'-P-O5'	-5.11	96.33	104.00
6	a	2429	G	C2'-C3'-O3'	-5.11	106.04	113.70
6	a	1543	G	C4'-C3'-O3'	-5.10	105.35	113.00
7	A	379	C	O3'-P-O5'	-5.10	96.35	104.00
6	a	2501	C	O3'-P-O5'	-5.10	96.36	104.00
6	a	369	U	O3'-P-O5'	-5.09	96.36	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	1299	G	C2'-C3'-O3'	-5.09	106.07	113.70
6	a	1847	A	O3'-P-O5'	-5.08	96.37	104.00
7	A	872	A	C1'-O4'-C4'	-5.08	104.62	109.70
6	a	2725	A	C1'-C2'-O2'	-5.07	104.20	111.80
41	q	6	GLN	CB-CA-C	5.07	118.11	109.75
6	a	2528	U	O3'-P-O5'	-5.06	96.41	104.00
6	a	296	U	O3'-P-O5'	-5.06	96.41	104.00
6	a	1033	U	O3'-P-O5'	-5.06	96.41	104.00
6	a	577	G	O3'-P-O5'	-5.05	96.43	104.00
6	a	1436	G	O3'-P-O5'	-5.03	96.45	104.00
6	a	1773	A	O3'-P-O5'	-5.03	96.45	104.00
6	a	1185	G	O3'-P-O5'	-5.03	96.45	104.00
7	A	921	U	O3'-P-O5'	-5.02	96.47	104.00
7	A	794	A	C4'-C3'-O3'	-5.02	105.47	113.00
6	a	1866	A	O3'-P-O5'	-5.01	96.48	104.00
6	a	763	G	C4'-C3'-O3'	-5.01	105.48	113.00
6	a	1416	G	O3'-P-O5'	-5.01	96.48	104.00
6	a	1936	A	C1'-O4'-C4'	-5.01	104.69	109.70

There are no chirality outliers.

All (62) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	0	28	ARG	Sidechain
9	1	41	ARG	Sidechain
10	2	13	ARG	Sidechain
10	2	45	ARG	Sidechain
10	2	8	ARG	Sidechain
5	3	4	ARG	Sidechain
11	B	137	ARG	Sidechain
12	C	11	ARG	Sidechain
12	C	126	ARG	Sidechain
12	C	59	ARG	Sidechain
12	C	88	ARG	Sidechain
13	D	14	ARG	Sidechain
13	D	165	ARG	Sidechain
13	D	62	ARG	Sidechain
13	D	73	ARG	Sidechain
14	E	112	ARG	Sidechain
15	F	45	ARG	Sidechain
52	G	111	ARG	Sidechain
52	G	143	ARG	Sidechain

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Mol	Chain	Res	Type	Group
17	I	124	ARG	Sidechain
17	I	85	ARG	Sidechain
53	J	62	ARG	Sidechain
53	J	7	ARG	Sidechain
1	K	118	HIS	Mainchain
1	K	120	GLY	Mainchain
2	L	54	ARG	Sidechain
2	L	9	ARG	Sidechain
18	M	107	ARG	Sidechain
18	M	71	ARG	Sidechain
20	O	64	ARG	Sidechain
20	O	72	ARG	Sidechain
22	Q	27	ARG	Sidechain
22	Q	65	ARG	Sidechain
24	S	36	ARG	Sidechain
25	T	24	ARG	Sidechain
25	T	74	ARG	Sidechain
6	a	1287	A	Sidechain
6	a	2595	G	Sidechain
6	a	512	G	Sidechain
6	a	956	G	Sidechain
6	a	983	A	Sidechain
29	c	133	ARG	Sidechain
29	c	156	ARG	Sidechain
29	c	43	ARG	Sidechain
3	d	83	ARG	Sidechain
30	e	21	ARG	Sidechain
30	e	61	ARG	Sidechain
31	f	125	ARG	Sidechain
31	f	150	ARG	Sidechain
32	g	35	ARG	Sidechain
34	i	13	ARG	Sidechain
34	i	69	ARG	Sidechain
35	j	49	ARG	Sidechain
39	o	103	ARG	Sidechain
39	o	53	ARG	Sidechain
40	p	13	ARG	Sidechain
40	p	28	ARG	Sidechain
46	v	55	ARG	Sidechain
47	w	16	ASN	Peptide
47	w	28	ARG	Sidechain
47	w	74	ARG	Sidechain

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Mol	Chain	Res	Type	Group
48	x	52	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	K	877	0	884	4	0
2	L	957	0	1017	3	0
3	d	1566	0	1618	3	0
4	4	472	0	467	4	0
5	3	302	0	340	1	0
6	a	59130	0	29769	85	0
7	A	32612	0	16432	54	0
8	0	405	0	437	1	0
9	1	367	0	405	1	0
10	2	504	0	572	3	0
11	B	1753	0	1780	7	0
12	C	1624	0	1696	3	0
13	D	1643	0	1707	10	0
14	E	1152	0	1196	1	0
15	F	839	0	833	5	0
16	H	979	0	1031	3	0
17	I	1022	0	1070	4	0
18	M	891	0	952	4	0
19	N	805	0	844	1	0
20	O	714	0	734	2	0
21	P	643	0	661	4	0
22	Q	624	0	658	3	0
23	R	455	0	478	3	0
24	S	668	0	693	4	0
25	T	670	0	719	3	0
26	X	65	0	33	0	0
27	Z	1643	0	836	10	0
28	b	2549	0	1291	8	0
29	c	2082	0	2154	7	0
30	e	1552	0	1619	2	0
31	f	1410	0	1444	1	0
32	g	1323	0	1371	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	h	303	0	327	1	0
34	i	1129	0	1162	6	0
35	j	946	0	1023	3	0
36	k	1053	0	1129	5	0
37	m	945	0	989	2	0
38	n	892	0	923	2	0
39	o	917	0	962	1	0
40	p	947	0	1019	1	0
41	q	816	0	839	2	0
42	r	857	0	922	3	0
43	s	738	0	807	0	0
44	t	779	0	831	5	0
45	u	753	0	780	7	0
46	v	569	0	581	0	0
47	w	625	0	652	0	0
48	x	501	0	531	2	0
49	y	444	0	483	1	0
50	z	444	0	458	1	0
51	l	1075	0	1146	8	0
52	G	1164	0	1213	2	0
53	J	786	0	828	5	0
54	U	589	0	629	1	0
55	8	131	0	129	1	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
All	All	139703	0	94104	278	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 1.

All (278) 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)
51:l:77:PRO:HG2	51:l:80:VAL:HG21	1.53	0.88
12:C:77:ILE:HA	12:C:84:VAL:HG23	1.73	0.70
6:a:568:U:H1'	6:a:2030:6MZ:H9C1	1.75	0.69
45:u:6:ALA:HB3	45:u:65:VAL:HG22	1.75	0.68
6:a:1872:A:H3'	6:a:1873:G:O4'	1.97	0.65
32:g:89:LEU:CD2	32:g:162:VAL:HG22	2.31	0.61
6:a:1252:G:H1	40:p:37:GLN:HE21	1.49	0.61
45:u:4:ILE:HG12	45:u:50:MET:HE1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:36:C:N4	28:b:49:C:O2	2.35	0.59
6:a:548:G:H2'	6:a:549:G:H1'	1.85	0.59
34:i:18:VAL:HG21	34:i:142:ILE:HD12	1.85	0.58
7:A:664:G:H22	7:A:741:G:H1	1.50	0.58
52:G:75:VAL:HG11	52:G:86:GLN:HB3	1.86	0.58
51:l:1:MET:HE1	51:l:44:ARG:N	2.18	0.58
53:J:18:ILE:HD12	53:J:70:HIS:HB2	1.85	0.57
29:c:29:PRO:HG2	29:c:34:LEU:HD11	1.84	0.57
6:a:1778:U:H2'	6:a:1784:A:N6	2.19	0.56
45:u:63:ILE:HG22	45:u:65:VAL:HG23	1.87	0.56
12:C:35:SER:OG	12:C:59:ARG:NH2	2.39	0.56
2:L:4:VAL:HG13	22:Q:34:TYR:HB3	1.87	0.56
51:l:53:MET:HE1	51:l:103:TYR:CD2	2.40	0.56
6:a:1028:A:N6	6:a:1125:G:H2'	2.21	0.55
6:a:894:U:H2'	6:a:895:U:O4'	2.06	0.55
27:Z:66:C:H2'	27:Z:67:C:C6	2.42	0.55
6:a:930:G:H1'	49:y:25:LEU:HD11	1.90	0.54
52:G:75:VAL:CG1	52:G:86:GLN:HB3	2.37	0.54
7:A:382:A:H2'	7:A:383:A:C8	2.43	0.54
6:a:1115:G:O2'	6:a:1116:G:O5'	2.22	0.54
53:J:12:ALA:HB3	53:J:18:ILE:HG13	1.90	0.54
6:a:1434:A:H2'	6:a:1435:G:C8	2.43	0.53
7:A:1302:C:C5	18:M:17:ILE:HG13	2.44	0.53
2:L:55:VAL:HG21	2:L:80:ILE:HD11	1.88	0.53
7:A:754:C:OP1	20:O:72:ARG:NH2	2.42	0.53
42:r:7:HIS:CD2	42:r:10:ALA:HB2	2.44	0.53
6:a:570:G:H2'	6:a:2030:6MZ:N7	2.24	0.52
1:K:111:THR:HG23	54:U:3:VAL:HG22	1.91	0.52
17:I:52:LEU:HD11	17:I:63:LEU:HD11	1.92	0.52
6:a:221:A:N1	6:a:265:A:O2'	2.41	0.52
30:e:5:LEU:HD11	30:e:12:LEU:HB2	1.92	0.52
7:A:532:A:N6	7:A:1206:G:O2'	2.42	0.52
7:A:1372:U:OP1	17:I:73:SER:N	2.43	0.52
45:u:81:PRO:HG2	51:l:20:LEU:HD13	1.92	0.52
6:a:1720:U:H2'	6:a:1721:G:O4'	2.10	0.52
21:P:18:GLN:OE1	21:P:35:ARG:NE	2.43	0.52
13:D:172:GLU:HG3	13:D:183:LYS:HD2	1.92	0.51
6:a:1509:A:O2'	6:a:1510:G:H8	1.93	0.51
6:a:714:U:OP2	20:O:88:ARG:NH2	2.44	0.51
6:a:2395:C:H2'	6:a:2396:G:O4'	2.10	0.51
7:A:203:G:O2'	7:A:465:A:N1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:1:MET:HE3	35:j:32:TYR:CZ	2.45	0.51
5:3:16:ILE:HD13	5:3:25:VAL:HG22	1.92	0.50
48:x:9:LYS:HB2	48:x:14:LEU:HD12	1.94	0.50
11:B:87:CYS:SG	11:B:221:VAL:HB	2.52	0.50
28:b:76:G:OP1	45:u:9:ARG:NH1	2.42	0.50
6:a:12:U:O2	6:a:12:U:H2'	2.10	0.50
7:A:404:G:N7	13:D:2:ALA:HB3	2.26	0.50
7:A:1371:G:H4'	17:I:71:GLY:HA3	1.93	0.50
29:c:107:PRO:HD2	29:c:110:LEU:HD22	1.93	0.50
35:j:1:MET:HE3	35:j:32:TYR:CE2	2.47	0.50
44:t:54:GLN:N	44:t:55:PRO:HD2	2.26	0.50
6:a:2328:A:H2'	6:a:2329:U:C6	2.46	0.50
7:A:946:A:H2'	7:A:947:G:C8	2.47	0.50
53:J:6:ILE:HB	53:J:76:ILE:HB	1.94	0.50
41:q:29:THR:O	41:q:63:VAL:O	2.30	0.50
32:g:156:PRO:O	32:g:171:THR:HA	2.13	0.49
6:a:1937:A:H1'	6:a:1939:5MU:H72	1.94	0.49
51:l:66:ARG:NH1	51:l:104:GLU:OE2	2.45	0.49
6:a:1021:A:H3'	6:a:1021:A:N3	2.28	0.49
28:b:29:A:H2'	28:b:30:C:O4'	2.13	0.49
6:a:2327:A:H2'	6:a:2328:A:C8	2.48	0.49
7:A:1273:C:H2'	7:A:1274:A:O4'	2.13	0.49
6:a:549:G:H2'	6:a:550:C:C6	2.48	0.48
27:Z:11:A:H2'	27:Z:12:G:C8	2.48	0.48
15:F:42:TRP:CE2	15:F:102:MET:HG3	2.48	0.48
16:H:38:ASN:OD1	16:H:49:PHE:CZ	2.66	0.48
27:Z:23:C:H2'	27:Z:24:U:C6	2.48	0.48
7:A:1323:G:H2'	7:A:1324:A:C8	2.47	0.48
34:i:31:GLU:CG	34:i:142:ILE:HG23	2.43	0.48
6:a:2291:U:H2'	6:a:2292:U:C6	2.49	0.48
32:g:44:LYS:HB2	32:g:51:THR:HB	1.95	0.48
36:k:77:ILE:HD13	36:k:108:ALA:HB1	1.96	0.48
7:A:373:A:C2	7:A:374:A:C8	3.02	0.48
7:A:673:A:H2'	7:A:674:G:C8	2.48	0.48
7:A:945:G:C2	7:A:946:A:C8	3.01	0.48
4:4:28:VAL:HG21	4:4:32:LEU:HD21	1.95	0.48
51:l:53:MET:HG3	51:l:120:ALA:HB2	1.95	0.48
4:4:63:ARG:NH2	7:A:1312:G:OP2	2.47	0.47
10:2:54:ASP:HB3	36:k:57:LEU:HD22	1.95	0.47
36:k:77:ILE:HD12	36:k:77:ILE:N	2.29	0.47
45:u:75:GLN:HB2	45:u:92:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:110:ARG:HB3	2:L:119:VAL:HG21	1.95	0.47
7:A:1033:G:H3'	7:A:1034:G:H8	1.79	0.47
53:J:12:ALA:HB3	53:J:18:ILE:CG1	2.44	0.47
6:a:2552:OMU:H6	6:a:2552:OMU:O5'	2.14	0.47
7:A:188:C:H2'	7:A:189:A:O4'	2.14	0.47
11:B:94:HIS:O	11:B:95:ARG:C	2.57	0.47
7:A:543:U:OP1	13:D:14:ARG:HD2	2.15	0.47
10:2:62:LEU:HB3	10:2:65:ALA:HB2	1.96	0.47
36:k:77:ILE:CD1	36:k:108:ALA:HB1	2.45	0.47
44:t:86:ARG:HG3	44:t:95:PHE:CD1	2.49	0.47
7:A:1004:A:H2'	7:A:1005:A:O4'	2.15	0.47
6:a:644:A:H2'	6:a:645:C:O4'	2.14	0.47
6:a:1857:G:H22	6:a:1884:G:HO2'	1.61	0.47
6:a:2547:A:H2'	6:a:2548:U:C6	2.49	0.47
6:a:2420:C:H5'	8:0:54:ILE:HD11	1.97	0.47
25:T:24:ARG:HB3	25:T:61:GLN:HE22	1.80	0.46
7:A:71:A:N1	7:A:99:C:O2'	2.42	0.46
6:a:1434:A:H2'	6:a:1435:G:H8	1.80	0.46
7:A:677:U:H3	7:A:713:G:H22	1.64	0.46
21:P:61:VAL:HG21	21:P:67:ILE:HD11	1.97	0.46
27:Z:18:G:C2	27:Z:58:A:C4	3.04	0.46
4:4:2:LYS:HE3	28:b:40:U:H2'	1.97	0.46
7:A:986:U:H2'	7:A:987:G:O4'	2.15	0.46
28:b:29:A:OP2	38:n:32:PRO:HD2	2.16	0.46
41:q:5:PHE:HB3	41:q:59:ILE:HD12	1.98	0.46
7:A:1086:U:H3	7:A:1099:G:H22	1.64	0.46
6:a:543:G:H8	6:a:543:G:H5''	1.80	0.46
14:E:56:VAL:N	14:E:57:PRO:HD2	2.30	0.46
23:R:32:TYR:HB3	23:R:55:LEU:HD21	1.97	0.46
13:D:105:MET:HE1	13:D:143:VAL:HB	1.98	0.46
11:B:70:VAL:HG21	11:B:161:LEU:HD11	1.97	0.46
6:a:493:G:H2'	6:a:494:G:O4'	2.16	0.45
6:a:1853:A:N1	6:a:2087:G:H1'	2.32	0.45
6:a:2038:G:H2'	6:a:2039:U:O4'	2.16	0.45
7:A:1477:U:H2'	7:A:1478:U:C6	2.51	0.45
11:B:130:THR:O	11:B:132:LYS:N	2.48	0.45
7:A:1391:U:H2'	7:A:1392:G:C8	2.51	0.45
48:x:9:LYS:HB2	48:x:14:LEU:CD1	2.46	0.45
6:a:1425:G:H2'	6:a:1426:G:C8	2.52	0.45
6:a:2491:U:H5''	6:a:2570:G:H5''	1.99	0.45
44:t:86:ARG:HG3	44:t:95:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:483:A:H5''	44:t:47:LYS:HD2	1.97	0.45
6:a:2756:U:H1'	6:a:2757:A:H5''	1.99	0.45
7:A:415:A:H3'	7:A:416:G:H8	1.82	0.45
16:H:29:SER:HB3	16:H:57:PRO:HB2	1.99	0.45
7:A:87:C:H2'	7:A:88:U:C6	2.52	0.45
7:A:299:G:H2'	7:A:300:A:C8	2.52	0.45
7:A:371:A:H2'	7:A:372:C:O4'	2.17	0.45
39:o:100:LEU:HD11	39:o:110:ILE:HD11	1.99	0.45
10:2:45:ARG:N	10:2:46:PRO:HD2	2.32	0.45
6:a:276:U:H2'	6:a:277:G:C8	2.52	0.44
6:a:723:C:H2'	6:a:724:U:O4'	2.17	0.44
15:F:102:MET:HE3	23:R:24:LYS:O	2.18	0.44
6:a:57:C:H2'	6:a:58:G:O4'	2.16	0.44
12:C:22:TRP:NE1	12:C:36:ASP:OD2	2.48	0.44
15:F:42:TRP:CD2	15:F:102:MET:HG3	2.53	0.44
19:N:46:LEU:HD13	24:S:13:LEU:HD13	1.99	0.44
7:A:451:A:H61	7:A:481:G:H5'	1.83	0.44
7:A:1424:U:H2'	7:A:1425:U:O4'	2.18	0.44
21:P:4:ILE:HG12	21:P:21:VAL:HG22	1.99	0.44
6:a:476:G:H4'	6:a:502:A:N1	2.32	0.44
6:a:2273:A:H2'	6:a:2274:A:C8	2.53	0.44
6:a:888:C:H2'	6:a:889:C:O4'	2.17	0.44
18:M:16:VAL:HG22	18:M:34:LEU:HD12	1.99	0.44
27:Z:25:C:H2'	27:Z:26:G:O4'	2.17	0.44
7:A:429:U:H3'	13:D:9:LEU:HD12	2.00	0.44
7:A:604:G:H2'	7:A:605:U:O4'	2.17	0.44
51:l:77:PRO:O	51:l:80:VAL:HB	2.17	0.44
6:a:876:C:H2'	6:a:877:A:O4'	2.17	0.44
6:a:1744:A:H3'	6:a:1745:A:H8	1.83	0.44
37:m:24:MET:HE1	37:m:40:LYS:HD3	1.99	0.44
6:a:613:A:H2'	6:a:614:A:O4'	2.18	0.43
32:g:94:TYR:HA	32:g:106:SER:O	2.17	0.43
6:a:2233:U:H2'	6:a:2234:G:C8	2.53	0.43
6:a:2243:U:H2'	6:a:2244:U:C6	2.53	0.43
28:b:24:G:N7	28:b:56:G:H2'	2.33	0.43
38:n:39:VAL:HB	38:n:49:VAL:HG22	1.99	0.43
6:a:1327:A:H2'	6:a:1328:A:O4'	2.18	0.43
1:K:67:ALA:HB2	1:K:96:THR:HG23	2.00	0.43
6:a:1548:A:H2'	6:a:1549:A:C8	2.53	0.43
7:A:176:C:H2'	7:A:177:G:N3	2.34	0.43
7:A:152:A:N6	7:A:170:U:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:28:LYS:N	11:B:29:PRO:CD	2.82	0.43
51:I:77:PRO:HG2	51:I:80:VAL:CG2	2.37	0.43
13:D:107:PHE:HB3	13:D:145:ILE:HD11	2.01	0.43
29:c:31:ALA:N	29:c:32:PRO:CD	2.82	0.43
6:a:1510:G:H2'	6:a:1511:G:O4'	2.19	0.43
7:A:1228:C:H1'	18:M:116:ILE:HD11	2.01	0.43
11:B:111:ILE:HD13	11:B:148:LEU:HB3	2.01	0.43
6:a:1944:U:C5	6:a:1955:U:C2	3.07	0.43
7:A:151:A:H2'	7:A:152:A:O4'	2.19	0.43
7:A:977:A:O2'	7:A:979:C:OP2	2.34	0.43
6:a:84:A:N1	6:a:98:G:O2'	2.46	0.42
6:a:139:U:H5''	6:a:140:C:H5	1.83	0.42
6:a:355:U:H2'	6:a:356:G:H8	1.83	0.42
6:a:720:U:H2'	6:a:721:A:C8	2.54	0.42
6:a:1109:C:H2'	6:a:1110:G:C4	2.54	0.42
29:c:5:LYS:HD2	29:c:17:VAL:HG22	2.01	0.42
7:A:580:C:H2'	7:A:581:G:O4'	2.19	0.42
7:A:1036:A:H2'	7:A:1037:C:O4'	2.19	0.42
13:D:101:VAL:HG12	13:D:105:MET:HE2	2.02	0.42
6:a:1799:G:N7	29:c:178:SER:OG	2.50	0.42
24:S:25:SER:HB2	24:S:28:LYS:HE3	2.00	0.42
32:g:37:LEU:HD12	32:g:43:VAL:HG21	2.02	0.42
6:a:1182:G:H2'	6:a:1183:U:O4'	2.20	0.42
6:a:2228:G:H2'	6:a:2229:U:C6	2.54	0.42
7:A:1029:U:O2'	7:A:1032:G:N1	2.50	0.42
7:A:1428:A:H2'	7:A:1429:A:O4'	2.18	0.42
6:a:639:U:H2'	6:a:640:C:C6	2.54	0.42
7:A:131:A:H2'	7:A:132:C:C6	2.55	0.42
7:A:160:A:H2'	7:A:161:A:O4'	2.20	0.42
7:A:769:G:H4'	7:A:1513:A:H4'	2.01	0.42
21:P:12:LYS:HG2	21:P:13:LYS:HG2	2.02	0.42
27:Z:18:G:N2	27:Z:58:A:O4'	2.50	0.42
6:a:572:A:C2	6:a:2033:A:C2	3.08	0.42
6:a:1932:A:H2'	6:a:1933:G:O4'	2.18	0.42
50:z:43:ILE:HG22	50:z:49:TYR:HB2	2.02	0.42
1:K:23:ILE:HG12	1:K:96:THR:HG21	2.02	0.42
3:d:1:MET:HE2	3:d:205:PRO:HG2	2.01	0.42
6:a:2:G:H2'	6:a:3:U:C6	2.54	0.42
6:a:465:G:OP1	9:1:12:ARG:NH1	2.52	0.42
6:a:1045:C:O2	6:a:1045:C:O4'	2.37	0.42
7:A:860:A:H2'	7:A:861:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:66:PHE:CD2	16:H:67:GLN:HG2	2.55	0.42
24:S:80:TYR:CZ	24:S:82:GLY:HA2	2.55	0.42
6:a:504:A:O2'	6:a:505:A:P	2.78	0.42
6:a:1011:G:H1'	6:a:1013:C:O4'	2.20	0.42
7:A:608:A:H2'	7:A:609:A:O4'	2.19	0.42
6:a:373:U:O2'	6:a:423:A:H1'	2.20	0.41
6:a:547:A:H4'	6:a:548:G:O4'	2.20	0.41
6:a:1582:C:H2'	6:a:1583:A:O4'	2.19	0.41
7:A:140:U:H2'	7:A:141:G:O4'	2.20	0.41
15:F:91:ARG:HG3	15:F:91:ARG:HH11	1.84	0.41
22:Q:78:VAL:HG11	22:Q:81:LYS:HE3	2.02	0.41
6:a:2251:OMG:HM23	6:a:2251:OMG:H1'	1.93	0.41
6:a:2312:U:H5'	31:f:85:ILE:HD11	2.01	0.41
27:Z:59:A:H2'	27:Z:60:U:O4'	2.20	0.41
35:j:63:VAL:HG12	35:j:107:LEU:HD11	2.01	0.41
4:4:64:PHE:CG	24:S:9:PRO:HD3	2.55	0.41
27:Z:21:A:N6	27:Z:47:U:O2'	2.53	0.41
3:d:35:THR:HG22	3:d:73:VAL:HG21	2.01	0.41
6:a:1028:A:H61	6:a:1125:G:H2'	1.85	0.41
7:A:1152:A:OP1	53:J:70:HIS:ND1	2.48	0.41
13:D:48:LEU:HD21	13:D:56:ARG:HG3	2.02	0.41
28:b:48:U:H2'	28:b:49:C:C6	2.55	0.41
28:b:106:G:H2'	28:b:107:G:O4'	2.20	0.41
34:i:77:HIS:HA	34:i:83:GLY:O	2.20	0.41
44:t:26:LYS:HD3	44:t:37:GLU:HB3	2.02	0.41
27:Z:16:C:H3'	27:Z:17:C:C6	2.56	0.41
33:h:31:VAL:HB	33:h:32:PRO:HD3	2.02	0.41
36:k:77:ILE:HD11	36:k:101:ILE:HG21	2.03	0.41
42:r:4:ILE:HG12	42:r:106:VAL:HG22	2.02	0.41
42:r:59:GLU:OE1	42:r:66:ILE:HB	2.20	0.41
45:u:51:GLN:HG2	45:u:86:LEU:HD11	2.02	0.41
55:8:1:GLY:O	55:8:2:HIS:C	2.64	0.41
6:a:527:C:N3	6:a:2779:U:H2'	2.35	0.41
6:a:890:C:H3'	6:a:891:G:O4'	2.21	0.41
6:a:1141:U:H4'	6:a:1142:A:O4'	2.20	0.41
7:A:1371:G:O3'	17:I:71:GLY:HA3	2.19	0.41
6:a:858:G:O2'	6:a:2268:A:N3	2.53	0.41
13:D:188:ARG:NH2	13:D:195:ILE:O	2.54	0.41
25:T:55:GLN:N	25:T:56:PRO:HD2	2.35	0.41
34:i:110:PRO:O	34:i:115:GLY:HA3	2.19	0.41
34:i:125:TYR:OH	34:i:132:HIS:NE2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:1248:G:OP1	30:e:44:ARG:NH2	2.52	0.41
29:c:181:MET:HB3	29:c:268:VAL:HB	2.02	0.41
32:g:27:LYS:HG3	32:g:32:GLU:HG2	2.03	0.41
6:a:1050:A:C2	6:a:2751:G:C4	3.09	0.41
7:A:79:G:H1	7:A:90:C:H42	1.68	0.41
15:F:18:VAL:HB	15:F:19:PRO:HD3	2.02	0.41
37:m:38:LEU:N	37:m:39:PRO:CD	2.84	0.41
3:d:62:LYS:N	3:d:63:PRO:CD	2.84	0.41
6:a:1607:C:H4'	6:a:1608:A:O5'	2.21	0.41
25:T:42:GLY:HA2	25:T:86:LEU:HD11	2.03	0.41
6:a:277:G:H1'	6:a:278:A:C5	2.56	0.40
11:B:129:LEU:HB3	11:B:133:GLU:HB2	2.03	0.40
22:Q:21:ILE:HG13	22:Q:46:VAL:HB	2.01	0.40
6:a:2757:A:N1	32:g:67:THR:HG21	2.36	0.40
7:A:404:G:O2'	7:A:498:A:N1	2.48	0.40
27:Z:8:U:O2'	27:Z:21:A:N1	2.49	0.40
1:K:118:HIS:HE1	23:R:71:THR:CG2	2.34	0.40
6:a:2040:G:H2'	6:a:2041:U:O4'	2.21	0.40
18:M:11:ASP:HB3	18:M:46:SER:HB3	2.02	0.40
29:c:5:LYS:NZ	29:c:16:VAL:O	2.48	0.40
6:a:247:G:H4'	6:a:386:G:C5	2.56	0.40
34:i:31:GLU:HB3	34:i:142:ILE:HG23	2.03	0.40
7:A:649:A:H2'	7:A:650:G:O4'	2.21	0.40
13:D:171:LEU:HD23	13:D:182:PHE:HA	2.04	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	K	113/129 (88%)	110 (97%)	3 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
3	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
4	4	55/70 (79%)	53 (96%)	2 (4%)	0	100	100
5	3	36/38 (95%)	36 (100%)	0	0	100	100
8	0	47/55 (86%)	47 (100%)	0	0	100	100
9	1	43/46 (94%)	43 (100%)	0	0	100	100
10	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
11	B	222/241 (92%)	216 (97%)	6 (3%)	0	100	100
12	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
13	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
14	E	154/167 (92%)	153 (99%)	1 (1%)	0	100	100
15	F	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
16	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
17	I	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
18	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
19	N	98/101 (97%)	98 (100%)	0	0	100	100
20	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	P	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
22	Q	75/84 (89%)	71 (95%)	4 (5%)	0	100	100
23	R	53/75 (71%)	53 (100%)	0	0	100	100
24	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
25	T	84/87 (97%)	84 (100%)	0	0	100	100
29	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
30	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
31	f	175/179 (98%)	172 (98%)	3 (2%)	0	100	100
32	g	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
33	h	39/149 (26%)	37 (95%)	2 (5%)	0	100	100
34	i	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
35	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
36	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
37	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
39	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
40	p	115/118 (98%)	115 (100%)	0	0	100	100
41	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
42	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
43	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
44	t	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
45	u	92/94 (98%)	92 (100%)	0	0	100	100
46	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
47	w	75/78 (96%)	75 (100%)	0	0	100	100
48	x	60/63 (95%)	60 (100%)	0	0	100	100
49	y	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
50	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
51	l	132/136 (97%)	129 (98%)	3 (2%)	0	100	100
52	G	143/179 (80%)	137 (96%)	6 (4%)	0	100	100
53	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	39
54	U	68/71 (96%)	68 (100%)	0	0	100	100
55	8	14/20 (70%)	12 (86%)	2 (14%)	0	100	100
All	All	5466/5933 (92%)	5345 (98%)	120 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
53	J	57	VAL

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	K	89/98 (91%)	87 (98%)	2 (2%)	45	77
2	L	102/103 (99%)	102 (100%)	0	100	100
3	d	163/163 (100%)	162 (99%)	1 (1%)	78	93
4	4	54/62 (87%)	54 (100%)	0	100	100
5	3	34/34 (100%)	34 (100%)	0	100	100
8	0	45/49 (92%)	45 (100%)	0	100	100
9	1	37/38 (97%)	37 (100%)	0	100	100
10	2	51/52 (98%)	50 (98%)	1 (2%)	48	78
11	B	186/199 (94%)	186 (100%)	0	100	100
12	C	170/190 (90%)	169 (99%)	1 (1%)	78	93
13	D	172/173 (99%)	167 (97%)	5 (3%)	37	71
14	E	119/126 (94%)	118 (99%)	1 (1%)	73	90
15	F	90/116 (78%)	89 (99%)	1 (1%)	65	88
16	H	104/105 (99%)	104 (100%)	0	100	100
17	I	105/107 (98%)	104 (99%)	1 (1%)	68	89
18	M	93/96 (97%)	93 (100%)	0	100	100
19	N	83/84 (99%)	83 (100%)	0	100	100
20	O	76/77 (99%)	76 (100%)	0	100	100
21	P	65/65 (100%)	65 (100%)	0	100	100
22	Q	71/78 (91%)	71 (100%)	0	100	100
23	R	48/65 (74%)	48 (100%)	0	100	100
24	S	72/79 (91%)	72 (100%)	0	100	100
25	T	65/66 (98%)	65 (100%)	0	100	100
29	c	216/218 (99%)	216 (100%)	0	100	100
30	e	165/165 (100%)	165 (100%)	0	100	100
31	f	148/150 (99%)	146 (99%)	2 (1%)	59	85
32	g	137/138 (99%)	134 (98%)	3 (2%)	45	77
33	h	32/114 (28%)	32 (100%)	0	100	100
34	i	116/116 (100%)	116 (100%)	0	100	100
35	j	104/104 (100%)	104 (100%)	0	100	100
36	k	103/103 (100%)	103 (100%)	0	100	100
37	m	98/103 (95%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	n	86/87 (99%)	86 (100%)	0	100	100
39	o	99/100 (99%)	99 (100%)	0	100	100
40	p	89/90 (99%)	89 (100%)	0	100	100
41	q	84/84 (100%)	84 (100%)	0	100	100
42	r	93/93 (100%)	91 (98%)	2 (2%)	45	77
43	s	80/84 (95%)	79 (99%)	1 (1%)	61	86
44	t	83/85 (98%)	79 (95%)	4 (5%)	23	55
45	u	78/78 (100%)	78 (100%)	0	100	100
46	v	56/63 (89%)	56 (100%)	0	100	100
47	w	67/68 (98%)	67 (100%)	0	100	100
48	x	54/55 (98%)	54 (100%)	0	100	100
49	y	48/49 (98%)	48 (100%)	0	100	100
50	z	47/48 (98%)	47 (100%)	0	100	100
51	l	107/107 (100%)	107 (100%)	0	100	100
52	G	122/147 (83%)	122 (100%)	0	100	100
53	J	86/90 (96%)	86 (100%)	0	100	100
54	U	60/61 (98%)	60 (100%)	0	100	100
55	8	15/19 (79%)	14 (93%)	1 (7%)	15	43
All	All	4567/4844 (94%)	4541 (99%)	26 (1%)	76	93

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	94	GLU
1	K	129	VAL
3	d	110	THR
10	2	31	HIS
12	C	178	LEU
13	D	34	ILE
13	D	35	GLU
13	D	44	ARG
13	D	45	LYS
13	D	188	ARG
14	E	162	GLU
15	F	62	MET
17	I	85	ARG

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Mol	Chain	Res	Type
31	f	120	LYS
31	f	150	ARG
32	g	72	LEU
32	g	73	ASN
32	g	76	VAL
42	r	31	GLN
42	r	66	ILE
43	s	93	LEU
44	t	17	LYS
44	t	40	ASN
44	t	52	LEU
44	t	54	GLN
55	8	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	118	HIS
3	d	32	ASN
3	d	140	HIS
3	d	173	GLN
4	4	20	ASN
4	4	30	HIS
4	4	33	ASN
8	0	45	GLN
10	2	31	HIS
11	B	89	GLN
11	B	103	ASN
11	B	120	GLN
12	C	139	GLN
12	C	140	ASN
13	D	40	GLN
13	D	196	ASN
14	E	70	ASN
14	E	82	GLN
14	E	97	GLN
14	E	132	ASN
15	F	3	HIS
15	F	55	HIS
15	F	68	GLN
16	H	21	ASN
17	I	37	GLN

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Mol	Chain	Res	Type
17	I	110	GLN
19	N	4	GLN
19	N	35	ASN
19	N	66	GLN
20	O	80	GLN
21	P	59	HIS
24	S	14	HIS
25	T	84	ASN
29	c	25	HIS
29	c	115	GLN
29	c	197	ASN
30	e	136	GLN
31	f	27	GLN
31	f	37	ASN
32	g	22	GLN
32	g	30	ASN
32	g	73	ASN
32	g	104	ASN
32	g	116	GLN
33	h	2	GLN
34	i	76	HIS
34	i	80	HIS
34	i	128	ASN
34	i	138	GLN
36	k	35	HIS
39	o	10	GLN
39	o	12	GLN
40	p	37	GLN
40	p	52	GLN
41	q	6	GLN
41	q	66	HIS
42	r	7	HIS
42	r	9	HIS
42	r	31	GLN
42	r	40	ASN
43	s	92	ASN
44	t	40	ASN
45	u	24	ASN
45	u	49	ASN
47	w	6	GLN
47	w	36	HIS
48	x	27	ASN

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Mol	Chain	Res	Type
48	x	36	GLN
48	x	45	GLN
48	x	58	ASN
49	y	9	GLN
51	l	60	GLN
52	G	68	ASN
52	G	86	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	X	2/3 (66%)	0	0
27	Z	76/77 (98%)	17 (22%)	3 (3%)
28	b	118/120 (98%)	10 (8%)	0
6	a	2749/2904 (94%)	305 (11%)	0
7	A	1516/1542 (98%)	209 (13%)	32 (2%)
All	All	4461/4646 (96%)	541 (12%)	35 (0%)

All (541) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	a	10	A
6	a	34	U
6	a	58	G
6	a	62	U
6	a	63	A
6	a	71	A
6	a	74	A
6	a	75	G
6	a	101	A
6	a	102	U
6	a	118	A
6	a	119	A
6	a	120	U
6	a	139	U
6	a	142	A
6	a	163	C
6	a	165	A
6	a	181	A
6	a	196	A
6	a	199	A

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Mol	Chain	Res	Type
6	a	200	U
6	a	215	G
6	a	216	A
6	a	221	A
6	a	222	A
6	a	248	G
6	a	272	A
6	a	278	A
6	a	282	A
6	a	285	G
6	a	286	U
6	a	289	G
6	a	294	A
6	a	310	A
6	a	311	A
6	a	329	G
6	a	330	A
6	a	357	C
6	a	361	G
6	a	362	A
6	a	386	G
6	a	396	G
6	a	404	A
6	a	405	U
6	a	411	G
6	a	412	A
6	a	481	G
6	a	491	G
6	a	503	A
6	a	504	A
6	a	505	A
6	a	509	C
6	a	532	A
6	a	533	G
6	a	543	G
6	a	544	C
6	a	545	U
6	a	546	U
6	a	549	G
6	a	563	A
6	a	573	U
6	a	575	A

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Mol	Chain	Res	Type
6	a	586	A
6	a	603	A
6	a	614	A
6	a	615	U
6	a	627	A
6	a	637	A
6	a	645	C
6	a	646	U
6	a	647	G
6	a	654	A
6	a	655	A
6	a	686	U
6	a	717	C
6	a	730	A
6	a	738	G
6	a	747	5MU
6	a	764	A
6	a	765	C
6	a	775	G
6	a	776	G
6	a	782	A
6	a	784	G
6	a	785	G
6	a	792	A
6	a	805	G
6	a	812	C
6	a	827	U
6	a	828	U
6	a	846	U
6	a	847	U
6	a	859	G
6	a	881	G
6	a	883	G
6	a	884	U
6	a	891	G
6	a	893	C
6	a	895	U
6	a	896	A
6	a	897	C
6	a	898	C
6	a	910	A
6	a	914	G

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Mol	Chain	Res	Type
6	a	915	C
6	a	931	U
6	a	946	C
6	a	961	C
6	a	962	G
6	a	974	G
6	a	983	A
6	a	984	A
6	a	985	C
6	a	996	A
6	a	1009	A
6	a	1012	U
6	a	1013	C
6	a	1022	G
6	a	1026	G
6	a	1033	U
6	a	1045	C
6	a	1046	A
6	a	1108	U
6	a	1110	G
6	a	1111	A
6	a	1112	G
6	a	1115	G
6	a	1116	G
6	a	1122	G
6	a	1128	G
6	a	1129	A
6	a	1132	U
6	a	1133	A
6	a	1134	A
6	a	1135	C
6	a	1142	A
6	a	1171	G
6	a	1187	G
6	a	1253	A
6	a	1256	G
6	a	1271	G
6	a	1272	A
6	a	1301	A
6	a	1320	C
6	a	1321	A
6	a	1352	U

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Mol	Chain	Res	Type
6	a	1365	A
6	a	1379	U
6	a	1383	A
6	a	1386	C
6	a	1403	A
6	a	1411	U
6	a	1416	G
6	a	1419	A
6	a	1420	A
6	a	1421	G
6	a	1428	C
6	a	1452	G
6	a	1453	A
6	a	1455	G
6	a	1482	G
6	a	1493	C
6	a	1509	A
6	a	1510	G
6	a	1515	A
6	a	1534	U
6	a	1535	A
6	a	1536	C
6	a	1537	G
6	a	1569	A
6	a	1578	U
6	a	1585	C
6	a	1608	A
6	a	1609	A
6	a	1647	U
6	a	1648	U
6	a	1649	G
6	a	1674	G
6	a	1715	G
6	a	1729	U
6	a	1730	C
6	a	1731	G
6	a	1733	G
6	a	1738	G
6	a	1764	C
6	a	1773	A
6	a	1800	C
6	a	1801	A

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Mol	Chain	Res	Type
6	a	1808	A
6	a	1809	A
6	a	1816	C
6	a	1829	A
6	a	1847	A
6	a	1848	A
6	a	1858	A
6	a	1870	C
6	a	1871	A
6	a	1873	G
6	a	1906	G
6	a	1907	G
6	a	1913	A
6	a	1914	C
6	a	1929	G
6	a	1930	G
6	a	1937	A
6	a	1938	A
6	a	1939	5MU
6	a	1955	U
6	a	1967	C
6	a	1970	A
6	a	1971	U
6	a	1972	G
6	a	1991	U
6	a	1993	U
6	a	2020	A
6	a	2023	C
6	a	2031	A
6	a	2033	A
6	a	2043	C
6	a	2055	C
6	a	2056	G
6	a	2060	A
6	a	2061	G
6	a	2062	A
6	a	2069	G7M
6	a	2198	A
6	a	2203	U
6	a	2204	G
6	a	2211	A
6	a	2212	A

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Mol	Chain	Res	Type
6	a	2225	A
6	a	2238	G
6	a	2239	G
6	a	2268	A
6	a	2278	A
6	a	2282	G
6	a	2283	C
6	a	2287	A
6	a	2305	U
6	a	2308	G
6	a	2309	A
6	a	2312	U
6	a	2322	A
6	a	2324	U
6	a	2325	G
6	a	2333	A
6	a	2335	A
6	a	2347	C
6	a	2350	C
6	a	2361	G
6	a	2377	A
6	a	2383	G
6	a	2385	C
6	a	2402	U
6	a	2403	C
6	a	2406	A
6	a	2424	C
6	a	2425	A
6	a	2429	G
6	a	2430	A
6	a	2435	A
6	a	2441	U
6	a	2448	A
6	a	2459	A
6	a	2468	A
6	a	2469	A
6	a	2470	G
6	a	2476	A
6	a	2491	U
6	a	2502	G
6	a	2505	G
6	a	2506	U

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Mol	Chain	Res	Type
6	a	2518	A
6	a	2529	G
6	a	2535	G
6	a	2547	A
6	a	2566	A
6	a	2567	G
6	a	2573	C
6	a	2574	G
6	a	2602	A
6	a	2609	U
6	a	2613	U
6	a	2629	U
6	a	2663	G
6	a	2689	U
6	a	2690	U
6	a	2714	G
6	a	2716	C
6	a	2726	A
6	a	2744	G
6	a	2748	A
6	a	2750	A
6	a	2757	A
6	a	2765	A
6	a	2778	A
6	a	2790	U
6	a	2791	G
6	a	2798	U
6	a	2820	A
6	a	2821	A
6	a	2867	G
6	a	2868	A
6	a	2883	A
6	a	2884	U
7	A	4	U
7	A	5	U
7	A	6	G
7	A	8	A
7	A	9	G
7	A	13	U
7	A	14	U
7	A	32	A
7	A	39	G

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Mol	Chain	Res	Type
7	A	47	C
7	A	48	C
7	A	51	A
7	A	70	U
7	A	71	A
7	A	74	A
7	A	83	C
7	A	84	U
7	A	85	U
7	A	86	G
7	A	87	C
7	A	88	U
7	A	94	G
7	A	95	C
7	A	120	A
7	A	122	G
7	A	131	A
7	A	141	G
7	A	144	G
7	A	164	G
7	A	166	U
7	A	182	A
7	A	183	C
7	A	197	A
7	A	202	G
7	A	204	G
7	A	226	G
7	A	240	G
7	A	245	U
7	A	247	G
7	A	251	G
7	A	266	G
7	A	267	C
7	A	280	C
7	A	281	G
7	A	289	G
7	A	321	A
7	A	328	C
7	A	329	A
7	A	339	C
7	A	347	G
7	A	352	C

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Mol	Chain	Res	Type
7	A	354	G
7	A	355	C
7	A	367	U
7	A	372	C
7	A	384	G
7	A	406	G
7	A	411	A
7	A	412	A
7	A	413	G
7	A	414	A
7	A	417	G
7	A	421	U
7	A	422	C
7	A	424	G
7	A	429	U
7	A	436	C
7	A	438	U
7	A	439	U
7	A	453	G
7	A	457	G
7	A	458	U
7	A	459	A
7	A	463	U
7	A	465	A
7	A	467	U
7	A	468	A
7	A	469	C
7	A	478	A
7	A	479	U
7	A	481	G
7	A	484	G
7	A	486	U
7	A	511	C
7	A	518	C
7	A	531	U
7	A	532	A
7	A	536	C
7	A	547	A
7	A	559	A
7	A	572	A
7	A	573	A
7	A	576	C

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Mol	Chain	Res	Type
7	A	577	G
7	A	587	G
7	A	588	G
7	A	596	A
7	A	633	G
7	A	642	A
7	A	648	A
7	A	650	G
7	A	653	U
7	A	665	A
7	A	721	G
7	A	723	U
7	A	724	G
7	A	734	G
7	A	746	A
7	A	748	G
7	A	755	G
7	A	777	A
7	A	793	U
7	A	794	A
7	A	815	A
7	A	817	C
7	A	832	G
7	A	890	G
7	A	914	A
7	A	926	G
7	A	934	C
7	A	935	A
7	A	960	U
7	A	966	2MG
7	A	969	A
7	A	975	A
7	A	976	G
7	A	977	A
7	A	984	C
7	A	992	U
7	A	993	G
7	A	994	A
7	A	996	A
7	A	1003	G
7	A	1004	A
7	A	1006	G

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Mol	Chain	Res	Type
7	A	1007	U
7	A	1008	U
7	A	1009	U
7	A	1024	G
7	A	1027	C
7	A	1030	U
7	A	1031	C
7	A	1033	G
7	A	1034	G
7	A	1035	A
7	A	1036	A
7	A	1039	G
7	A	1046	A
7	A	1065	U
7	A	1094	G
7	A	1095	U
7	A	1101	A
7	A	1129	C
7	A	1130	A
7	A	1132	C
7	A	1137	C
7	A	1139	G
7	A	1145	A
7	A	1146	A
7	A	1184	G
7	A	1196	A
7	A	1197	A
7	A	1211	U
7	A	1212	U
7	A	1213	A
7	A	1225	A
7	A	1226	C
7	A	1227	A
7	A	1238	A
7	A	1256	A
7	A	1260	G
7	A	1275	A
7	A	1280	A
7	A	1286	U
7	A	1287	A
7	A	1300	G
7	A	1302	C

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Mol	Chain	Res	Type
7	A	1317	C
7	A	1319	A
7	A	1320	C
7	A	1331	G
7	A	1338	G
7	A	1346	A
7	A	1353	G
7	A	1363	A
7	A	1370	G
7	A	1378	C
7	A	1379	G
7	A	1381	U
7	A	1397	C
7	A	1398	A
7	A	1419	G
7	A	1429	A
7	A	1441	A
7	A	1451	U
7	A	1452	C
7	A	1453	G
7	A	1492	A
7	A	1493	A
7	A	1494	G
7	A	1497	G
7	A	1503	A
7	A	1505	G
7	A	1506	U
7	A	1517	G
7	A	1529	G
7	A	1530	G
7	A	1533	C
7	A	1534	A
27	Z	6	G
27	Z	7	G
27	Z	8	U
27	Z	9	G
27	Z	16	C
27	Z	17	C
27	Z	17(A)	U
27	Z	18	G
27	Z	19	G
27	Z	20	U

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Mol	Chain	Res	Type
27	Z	22	G
27	Z	46	G
27	Z	47	U
27	Z	51	C
27	Z	58	A
27	Z	65	C
27	Z	76	A
28	b	35	C
28	b	36	C
28	b	37	C
28	b	45	A
28	b	56	G
28	b	67	G
28	b	89	U
28	b	90	C
28	b	99	A
28	b	109	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	5	U
7	A	7	A
7	A	13	U
7	A	62	U
7	A	70	U
7	A	94	G
7	A	119	A
7	A	199	A
7	A	280	C
7	A	438	U
7	A	532	A
7	A	587	G
7	A	641	U
7	A	653	U
7	A	793	U
7	A	858	G
7	A	992	U
7	A	993	G
7	A	1006	G
7	A	1034	G
7	A	1035	A

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Mol	Chain	Res	Type
7	A	1124	G
7	A	1129	C
7	A	1145	A
7	A	1211	U
7	A	1225	A
7	A	1319	A
7	A	1320	C
7	A	1337	G
7	A	1397	C
7	A	1447	A
7	A	1505	G
27	Z	7	G
27	Z	46	G
27	Z	60	U

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

40 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	5MU	a	747	6	19,22,23	0.29	0	28,32,35	0.42	0
6	2MG	a	2445	6	23,26,27	0.54	0	32,38,41	0.53	0
6	3TD	a	1915	6	18,22,23	0.83	1 (5%)	22,32,35	0.65	0
6	1MG	a	745	6	22,26,27	0.85	2 (9%)	33,39,42	0.47	0
6	PSU	a	746	6	18,21,22	0.87	1 (5%)	22,30,33	0.70	0
6	PSU	a	1917	6	18,21,22	0.88	1 (5%)	22,30,33	0.60	0
6	PSU	a	2457	6	18,21,22	0.96	1 (5%)	22,30,33	0.63	0
6	5MC	a	1962	6	18,22,23	0.47	0	26,32,35	0.65	0
7	2MG	A	1516	7	23,26,27	0.39	0	32,38,41	0.52	0
6	G7M	a	2069	6	23,26,27	0.58	0	35,39,42	0.68	1 (2%)
7	MA6	A	1518	7	23,26,27	0.34	0	34,38,41	0.67	1 (2%)
7	MA6	A	1519	7	23,26,27	0.34	0	34,38,41	0.84	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PSU	a	1911	6	18,21,22	0.87	1 (5%)	22,30,33	0.62	0
6	2MA	a	2503	6	22,25,26	0.48	0	33,37,40	0.79	3 (9%)
7	2MG	A	966	7	23,26,27	0.42	0	32,38,41	0.38	0
7	2MG	A	1207	7	23,26,27	0.38	0	32,38,41	0.43	0
6	H2U	a	2449	6	18,21,22	0.96	2 (11%)	21,30,33	1.03	2 (9%)
51	MS6	l	82	51	5,7,8	0.22	0	2,7,9	0.27	0
6	5MU	a	1939	6	19,22,23	0.41	0	28,32,35	0.45	0
6	OMC	a	2498	6	19,22,23	0.41	0	26,31,34	0.47	0
6	2MG	a	1835	6	23,26,27	0.35	0	32,38,41	0.43	0
6	OMU	a	2552	6	19,22,23	0.37	0	26,31,34	0.42	0
2	D2T	L	89	2	7,9,10	0.99	0	6,11,13	1.77	3 (50%)
7	4OC	A	1402	7	20,23,24	0.37	0	26,32,35	0.58	0
6	OMG	a	2251	27,6	23,26,27	0.43	0	33,38,41	0.56	0
7	G7M	A	527	7	23,26,27	0.75	1 (4%)	35,39,42	0.65	0
7	5MC	A	1407	7	18,22,23	0.34	0	26,32,35	0.67	0
6	PSU	a	2504	6	18,21,22	0.93	1 (5%)	22,30,33	0.73	1 (4%)
6	6MZ	a	2030	6	22,25,26	0.71	0	30,36,39	0.70	0
7	5MC	A	967	7	18,22,23	0.37	0	26,32,35	0.64	0
51	4D4	l	81	51	9,11,12	1.89	2 (22%)	8,13,15	1.31	0
7	UR3	A	1498	7	19,22,23	0.38	0	26,32,35	0.73	1 (3%)
6	PSU	a	955	6	18,21,22	0.85	1 (5%)	22,30,33	0.78	0
6	PSU	a	2580	6	18,21,22	0.97	1 (5%)	22,30,33	0.86	1 (4%)
1	IAS	K	119	1	6,7,8	1.37	1 (16%)	6,8,10	0.88	0
7	PSU	A	516	7	18,21,22	0.95	1 (5%)	22,30,33	0.72	0
6	PSU	a	2605	6	18,21,22	1.00	2 (11%)	22,30,33	0.85	1 (4%)
3	MEQ	d	150	3	8,9,10	0.57	0	5,10,12	1.10	0
6	6MZ	a	1618	6	22,25,26	0.44	0	30,36,39	0.58	0
6	PSU	a	2604	6	18,21,22	0.92	1 (5%)	22,30,33	0.93	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5MU	a	747	6	-	0/7/25/26	0/2/2/2
6	2MG	a	2445	6	-	0/9/27/28	0/3/3/3
6	3TD	a	1915	6	-	0/7/25/26	0/2/2/2
6	1MG	a	745	6	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	a	746	6	-	3/7/25/26	0/2/2/2
6	PSU	a	1917	6	-	0/7/25/26	0/2/2/2
6	PSU	a	2457	6	-	0/7/25/26	0/2/2/2
6	5MC	a	1962	6	-	0/7/25/26	0/2/2/2
7	2MG	A	1516	7	-	0/9/27/28	0/3/3/3
6	G7M	a	2069	6	-	2/7/25/26	0/3/3/3
7	MA6	A	1518	7	-	0/11/29/30	0/3/3/3
7	MA6	A	1519	7	-	3/11/29/30	0/3/3/3
6	PSU	a	1911	6	-	0/7/25/26	0/2/2/2
6	2MA	a	2503	6	-	3/7/25/26	0/3/3/3
7	2MG	A	966	7	-	0/9/27/28	0/3/3/3
7	2MG	A	1207	7	-	0/9/27/28	0/3/3/3
6	H2U	a	2449	6	-	0/7/38/39	0/2/2/2
51	MS6	l	82	51	-	1/4/6/8	-
6	5MU	a	1939	6	-	0/7/25/26	0/2/2/2
6	OMC	a	2498	6	-	0/9/27/28	0/2/2/2
6	2MG	a	1835	6	-	0/9/27/28	0/3/3/3
6	OMU	a	2552	6	-	0/9/27/28	0/2/2/2
2	D2T	L	89	2	-	4/7/12/14	-
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
6	OMG	a	2251	27,6	-	1/9/27/28	0/3/3/3
7	G7M	A	527	7	-	1/7/25/26	0/3/3/3
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
6	PSU	a	2504	6	-	0/7/25/26	0/2/2/2
6	6MZ	a	2030	6	-	2/9/27/28	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
51	4D4	l	81	51	-	1/11/12/14	-
7	UR3	A	1498	7	-	0/7/25/26	0/2/2/2
6	PSU	a	955	6	-	0/7/25/26	0/2/2/2
6	PSU	a	2580	6	-	0/7/25/26	0/2/2/2
1	IAS	K	119	1	-	0/7/7/8	-
7	PSU	A	516	7	-	0/7/25/26	0/2/2/2
6	PSU	a	2605	6	-	0/7/25/26	0/2/2/2
3	MEQ	d	150	3	-	2/8/9/11	-
6	6MZ	a	1618	6	-	0/9/27/28	0/3/3/3
6	PSU	a	2604	6	-	0/7/25/26	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	l	81	4D4	CZ-NE	4.05	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	516	PSU	C6-C5	3.64	1.39	1.35
6	a	1915	3TD	C6-C5	3.32	1.39	1.35
6	a	1917	PSU	C6-C5	3.32	1.39	1.35
6	a	1911	PSU	C6-C5	3.27	1.39	1.35
6	a	2580	PSU	C6-C5	3.18	1.39	1.35
6	a	2457	PSU	C6-C5	3.17	1.39	1.35
6	a	2604	PSU	C6-C5	3.10	1.38	1.35
6	a	746	PSU	C6-C5	3.05	1.38	1.35
6	a	2605	PSU	C6-C5	3.00	1.38	1.35
6	a	2504	PSU	C6-C5	2.86	1.38	1.35
51	l	81	4D4	CZ-NH2	2.86	1.43	1.32
1	K	119	IAS	CB-CG	2.73	1.56	1.49
7	A	527	G7M	C8-N7	2.62	1.37	1.33
6	a	2449	H2U	C1'-N1	2.42	1.51	1.46
6	a	2449	H2U	C2-N3	-2.25	1.34	1.38
6	a	2605	PSU	C4-C5	-2.23	1.37	1.44
6	a	745	1MG	C5-C6	-2.17	1.40	1.45
6	a	955	PSU	C6-C5	2.10	1.37	1.35
6	a	745	1MG	C1'-N9	-2.03	1.41	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1518	MA6	C2-N1-C6	3.00	118.84	111.75
7	A	1519	MA6	C2-N1-C6	2.96	118.75	111.75
6	a	2580	PSU	C3'-C2'-C1'	2.84	104.94	101.64
6	a	2449	H2U	N3-C2-N1	2.73	119.54	116.65
6	a	2449	H2U	O2-C2-N1	-2.53	119.93	123.11
2	L	89	D2T	OD1-CG-CB	-2.51	117.17	122.44
6	a	2503	2MA	C5-C4-N3	-2.41	124.48	127.19
6	a	2604	PSU	C2'-C3'-C4'	-2.36	98.05	102.64
6	a	2503	2MA	N3-C4-N9	2.23	130.08	126.99
2	L	89	D2T	O-C-CA	-2.20	119.01	124.78
6	a	2503	2MA	O3'-C3'-C2'	-2.17	104.80	111.82
6	a	2504	PSU	C2'-C3'-C4'	-2.14	98.49	102.64
6	a	2605	PSU	C2'-C3'-C4'	-2.11	98.54	102.64
2	L	89	D2T	OD2-CG-CB	2.11	117.71	113.15
6	a	2604	PSU	C5-C6-N1	-2.08	118.99	122.11
6	a	2069	G7M	N9-C8-N7	-2.00	107.25	112.21
7	A	1498	UR3	C4-N3-C2	-2.00	122.68	124.56

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	89	D2T	CA-CB-CG-OD1
2	L	89	D2T	CA-CB-CG-OD2
6	a	746	PSU	C2'-C1'-C5-C4
6	a	746	PSU	C2'-C1'-C5-C6
6	a	746	PSU	O4'-C1'-C5-C6
3	d	150	MEQ	NE2-CD-CG-CB
3	d	150	MEQ	OE1-CD-CG-CB
6	a	2030	6MZ	O4'-C4'-C5'-O5'
7	A	1519	MA6	O4'-C4'-C5'-O5'
7	A	1519	MA6	C5-C6-N6-C10
2	L	89	D2T	CG-CB-SB-CB1
6	a	2030	6MZ	C3'-C4'-C5'-O5'
6	a	2503	2MA	C4'-C5'-O5'-P
7	A	1519	MA6	C3'-C4'-C5'-O5'
2	L	89	D2T	SB-CB-CG-OD2
7	A	527	G7M	C3'-C4'-C5'-O5'
6	a	2251	OMG	C1'-C2'-O2'-CM2
6	a	2069	G7M	O4'-C4'-C5'-O5'
51	l	82	MS6	CB-CG-SD-CE
6	a	2069	G7M	C4'-C5'-O5'-P
6	a	2503	2MA	O4'-C4'-C5'-O5'
6	a	2503	2MA	O4'-C1'-N9-C8
51	l	81	4D4	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	a	1939	5MU	1	0
6	a	2552	OMU	1	0
6	a	2251	OMG	1	0
6	a	2030	6MZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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](#)

There are no chain breaks in this entry.

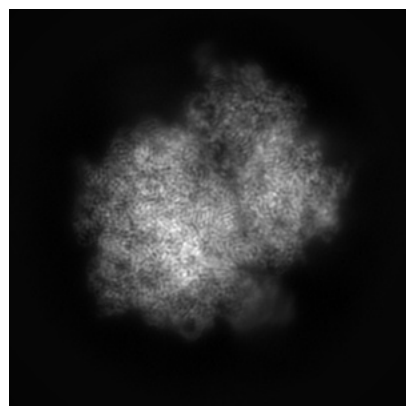
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55844. These allow visual inspection of the internal detail of the map and identification of artifacts.

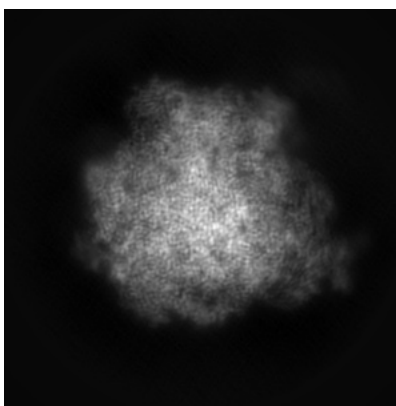
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

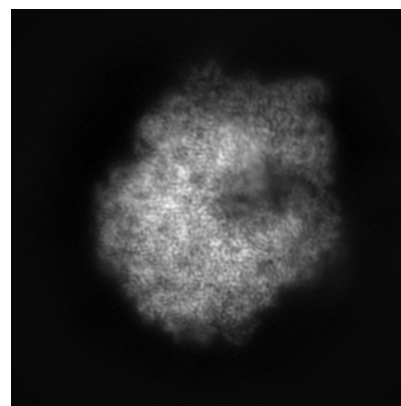
6.1.1 Primary map



X

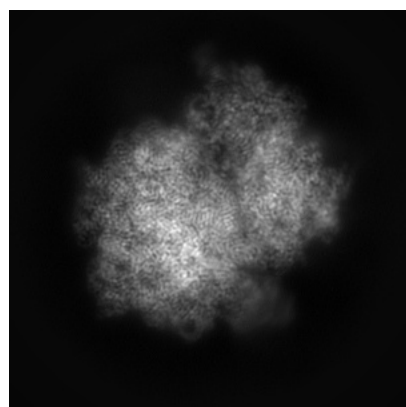


Y

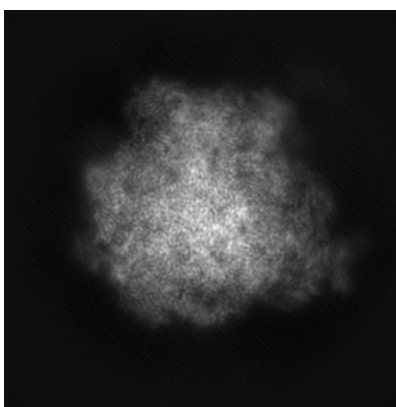


Z

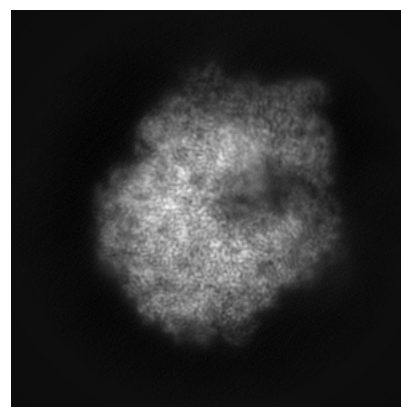
6.1.2 Raw map



X



Y

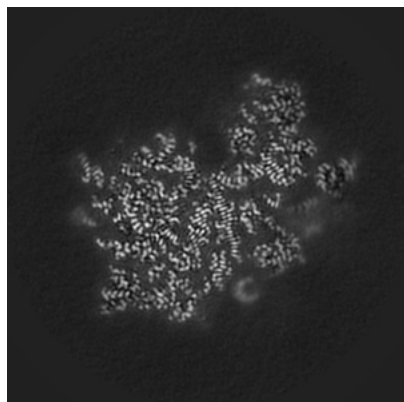


Z

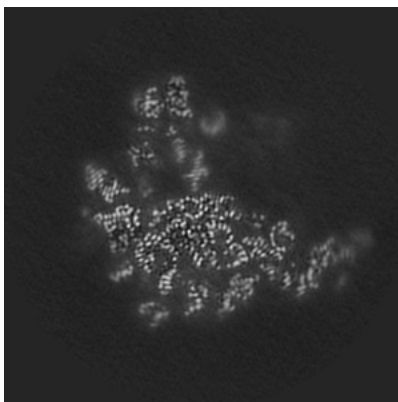
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

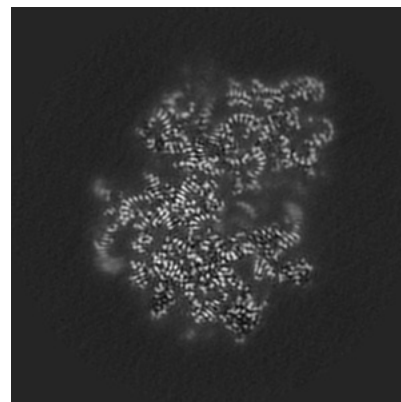
6.2.1 Primary map



X Index: 208

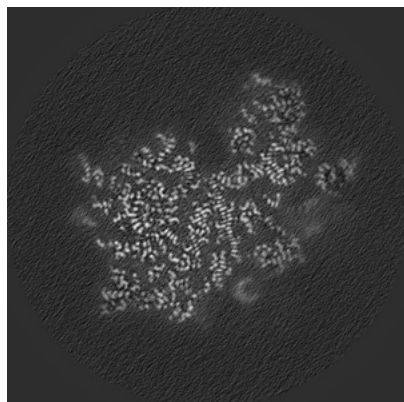


Y Index: 208

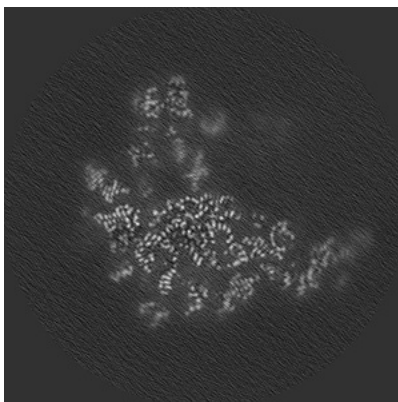


Z Index: 208

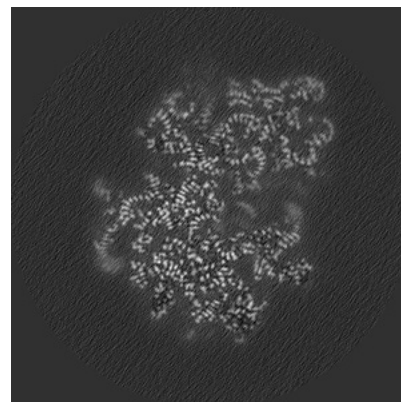
6.2.2 Raw map



X Index: 208



Y Index: 208

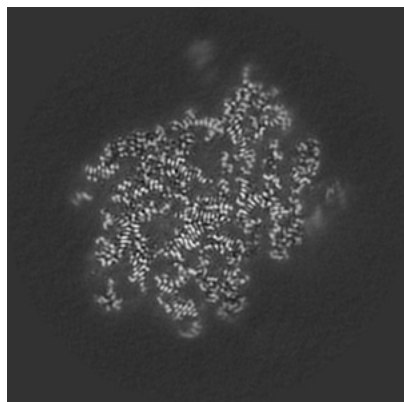


Z Index: 208

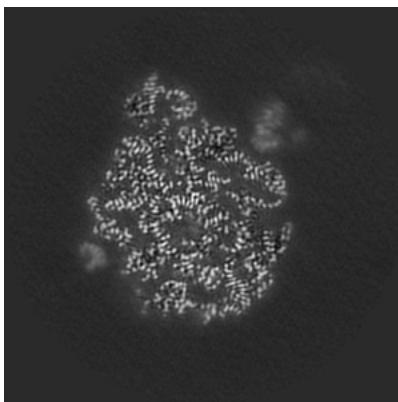
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

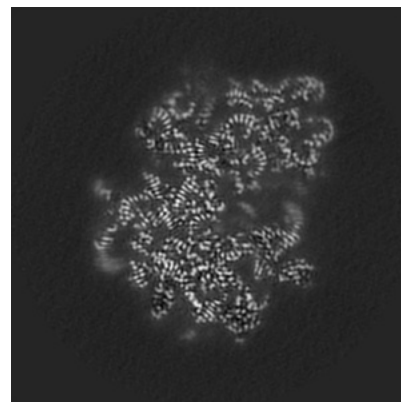
6.3.1 Primary map



X Index: 179

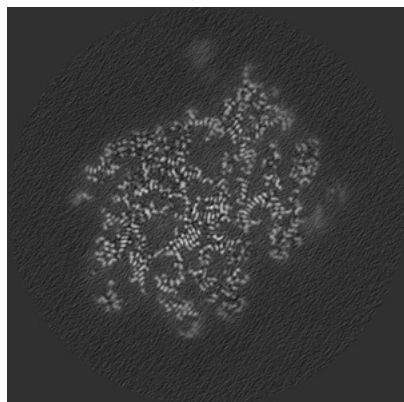


Y Index: 171

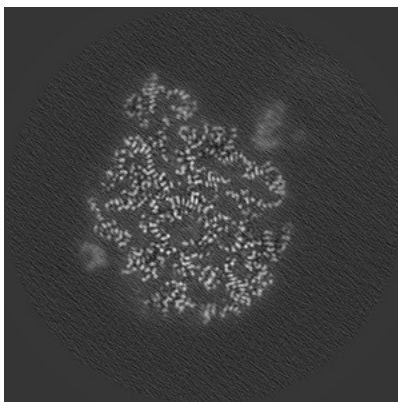


Z Index: 209

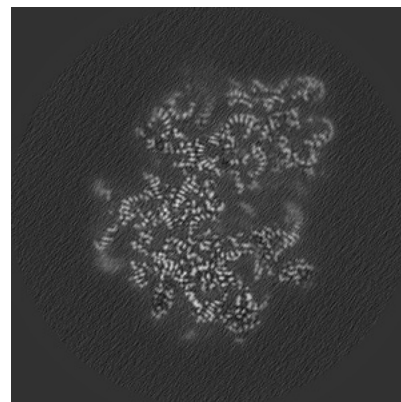
6.3.2 Raw map



X Index: 178



Y Index: 170

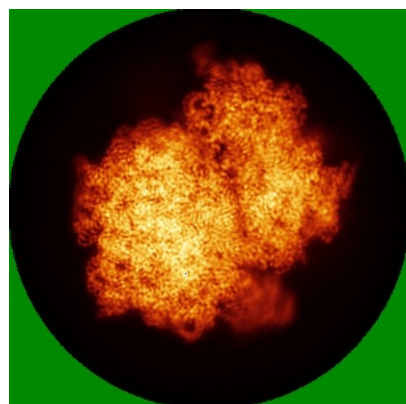


Z Index: 209

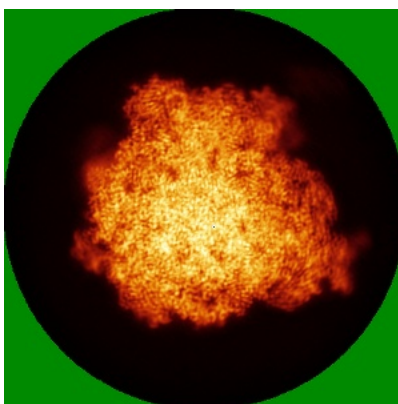
The images above show the largest variance slices of the map in three orthogonal directions.

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

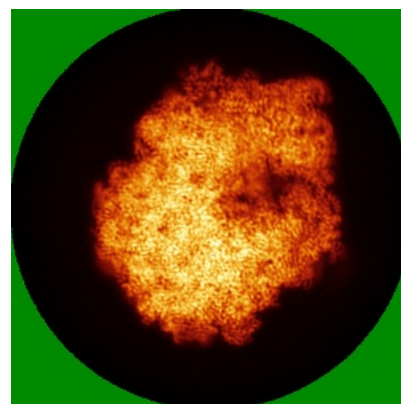
6.4.1 Primary map



X

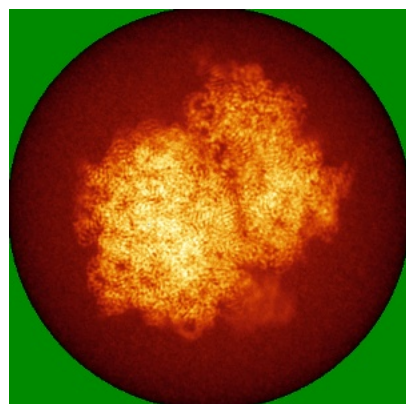


Y

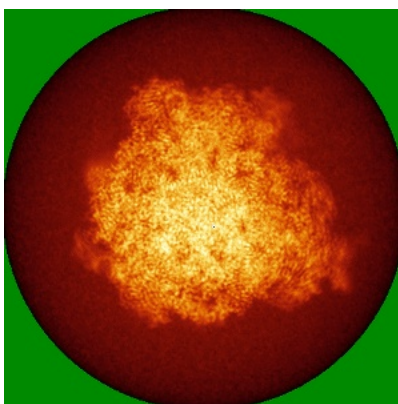


Z

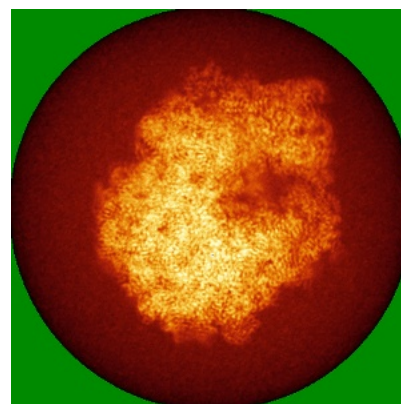
6.4.2 Raw map



X



Y

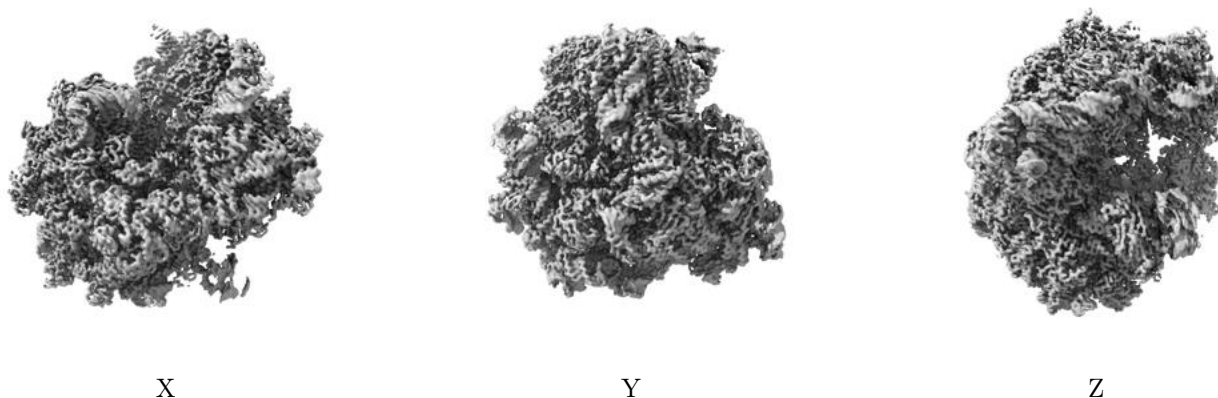


Z

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.

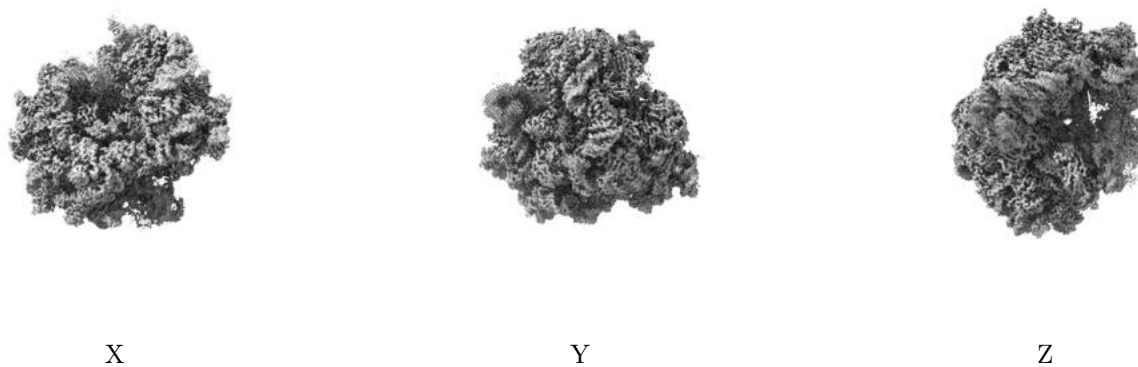
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

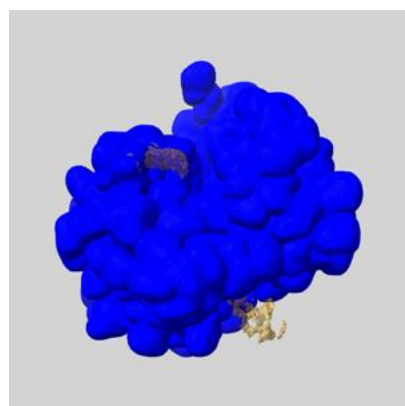
6.6 Mask visualisation [i](#)

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

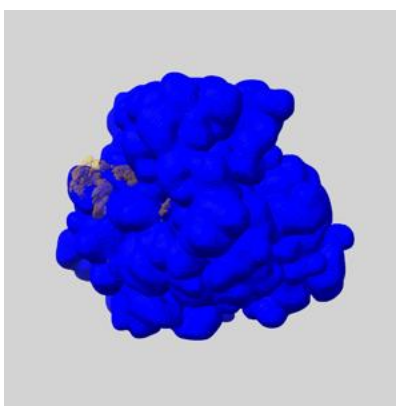
A mask typically either:

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

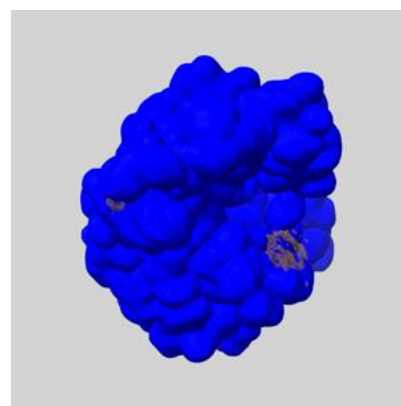
6.6.1 emd_55844_msk_1.map [i](#)



X



Y

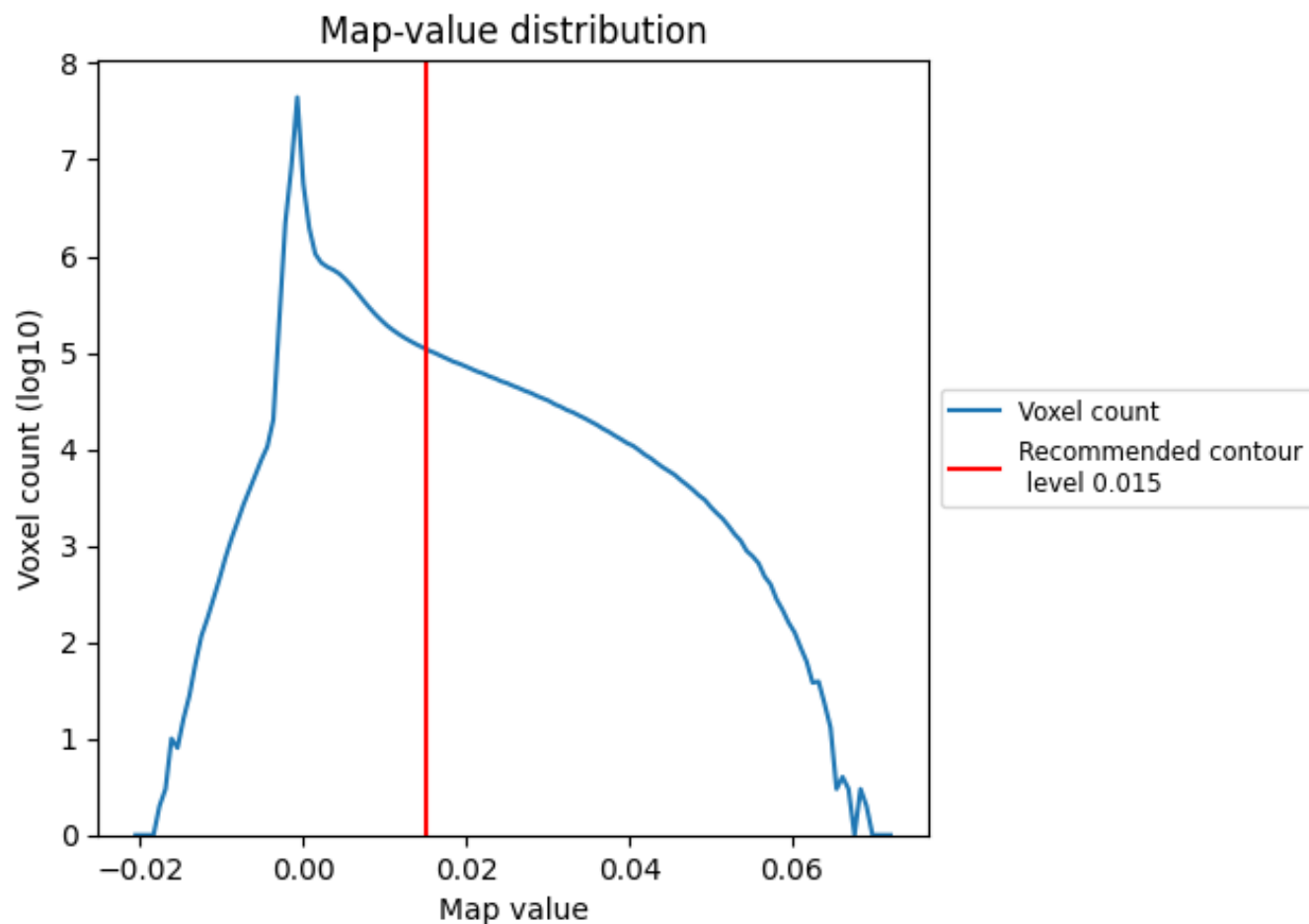


Z

7 Map analysis [i](#)

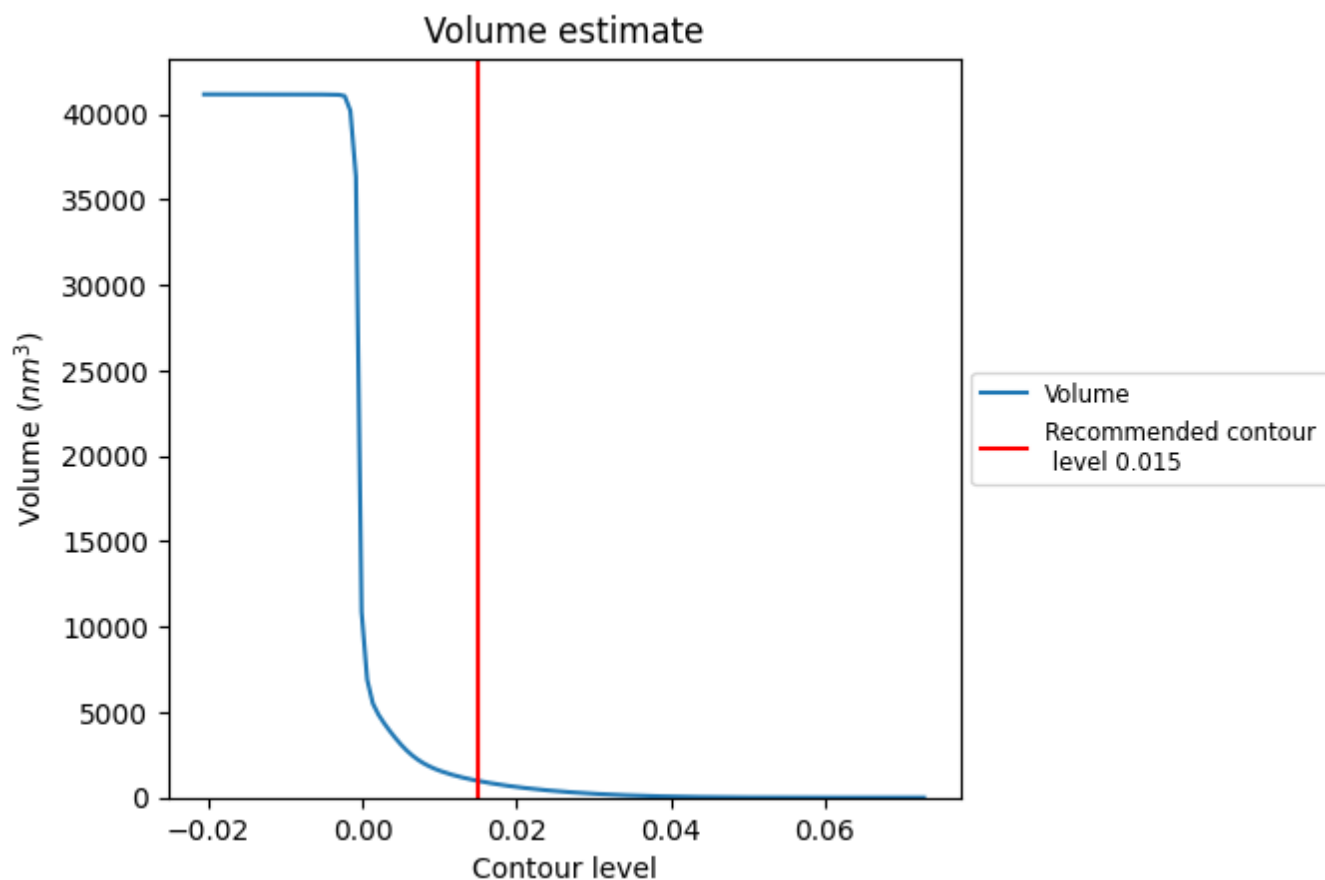
This section contains the results of statistical analysis of the map.

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.

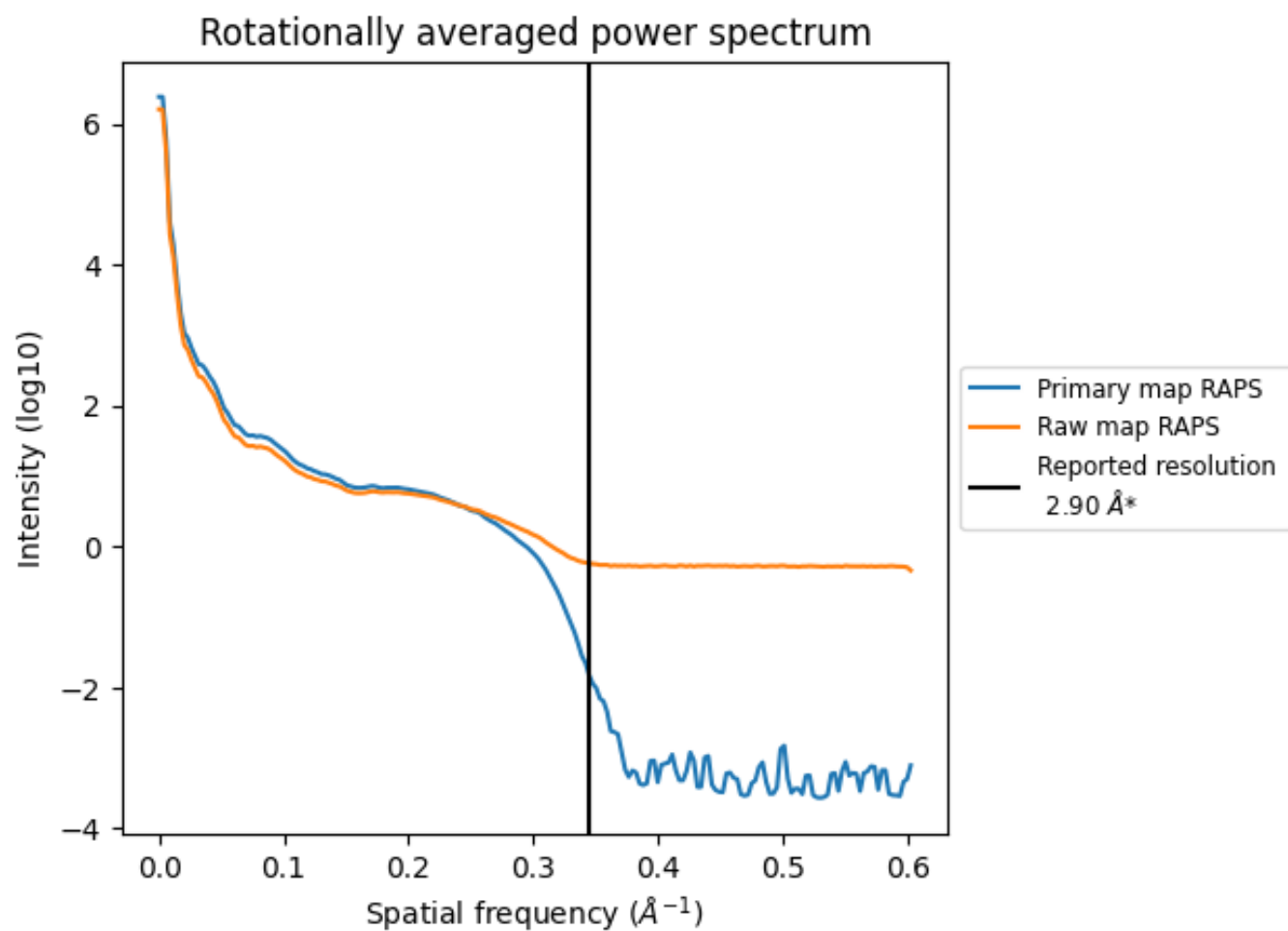
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 976 nm^3 ; this corresponds to an approximate mass of 882 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

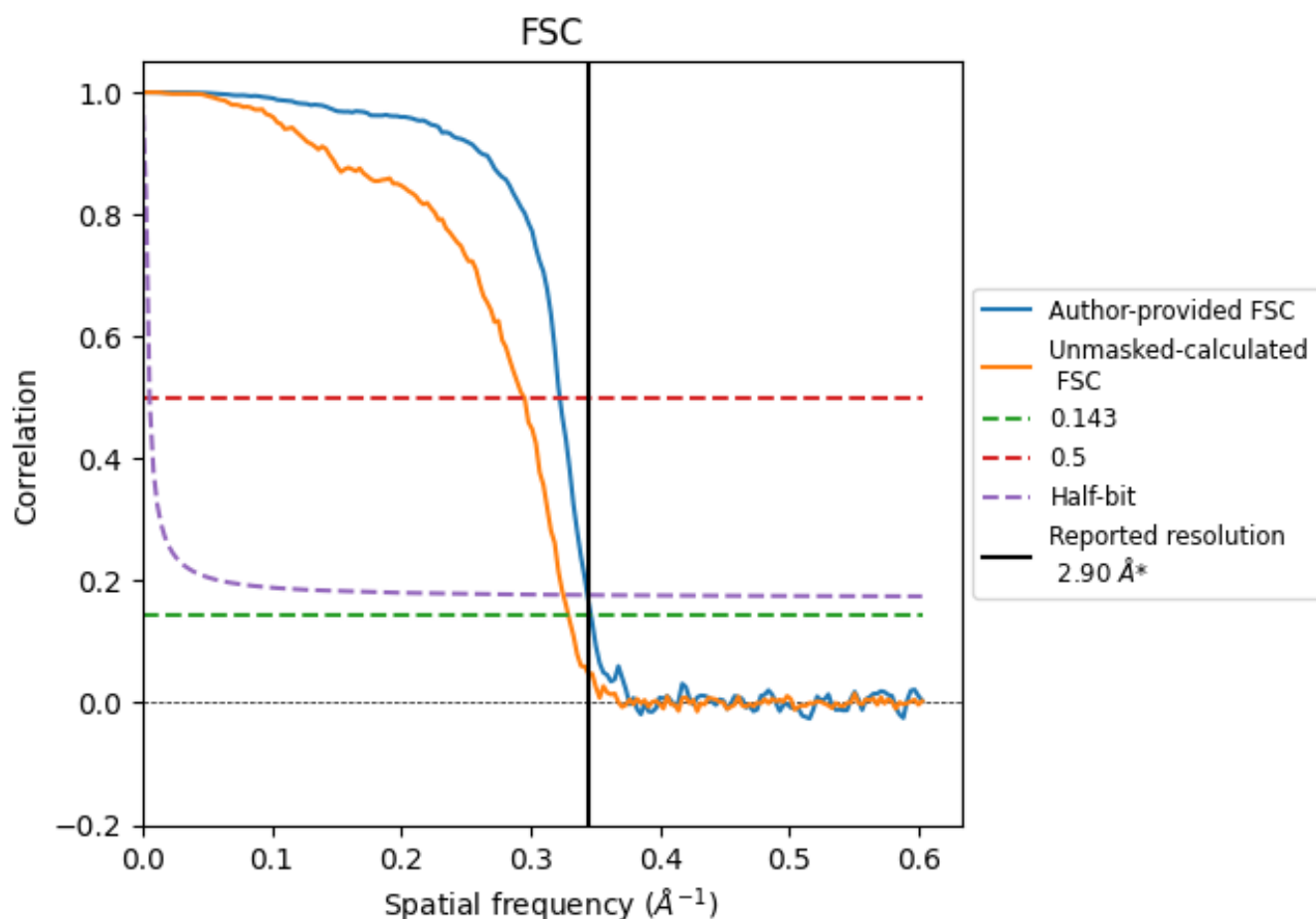


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

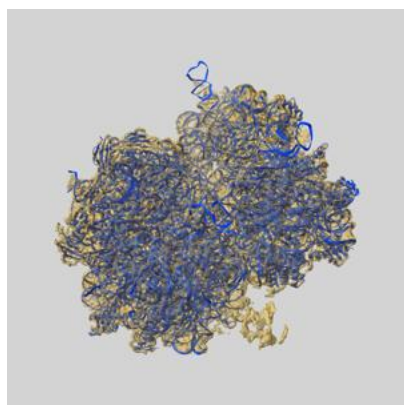
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.10	2.91
Unmasked-calculated*	3.04	3.39	3.08

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

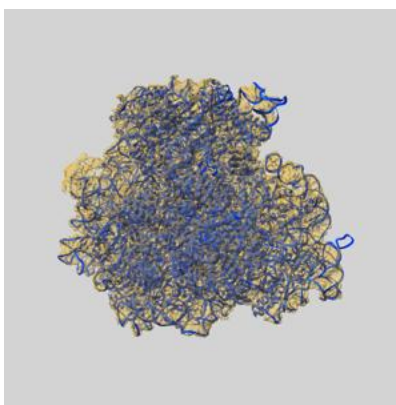
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55844 and PDB model 9TEW. Per-residue inclusion information can be found in section [3](#) on page [15](#).

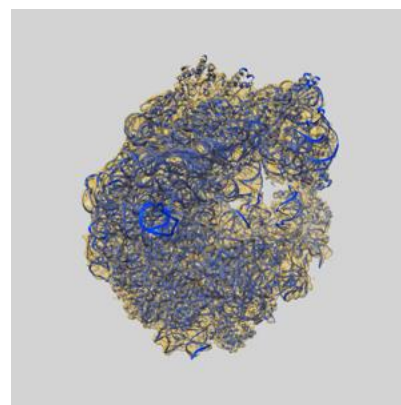
9.1 Map-model overlay [i](#)



X



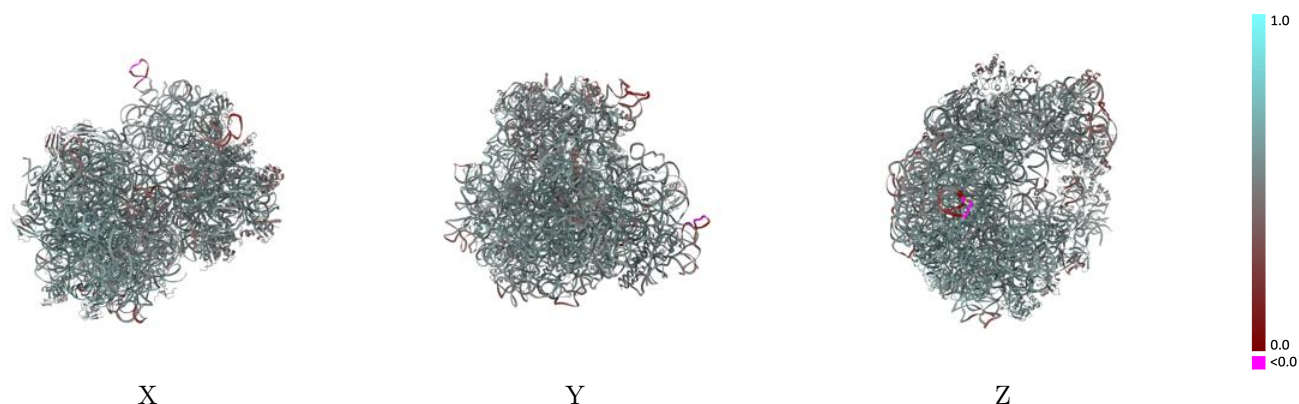
Y



Z

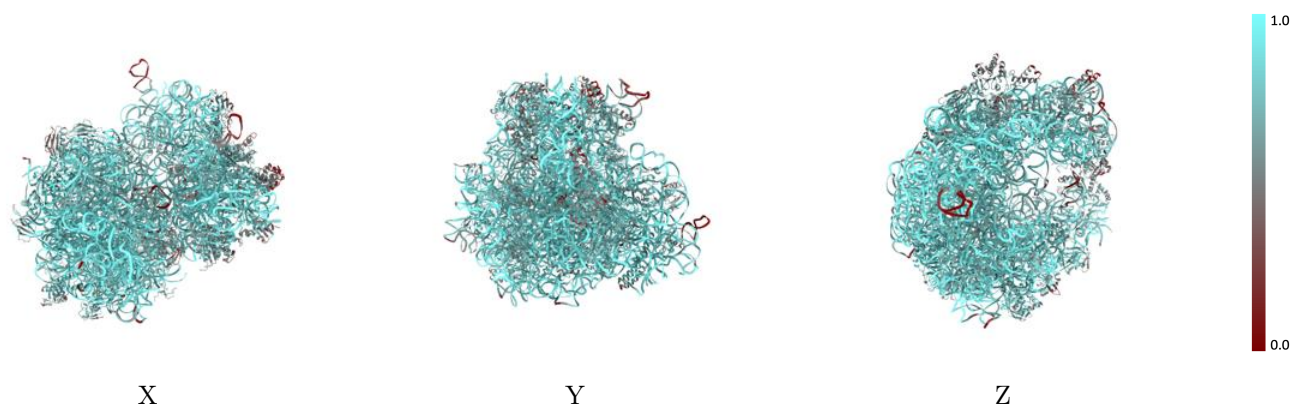
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



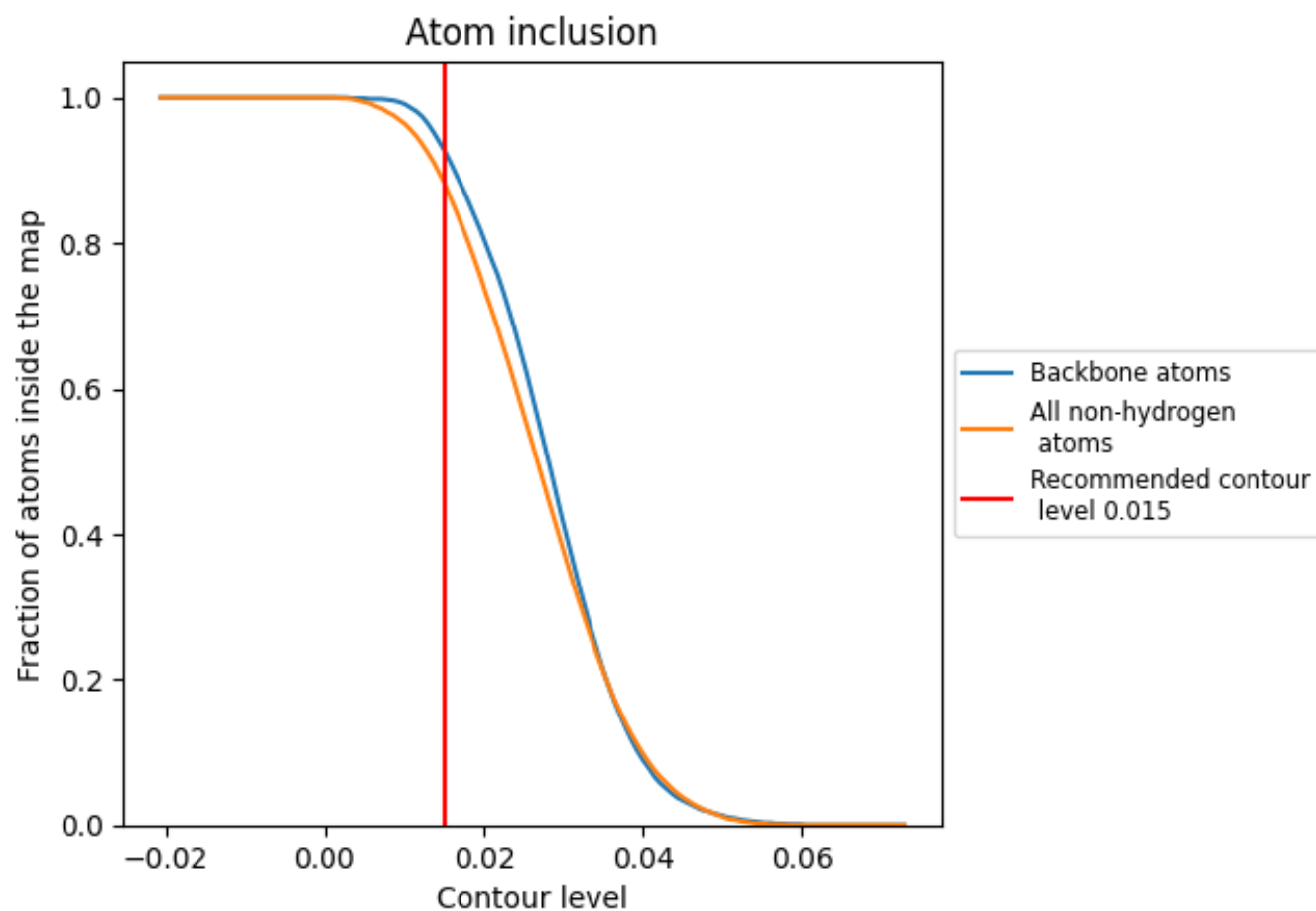
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.5500
0	 0.8090	 0.5540
1	 0.9620	 0.5950
2	 0.9270	 0.6010
3	 0.8500	 0.5730
4	 0.3880	 0.4760
8	 0.7620	 0.5420
A	 0.9280	 0.5370
B	 0.5490	 0.4800
C	 0.6770	 0.5290
D	 0.6380	 0.5200
E	 0.7970	 0.5500
F	 0.6710	 0.5120
G	 0.6340	 0.4860
H	 0.7530	 0.5450
I	 0.6910	 0.4980
J	 0.5620	 0.4820
K	 0.7600	 0.5320
L	 0.7470	 0.5430
M	 0.6880	 0.5010
N	 0.7360	 0.5290
O	 0.7320	 0.5310
P	 0.7700	 0.5440
Q	 0.7120	 0.5230
R	 0.7250	 0.5260
S	 0.6560	 0.4990
T	 0.7500	 0.5140
U	 0.5650	 0.4730
X	 1.0000	 0.5920
Z	 0.8540	 0.4990
a	 0.9570	 0.5670
b	 0.9450	 0.5580
c	 0.8820	 0.5850
d	 0.8450	 0.5780
e	 0.7620	 0.5530



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Chain	Atom inclusion	Q-score
f	 0.6560	 0.5060
g	 0.6200	 0.4910
h	 0.6770	 0.5180
i	 0.8360	 0.5730
j	 0.8030	 0.5720
k	 0.8250	 0.5720
l	 0.8370	 0.5700
m	 0.8930	 0.5880
n	 0.7530	 0.5290
o	 0.7900	 0.5650
p	 0.8790	 0.5830
q	 0.7830	 0.5670
r	 0.8250	 0.5700
s	 0.7760	 0.5430
t	 0.7240	 0.5410
u	 0.7370	 0.5400
v	 0.8670	 0.5760
w	 0.8740	 0.5770
x	 0.7240	 0.5150
y	 0.8060	 0.5630
z	 0.8220	 0.5750