



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2025 – 12:47 pm GMT

PDB ID : 7NAW / pdb\_00007naw  
EMDB ID : EMD-12250  
Title : Bacterial 30S ribosomal subunit assembly complex state B (Consensus Refinement)  
Authors : Schedlbauer, A.; Iturrioz, I.; Ochoa-Lizarralde, B.; Diercks, T.; Kaminishi, T.; Capuni, R.; Astigarraga, E.; Gil-Carton, D.; Fucini, P.; Connell, S.  
Deposited on : 2021-01-25  
Resolution : 4.05 Å (reported)  
Based on initial model : 4YBB

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

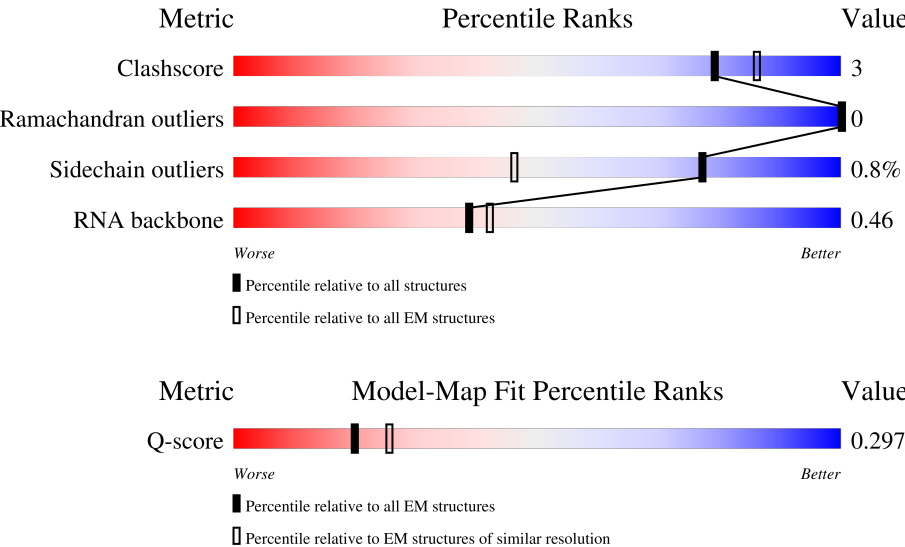
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.05 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.



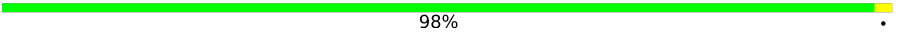



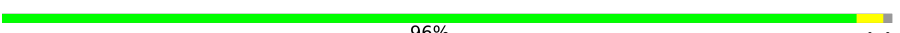












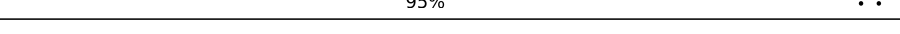

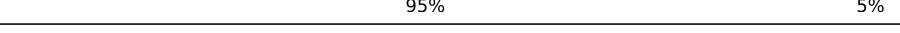
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	6569 ( 3.55 - 4.55 )

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  $\geq 3$ , 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	A	1542	<div> <div>41%</div> <div>36%</div> <div>13%</div> <div>•</div> <div>7%</div> </div>
2	B	241	<div> <div>17%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
3	C	233	<div> <div>•</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	X	151	
23	Y	273	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1427	Total	C	N	O	P	0	0
			30625	13663	5617	9918	1427		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	52	Total	C	N	O	S	0	0
			430	269	89	71	1		

- Molecule 22 is a protein called Ribosome maturation factor RimP.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	151	Total	C	N	O	S	0	0
			1174	742	197	230	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	151	ALA	-	expression tag	UNP A0A0J3VRH1

- Molecule 23 is a protein called Ribosomal RNA small subunit methyltransferase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	252	Total	C	N	O	S	0	0
			1963	1252	338	360	13		

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	A	31	Total	Mg	0
			31	31	

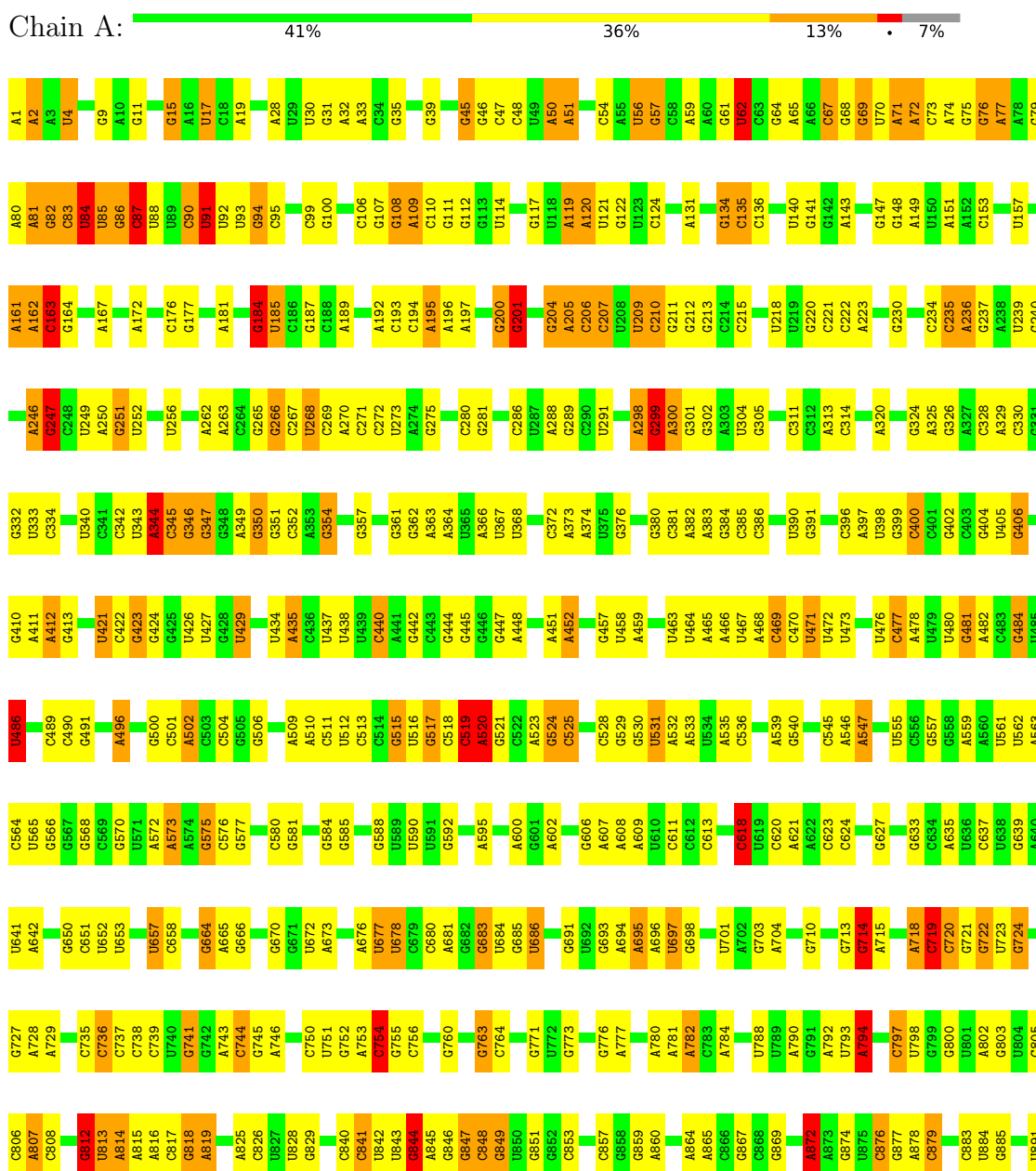
- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	B	1	Total	Zn	0
			1	1	

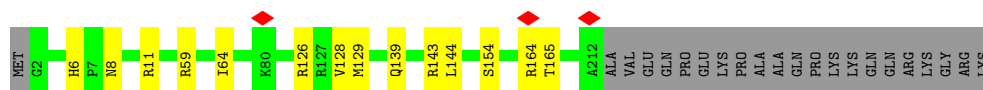
### 3 Residue-property plots

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

#### • Molecule 1: 16S rRNA







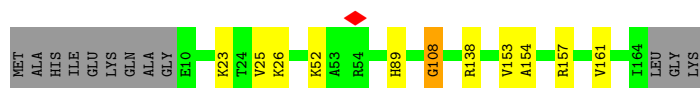
- Molecule 4: Small ribosomal subunit protein uS4

Chain D: 98%



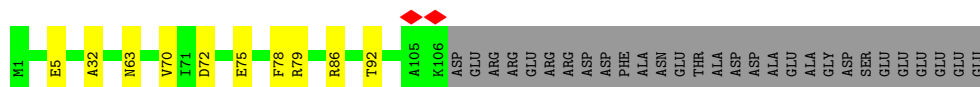
- Molecule 5: Small ribosomal subunit protein uS5

Chain E: 86% 6% 7%



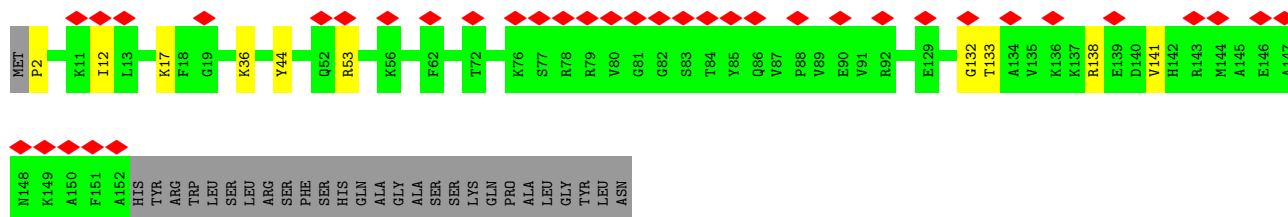
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform

Chain F: 71% 7% 21%



- Molecule 7: Small ribosomal subunit protein uS7

Chain G: 21% 79% 6% 16%



- Molecule 8: Small ribosomal subunit protein uS8

Chain H: 96%

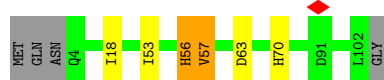


- Molecule 9: Small ribosomal subunit protein uS9

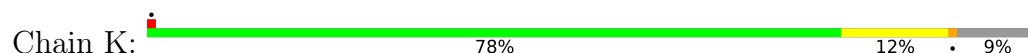
Chain I: 89% 8%



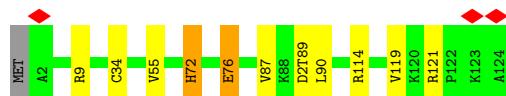
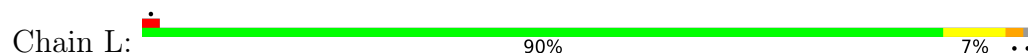
- Molecule 10: Small ribosomal subunit protein uS10



- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein uS12



- Molecule 13: Small ribosomal subunit protein uS13



- Molecule 14: Small ribosomal subunit protein uS14

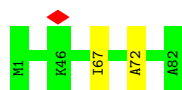


- Molecule 15: Small ribosomal subunit protein uS15



- Molecule 16: Small ribosomal subunit protein bS16

Chain P:  98%




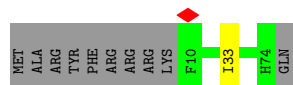
- Molecule 17: Small ribosomal subunit protein uS17

Chain Q:  93%




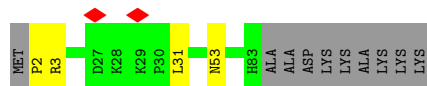
- Molecule 18: Small ribosomal subunit protein bS18

Chain R:  85%



- Molecule 19: Small ribosomal subunit protein uS19

Chain S:  85%



- Molecule 20: Small ribosomal subunit protein bS20

Chain T:  95%



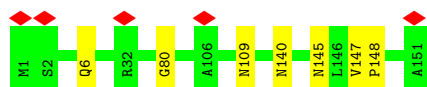
- Molecule 21: Small ribosomal subunit protein bS21

Chain U:  73%

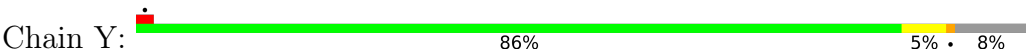


- Molecule 22: Ribosome maturation factor RimP

Chain X:  95%



- Molecule 23: Ribosomal RNA small subunit methyltransferase A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23278	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 ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	416.64, 416.64, 416.64	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, MA6, MG, ZN, D2T, 2MG

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	A	0.84	0/34130	1.28	154/53237 (0.3%)
2	B	0.52	0/1784	0.83	0/2403
3	C	0.73	0/1680	1.24	1/2263 (0.0%)
4	D	0.74	0/1665	1.24	0/2227
5	E	0.74	0/1157	1.31	1/1557 (0.1%)
6	F	0.73	0/881	1.27	2/1189 (0.2%)
7	G	0.82	1/1195 (0.1%)	1.32	2/1602 (0.1%)
8	H	0.72	0/989	1.21	3/1326 (0.2%)
9	I	0.77	0/1034	1.26	1/1375 (0.1%)
10	J	0.78	0/805	1.37	7/1089 (0.6%)
11	K	0.87	0/893	1.56	9/1205 (0.7%)
12	L	0.83	0/960	1.36	3/1286 (0.2%)
13	M	0.83	0/892	1.30	1/1193 (0.1%)
14	N	0.78	0/817	1.26	0/1088
15	O	0.75	0/722	1.26	2/964 (0.2%)
16	P	0.79	0/659	1.32	0/884
17	Q	0.73	0/657	1.29	2/881 (0.2%)
18	R	0.79	0/544	1.30	0/731
19	S	0.77	0/675	1.35	3/908 (0.3%)
20	T	0.73	0/676	1.28	0/895
21	U	0.83	0/436	1.22	0/577
22	X	0.73	0/1192	1.33	3/1619 (0.2%)
23	Y	0.79	1/2006 (0.0%)	1.34	6/2730 (0.2%)
All	All	0.80	2/56449 (0.0%)	1.28	200/83229 (0.2%)

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	A	0	436
2	B	0	1
3	C	0	1
4	D	0	3
5	E	0	1
6	F	0	2
7	G	0	1
8	H	0	1
9	I	0	4
11	K	0	1
12	L	0	2
14	N	0	1
20	T	0	1
23	Y	0	5
All	All	0	460

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	229	LEU	C-O	-6.35	1.15	1.24
7	G	2	PRO	N-CD	5.18	1.55	1.47

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1242	G	C3'-C2'-O2'	10.52	126.48	110.70
1	A	1208	C	C2'-C3'-O3'	10.33	129.19	113.70
1	A	1303	C	C4'-C3'-O3'	9.69	127.54	113.00
10	J	57	VAL	N-CA-C	9.46	129.01	109.34
10	J	56	HIS	N-CA-C	-9.28	95.97	110.36
7	G	132	GLY	N-CA-C	9.06	123.01	112.50
1	A	819	A	C5'-C4'-C3'	-8.43	102.56	115.20
5	E	108	GLY	CA-C-O	-8.39	114.03	121.58
1	A	816	A	C5'-C4'-C3'	-8.17	103.74	116.00
1	A	196	A	O3'-P-O5'	-7.76	92.35	104.00
22	X	109	ASN	N-CA-C	-7.57	101.07	111.28
1	A	1242	G	C2'-C3'-O3'	7.17	124.45	113.70
10	J	57	VAL	CB-CA-C	-6.91	99.95	111.29
1	A	1531	A	C2'-C3'-O3'	6.86	119.79	109.50
12	L	76	GLU	N-CA-C	6.84	119.61	111.33
1	A	62	U	C5'-C4'-C3'	-6.82	105.78	116.00
1	A	350	G	C2'-C3'-O3'	-6.79	103.51	113.70
11	K	15	GLN	CA-C-N	6.71	132.27	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	15	GLN	C-N-CA	6.71	132.27	122.94
1	A	517	G	C2'-C3'-O3'	6.67	119.50	109.50
11	K	16	VAL	CA-C-N	-6.63	113.40	122.95
11	K	16	VAL	C-N-CA	-6.63	113.40	122.95
1	A	1141	C	C2'-C3'-O3'	6.58	119.37	109.50
12	L	72	HIS	CA-CB-CG	6.57	120.37	113.80
1	A	953	G	C2'-C3'-O3'	6.53	123.50	113.70
1	A	298	A	C2'-C3'-O3'	6.51	123.47	113.70
10	J	56	HIS	CA-C-O	-6.51	113.94	121.82
1	A	1238	A	C3'-C2'-O2'	-6.51	100.94	110.70
1	A	1015	G	C5'-C4'-C3'	-6.48	106.28	116.00
1	A	67	C	C4'-C3'-C2'	-6.37	96.23	102.60
11	K	17	SER	N-CA-C	6.34	120.94	107.70
1	A	344	A	C4'-C3'-O3'	6.32	118.88	109.40
19	S	2	PRO	CA-N-CD	-6.30	103.18	112.00
1	A	519	C	C2'-C3'-O3'	-6.29	104.26	113.70
1	A	1286	U	N1-C1'-C2'	6.26	121.39	112.00
1	A	1208	C	C3'-C2'-O2'	6.25	120.07	110.70
1	A	1238	A	C5'-C4'-C3'	6.23	125.34	116.00
1	A	209	U	C2'-C3'-O3'	6.21	118.81	109.50
23	Y	21	ASN	CA-CB-CG	6.19	118.79	112.60
1	A	1092	A	O4'-C4'-C3'	6.18	110.18	104.00
1	A	1227	A	C5'-C4'-C3'	-6.17	106.74	116.00
1	A	1210	C	C2'-C3'-O3'	-6.15	104.48	113.70
1	A	722	G	C5'-C4'-C3'	-6.14	106.78	116.00
1	A	28	A	C5'-C4'-C3'	-6.13	106.81	116.00
1	A	176	C	O3'-P-O5'	-6.12	94.82	104.00
1	A	1228	C	C5'-C4'-C3'	-6.11	106.84	116.00
11	K	103	ALA	N-CA-C	-6.07	103.01	111.39
1	A	1140	C	O3'-P-O5'	-6.07	94.90	104.00
1	A	1019	A	C4'-C3'-C2'	-6.05	96.55	102.60
1	A	1238	A	C1'-C2'-O2'	6.05	117.47	108.40
15	O	25	THR	CA-C-N	5.99	128.23	120.44
15	O	25	THR	C-N-CA	5.99	128.23	120.44
1	A	1536	C	C2'-C3'-O3'	5.98	118.47	109.50
19	S	53	ASN	N-CA-C	-5.97	105.76	113.16
1	A	83	C	C5'-C4'-C3'	-5.95	107.07	116.00
1	A	496	A	C1'-O4'-C4'	-5.94	103.96	109.90
1	A	1242	G	C4'-C3'-O3'	-5.91	104.14	113.00
1	A	1005	A	O3'-P-O5'	-5.90	95.15	104.00
10	J	63	ASP	CA-C-O	-5.89	115.15	121.45
11	K	100	LEU	N-CA-C	-5.88	105.20	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1332	A	O4'-C1'-C2'	-5.86	101.74	107.60
1	A	112	G	C4'-C3'-C2'	-5.86	96.74	102.60
1	A	1270	G	C5'-C4'-C3'	-5.85	107.23	116.00
1	A	1141	C	O3'-P-O5'	-5.83	95.26	104.00
1	A	354	G	C5'-C4'-C3'	-5.82	107.27	116.00
23	Y	229	LEU	CA-C-O	-5.81	112.93	119.79
1	A	763	G	C3'-C2'-C1'	5.80	107.11	101.30
1	A	163	C	O4'-C1'-C2'	-5.79	101.81	107.60
1	A	1140	C	C2'-C3'-O3'	5.79	118.19	109.50
1	A	754	C	C5'-C4'-C3'	-5.79	107.32	116.00
23	Y	116	TYR	N-CA-C	5.77	120.13	113.38
1	A	84	U	O3'-P-O5'	-5.75	95.38	104.00
1	A	31	G	C2'-C3'-O3'	5.75	118.12	109.50
1	A	545	C	C4'-C3'-C2'	-5.74	96.86	102.60
1	A	750	C	C4'-C3'-C2'	-5.73	96.87	102.60
1	A	410	G	C2'-C3'-O3'	-5.73	105.10	113.70
1	A	19	A	C4'-C3'-C2'	-5.71	96.89	102.60
23	Y	226	ARG	N-CA-C	-5.70	105.15	111.71
1	A	1016	A	C5'-C4'-C3'	-5.68	107.48	116.00
1	A	982	U	C4'-C3'-O3'	-5.67	100.89	109.40
1	A	844	G	C3'-C2'-C1'	5.67	106.97	101.30
3	C	6	HIS	CB-CG-CD2	-5.66	123.84	131.20
12	L	72	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	45	G	C3'-C2'-C1'	5.66	106.96	101.30
1	A	221	C	O4'-C1'-C2'	-5.63	101.97	107.60
1	A	404	G	C4'-C3'-C2'	-5.63	96.97	102.60
1	A	15	G	O4'-C4'-C3'	5.62	109.62	104.00
1	A	618	C	O4'-C4'-C3'	5.62	109.62	104.00
1	A	907	A	C5'-C4'-C3'	-5.62	107.58	116.00
1	A	1530	G	C4'-C3'-O3'	5.61	117.82	109.40
1	A	162	A	C4'-C3'-O3'	5.61	121.41	113.00
1	A	1008	U	O4'-C1'-N1	5.60	116.90	108.50
1	A	812	G	C1'-O4'-C4'	-5.60	104.10	109.70
1	A	1103	C	C2'-C3'-O3'	5.60	122.09	113.70
1	A	77	A	C1'-O4'-C4'	-5.59	104.31	109.90
1	A	814	A	C5'-C4'-C3'	-5.59	107.61	116.00
1	A	311	C	C4'-C3'-C2'	-5.57	97.03	102.60
11	K	75	LYS	N-CA-C	-5.56	105.22	111.28
1	A	1277	C	C4'-C3'-C2'	-5.53	97.07	102.60
1	A	1021	A	C1'-O4'-C4'	-5.52	104.38	109.90
1	A	973	G	C4'-C3'-O3'	-5.51	104.73	113.00
1	A	840	C	O3'-P-O5'	5.50	112.25	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1004	A	C5'-C4'-C3'	-5.50	107.75	116.00
1	A	1191	A	C4'-C3'-O3'	5.49	121.24	113.00
1	A	1279	G	N9-C1'-C2'	5.49	120.24	112.00
17	Q	6	ARG	CD-NE-CZ	5.49	132.09	124.40
1	A	523	A	C5'-C4'-C3'	-5.49	107.77	116.00
1	A	1312	G	C4'-C3'-C2'	-5.49	97.11	102.60
1	A	211	G	C2'-C3'-O3'	-5.48	105.48	113.70
6	F	63	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	1236	A	C5'-C4'-C3'	-5.47	107.80	116.00
1	A	794	A	C5'-C4'-C3'	-5.44	107.83	116.00
1	A	1197	A	C5'-C4'-C3'	-5.44	107.84	116.00
1	A	720	C	C5'-C4'-C3'	-5.43	107.85	116.00
1	A	108	G	O3'-P-O5'	-5.43	95.85	104.00
1	A	1169	A	C4'-C3'-C2'	-5.43	97.17	102.60
1	A	429	U	O4'-C1'-C2'	-5.42	100.38	105.80
1	A	515	G	C5'-C4'-C3'	-5.41	107.88	116.00
1	A	1084	G	C2'-C3'-O3'	-5.41	105.59	113.70
1	A	1287	A	C5'-C4'-C3'	-5.40	107.90	116.00
1	A	196	A	O4'-C4'-C3'	5.39	109.39	104.00
1	A	1167	A	C3'-C2'-C1'	5.38	106.68	101.30
1	A	741	G	C5'-C4'-C3'	-5.38	107.93	116.00
1	A	1521	C	C4'-C3'-C2'	-5.38	97.22	102.60
1	A	412	A	C1'-O4'-C4'	-5.38	104.52	109.90
1	A	529	G	C5'-C4'-C3'	-5.37	107.94	116.00
1	A	1341	U	C3'-C2'-C1'	5.37	106.67	101.30
1	A	1198	G	O5'-C5'-C4'	5.36	119.55	111.50
1	A	1158	C	N1-C1'-C2'	5.36	120.04	112.00
1	A	953	G	C4'-C3'-C2'	-5.35	97.25	102.60
1	A	502	A	C5'-C4'-C3'	-5.34	107.98	116.00
8	H	88	ARG	CA-C-N	5.34	128.17	120.38
8	H	88	ARG	C-N-CA	5.34	128.17	120.38
1	A	1146	A	C5'-C4'-C3'	-5.33	108.00	116.00
1	A	513	C	C4'-C3'-C2'	-5.33	97.27	102.60
1	A	330	C	C5'-C4'-C3'	-5.33	108.01	116.00
1	A	427	U	C5'-C4'-C3'	-5.33	108.01	116.00
1	A	879	C	C4'-C3'-C2'	-5.31	97.29	102.60
1	A	1037	C	C5'-C4'-C3'	-5.31	108.03	116.00
1	A	1279	G	C4'-C3'-O3'	-5.30	105.04	113.00
1	A	301	G	C5'-C4'-C3'	-5.30	108.05	116.00
1	A	797	C	C5'-C4'-C3'	-5.29	108.06	116.00
7	G	133	THR	N-CA-C	5.28	117.46	111.02
1	A	381	C	C4'-C3'-C2'	-5.28	97.32	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1094	G	O5'-C5'-C4'	-5.28	103.78	111.70
1	A	196	A	C4'-C3'-O3'	-5.27	105.09	113.00
1	A	298	A	C4'-C3'-C2'	-5.27	97.33	102.60
1	A	1513	A	C4'-C3'-C2'	-5.26	97.33	102.60
1	A	268	U	C3'-C2'-C1'	5.23	106.53	101.30
1	A	959	A	C4'-C3'-C2'	-5.23	97.37	102.60
1	A	618	C	C5'-C4'-C3'	-5.22	108.17	116.00
1	A	1014	A	O4'-C4'-C3'	5.20	109.20	104.00
13	M	14	HIS	CA-C-O	-5.20	115.63	121.40
1	A	818	G	O4'-C1'-C2'	-5.19	100.61	105.80
1	A	1108	G	C4'-C3'-C2'	-5.17	97.43	102.60
1	A	843	U	O4'-C4'-C3'	5.16	109.16	104.00
1	A	1178	G	C4'-C3'-C2'	-5.15	97.45	102.60
1	A	406	G	C5'-C4'-C3'	-5.15	108.28	116.00
1	A	851	G	C5'-C4'-C3'	-5.15	108.27	116.00
1	A	973	G	C5'-C4'-C3'	-5.15	108.28	116.00
1	A	106	C	C4'-C3'-C2'	-5.14	97.46	102.60
19	S	3	ARG	CD-NE-CZ	5.14	131.60	124.40
1	A	440	C	C4'-C3'-C2'	-5.14	97.46	102.60
8	H	100	GLY	CA-C-O	-5.14	117.14	122.28
17	Q	31	HIS	CB-CG-CD2	-5.13	124.53	131.20
22	X	80	GLY	N-CA-C	5.13	119.13	112.25
11	K	16	VAL	O-C-N	-5.13	117.61	123.10
1	A	1135	U	C5'-C4'-C3'	-5.13	108.31	116.00
1	A	1149	C	C5'-C4'-C3'	-5.12	108.31	116.00
1	A	782	A	C4'-C3'-C2'	-5.12	97.48	102.60
1	A	405	U	C3'-C2'-O2'	5.11	118.36	110.70
9	I	27	LYS	CA-C-O	-5.10	115.77	121.23
1	A	996	A	C1'-O4'-C4'	-5.10	104.80	109.90
1	A	221	C	C5'-C4'-C3'	-5.10	108.35	116.00
1	A	452	A	C5'-C4'-C3'	-5.10	108.35	116.00
1	A	1351	U	C5'-C4'-C3'	-5.10	108.35	116.00
1	A	1525	G	C3'-C2'-C1'	5.10	106.40	101.30
1	A	275	G	C5'-C4'-C3'	-5.09	108.37	116.00
1	A	872	A	O3'-P-O5'	-5.09	96.37	104.00
1	A	977	A	C1'-O4'-C4'	-5.08	104.82	109.90
1	A	1221	G	C4'-C3'-C2'	-5.07	97.53	102.60
1	A	1239	A	C5'-C4'-C3'	-5.07	107.60	115.20
1	A	247	G	C4'-C3'-C2'	-5.07	97.53	102.60
1	A	364	A	C5'-C4'-C3'	-5.06	108.41	116.00
1	A	1062	U	O4'-C4'-C3'	5.06	109.06	104.00
1	A	262	A	O4'-C4'-C3'	5.06	109.06	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	57	VAL	N-CA-CB	-5.05	102.90	111.23
1	A	925	G	C2'-C3'-O3'	-5.04	101.94	109.50
1	A	263	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	A	714	G	O4'-C1'-N9	5.04	116.05	108.50
10	J	70	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	A	1038	C	C3'-C2'-C1'	5.02	106.32	101.30
1	A	1324	A	C4'-C3'-C2'	-5.01	97.59	102.60
22	X	140	ASN	CA-CB-CG	5.01	117.61	112.60
1	A	343	U	C4'-C3'-C2'	-5.01	97.59	102.60
6	F	72	ASP	CA-CB-CG	5.01	117.61	112.60
23	Y	176	VAL	CA-C-N	5.00	123.26	119.66
23	Y	176	VAL	C-N-CA	5.00	123.26	119.66
1	A	756	C	C4'-C3'-C2'	-5.00	97.60	102.60
1	A	1179	A	C5'-C4'-O4'	5.00	117.30	109.80

There are no chirality outliers.

All (460) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	A	Sidechain
1	A	100	G	Sidechain
1	A	1000	A	Sidechain
1	A	1004	A	Sidechain
1	A	1008	U	Sidechain
1	A	1011	C	Sidechain
1	A	1012	A	Sidechain
1	A	1013	G	Sidechain
1	A	1014	A	Sidechain
1	A	1016	A	Sidechain
1	A	1021	A	Sidechain
1	A	1024	G	Sidechain
1	A	1027	C	Sidechain
1	A	1030	U	Sidechain
1	A	1032	G	Sidechain
1	A	1036	A	Sidechain
1	A	1039	G	Sidechain
1	A	1041	G	Sidechain
1	A	1042	A	Sidechain
1	A	1047	G	Sidechain
1	A	1048	G	Sidechain
1	A	1053	G	Sidechain
1	A	1055	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1060	U	Sidechain
1	A	1067	A	Sidechain
1	A	107	G	Sidechain
1	A	1074	G	Sidechain
1	A	1075	U	Sidechain
1	A	1077	G	Sidechain
1	A	1078	U	Sidechain
1	A	108	G	Sidechain
1	A	1086	U	Sidechain
1	A	1089	G	Sidechain
1	A	109	A	Sidechain
1	A	1095	U	Sidechain
1	A	1097	C	Sidechain
1	A	1098	C	Sidechain
1	A	1099	G	Sidechain
1	A	11	G	Sidechain
1	A	110	C	Sidechain
1	A	1100	C	Sidechain
1	A	1101	A	Sidechain
1	A	1106	G	Sidechain
1	A	111	G	Sidechain
1	A	1115	U	Sidechain
1	A	1116	U	Sidechain
1	A	1119	C	Sidechain
1	A	1120	C	Sidechain
1	A	1121	U	Sidechain
1	A	1125	U	Sidechain
1	A	1126	U	Sidechain
1	A	1128	C	Sidechain
1	A	1129	C	Sidechain
1	A	1139	G	Sidechain
1	A	114	U	Sidechain
1	A	1140	C	Sidechain
1	A	1141	C	Sidechain
1	A	1142	G	Sidechain
1	A	1144	G	Sidechain
1	A	1146	A	Sidechain
1	A	1147	C	Sidechain
1	A	1148	U	Sidechain
1	A	1150	A	Sidechain
1	A	1153	G	Sidechain
1	A	1160	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1161	C	Sidechain
1	A	1162	C	Sidechain
1	A	1166	G	Sidechain
1	A	1167	A	Sidechain
1	A	1169	A	Sidechain
1	A	117	G	Sidechain
1	A	1173	U	Sidechain
1	A	1176	A	Sidechain
1	A	1179	A	Sidechain
1	A	1180	A	Sidechain
1	A	1187	G	Sidechain
1	A	1188	A	Sidechain
1	A	119	A	Sidechain
1	A	1192	C	Sidechain
1	A	1194	U	Sidechain
1	A	120	A	Sidechain
1	A	1200	C	Sidechain
1	A	1204	A	Sidechain
1	A	1205	U	Sidechain
1	A	1210	C	Sidechain
1	A	1217	C	Sidechain
1	A	1220	G	Sidechain
1	A	1223	C	Sidechain
1	A	1233	G	Sidechain
1	A	1234	C	Sidechain
1	A	124	C	Sidechain
1	A	1246	A	Sidechain
1	A	1253	G	Sidechain
1	A	1258	G	Sidechain
1	A	1260	G	Sidechain
1	A	1264	U	Sidechain
1	A	1266	G	Sidechain
1	A	1268	G	Sidechain
1	A	1269	A	Sidechain
1	A	1279	G	Sidechain
1	A	1284	C	Sidechain
1	A	1285	A	Sidechain
1	A	1289	A	Sidechain
1	A	1300	G	Sidechain
1	A	1304	G	Sidechain
1	A	1307	U	Sidechain
1	A	1311	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1316	G	Sidechain
1	A	1317	C	Sidechain
1	A	1321	U	Sidechain
1	A	1323	G	Sidechain
1	A	1324	A	Sidechain
1	A	1326	U	Sidechain
1	A	1327	C	Sidechain
1	A	1331	G	Sidechain
1	A	1333	A	Sidechain
1	A	1334	G	Sidechain
1	A	1335	U	Sidechain
1	A	1338	G	Sidechain
1	A	1339	A	Sidechain
1	A	134	G	Sidechain
1	A	1343	G	Sidechain
1	A	1345	U	Sidechain
1	A	135	C	Sidechain
1	A	1350	A	Sidechain
1	A	1351	U	Sidechain
1	A	1352	C	Sidechain
1	A	1353	G	Sidechain
1	A	1358	U	Sidechain
1	A	136	C	Sidechain
1	A	1360	A	Sidechain
1	A	1362	A	Sidechain
1	A	1365	G	Sidechain
1	A	1366	C	Sidechain
1	A	1367	C	Sidechain
1	A	1372	U	Sidechain
1	A	1378	C	Sidechain
1	A	1379	G	Sidechain
1	A	1381	U	Sidechain
1	A	1384	C	Sidechain
1	A	141	G	Sidechain
1	A	149	A	Sidechain
1	A	15	G	Sidechain
1	A	151	A	Sidechain
1	A	1512	U	Sidechain
1	A	1521	C	Sidechain
1	A	1525	G	Sidechain
1	A	1527	U	Sidechain
1	A	153	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1535	C	Sidechain
1	A	1539	C	Sidechain
1	A	157	U	Sidechain
1	A	161	A	Sidechain
1	A	163	C	Sidechain
1	A	167	A	Sidechain
1	A	17	U	Sidechain
1	A	172	A	Sidechain
1	A	177	G	Sidechain
1	A	184	G	Sidechain
1	A	185	U	Sidechain
1	A	187	G	Sidechain
1	A	189	A	Sidechain
1	A	192	A	Sidechain
1	A	194	C	Sidechain
1	A	195	A	Sidechain
1	A	2	A	Sidechain
1	A	201	G	Sidechain
1	A	204	G	Sidechain
1	A	205	A	Sidechain
1	A	207	C	Sidechain
1	A	210	C	Sidechain
1	A	215	C	Sidechain
1	A	218	U	Sidechain
1	A	220	G	Sidechain
1	A	222	C	Sidechain
1	A	223	A	Sidechain
1	A	230	G	Sidechain
1	A	234	C	Sidechain
1	A	235	C	Sidechain
1	A	236	A	Sidechain
1	A	237	G	Sidechain
1	A	239	U	Sidechain
1	A	249	U	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	252	U	Sidechain
1	A	256	U	Sidechain
1	A	265	G	Sidechain
1	A	266	G	Sidechain
1	A	273	U	Sidechain
1	A	286	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	288	A	Sidechain
1	A	291	U	Sidechain
1	A	299	G	Sidechain
1	A	30	U	Sidechain
1	A	300	A	Sidechain
1	A	302	G	Sidechain
1	A	313	A	Sidechain
1	A	314	C	Sidechain
1	A	324	G	Sidechain
1	A	325	A	Sidechain
1	A	326	G	Sidechain
1	A	33	A	Sidechain
1	A	333	U	Sidechain
1	A	340	U	Sidechain
1	A	342	C	Sidechain
1	A	344	A	Sidechain
1	A	345	C	Sidechain
1	A	346	G	Sidechain
1	A	347	G	Sidechain
1	A	35	G	Sidechain
1	A	357	G	Sidechain
1	A	361	G	Sidechain
1	A	362	G	Sidechain
1	A	363	A	Sidechain
1	A	366	A	Sidechain
1	A	368	U	Sidechain
1	A	373	A	Sidechain
1	A	374	A	Sidechain
1	A	376	G	Sidechain
1	A	380	G	Sidechain
1	A	386	C	Sidechain
1	A	390	U	Sidechain
1	A	391	G	Sidechain
1	A	396	C	Sidechain
1	A	4	U	Sidechain
1	A	400	C	Sidechain
1	A	402	G	Sidechain
1	A	423	G	Sidechain
1	A	424	G	Sidechain
1	A	426	U	Sidechain
1	A	434	U	Sidechain
1	A	435	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	437	U	Sidechain
1	A	438	U	Sidechain
1	A	442	G	Sidechain
1	A	444	G	Sidechain
1	A	445	G	Sidechain
1	A	447	G	Sidechain
1	A	448	A	Sidechain
1	A	465	A	Sidechain
1	A	466	A	Sidechain
1	A	469	C	Sidechain
1	A	471	U	Sidechain
1	A	476	U	Sidechain
1	A	477	C	Sidechain
1	A	480	U	Sidechain
1	A	481	G	Sidechain
1	A	486	U	Sidechain
1	A	489	C	Sidechain
1	A	490	C	Sidechain
1	A	491	G	Sidechain
1	A	496	A	Sidechain
1	A	50	A	Sidechain
1	A	500	G	Sidechain
1	A	501	C	Sidechain
1	A	502	A	Sidechain
1	A	504	C	Sidechain
1	A	506	G	Sidechain
1	A	509	A	Sidechain
1	A	51	A	Sidechain
1	A	510	A	Sidechain
1	A	516	U	Sidechain
1	A	517	G	Sidechain
1	A	519	C	Sidechain
1	A	520	A	Sidechain
1	A	524	G	Sidechain
1	A	525	C	Sidechain
1	A	528	C	Sidechain
1	A	531	U	Sidechain
1	A	532	A	Sidechain
1	A	533	A	Sidechain
1	A	535	A	Sidechain
1	A	536	C	Sidechain
1	A	546	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	547	A	Sidechain
1	A	555	U	Sidechain
1	A	557	G	Sidechain
1	A	56	U	Sidechain
1	A	563	A	Sidechain
1	A	566	G	Sidechain
1	A	568	G	Sidechain
1	A	57	G	Sidechain
1	A	570	G	Sidechain
1	A	573	A	Sidechain
1	A	575	G	Sidechain
1	A	580	C	Sidechain
1	A	581	G	Sidechain
1	A	584	G	Sidechain
1	A	585	G	Sidechain
1	A	588	G	Sidechain
1	A	59	A	Sidechain
1	A	590	U	Sidechain
1	A	592	G	Sidechain
1	A	595	A	Sidechain
1	A	600	A	Sidechain
1	A	602	A	Sidechain
1	A	606	G	Sidechain
1	A	609	A	Sidechain
1	A	61	G	Sidechain
1	A	611	C	Sidechain
1	A	613	C	Sidechain
1	A	618	C	Sidechain
1	A	62	U	Sidechain
1	A	620	C	Sidechain
1	A	621	A	Sidechain
1	A	623	C	Sidechain
1	A	624	C	Sidechain
1	A	627	G	Sidechain
1	A	635	A	Sidechain
1	A	637	C	Sidechain
1	A	641	U	Sidechain
1	A	642	A	Sidechain
1	A	657	U	Sidechain
1	A	658	C	Sidechain
1	A	664	G	Sidechain
1	A	666	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	670	G	Sidechain
1	A	672	U	Sidechain
1	A	673	A	Sidechain
1	A	676	A	Sidechain
1	A	677	U	Sidechain
1	A	678	U	Sidechain
1	A	680	C	Sidechain
1	A	681	A	Sidechain
1	A	686	U	Sidechain
1	A	691	G	Sidechain
1	A	693	G	Sidechain
1	A	694	A	Sidechain
1	A	695	A	Sidechain
1	A	697	U	Sidechain
1	A	698	G	Sidechain
1	A	701	U	Sidechain
1	A	71	A	Sidechain
1	A	710	G	Sidechain
1	A	714	G	Sidechain
1	A	715	A	Sidechain
1	A	719	C	Sidechain
1	A	720	C	Sidechain
1	A	722	G	Sidechain
1	A	724	G	Sidechain
1	A	727	G	Sidechain
1	A	728	A	Sidechain
1	A	729	A	Sidechain
1	A	736	C	Sidechain
1	A	737	C	Sidechain
1	A	738	C	Sidechain
1	A	739	C	Sidechain
1	A	744	C	Sidechain
1	A	745	G	Sidechain
1	A	746	A	Sidechain
1	A	75	G	Sidechain
1	A	751	U	Sidechain
1	A	752	G	Sidechain
1	A	754	C	Sidechain
1	A	76	G	Sidechain
1	A	760	G	Sidechain
1	A	771	G	Sidechain
1	A	773	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	776	G	Sidechain
1	A	780	A	Sidechain
1	A	788	U	Sidechain
1	A	79	G	Sidechain
1	A	790	A	Sidechain
1	A	794	A	Sidechain
1	A	797	C	Sidechain
1	A	798	U	Sidechain
1	A	800	G	Sidechain
1	A	802	A	Sidechain
1	A	803	G	Sidechain
1	A	805	C	Sidechain
1	A	807	A	Sidechain
1	A	808	C	Sidechain
1	A	812	G	Sidechain
1	A	813	U	Sidechain
1	A	82	G	Sidechain
1	A	825	A	Sidechain
1	A	826	C	Sidechain
1	A	829	G	Sidechain
1	A	84	U	Sidechain
1	A	844	G	Sidechain
1	A	845	A	Sidechain
1	A	848	C	Sidechain
1	A	849	G	Sidechain
1	A	85	U	Sidechain
1	A	853	C	Sidechain
1	A	857	C	Sidechain
1	A	859	G	Sidechain
1	A	86	G	Sidechain
1	A	860	A	Sidechain
1	A	864	A	Sidechain
1	A	865	A	Sidechain
1	A	867	G	Sidechain
1	A	869	G	Sidechain
1	A	87	C	Sidechain
1	A	872	A	Sidechain
1	A	874	G	Sidechain
1	A	876	C	Sidechain
1	A	878	A	Sidechain
1	A	879	C	Sidechain
1	A	883	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	891	U	Sidechain
1	A	897	C	Sidechain
1	A	898	G	Sidechain
1	A	899	C	Sidechain
1	A	900	A	Sidechain
1	A	901	A	Sidechain
1	A	903	G	Sidechain
1	A	906	A	Sidechain
1	A	91	U	Sidechain
1	A	910	C	Sidechain
1	A	915	A	Sidechain
1	A	917	G	Sidechain
1	A	92	U	Sidechain
1	A	920	U	Sidechain
1	A	93	U	Sidechain
1	A	933	G	Sidechain
1	A	939	G	Sidechain
1	A	94	G	Sidechain
1	A	946	A	Sidechain
1	A	947	G	Sidechain
1	A	95	C	Sidechain
1	A	953	G	Sidechain
1	A	958	A	Sidechain
1	A	961	U	Sidechain
1	A	963	G	Sidechain
1	A	975	A	Sidechain
1	A	978	A	Sidechain
1	A	980	C	Sidechain
1	A	981	U	Sidechain
1	A	982	U	Sidechain
1	A	984	C	Sidechain
1	A	985	C	Sidechain
1	A	986	U	Sidechain
1	A	99	C	Sidechain
1	A	991	U	Sidechain
2	B	139	ARG	Sidechain
3	C	11	ARG	Sidechain
4	D	128	ARG	Sidechain
4	D	26	ARG	Sidechain
4	D	3	ARG	Sidechain
5	E	108	GLY	Mainchain
6	F	79	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	F	86	ARG	Sidechain
7	G	53	ARG	Sidechain
8	H	77	ARG	Sidechain
9	I	130	ARG	Sidechain
9	I	18	ARG	Sidechain
9	I	45	ARG	Sidechain
9	I	64	TYR	Sidechain
11	K	46	THR	Mainchain
12	L	72	HIS	Sidechain
12	L	9	ARG	Sidechain
14	N	59	ARG	Sidechain
20	T	74	ARG	Sidechain
23	Y	116	TYR	Sidechain
23	Y	147	ARG	Sidechain
23	Y	157	TYR	Sidechain
23	Y	166	TYR	Sidechain
23	Y	222	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	A	30625	0	15353	166	0
2	B	1753	0	1780	26	0
3	C	1653	0	1727	15	0
4	D	1643	0	1707	1	0
5	E	1144	0	1175	16	0
6	F	862	0	864	5	0
7	G	1181	0	1238	2	0
8	H	979	0	1031	1	0
9	I	1022	0	1070	6	0
10	J	795	0	836	5	0
11	K	877	0	887	4	0
12	L	957	0	1017	7	0
13	M	883	0	941	1	0
14	N	805	0	844	2	0
15	O	714	0	734	3	0
16	P	649	0	666	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	648	0	691	0	0
18	R	535	0	552	0	0
19	S	658	0	683	1	0
20	T	670	0	719	1	0
21	U	430	0	458	0	0
22	X	1174	0	1174	2	0
23	Y	1963	0	1977	6	0
24	A	31	0	0	0	0
25	B	1	0	0	0	0
All	All	52652	0	38124	236	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 3.

All (236) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:A:C8	5:E:23:LYS:NZ	2.13	1.12
1:A:920:U:H5'	1:A:1080:A:H61	0.94	1.09
1:A:421:U:O2	3:C:126:ARG:NE	1.86	1.08
1:A:421:U:O2	3:C:126:ARG:CZ	2.02	1.08
1:A:920:U:H5'	1:A:1080:A:N6	1.70	1.04
1:A:421:U:C2	3:C:126:ARG:NH2	2.28	1.02
1:A:1078:U:O3'	5:E:138:ARG:NH1	1.58	0.99
1:A:1537:U:OP2	3:C:164:ARG:NH1	1.97	0.97
1:A:920:U:C5'	1:A:1080:A:H61	1.82	0.91
1:A:1081:A:N9	5:E:23:LYS:NZ	1.82	0.91
1:A:927:G:O6	1:A:1390:U:O2	1.92	0.88
2:B:111:ILE:HD12	2:B:152:LYS:HA	1.59	0.84
1:A:920:U:C5'	1:A:1080:A:N6	2.41	0.83
1:A:421:U:O2	3:C:126:ARG:NH2	2.08	0.82
1:A:927:G:C6	1:A:1390:U:O2	2.34	0.81
1:A:1237:C:H3'	1:A:1238:A:H5'	1.66	0.78
1:A:921:U:H5''	1:A:1082:A:OP1	1.84	0.77
2:B:23:TRP:HZ3	2:B:25:PRO:HA	1.48	0.76
1:A:928:G:N2	1:A:1389:C:O2	2.13	0.76
1:A:928:G:N1	1:A:1389:C:N3	2.27	0.76
1:A:927:G:N1	1:A:1390:U:O2	2.19	0.76
1:A:1078:U:H1'	5:E:89:HIS:HE1	1.50	0.76
1:A:927:G:N2	1:A:1391:U:O5'	2.20	0.73
1:A:966:2MG:HM23	1:A:967:5MC:H1'	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:G:O4'	10:J:57:VAL:HG21	1.92	0.70
2:B:187:VAL:HG13	2:B:191:SER:HB2	1.74	0.68
1:A:1537:U:OP1	3:C:164:ARG:NH2	2.25	0.67
2:B:68:LEU:HB3	2:B:161:LEU:HD23	1.77	0.67
1:A:921:U:H5'	1:A:1081:A:O3'	1.95	0.67
1:A:17:U:H4'	1:A:1080:A:O4'	1.97	0.64
1:A:928:G:H2'	1:A:929:G:C8	2.33	0.64
23:Y:41:MET:HE2	23:Y:111:PHE:CE1	2.34	0.63
1:A:928:G:O6	1:A:1389:C:N4	2.29	0.62
2:B:23:TRP:CZ3	2:B:25:PRO:HA	2.34	0.61
1:A:1537:U:P	3:C:164:ARG:HH12	2.24	0.61
1:A:927:G:O2'	1:A:1392:G:N7	2.34	0.61
1:A:928:G:H2'	1:A:929:G:H8	1.67	0.59
1:A:17:U:O4'	1:A:1080:A:H1'	2.02	0.59
9:I:84:THR:HG21	9:I:103:PHE:HB3	1.85	0.59
1:A:17:U:C1'	1:A:1080:A:H1'	2.34	0.58
1:A:967:5MC:H2'	1:A:968:A:C8	2.38	0.58
3:C:139:GLN:O	3:C:143:ARG:HG3	2.04	0.58
6:F:5:GLU:HG3	6:F:92:THR:HG21	1.86	0.57
5:E:153:VAL:HG13	5:E:157:ARG:NH1	2.18	0.56
12:L:114:ARG:NE	12:L:121:ARG:HA	2.19	0.56
1:A:921:U:C5'	1:A:1082:A:OP1	2.53	0.56
1:A:1078:U:H1'	5:E:89:HIS:CE1	2.37	0.56
1:A:1081:A:N9	5:E:23:LYS:HZ2	1.31	0.56
1:A:1008:U:C5	1:A:1022:A:C2	2.94	0.56
1:A:1238:A:N7	1:A:1299:A:N1	2.53	0.56
1:A:1537:U:OP2	3:C:164:ARG:CZ	2.52	0.56
2:B:68:LEU:HD23	2:B:161:LEU:CD2	2.36	0.55
2:B:173:ILE:HG23	2:B:183:VAL:HG21	1.89	0.55
1:A:920:U:C6	1:A:1080:A:H2	2.20	0.55
1:A:920:U:C4'	1:A:1080:A:N6	2.58	0.55
1:A:664:G:H22	1:A:741:G:H1	1.55	0.54
1:A:1537:U:P	3:C:164:ARG:NH1	2.81	0.54
12:L:114:ARG:HB2	12:L:119:VAL:HG13	1.89	0.54
1:A:1080:A:C5'	5:E:52:LYS:NZ	2.71	0.54
5:E:157:ARG:HD2	8:H:43:GLU:O	2.08	0.53
22:X:6:GLN:CD	22:X:6:GLN:H	2.16	0.53
12:L:114:ARG:HE	12:L:121:ARG:HA	1.73	0.53
1:A:926:G:O2'	1:A:1392:G:O6	2.17	0.53
2:B:111:ILE:HD13	2:B:148:LEU:HD13	1.89	0.53
1:A:162:A:C5	1:A:163:C:H1'	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ILE:HD13	2:B:39:HIS:CE1	2.44	0.52
1:A:1519:MA6:H1'	23:Y:186:LYS:HD2	1.91	0.52
2:B:72:THR:HG22	2:B:94:HIS:O	2.09	0.52
1:A:17:U:H1'	1:A:1080:A:H1'	1.89	0.52
2:B:23:TRP:HB3	2:B:39:HIS:CD2	2.45	0.52
2:B:81:LYS:HG3	2:B:91:PHE:CZ	2.45	0.51
1:A:519:C:C6	1:A:520:A:H1'	2.46	0.51
1:A:713:G:H2'	1:A:714:G:C8	2.45	0.51
1:A:919:A:O2'	1:A:1080:A:N1	2.41	0.51
1:A:1005:A:C5	1:A:1006:G:H1'	2.46	0.50
1:A:1097:C:H2'	1:A:1098:C:C6	2.47	0.50
11:K:31:ILE:HG12	11:K:46:THR:HG22	1.93	0.50
19:S:31:LEU:HD23	19:S:31:LEU:H	1.77	0.50
1:A:1239:A:H1'	1:A:1241:G:C4	2.47	0.49
20:T:36:TYR:CZ	20:T:79:LEU:HD21	2.48	0.49
12:L:114:ARG:HB2	12:L:119:VAL:CG1	2.41	0.49
1:A:695:A:OP1	11:K:53:ARG:HG2	2.12	0.49
1:A:17:U:C4'	1:A:1080:A:O4'	2.60	0.49
1:A:268:U:H2'	1:A:269:C:C6	2.48	0.49
1:A:1081:A:C8	5:E:23:LYS:CE	2.96	0.48
1:A:1303:C:N4	1:A:1304:G:C6	2.82	0.48
2:B:187:VAL:O	2:B:201:PRO:HA	2.14	0.48
1:A:1537:U:P	3:C:164:ARG:HH22	2.36	0.48
12:L:114:ARG:HH21	12:L:121:ARG:HB2	1.79	0.48
1:A:876:C:H2'	1:A:877:G:C8	2.48	0.48
6:F:32:ALA:HB2	6:F:70:VAL:HG11	1.96	0.48
5:E:153:VAL:CG1	5:E:157:ARG:NH1	2.77	0.48
1:A:17:U:O4'	1:A:1080:A:C1'	2.62	0.47
1:A:269:C:H2'	1:A:270:A:C8	2.49	0.47
1:A:847:G:H2'	1:A:848:C:C6	2.50	0.47
1:A:1316:G:H2'	1:A:1317:C:H5''	1.97	0.47
1:A:921:U:H2'	1:A:922:G:C8	2.49	0.47
1:A:1032:G:C4	1:A:1033:G:H1'	2.50	0.47
1:A:1386:G:H2'	1:A:1387:G:C8	2.49	0.47
4:D:28:ILE:H	4:D:28:ILE:HD12	1.80	0.47
1:A:1080:A:C5'	5:E:52:LYS:HZ1	2.28	0.47
1:A:1028:C:H2'	1:A:1029:U:C6	2.49	0.47
1:A:1196:A:H3'	1:A:1197:A:C5'	2.45	0.47
2:B:148:LEU:CD2	2:B:151:ILE:HD11	2.44	0.47
10:J:53:ILE:HG22	14:N:85:ARG:HD2	1.96	0.47
1:A:651:C:H2'	1:A:652:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1369:C:OP2	9:I:114:LYS:HE2	2.15	0.47
1:A:973:G:C4'	10:J:57:VAL:HG21	2.45	0.46
1:A:463:U:H2'	1:A:464:U:C6	2.50	0.46
1:A:683:G:H2'	1:A:684:U:C6	2.50	0.46
1:A:925:G:C2	1:A:927:G:H1'	2.50	0.46
1:A:1287:A:H2'	1:A:1288:A:C8	2.50	0.46
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.46
1:A:1078:U:C1'	5:E:89:HIS:HE1	2.26	0.46
1:A:1180:A:OP1	9:I:105:THR:HG22	2.16	0.46
1:A:966:2MG:H5''	1:A:969:A:N7	2.31	0.46
1:A:1005:A:C6	1:A:1006:G:H1'	2.50	0.46
1:A:928:G:C6	1:A:929:G:C6	3.04	0.46
1:A:384:G:H2'	1:A:385:C:C6	2.51	0.46
1:A:421:U:C2	3:C:126:ARG:NE	2.79	0.46
1:A:1229:A:H2'	1:A:1230:C:C6	2.51	0.45
1:A:80:A:H3'	1:A:81:A:H4'	1.98	0.45
1:A:1519:MA6:H3'	1:A:1520:C:O4'	2.16	0.45
1:A:477:C:H2'	1:A:478:A:C8	2.51	0.45
1:A:161:A:H2'	1:A:162:A:C8	2.52	0.45
1:A:1167:A:H2'	1:A:1169:A:C8	2.52	0.45
1:A:967:5MC:H4'	9:I:127:PHE:CE1	2.52	0.45
1:A:1016:A:N7	1:A:1017:U:H1'	2.32	0.45
1:A:56:U:H2'	1:A:57:G:C8	2.51	0.45
9:I:84:THR:HG21	9:I:103:PHE:CB	2.46	0.45
7:G:138:ARG:O	7:G:141:VAL:HG12	2.16	0.45
13:M:15:ALA:HB2	13:M:43:VAL:O	2.17	0.44
23:Y:127:PHE:HA	23:Y:130:THR:HG23	1.98	0.44
1:A:184:G:H2'	1:A:185:U:C6	2.53	0.44
12:L:87:VAL:HG11	12:L:90:LEU:HD12	1.99	0.44
5:E:154:ALA:HB1	5:E:161:VAL:HG22	2.00	0.44
1:A:299:G:H2'	1:A:300:A:C8	2.53	0.44
6:F:5:GLU:CD	6:F:92:THR:HG21	2.42	0.44
1:A:841:C:C2	1:A:846:G:C6	3.06	0.44
1:A:1389:C:H3'	1:A:1390:U:C6	2.52	0.44
1:A:743:A:H2'	1:A:744:C:C6	2.52	0.44
1:A:1387:G:H2'	1:A:1388:C:O4'	2.18	0.44
1:A:45:G:H2'	1:A:46:G:C8	2.53	0.44
1:A:718:A:C2	1:A:719:C:C5	3.06	0.44
2:B:9:MET:HB3	2:B:14:VAL:HB	2.00	0.44
2:B:154:MET:HG2	2:B:156:GLY:O	2.18	0.44
1:A:1141:C:C2	1:A:1142:G:C8	3.05	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:17:LYS:HE3	7:G:44:TYR:CE2	2.52	0.43
1:A:657:U:H1'	15:O:23:GLY:CA	2.48	0.43
1:A:1537:U:P	3:C:164:ARG:NH2	2.91	0.43
1:A:524:G:H2'	1:A:525:C:C6	2.54	0.43
2:B:72:THR:OG1	2:B:169:GLU:OE2	2.27	0.43
3:C:154:SER:HA	3:C:165:THR:HG22	1.99	0.43
23:Y:41:MET:HE3	23:Y:109:ARG:CB	2.48	0.43
1:A:1306:A:C5	1:A:1332:A:C2	3.06	0.43
2:B:186:ILE:HG21	2:B:213:TYR:CE2	2.54	0.43
1:A:147:G:H2'	1:A:148:G:C8	2.54	0.43
1:A:1324:A:C4'	1:A:1362:A:H4'	2.49	0.43
1:A:200:G:H2'	1:A:201:G:H5'	2.01	0.43
1:A:484:G:C5	1:A:486:U:H1'	2.54	0.43
1:A:1218:C:H2'	1:A:1219:A:C8	2.54	0.43
2:B:208:ARG:H	2:B:208:ARG:HG2	1.67	0.42
6:F:5:GLU:CG	6:F:92:THR:HG21	2.48	0.42
6:F:75:GLU:HA	6:F:78:PHE:CD1	2.54	0.42
1:A:901:A:H3'	1:A:902:G:O4'	2.19	0.42
1:A:973:G:H4'	10:J:57:VAL:HG11	2.01	0.42
2:B:68:LEU:HA	2:B:90:PHE:O	2.19	0.42
23:Y:41:MET:HE2	23:Y:111:PHE:CD1	2.54	0.42
9:I:80:ARG:O	9:I:84:THR:HG23	2.20	0.42
23:Y:42:VAL:HG13	23:Y:110:VAL:HG12	2.01	0.42
2:B:210:VAL:O	2:B:214:LEU:HG	2.19	0.42
1:A:270:A:H2'	1:A:271:C:C6	2.55	0.42
22:X:147:VAL:N	22:X:148:PRO:HD3	2.35	0.42
1:A:17:U:O2	1:A:1079:G:N2	2.52	0.42
1:A:1078:U:C1'	5:E:89:HIS:CE1	3.03	0.42
1:A:1084:G:H2'	1:A:1085:U:C5	2.55	0.42
1:A:1118:U:H1'	1:A:1179:A:C5	2.55	0.42
1:A:17:U:O2'	1:A:1079:G:N3	2.52	0.42
1:A:657:U:H1'	15:O:23:GLY:HA3	2.02	0.42
1:A:1070:U:H2'	1:A:1071:C:C6	2.55	0.42
1:A:1219:A:H2'	1:A:1220:G:C8	2.55	0.42
1:A:1518:MA6:H2'	1:A:1519:MA6:H8	2.00	0.42
12:L:34:CYS:SG	12:L:76:GLU:HA	2.60	0.42
1:A:399:G:H2'	1:A:400:C:C6	2.55	0.41
1:A:1255:G:C6	1:A:1279:G:C8	3.08	0.41
1:A:67:C:H2'	1:A:68:G:C8	2.55	0.41
1:A:920:U:C6	1:A:1080:A:C2	2.99	0.41
3:C:59:ARG:HG2	3:C:64:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:U:H2'	1:A:459:A:C8	2.55	0.41
1:A:1158:C:C5	1:A:1160:G:H1'	2.55	0.41
1:A:1213:A:C8	1:A:1215:G:C6	3.08	0.41
10:J:56:HIS:C	10:J:57:VAL:HG13	2.45	0.41
11:K:73:ALA:O	11:K:77:TYR:HD2	2.03	0.41
1:A:87:C:C2	1:A:88:U:C6	3.08	0.41
1:A:559:A:H1'	1:A:561:U:O2'	2.19	0.41
2:B:152:LYS:HG3	2:B:153:ASP:CG	2.45	0.41
1:A:206:C:H2'	1:A:207:C:C6	2.56	0.41
1:A:806:C:H2'	1:A:807:A:C8	2.55	0.41
1:A:928:G:C6	1:A:929:G:C5	3.09	0.41
2:B:90:PHE:CE2	2:B:154:MET:HA	2.55	0.41
2:B:162:PHE:HA	2:B:184:PHE:O	2.20	0.41
5:E:25:VAL:HG22	5:E:26:LYS:H	1.85	0.41
1:A:677:U:C4	1:A:678:U:C4	3.08	0.41
1:A:910:C:H2'	1:A:911:U:C6	2.55	0.41
2:B:20:THR:O	2:B:23:TRP:HD1	2.04	0.41
1:A:470:C:H2'	1:A:471:U:C6	2.55	0.41
1:A:781:A:C6	1:A:782:A:H1'	2.55	0.41
1:A:90:C:C2	1:A:91:U:C5	3.08	0.41
1:A:735:C:H2'	1:A:736:C:C6	2.55	0.41
1:A:763:G:H2'	1:A:764:C:C6	2.56	0.41
1:A:927:G:O6	1:A:1390:U:C2	2.70	0.41
1:A:246:A:N3	1:A:247:G:H1'	2.35	0.41
1:A:382:A:H2'	1:A:383:A:C8	2.55	0.41
1:A:696:A:C2	1:A:697:U:C2	3.08	0.41
1:A:1003:G:N2	1:A:1005:A:H5'	2.36	0.41
1:A:1261:A:C5	1:A:1262:C:C5	3.09	0.41
2:B:6:MET:HE2	2:B:43:LEU:HB2	2.03	0.41
1:A:1187:G:C2'	1:A:1188:A:H5'	2.51	0.41
1:A:1238:A:C2	1:A:1303:C:H4'	2.56	0.41
16:P:67:ILE:CD1	16:P:72:ALA:HB2	2.51	0.41
1:A:68:G:C6	1:A:69:G:H1'	2.56	0.40
1:A:304:U:H2'	1:A:305:G:C8	2.55	0.40
1:A:1388:C:H2'	1:A:1389:C:C6	2.56	0.40
1:A:235:C:H2'	1:A:236:A:C8	2.57	0.40
1:A:949:A:C5	1:A:950:U:C5	3.09	0.40
1:A:1005:A:C4	1:A:1006:G:H1'	2.57	0.40
1:A:1296:C:C5'	1:A:1297:G:OP2	2.69	0.40
14:N:16:LEU:C	14:N:16:LEU:HD23	2.45	0.40
15:O:71:LYS:HB2	15:O:78:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:A:C2	1:A:162:A:C4	3.10	0.40
1:A:607:A:C2	1:A:608:A:C4	3.09	0.40
11:K:53:ARG:HG2	11:K:54:GLY:N	2.36	0.40
1:A:71:A:H3'	1:A:72:A:H5''	2.04	0.40
1:A:349:A:C2	1:A:350:G:C4	3.10	0.40
1:A:957:U:O2	1:A:960:U:C2	2.74	0.40
1:A:1172:C:H2'	1:A:1173:U:C6	2.57	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	
2	B	222/241 (92%)	218 (98%)	4 (2%)	0	100	100
3	C	209/233 (90%)	201 (96%)	8 (4%)	0	100	100
4	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
5	E	153/167 (92%)	143 (94%)	10 (6%)	0	100	100
6	F	104/135 (77%)	104 (100%)	0	0	100	100
7	G	149/179 (83%)	137 (92%)	12 (8%)	0	100	100
8	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	I	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	J	97/103 (94%)	92 (95%)	5 (5%)	0	100	100
11	K	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
12	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	M	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
14	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
15	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
17	Q	78/84 (93%)	72 (92%)	6 (8%)	0	100	100
18	R	63/75 (84%)	61 (97%)	2 (3%)	0	100	100
19	S	80/92 (87%)	79 (99%)	1 (1%)	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	50/71 (70%)	50 (100%)	0	0	100	100
22	X	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
23	Y	250/273 (92%)	240 (96%)	10 (4%)	0	100	100
All	All	2754/3000 (92%)	2641 (96%)	113 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	172/190 (90%)	168 (98%)	4 (2%)	45	65
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	118/126 (94%)	118 (100%)	0	100	100
6	F	92/116 (79%)	92 (100%)	0	100	100
7	G	124/147 (84%)	122 (98%)	2 (2%)	58	74
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	87/90 (97%)	86 (99%)	1 (1%)	70	80
11	K	90/99 (91%)	86 (96%)	4 (4%)	24	47
12	L	102/103 (99%)	101 (99%)	1 (1%)	73	82
13	M	92/96 (96%)	91 (99%)	1 (1%)	70	80
14	N	83/84 (99%)	82 (99%)	1 (1%)	67	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	74/78 (95%)	74 (100%)	0	100	100
18	R	56/65 (86%)	55 (98%)	1 (2%)	54	72
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	43/61 (70%)	43 (100%)	0	100	100
22	X	130/130 (100%)	129 (99%)	1 (1%)	79	85
23	Y	216/234 (92%)	213 (99%)	3 (1%)	62	76
All	All	2324/2490 (93%)	2305 (99%)	19 (1%)	77	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	8	ASN
3	C	128	VAL
3	C	129	MET
3	C	144	LEU
7	G	12	ILE
7	G	36	LYS
10	J	18	ILE
11	K	23	ILE
11	K	36	ASP
11	K	79	ILE
11	K	110	ILE
12	L	55	VAL
13	M	11	ASP
14	N	34	VAL
18	R	33	ILE
22	X	145	ASN
23	Y	42	VAL
23	Y	51	LEU
23	Y	222	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	24	ASN

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Mol	Chain	Res	Type
2	B	94	HIS
2	B	120	GLN
2	B	122	GLN
2	B	178	ASN
3	C	102	ASN
5	E	89	HIS
6	F	55	HIS
7	G	52	GLN
11	K	24	HIS
15	O	50	HIS
16	P	26	ASN
18	R	54	GLN
19	S	52	HIS
19	S	53	ASN
20	T	3	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1425/1542 (92%)	310 (21%)	61 (4%)

All (310) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	4	U
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	62	U
1	A	64	G
1	A	65	A
1	A	69	G
1	A	70	U
1	A	72	A
1	A	73	C

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Mol	Chain	Res	Type
1	A	74	A
1	A	76	G
1	A	77	A
1	A	81	A
1	A	82	G
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C
1	A	90	C
1	A	91	U
1	A	94	G
1	A	109	A
1	A	119	A
1	A	120	A
1	A	121	U
1	A	122	G
1	A	131	A
1	A	134	G
1	A	135	C
1	A	140	U
1	A	143	A
1	A	163	C
1	A	164	G
1	A	184	G
1	A	193	C
1	A	195	A
1	A	197	A
1	A	200	G
1	A	201	G
1	A	204	G
1	A	205	A
1	A	206	C
1	A	210	C
1	A	212	G
1	A	213	G
1	A	240	G
1	A	246	A
1	A	247	G
1	A	251	G
1	A	266	G

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Mol	Chain	Res	Type
1	A	267	C
1	A	272	C
1	A	280	C
1	A	281	G
1	A	289	G
1	A	299	G
1	A	320	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	334	C
1	A	344	A
1	A	345	C
1	A	346	G
1	A	347	G
1	A	351	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	397	A
1	A	398	U
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	429	U
1	A	435	A
1	A	440	C
1	A	451	A
1	A	452	A
1	A	457	G
1	A	467	U
1	A	468	A
1	A	469	C
1	A	472	U
1	A	473	U
1	A	481	G
1	A	482	A

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Mol	Chain	Res	Type
1	A	484	G
1	A	486	U
1	A	511	C
1	A	512	U
1	A	515	G
1	A	518	C
1	A	519	C
1	A	520	A
1	A	521	G
1	A	530	G
1	A	531	U
1	A	547	A
1	A	562	U
1	A	564	C
1	A	565	U
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	C
1	A	577	G
1	A	618	C
1	A	633	G
1	A	639	G
1	A	650	G
1	A	653	U
1	A	665	A
1	A	683	G
1	A	686	U
1	A	703	G
1	A	704	A
1	A	718	A
1	A	719	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	753	A
1	A	754	C
1	A	755	G
1	A	777	A
1	A	784	A
1	A	792	A
1	A	793	U

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Mol	Chain	Res	Type
1	A	794	A
1	A	812	G
1	A	813	U
1	A	814	A
1	A	815	A
1	A	817	C
1	A	819	A
1	A	828	U
1	A	841	C
1	A	842	U
1	A	844	G
1	A	847	G
1	A	849	G
1	A	872	A
1	A	884	U
1	A	885	G
1	A	902	G
1	A	910	C
1	A	914	A
1	A	924	C
1	A	925	G
1	A	926	G
1	A	927	G
1	A	928	G
1	A	931	C
1	A	932	C
1	A	934	C
1	A	935	A
1	A	939	G
1	A	953	G
1	A	954	G
1	A	959	A
1	A	960	U
1	A	966	2MG
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C
1	A	993	G

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Mol	Chain	Res	Type
1	A	1000	A
1	A	1003	G
1	A	1004	A
1	A	1017	U
1	A	1018	G
1	A	1020	G
1	A	1021	A
1	A	1026	G
1	A	1028	C
1	A	1030	U
1	A	1031	C
1	A	1037	C
1	A	1038	C
1	A	1043	G
1	A	1045	C
1	A	1047	G
1	A	1053	G
1	A	1054	C
1	A	1064	G
1	A	1065	U
1	A	1067	A
1	A	1068	G
1	A	1085	U
1	A	1086	U
1	A	1092	A
1	A	1093	A
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1108	G
1	A	1125	U
1	A	1129	C
1	A	1130	A
1	A	1132	C
1	A	1136	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	G

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Mol	Chain	Res	Type
1	A	1150	A
1	A	1154	G
1	A	1159	U
1	A	1160	G
1	A	1168	U
1	A	1179	A
1	A	1184	G
1	A	1188	A
1	A	1189	U
1	A	1192	C
1	A	1193	G
1	A	1195	C
1	A	1196	A
1	A	1197	A
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1206	G
1	A	1207	2MG
1	A	1208	C
1	A	1209	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1239	A
1	A	1240	U
1	A	1241	G
1	A	1243	C
1	A	1250	A
1	A	1257	A
1	A	1258	G
1	A	1260	G
1	A	1279	G
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1296	C

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Mol	Chain	Res	Type
1	A	1297	G
1	A	1299	A
1	A	1300	G
1	A	1302	C
1	A	1303	C
1	A	1305	G
1	A	1317	C
1	A	1322	C
1	A	1332	A
1	A	1333	A
1	A	1337	G
1	A	1338	G
1	A	1342	C
1	A	1346	A
1	A	1363	A
1	A	1366	C
1	A	1379	G
1	A	1383	C
1	A	1385	G
1	A	1386	G
1	A	1387	G
1	A	1389	C
1	A	1391	U
1	A	1392	G
1	A	1393	U
1	A	1509	C
1	A	1516	2MG
1	A	1517	G
1	A	1518	MA6
1	A	1519	MA6
1	A	1520	C
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C
1	A	1535	C
1	A	1536	C
1	A	1537	U
1	A	1538	C
1	A	1540	U

All (61) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	64	G
1	A	73	C
1	A	85	U
1	A	86	G
1	A	119	A
1	A	134	G
1	A	181	A
1	A	200	G
1	A	209	U
1	A	266	G
1	A	280	C
1	A	298	A
1	A	344	A
1	A	345	C
1	A	351	G
1	A	411	A
1	A	421	U
1	A	422	C
1	A	451	A
1	A	467	U
1	A	481	G
1	A	518	C
1	A	564	C
1	A	575	G
1	A	685	G
1	A	723	U
1	A	753	A
1	A	792	A
1	A	812	G
1	A	818	G
1	A	884	U
1	A	909	A
1	A	924	C
1	A	953	G
1	A	977	A
1	A	983	A
1	A	1054	C
1	A	1067	A
1	A	1092	A
1	A	1101	A
1	A	1103	C
1	A	1129	C
1	A	1137	C

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	1159	U
1	A	1188	A
1	A	1195	C
1	A	1196	A
1	A	1206	G
1	A	1208	C
1	A	1213	A
1	A	1226	C
1	A	1238	A
1	A	1240	U
1	A	1257	A
1	A	1286	U
1	A	1332	A
1	A	1337	G
1	A	1516	2MG
1	A	1530	G
1	A	1531	A
1	A	1535	C

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

7 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
1	2MG	A	1207	1	18,26,27	1.10	1 (5%)	16,38,41	1.26	3 (18%)
12	D2T	L	89	12	7,9,10	1.97	3 (42%)	6,11,13	3.49	3 (50%)
1	MA6	A	1518	1	18,26,27	1.06	1 (5%)	19,38,41	2.01	7 (36%)
1	2MG	A	1516	1	18,26,27	0.97	1 (5%)	16,38,41	1.69	5 (31%)
1	5MC	A	967	1	18,22,23	0.98	2 (11%)	26,32,35	1.29	3 (11%)
1	2MG	A	966	1	18,26,27	1.00	1 (5%)	16,38,41	1.37	3 (18%)
1	MA6	A	1519	1	18,26,27	1.17	1 (5%)	19,38,41	2.01	7 (36%)

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
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
12	D2T	L	89	12	-	2/7/12/14	-
1	MA6	A	1518	1	-	4/7/29/30	0/3/3/3
1	2MG	A	1516	1	-	3/5/27/28	0/3/3/3
1	5MC	A	967	1	-	3/7/25/26	0/2/2/2
1	2MG	A	966	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	89	D2T	OD2-CG	-2.93	1.21	1.30
12	L	89	D2T	OD1-CG	2.91	1.31	1.22
12	L	89	D2T	O-C	2.78	1.31	1.19
1	A	1207	2MG	C6-N1	-2.63	1.34	1.37
1	A	967	5MC	C6-C5	2.53	1.38	1.34
1	A	1519	MA6	C5-C4	2.50	1.47	1.40
1	A	966	2MG	C6-N1	-2.43	1.34	1.37
1	A	1516	2MG	C6-N1	-2.39	1.34	1.37
1	A	967	5MC	C6-N1	-2.36	1.34	1.38
1	A	1518	MA6	C5-C4	2.34	1.47	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	89	D2T	OD1-CG-CB	-5.43	111.06	122.44
12	L	89	D2T	OD2-CG-CB	5.26	124.52	113.15
1	A	1519	MA6	N1-C6-N6	4.36	121.64	117.06
1	A	1516	2MG	CM2-N2-C2	-3.78	115.51	123.86
1	A	1518	MA6	N1-C6-N6	3.52	120.77	117.06
1	A	1518	MA6	C9-N6-C6	-3.45	109.06	119.51
12	L	89	D2T	O-C-CA	-3.41	115.83	124.78
1	A	1518	MA6	N3-C2-N1	-3.39	123.38	128.68
1	A	1519	MA6	C9-N6-C6	-3.37	109.32	119.51
1	A	1518	MA6	C10-N6-C6	-3.33	109.44	119.51
1	A	1519	MA6	C10-N6-C6	-3.28	109.58	119.51
1	A	967	5MC	C5-C6-N1	-3.17	120.08	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	N3-C2-N1	-3.16	123.75	128.68
1	A	966	2MG	C3'-C2'-C1'	3.07	105.60	100.98
1	A	1516	2MG	C3'-C2'-C1'	2.99	105.48	100.98
1	A	1518	MA6	C4-C5-N7	-2.77	106.52	109.40
1	A	1518	MA6	C3'-C2'-C1'	2.72	105.07	100.98
1	A	967	5MC	C5-C4-N3	-2.56	118.92	121.67
1	A	1516	2MG	O4'-C1'-C2'	-2.43	103.37	106.93
1	A	1519	MA6	C4-C5-N7	-2.40	106.89	109.40
1	A	966	2MG	C8-N7-C5	2.36	107.48	102.99
1	A	1207	2MG	C5-C6-N1	2.34	118.09	113.95
1	A	966	2MG	C5-C6-N1	2.32	118.04	113.95
1	A	1516	2MG	C5-C6-N1	2.26	117.94	113.95
1	A	1516	2MG	C8-N7-C5	2.23	107.23	102.99
1	A	1519	MA6	O2'-C2'-C3'	-2.16	104.83	111.82
1	A	1519	MA6	C10-N6-C9	-2.14	109.21	116.12
1	A	1207	2MG	C8-N7-C5	2.11	107.00	102.99
1	A	967	5MC	C3'-C2'-C1'	2.09	105.41	101.43
1	A	1518	MA6	C10-N6-C9	-2.09	109.38	116.12
1	A	1207	2MG	CM2-N2-C2	-2.02	119.41	123.86

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CA-CB-SB-CB1
1	A	1516	2MG	C4'-C5'-O5'-P
1	A	1519	MA6	C5-C6-N6-C9
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C10
1	A	1519	MA6	N1-C6-N6-C9
1	A	1516	2MG	C3'-C4'-C5'-O5'
1	A	967	5MC	C4'-C5'-O5'-P
1	A	1516	2MG	O4'-C4'-C5'-O5'
12	L	89	D2T	CG-CB-SB-CB1
1	A	1518	MA6	N1-C6-N6-C10

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1518	MA6	1	0
1	A	967	5MC	3	0
1	A	966	2MG	2	0
1	A	1519	MA6	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 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.

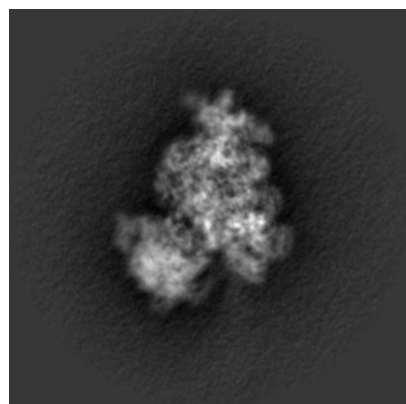
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12250. These allow visual inspection of the internal detail of the map and identification of artifacts.

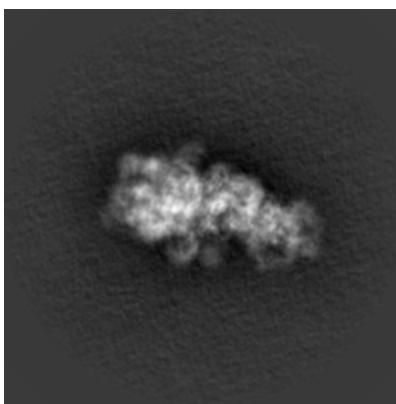
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

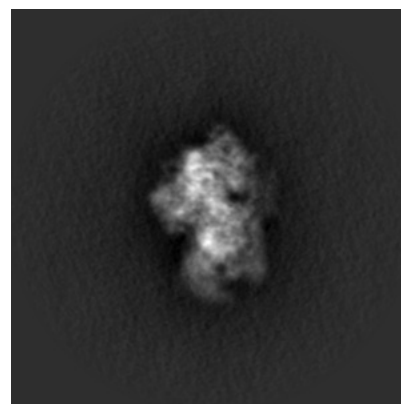
#### 6.1.1 Primary map



X

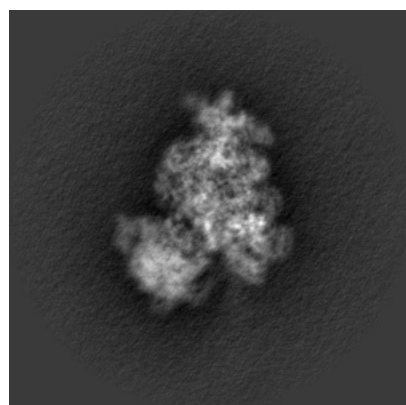


Y

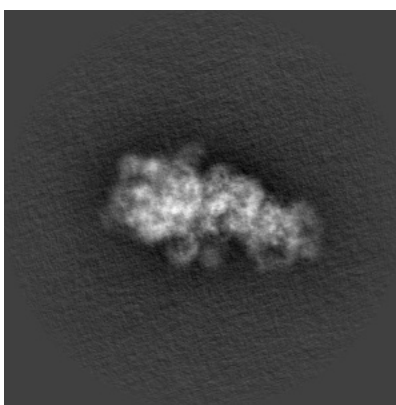


Z

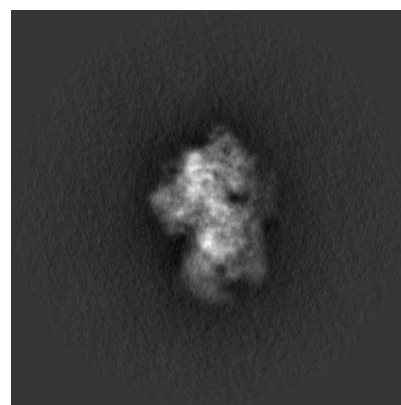
#### 6.1.2 Raw map



X



Y

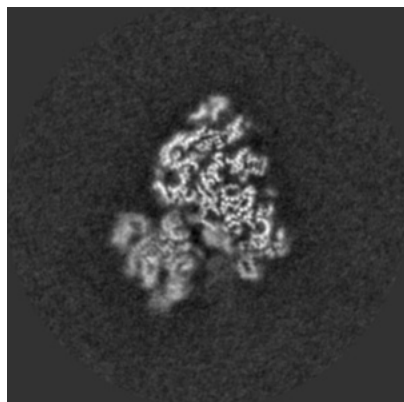


Z

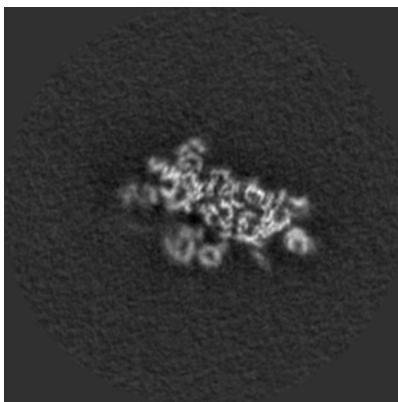
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

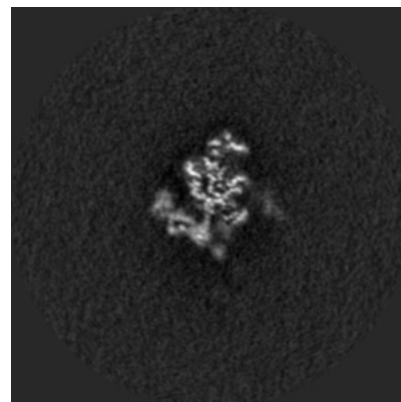
### 6.2.1 Primary map



X Index: 192

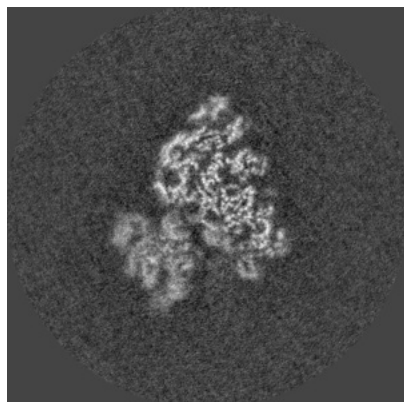


Y Index: 192

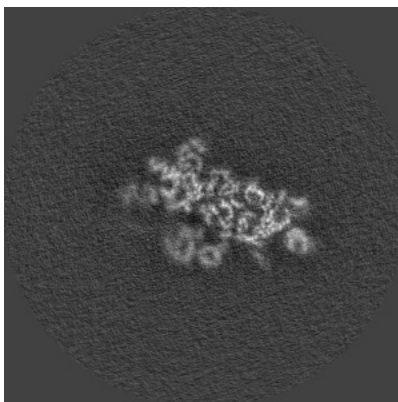


Z Index: 192

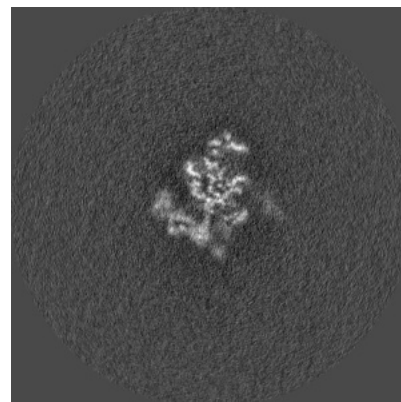
### 6.2.2 Raw map



X Index: 192



Y Index: 192

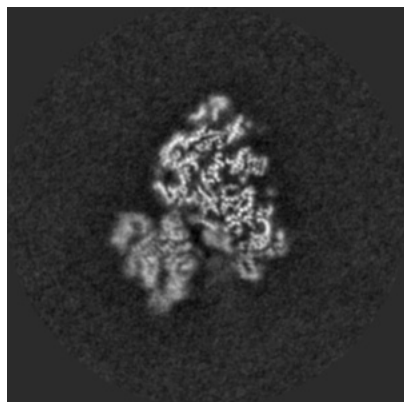


Z Index: 192

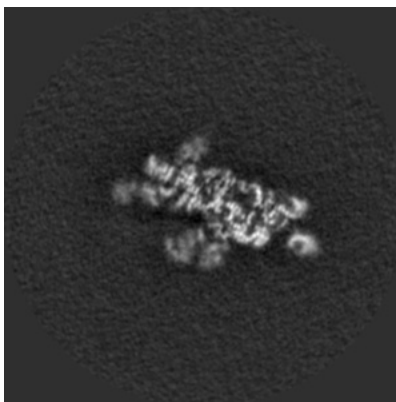
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

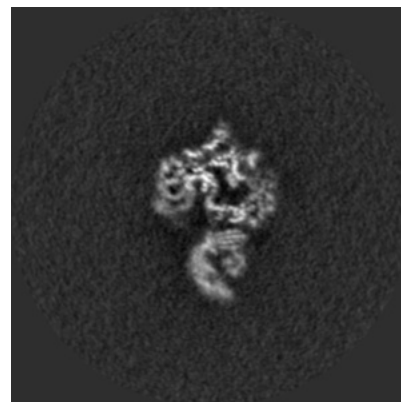
### 6.3.1 Primary map



X Index: 191

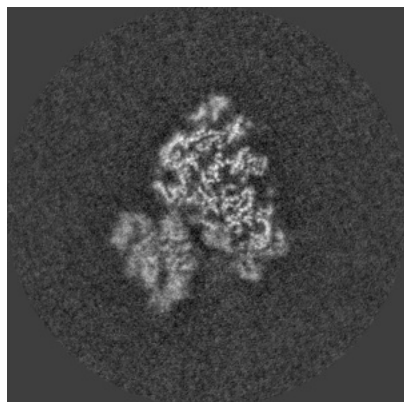


Y Index: 188

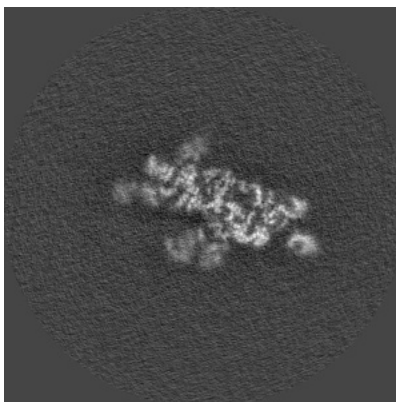


Z Index: 175

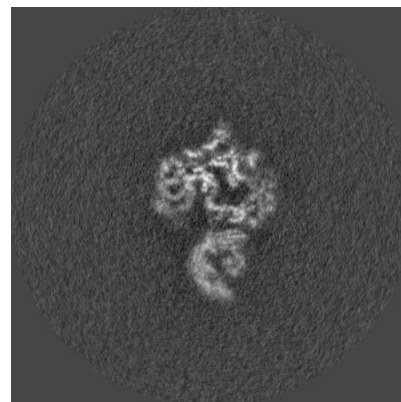
### 6.3.2 Raw map



X Index: 191



Y Index: 188

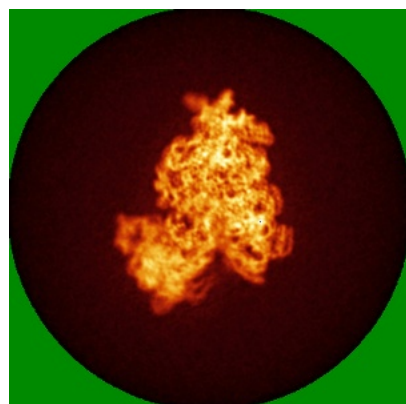


Z Index: 175

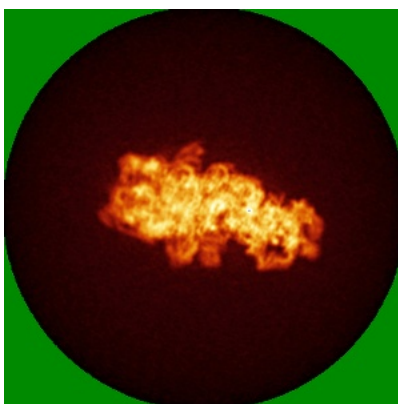
The images above show the largest variance slices of the map in three orthogonal directions.

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

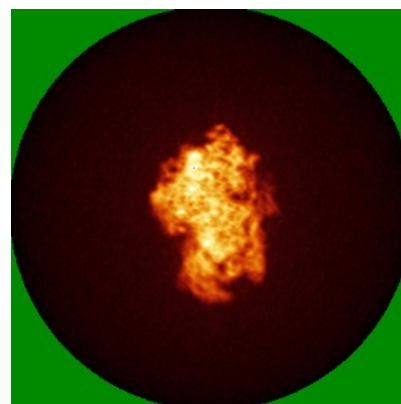
### 6.4.1 Primary map



X

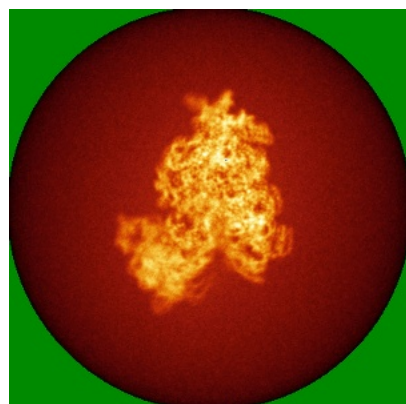


Y

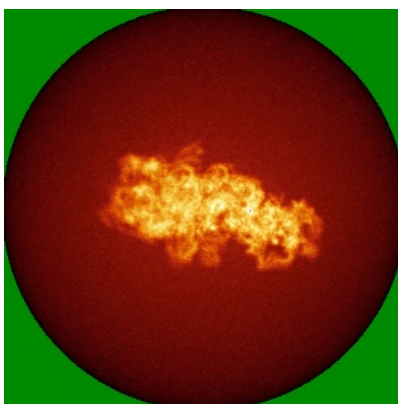


Z

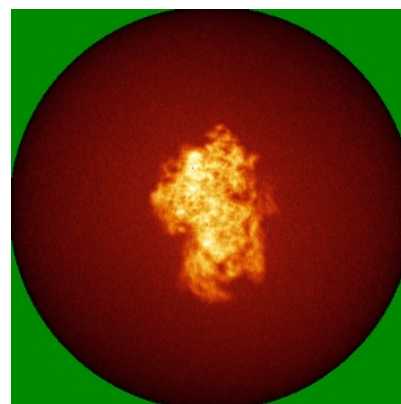
### 6.4.2 Raw map



X



Y

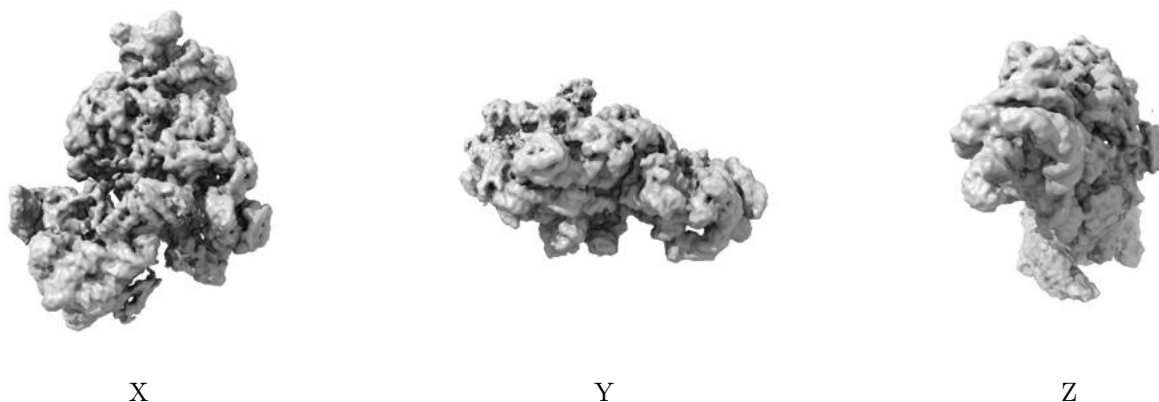


Z

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.

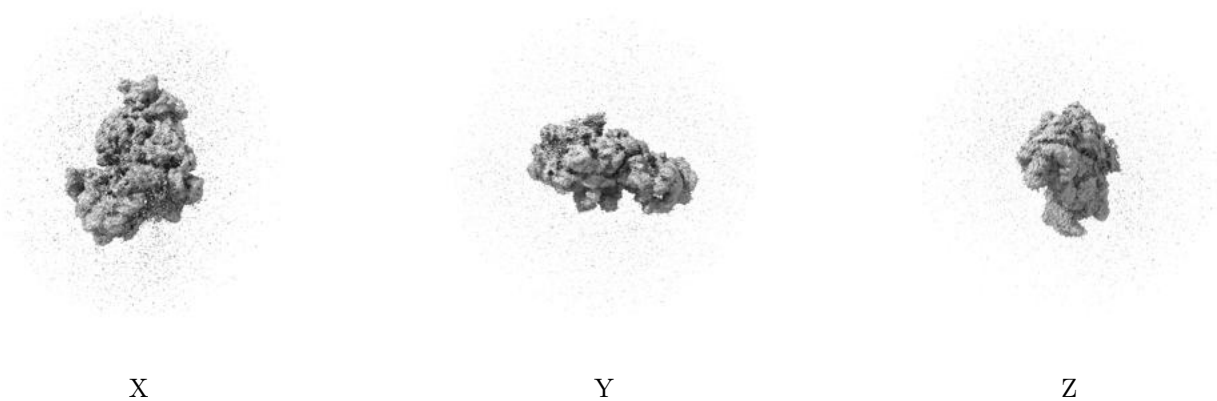
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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.

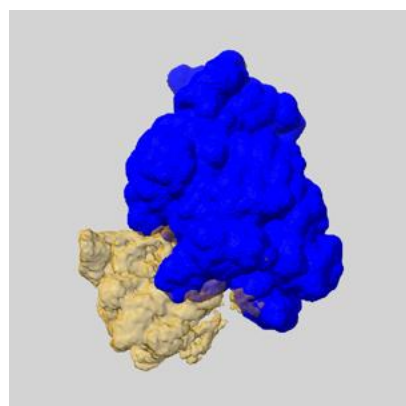
## 6.6 Mask visualisation [i](#)

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

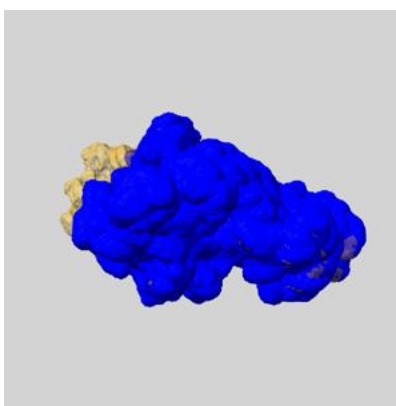
A mask typically either:

- 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\_12250\_msk\_1.map [i](#)



X

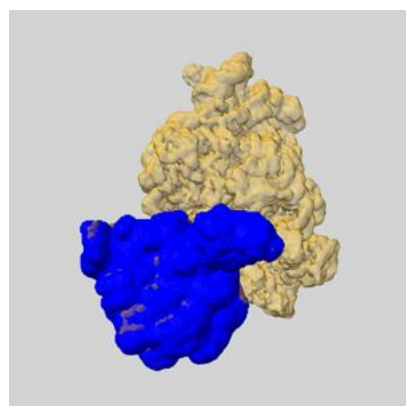


Y

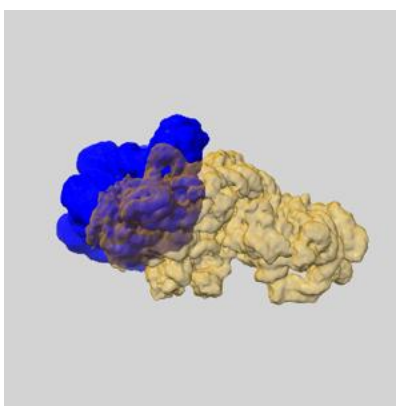


Z

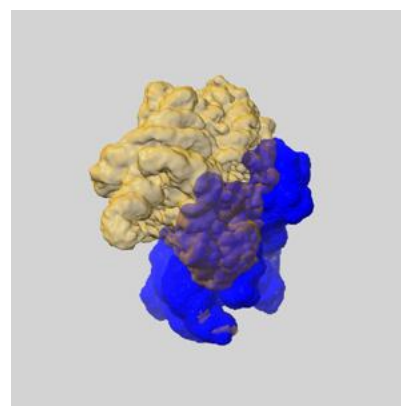
### 6.6.2 emd\_12250\_msk\_2.map [i](#)



X



Y

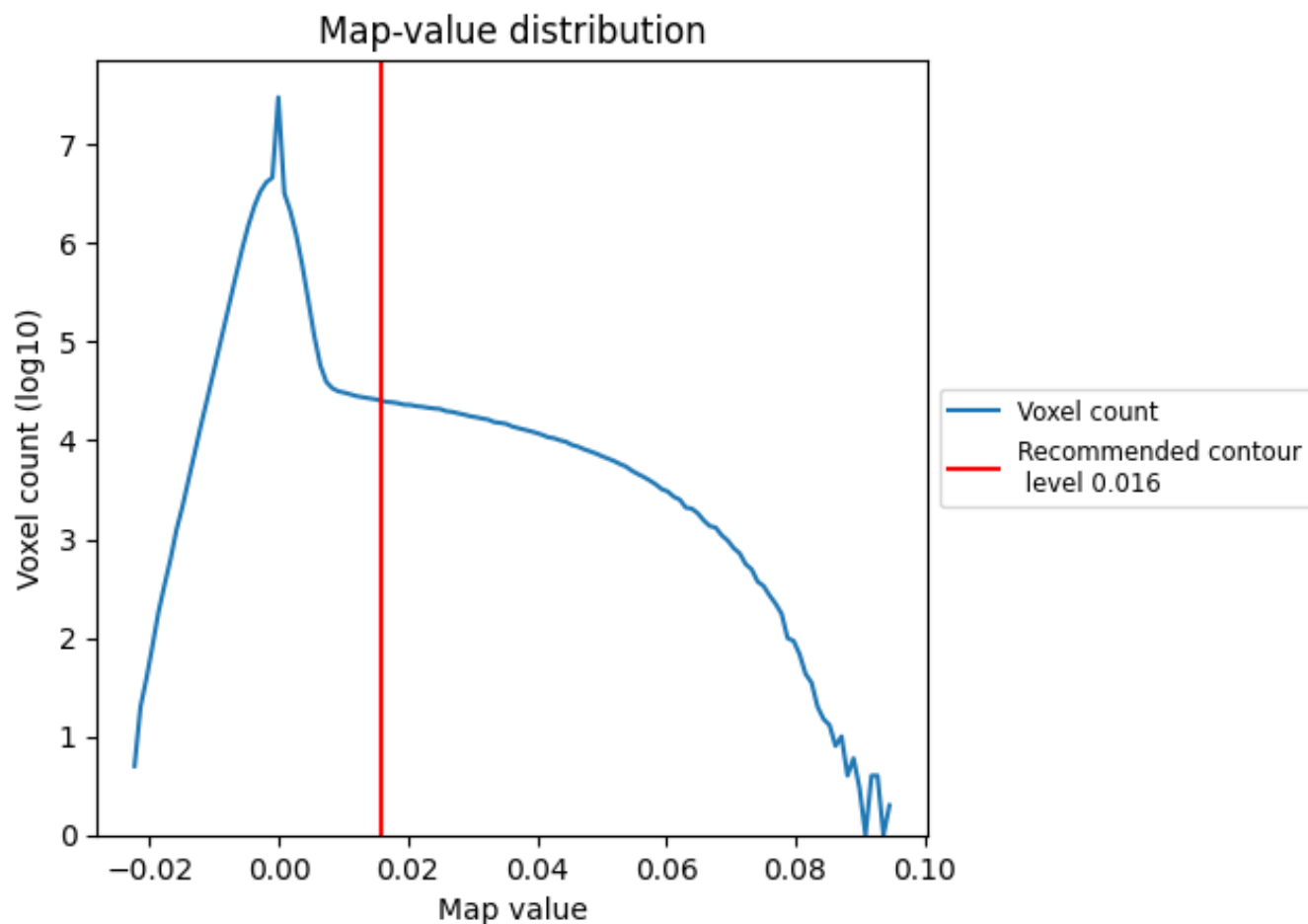


Z

## 7 Map analysis [i](#)

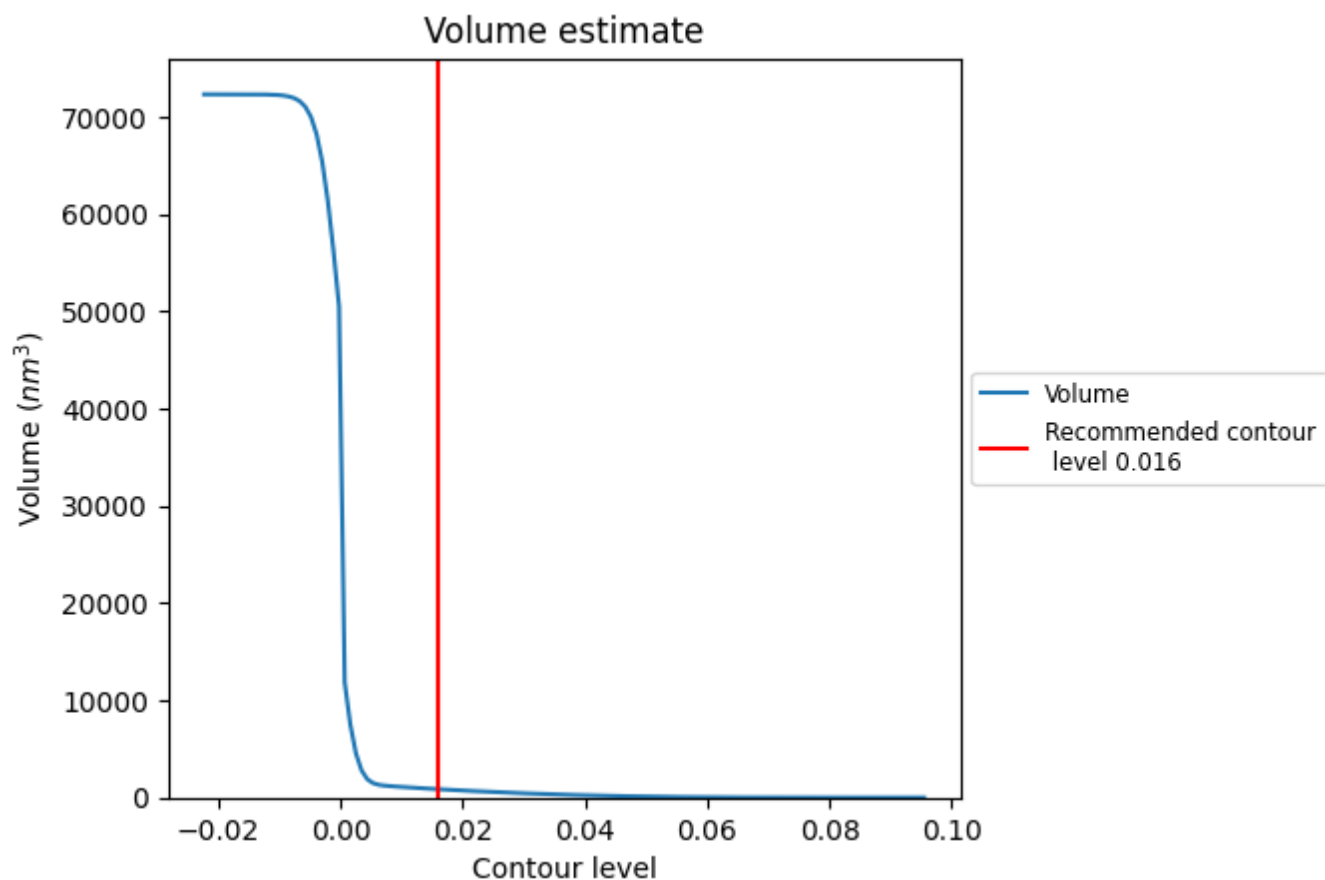
This section contains the results of statistical analysis of the map.

### 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.

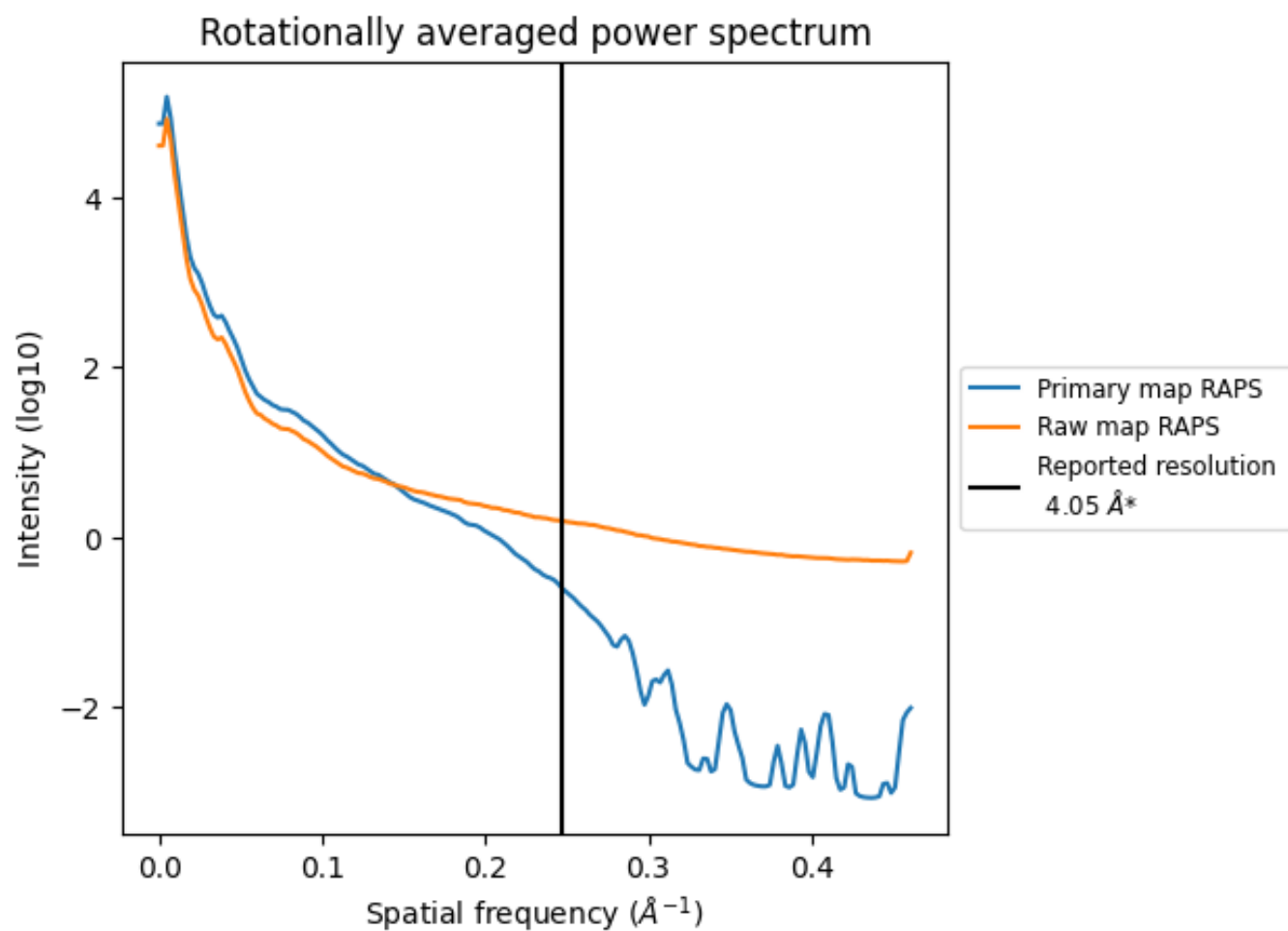
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 858 nm<sup>3</sup>; this corresponds to an approximate mass of 775 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

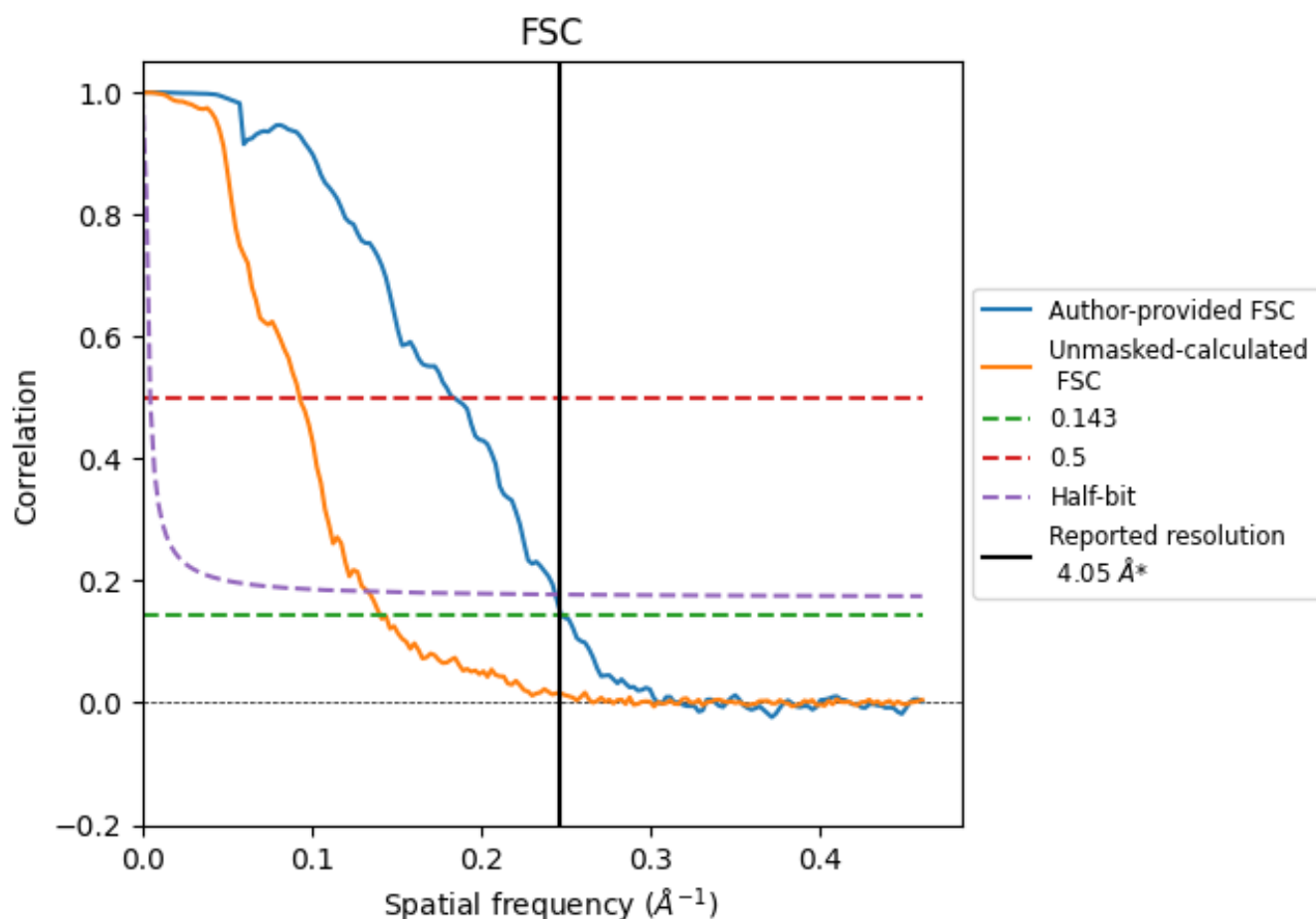


\*Reported resolution corresponds to spatial frequency of 0.247 Å<sup>-1</sup>

## 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 0.247  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

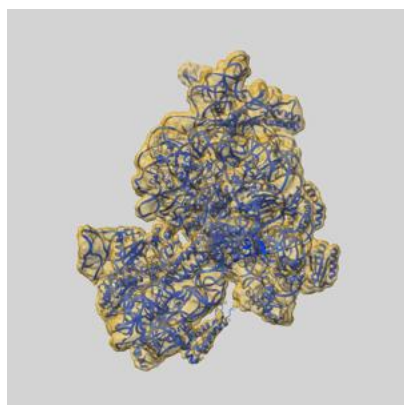
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.03	5.43	4.10
Unmasked-calculated*	7.11	10.75	7.50

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.11 differs from the reported value 4.05 by more than 10 %

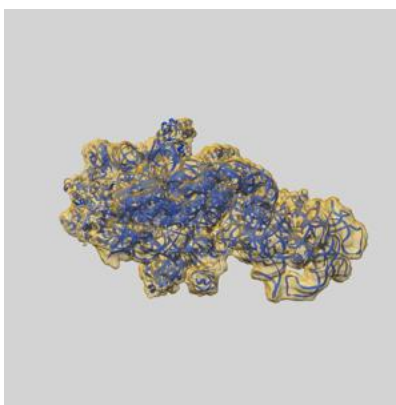
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12250 and PDB model 7NAW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

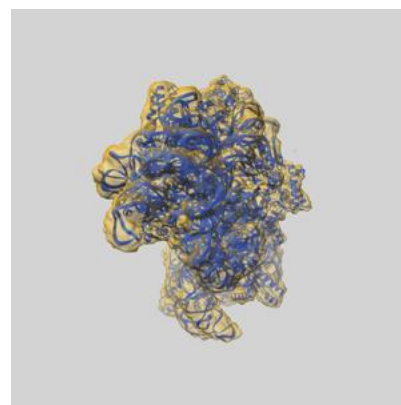
### 9.1 Map-model overlay [i](#)



X



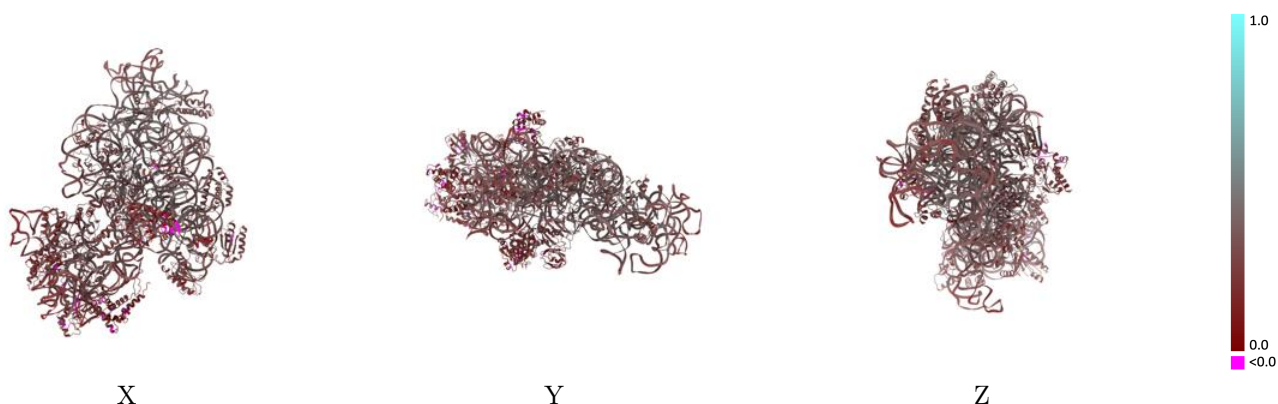
Y



Z

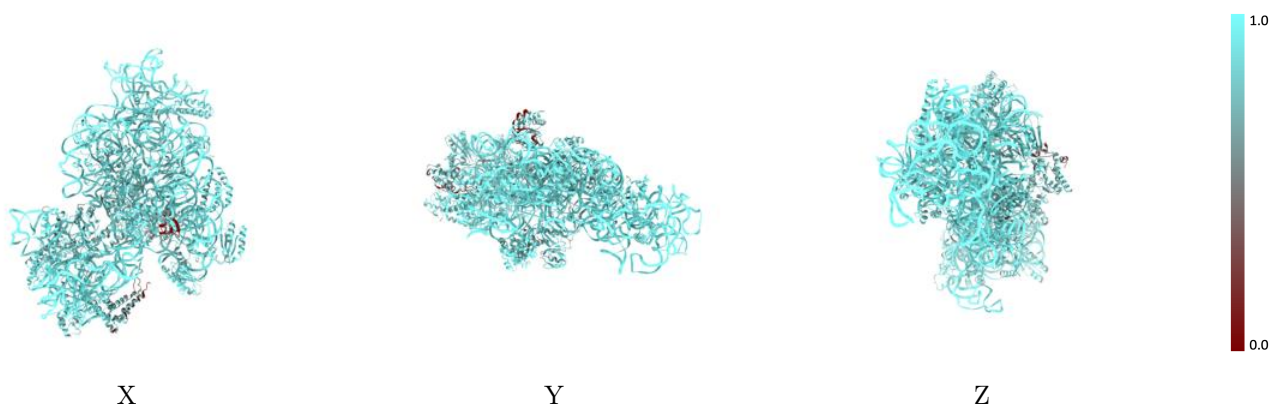
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



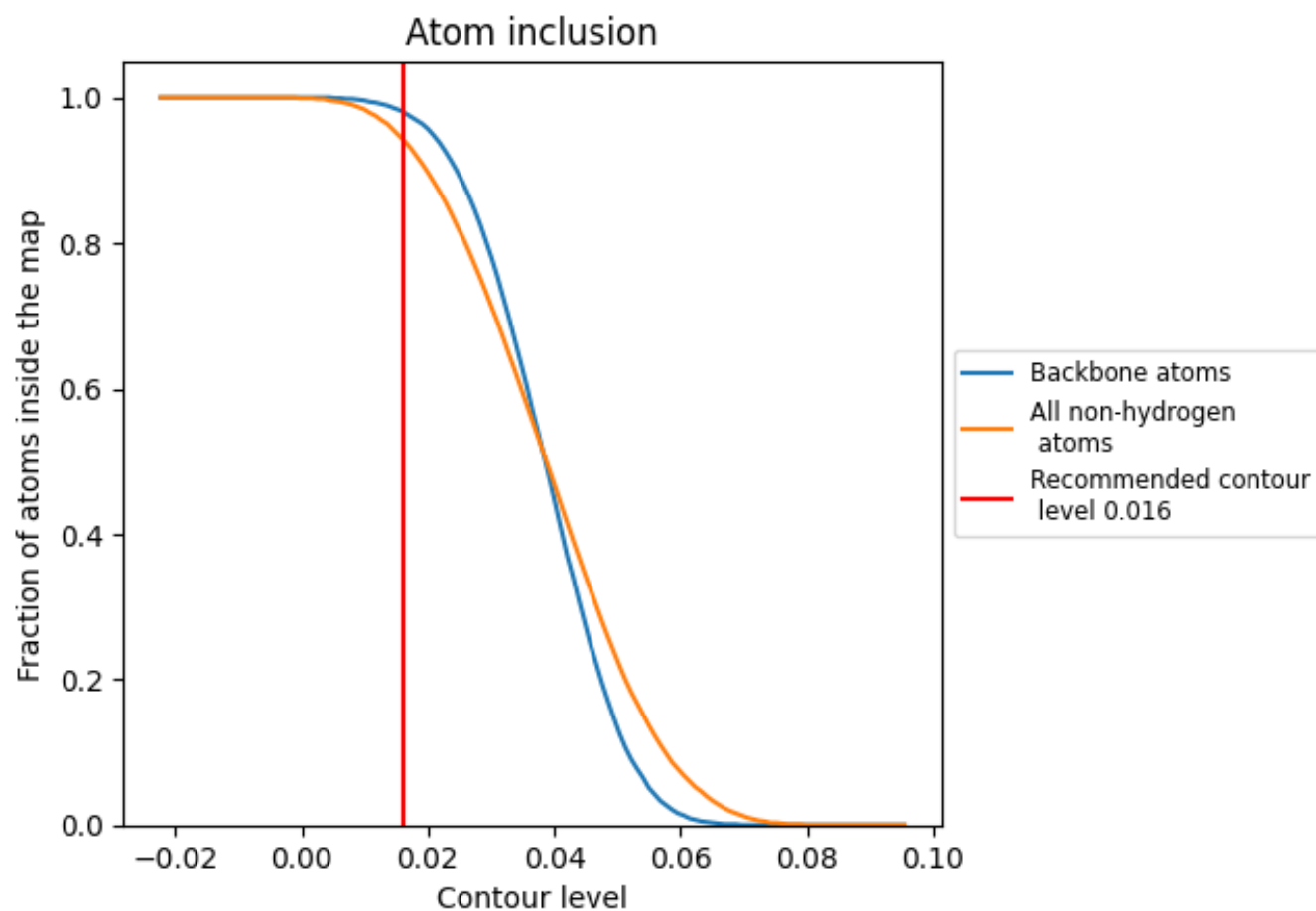
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.2970
A	 0.9950	 0.3280
B	 0.6620	 0.1870
C	 0.8600	 0.2700
D	 0.9320	 0.3150
E	 0.8920	 0.3300
F	 0.9020	 0.2820
G	 0.6260	 0.1530
H	 0.9050	 0.3360
I	 0.9070	 0.2190
J	 0.9060	 0.2310
K	 0.9270	 0.2520
L	 0.8720	 0.3040
M	 0.8940	 0.1640
N	 0.9120	 0.2440
O	 0.9320	 0.2920
P	 0.9490	 0.3540
Q	 0.9350	 0.3370
R	 0.8950	 0.2810
S	 0.9420	 0.1870
T	 0.9620	 0.2890
U	 0.8150	 0.2620
X	 0.9000	 0.2080
Y	 0.8760	 0.2100

