Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:51 AM JST

PDB ID	:	7WTU
EMDB ID	:	EMD-32801
Title	:	Cryo-EM structure of a human pre-40S ribosomal subunit - State RRP12-A1 (without CK1)
Authors	:	Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on	:	2022-02-05
Resolution	:	3.00 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:

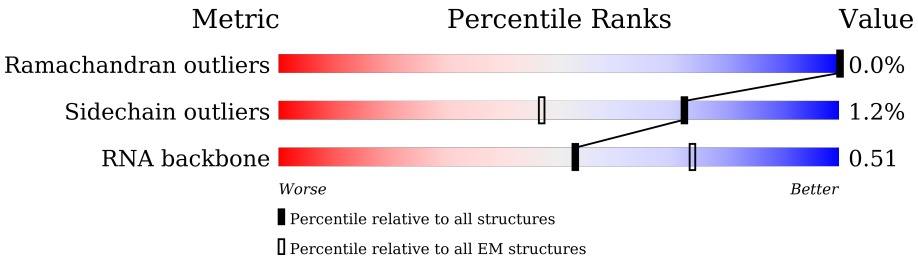
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.00 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1873	62% 21% 16%
2	R	135	59% 40%
3	b	84	98%
4	B	264	80% 19%
5	c	69	88% 12%
6	E	263	99%
7	e	59	34% 66%
8	F	204	92% 7%

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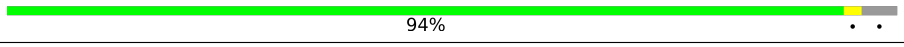
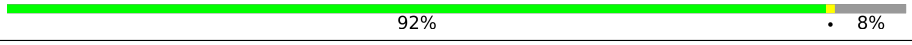
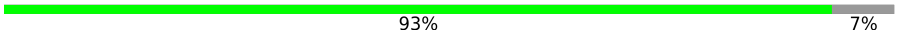
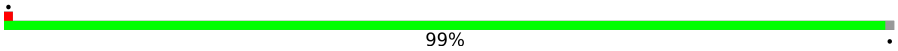
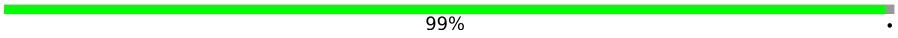
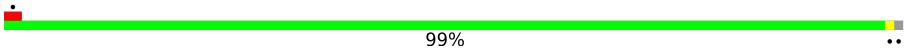
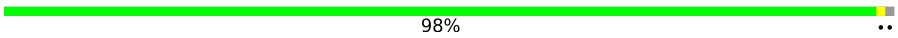
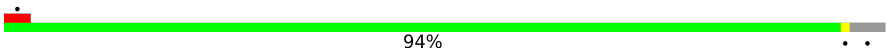
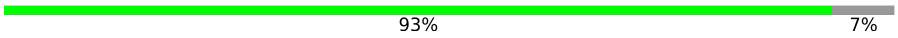
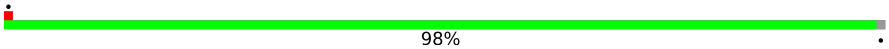
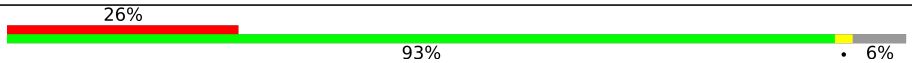
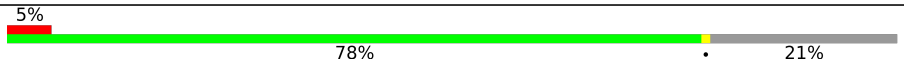
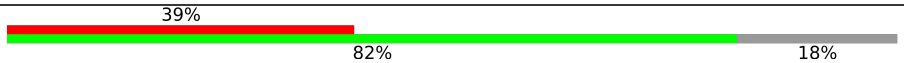
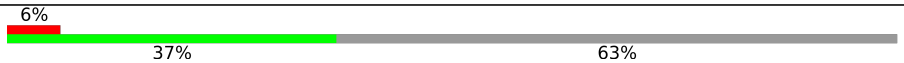
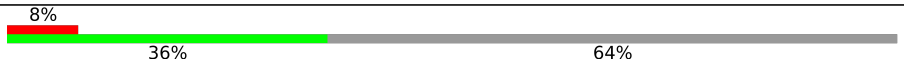
Mol	Chain	Length	Quality of chain
9	H	194	
10	G	249	
11	Z	125	
12	Y	133	
13	x	252	
14	X	143	
15	w	437	
16	W	130	
17	u	804	
18	t	475	
19	T	145	
20	S	152	
21	Q	146	
22	P	145	
23	O	151	
24	N	151	
25	L	158	
26	J	194	
27	I	208	
28	r	125	
29	q	281	
30	K	1297	
31	M	132	
32	f	156	
33	z	230	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 81215 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1575	33634	15011	6036	11012	1575	0	0

- Molecule 2 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	81	673	420	137	114	2	0	0

- Molecule 3 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	b	82	640	402	118	113	7	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	213	1729	1098	309	308	14	0	0

- Molecule 5 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	c	61	471	288	95	86	2	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	262	2076	1324	386	358	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	20	Total	C	N	O	S	0	0
			179	110	43	25	1		

- Molecule 8 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	189	Total	C	N	O	S	0	0
			1494	934	284	269	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 11 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 12 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 13 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	x	175	Total	C	N	O	S	0	0
			1372	881	249	238	4		

- Molecule 14 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 15 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	w	331	Total	C	N	O	S	0	0
			2610	1671	477	453	9		

- Molecule 16 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 17 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	u	642	Total	C	N	O	S	0	0
			5168	3315	928	901	24		

- Molecule 18 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	t	59	Total	C	N	O	S	0	0
			520	328	88	101	3		

- Molecule 19 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	127	Total	C	N	O	S	0	0
			1054	669	205	179	1		

- Molecule 21 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	125	Total	C	N	O	S	0	0
			998	637	185	173	3		

- Molecule 22 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	121	Total	C	N	O	S	0	0
			1006	643	186	170	7		

- Molecule 23 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 26 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 28 is a protein called Multifunctional methyltransferase subunit TRM112-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	r	118	Total	C	N	O	S	0	0
			940	601	166	166	7		

- Molecule 29 is a protein called Probable 18S rRNA (guanine-N(7))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	q	235	Total	C	N	O	S	0	0
			1869	1182	333	343	11		

- Molecule 30 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	1022	Total	C	N	O	S	0	0
			7949	5087	1383	1434	45		

- Molecule 31 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	108	Total	C	N	O	S	0	0
			837	530	147	153	7		

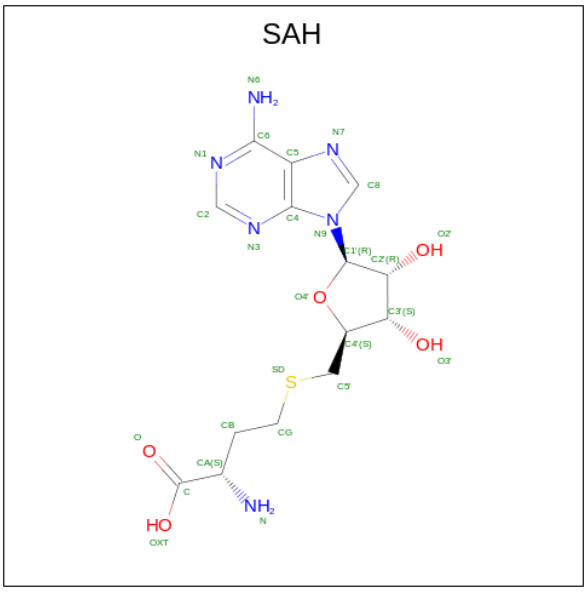
- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 33 is a protein called Ribosome biogenesis protein SLX9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	82	Total	C	N	O	S	0	0
			679	424	132	120	3		

- Molecule 34 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					AltConf
34	q	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

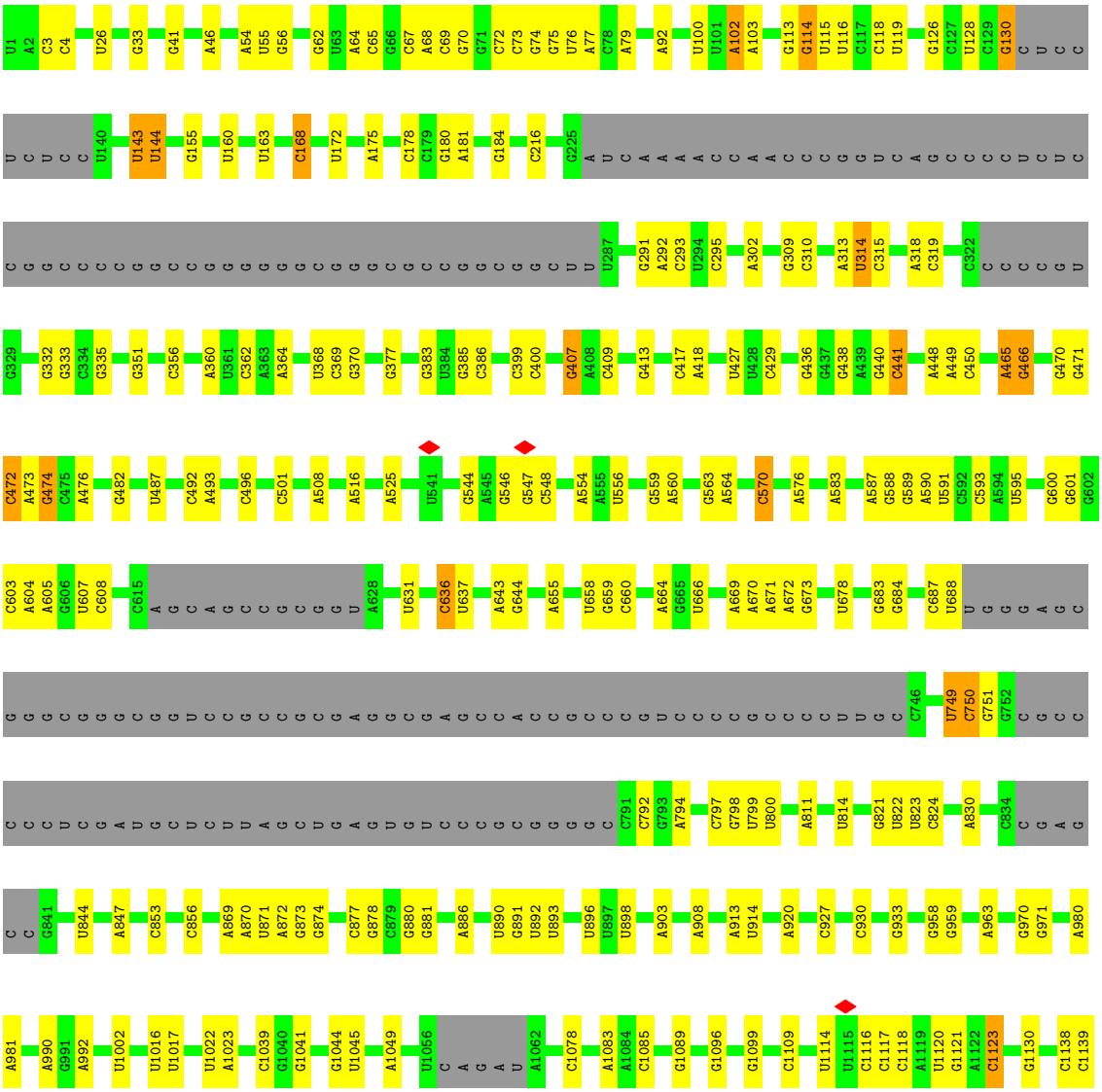
Mol	Chain	Residues	Atoms		AltConf
35	f	1	Total	Zn	0
			1	1	

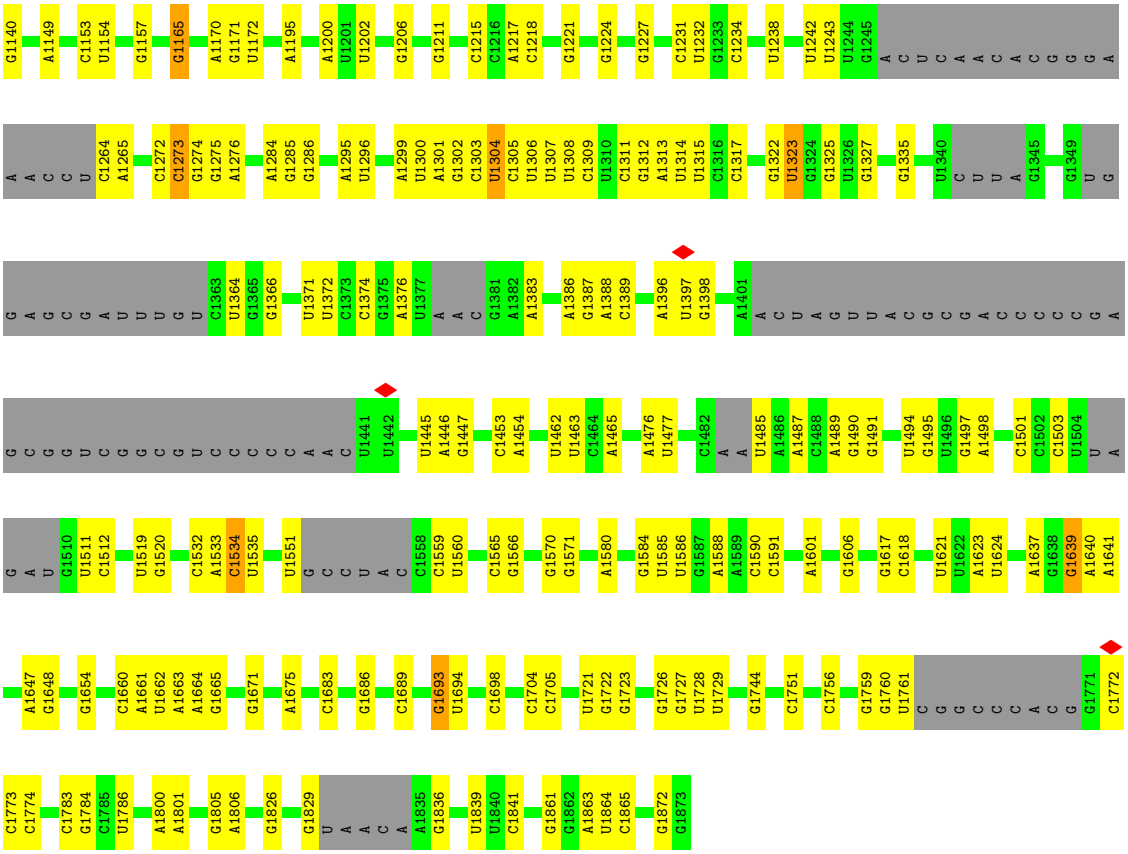
3 Residue-property plots (i)

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: 18S rRNA

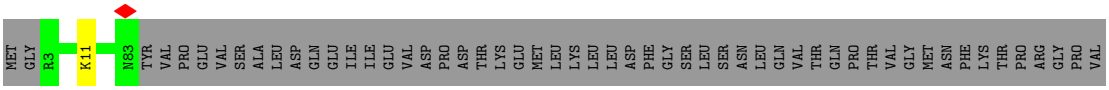
Chain 2:





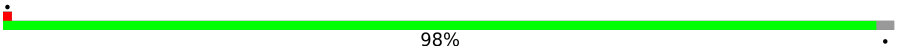
• Molecule 2: 40S ribosomal protein S17

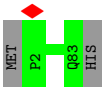
Chain R:



• Molecule 3: 40S ribosomal protein S27

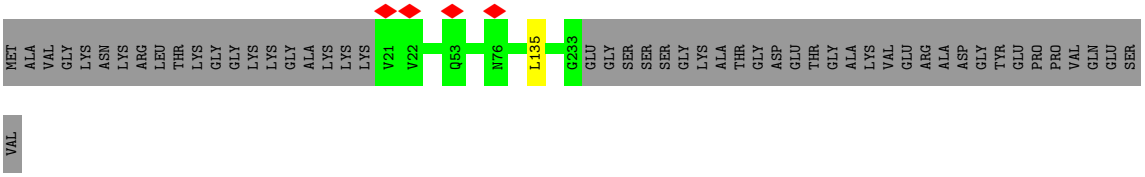
Chain b:





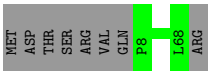
• Molecule 4: 40S ribosomal protein S3a

Chain B:



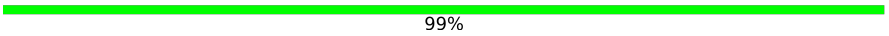
• Molecule 5: 40S ribosomal protein S28

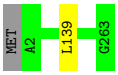
Chain c:



• Molecule 6: 40S ribosomal protein S4, X isoform

Chain E:



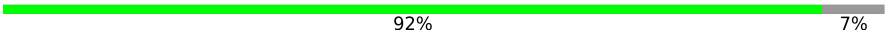


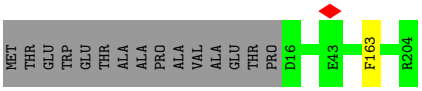
• Molecule 7: 40S ribosomal protein S30

Chain e:

• Molecule 8: 40S ribosomal protein S5

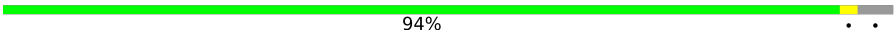
Chain F:

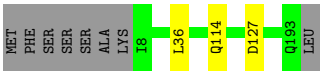




• Molecule 9: 40S ribosomal protein S7

Chain H:



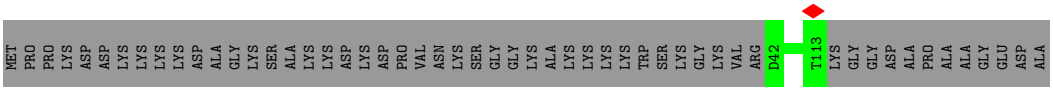


• Molecule 10: 40S ribosomal protein S6

Chain G:

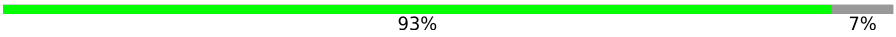
• Molecule 11: 40S ribosomal protein S25

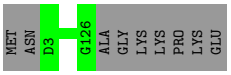
Chain Z:



• Molecule 12: 40S ribosomal protein S24

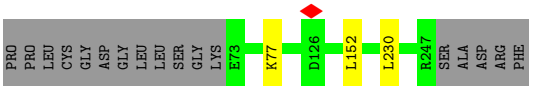
Chain Y:





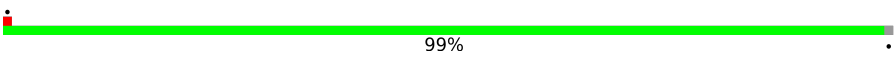
• Molecule 13: RNA-binding protein PNO1

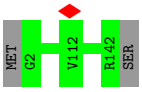
Chain x:



• Molecule 14: 40S ribosomal protein S23

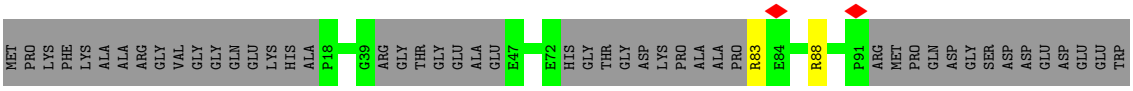
Chain X:

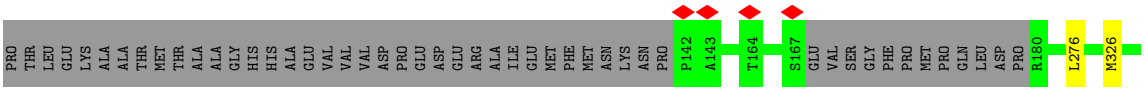


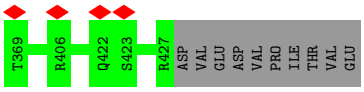


• Molecule 15: Bystin

Chain w:

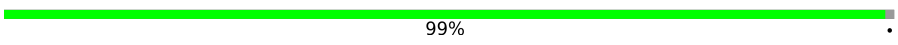






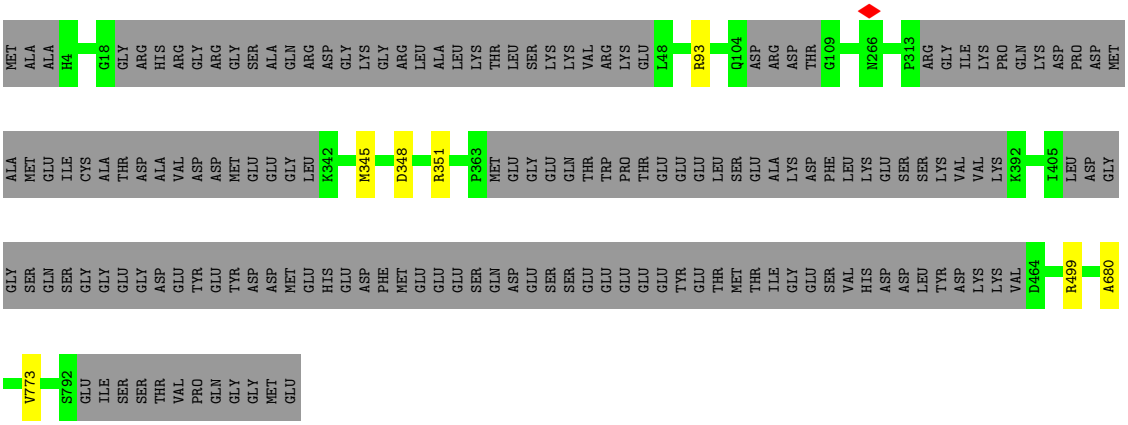
• Molecule 16: 40S ribosomal protein S15a

Chain W:



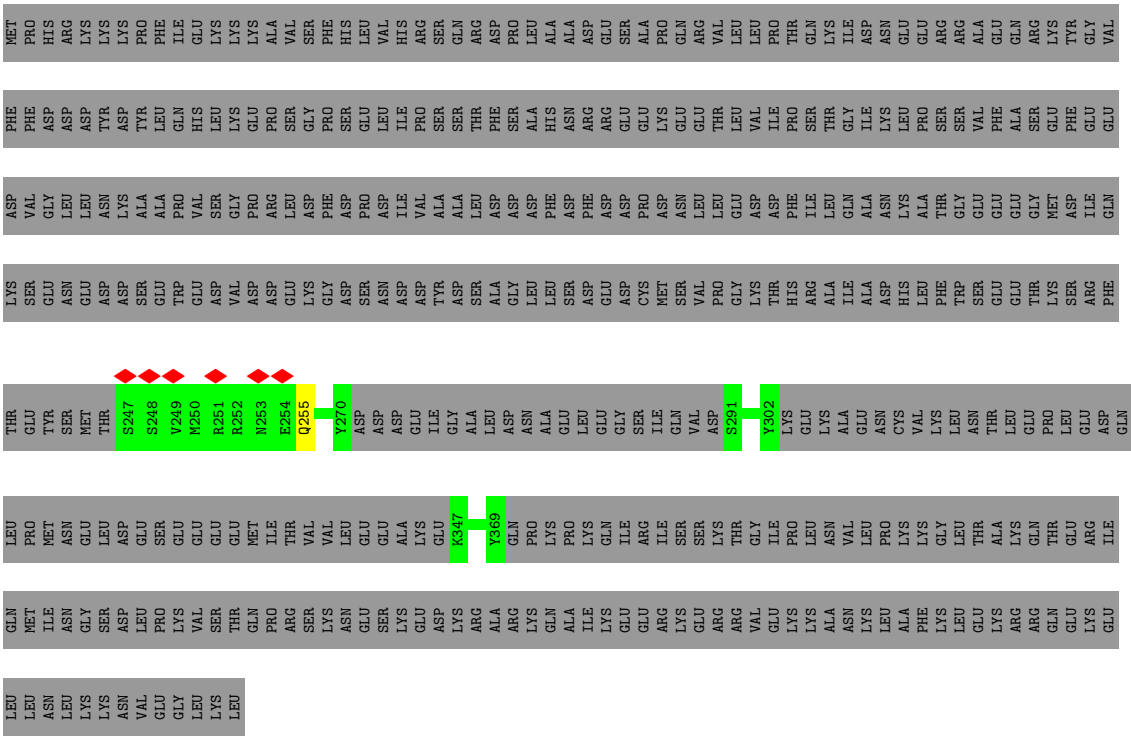
• Molecule 17: Pre-rRNA-processing protein TSR1 homolog

Chain u:



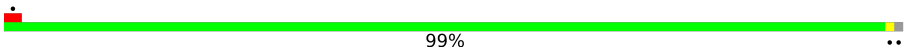
• Molecule 18: Protein LTV1 homolog

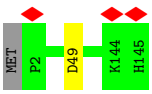
Chain t:



• Molecule 19: 40S ribosomal protein S19

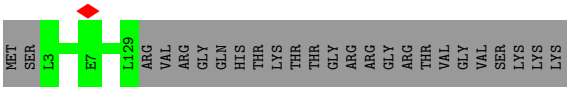
Chain T:





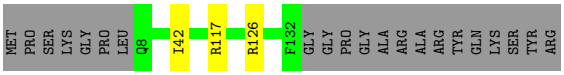
• Molecule 20: 40S ribosomal protein S18

Chain S:



• Molecule 21: 40S ribosomal protein S16

Chain Q:

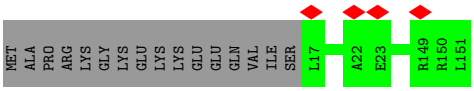


• Molecule 22: 40S ribosomal protein S15

Chain P:

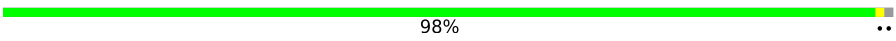
• Molecule 23: 40S ribosomal protein S14

Chain O:



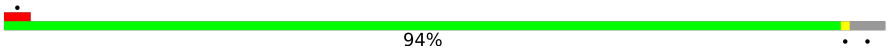
• Molecule 24: 40S ribosomal protein S13

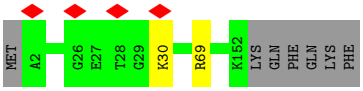
Chain N:



• Molecule 25: 40S ribosomal protein S11

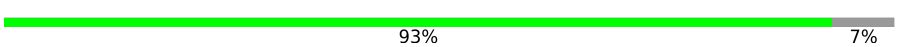
Chain L:

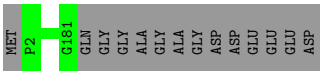




• Molecule 26: 40S ribosomal protein S9

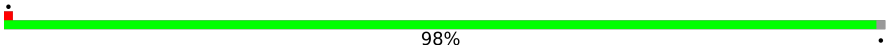
Chain J:

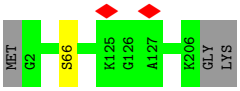




• Molecule 27: 40S ribosomal protein S8

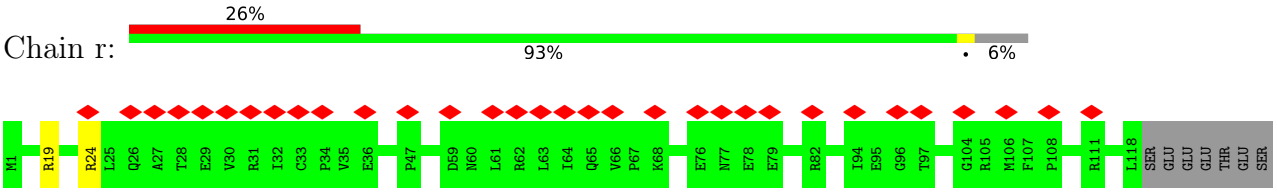
Chain I:





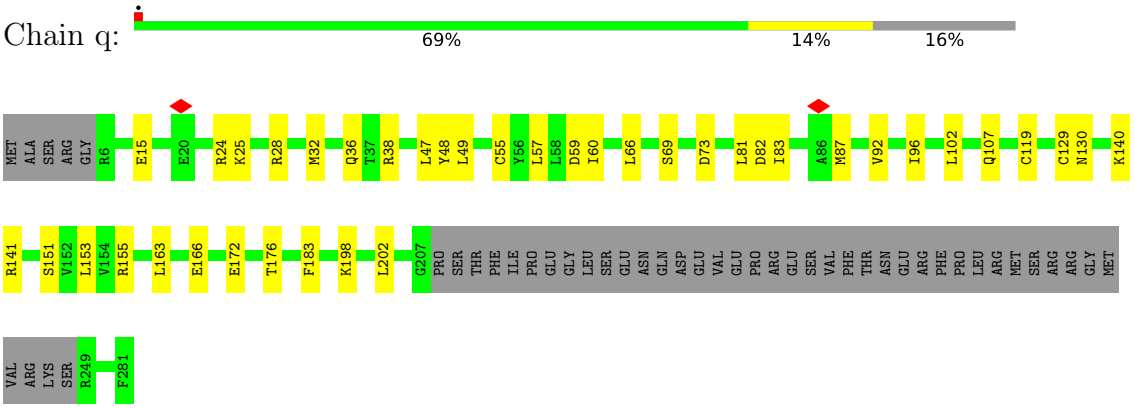
• Molecule 28: Multifunctional methyltransferase subunit TRM112-like protein

Chain r:



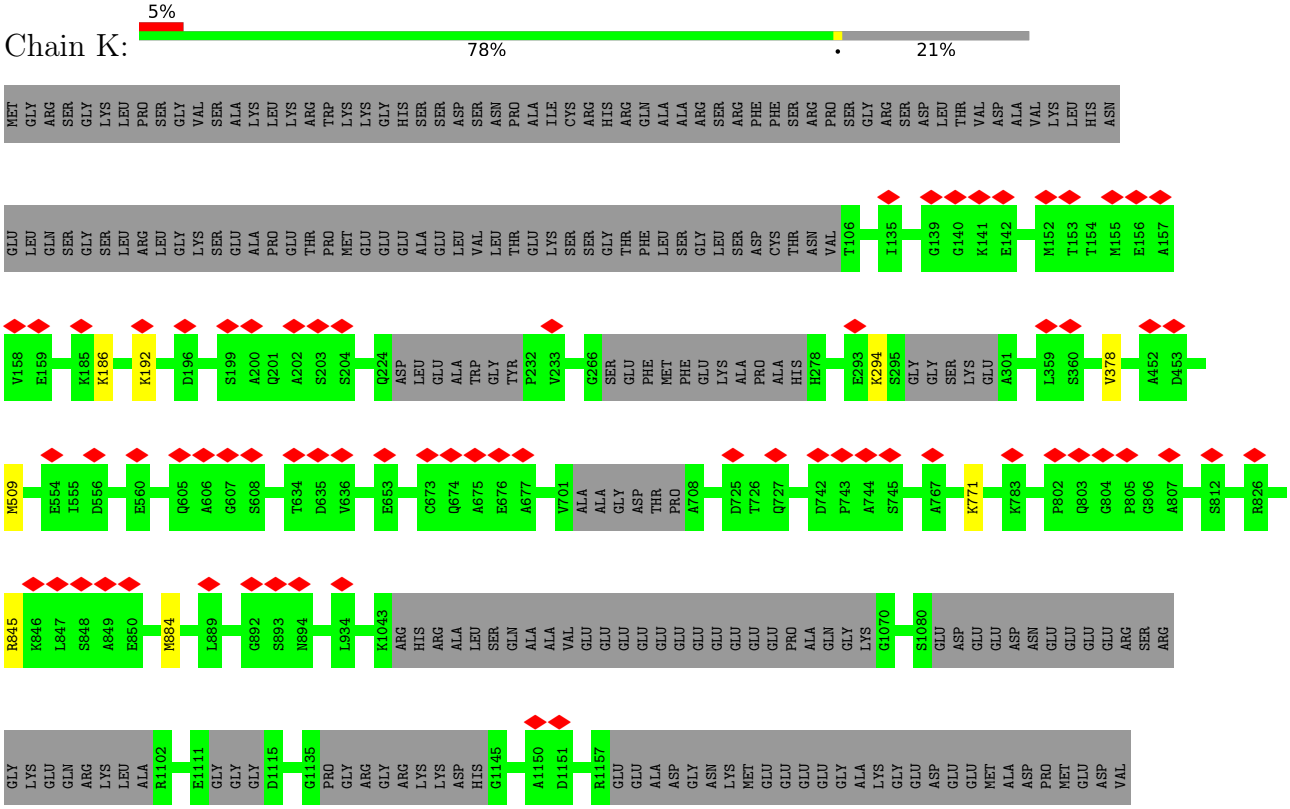
• Molecule 29: Probable 18S rRNA (guanine-N(7))-methyltransferase

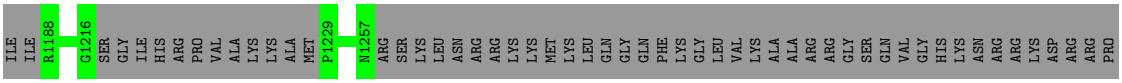
Chain q:



• Molecule 30: RRP12-like protein

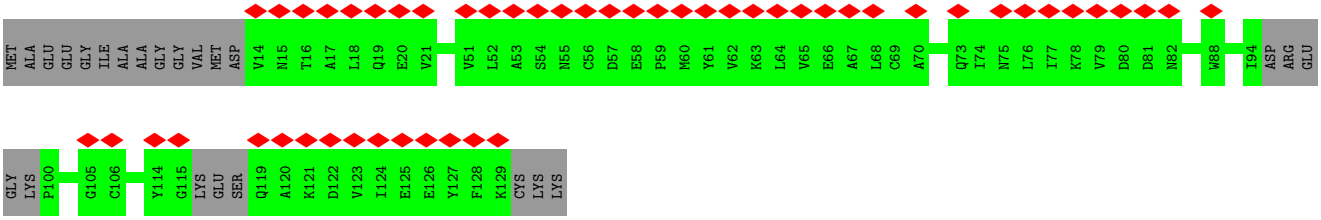
Chain K:





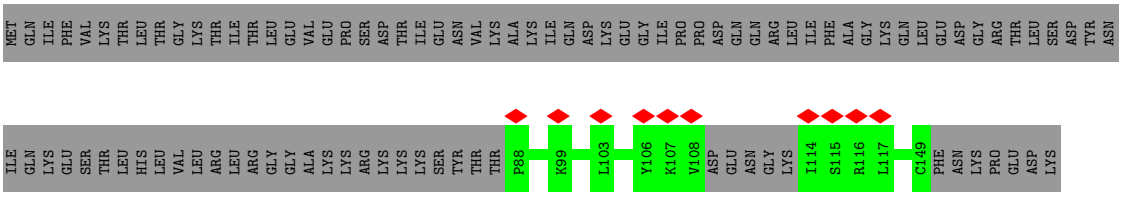
• Molecule 31: 40S ribosomal protein S12

Chain M:



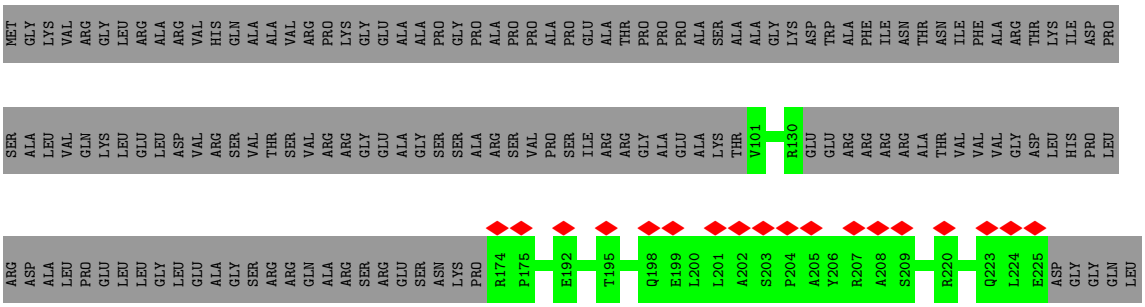
• Molecule 32: Ubiquitin-40S ribosomal protein S27a

Chain f:



• Molecule 33: Ribosome biogenesis protein SLX9 homolog

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104045	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.599	Depositor
Minimum map value	-0.389	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, SAH, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	2	0.56	0/37573	1.03	145/58534 (0.2%)
2	R	0.27	0/680	0.62	0/905
3	b	0.32	0/653	0.56	0/876
4	B	0.29	0/1756	0.63	1/2350 (0.0%)
5	c	0.31	0/473	0.72	0/633
6	E	0.38	0/2118	0.65	1/2849 (0.0%)
7	e	0.33	0/180	0.68	0/232
8	F	0.28	0/1515	0.59	0/2037
9	H	0.29	0/1524	0.65	2/2042 (0.1%)
10	G	0.34	0/1885	0.68	1/2510 (0.0%)
11	Z	0.31	0/580	0.70	0/780
12	Y	0.39	0/1031	0.63	0/1370
13	x	0.32	0/1394	0.66	2/1880 (0.1%)
14	X	0.36	0/1116	0.62	0/1490
15	w	0.28	0/2656	0.60	2/3586 (0.1%)
16	W	0.35	0/1050	0.62	0/1406
17	u	0.33	0/5296	0.59	1/7154 (0.0%)
18	t	0.27	0/531	0.60	0/713
19	T	0.27	0/1142	0.60	1/1530 (0.1%)
20	S	0.30	0/1071	0.64	0/1437
21	Q	0.32	0/1012	0.67	0/1356
22	P	0.29	0/1025	0.62	1/1369 (0.1%)
23	O	0.30	0/1022	0.69	0/1372
24	N	0.31	0/1226	0.61	0/1649
25	L	0.40	0/1250	0.64	0/1673
26	J	0.37	0/1524	0.67	0/2035
27	I	0.39	0/1711	0.67	0/2282
28	r	0.27	0/961	0.63	0/1301
29	q	0.61	0/1910	0.64	0/2572
30	K	0.27	0/8097	0.57	2/10950 (0.0%)
31	M	0.24	0/845	0.53	0/1134
32	f	0.25	0/474	0.61	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	z	0.29	0/686	0.62	0/914
All	All	0.44	0/85967	0.84	159/123547 (0.1%)

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
17	u	0	3
18	t	0	1
21	Q	0	1
27	I	0	1
30	K	0	1
All	All	0	7

There are no bond length outliers.

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1323	U	N3-C2-O2	-14.41	112.11	122.20
1	2	501	C	N1-C2-O2	12.63	126.48	118.90
1	2	501	C	C2-N1-C1'	12.40	132.44	118.80
1	2	293	C	N1-C2-O2	12.24	126.24	118.90
1	2	1773	C	N3-C2-O2	-11.85	113.61	121.90
1	2	356	C	N1-C2-O2	11.47	125.78	118.90
1	2	356	C	C2-N1-C1'	11.11	131.03	118.80
1	2	501	C	N3-C2-O2	-10.96	114.23	121.90
1	2	1774	C	N3-C2-O2	-10.38	114.63	121.90
1	2	293	C	C2-N1-C1'	10.14	129.96	118.80
1	2	427	U	N3-C2-O2	-10.00	115.20	122.20
1	2	356	C	N3-C2-O2	-9.39	115.32	121.90
1	2	1323	U	N1-C2-O2	9.32	129.33	122.80
1	2	293	C	N3-C2-O2	-9.10	115.53	121.90
1	2	1374	C	N3-C2-O2	-9.07	115.55	121.90
1	2	1773	C	N1-C2-O2	9.00	124.30	118.90
1	2	1865	C	N1-C2-O2	8.81	124.19	118.90
1	2	501	C	C6-N1-C1'	-8.78	110.26	120.80
1	2	1022	U	C2-N1-C1'	8.61	128.04	117.70
1	2	853	C	C2-N1-C1'	8.39	128.03	118.80
1	2	853	C	N1-C2-O2	8.21	123.83	118.90
1	2	853	C	N3-C2-O2	-8.15	116.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	356	C	C6-N1-C1'	-8.15	111.02	120.80
1	2	823	U	N3-C2-O2	-8.02	116.59	122.20
1	2	1865	C	N3-C2-O2	-7.89	116.37	121.90
1	2	1276	A	N1-C6-N6	-7.84	113.90	118.60
1	2	1865	C	C2-N1-C1'	7.78	127.36	118.80
1	2	1624	U	C2-N1-C1'	7.76	127.01	117.70
1	2	1590	C	N1-C2-O2	7.74	123.55	118.90
1	2	427	U	N1-C2-O2	7.61	128.12	122.80
1	2	1139	C	C2-N1-C1'	7.59	127.15	118.80
1	2	1139	C	N1-C2-O2	7.58	123.45	118.90
1	2	501	C	C6-N1-C2	-7.58	117.27	120.30
1	2	4	C	C2-N1-C1'	7.55	127.10	118.80
1	2	1139	C	N3-C2-O2	-7.50	116.65	121.90
1	2	293	C	C6-N1-C1'	-7.42	111.90	120.80
9	H	127	ASP	CB-CG-OD1	7.41	124.97	118.30
1	2	1139	C	C6-N1-C2	-7.36	117.36	120.30
1	2	427	U	C2-N1-C1'	7.35	126.52	117.70
1	2	1453	C	C2-N1-C1'	7.30	126.83	118.80
1	2	1453	C	N1-C2-O2	7.28	123.27	118.90
1	2	823	U	N1-C2-O2	7.26	127.88	122.80
1	2	1774	C	N1-C2-O2	7.22	123.23	118.90
1	2	1520	G	C4-N9-C1'	7.09	135.72	126.50
1	2	1772	C	N1-C2-O2	7.01	123.11	118.90
1	2	1016	U	N3-C2-O2	-6.93	117.35	122.20
1	2	856	C	C2-N1-C1'	6.93	126.42	118.80
1	2	1759	G	N1-C2-N2	-6.74	110.13	116.20
1	2	823	U	C2-N1-C1'	6.55	125.56	117.70
1	2	814	U	N3-C2-O2	-6.53	117.63	122.20
1	2	1306	U	C2-N1-C1'	6.42	125.41	117.70
1	2	472	C	C6-N1-C2	-6.40	117.74	120.30
1	2	1016	U	N1-C2-O2	6.39	127.27	122.80
1	2	114	G	P-O3'-C3'	6.38	127.36	119.70
1	2	102	A	P-O3'-C3'	6.36	127.33	119.70
1	2	1022	U	N1-C2-O2	6.33	127.23	122.80
1	2	1759	G	N1-C6-O6	-6.31	116.11	119.90
1	2	1760	G	N1-C2-N2	-6.31	110.52	116.20
1	2	1022	U	C6-N1-C1'	-6.27	112.43	121.20
1	2	356	C	C6-N1-C2	-6.19	117.82	120.30
6	E	139	LEU	CA-CB-CG	6.18	129.52	115.30
1	2	1624	U	N1-C2-O2	6.16	127.11	122.80
1	2	1590	C	N3-C2-O2	-6.15	117.59	121.90
19	T	49	ASP	CB-CG-OD1	6.12	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1078	C	N3-C2-O2	-6.11	117.62	121.90
1	2	1624	U	N3-C2-O2	-6.10	117.93	122.20
1	2	853	C	C6-N1-C2	-6.05	117.88	120.30
1	2	1323	U	N1-C2-N3	6.03	118.52	114.90
1	2	1520	G	C8-N9-C1'	-6.01	119.19	127.00
1	2	1590	C	C2-N1-C1'	5.96	125.36	118.80
1	2	1683	C	N1-C2-O2	5.95	122.47	118.90
1	2	1760	G	N3-C2-N2	5.95	124.06	119.90
1	2	1532	C	N1-C2-O2	5.93	122.46	118.90
1	2	1590	C	C6-N1-C2	-5.92	117.93	120.30
1	2	1759	G	N3-C2-N2	5.92	124.04	119.90
1	2	1532	C	N3-C2-O2	-5.90	117.77	121.90
1	2	1276	A	C5-C6-N6	5.88	128.40	123.70
1	2	314	U	N3-C2-O2	-5.87	118.09	122.20
1	2	119	U	N3-C2-O2	-5.85	118.10	122.20
1	2	178	C	N1-C2-O2	5.84	122.40	118.90
30	K	509	MET	CA-CB-CG	5.82	123.19	113.30
1	2	1234	C	C2-N1-C1'	5.73	125.10	118.80
1	2	1520	G	N3-C4-N9	5.70	129.42	126.00
17	u	773	VAL	C-N-CA	5.68	135.90	121.70
1	2	1453	C	N3-C2-O2	-5.66	117.94	121.90
15	w	276	LEU	CA-CB-CG	5.60	128.18	115.30
1	2	853	C	C6-N1-C1'	-5.60	114.08	120.80
1	2	4	C	C6-N1-C2	-5.59	118.06	120.30
1	2	1693	G	P-O3'-C3'	5.59	126.40	119.70
1	2	1016	U	C2-N1-C1'	5.58	124.40	117.70
1	2	750	C	C5-C6-N1	5.57	123.79	121.00
1	2	1751	C	N1-C2-O2	5.57	122.24	118.90
1	2	749	U	C2-N1-C1'	5.56	124.37	117.70
1	2	1311	C	N1-C2-O2	5.54	122.22	118.90
1	2	1109	C	N1-C2-O2	5.54	122.22	118.90
1	2	1374	C	C6-N1-C2	-5.51	118.09	120.30
1	2	659	G	C4-N9-C1'	5.50	133.65	126.50
1	2	1865	C	C6-N1-C2	-5.50	118.10	120.30
1	2	168	C	N1-C2-O2	5.47	122.18	118.90
1	2	1520	G	N3-C4-C5	-5.45	125.87	128.60
1	2	1774	C	C6-N1-C2	-5.45	118.12	120.30
1	2	465	A	P-O3'-C3'	5.44	126.23	119.70
1	2	293	C	C6-N1-C2	-5.43	118.13	120.30
1	2	474	G	C4-N9-C1'	5.43	133.56	126.50
1	2	144	U	C5-C6-N1	5.42	125.41	122.70
1	2	1123	C	C6-N1-C2	-5.42	118.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	666	U	C2-N1-C1'	5.42	124.20	117.70
9	H	36	LEU	CA-CB-CG	5.42	127.76	115.30
1	2	636	C	P-O3'-C3'	5.41	126.19	119.70
1	2	1591	C	N1-C2-O2	5.40	122.14	118.90
22	P	82	ASP	CB-CG-OD1	5.40	123.16	118.30
1	2	1273	C	O4'-C1'-N1	5.39	112.51	108.20
1	2	508	A	N1-C6-N6	-5.38	115.37	118.60
1	2	441	C	C2-N1-C1'	5.38	124.72	118.80
1	2	1311	C	C2-N1-C1'	5.37	124.70	118.80
1	2	4	C	N1-C2-O2	5.36	122.12	118.90
1	2	1751	C	N3-C2-O2	-5.36	118.15	121.90
1	2	4	C	C5-C6-N1	5.36	123.68	121.00
1	2	1759	G	C5-C6-O6	5.34	131.80	128.60
1	2	1485	U	N1-C2-O2	5.33	126.53	122.80
1	2	814	U	N1-C2-O2	5.32	126.53	122.80
1	2	1534	C	P-O3'-C3'	5.32	126.08	119.70
1	2	1683	C	C6-N1-C2	-5.28	118.19	120.30
1	2	407	G	C4-N9-C1'	5.26	133.34	126.50
1	2	118	C	N1-C2-O2	5.26	122.06	118.90
30	K	884	MET	CA-CB-CG	5.26	122.24	113.30
1	2	1304	U	P-O3'-C3'	5.26	126.01	119.70
1	2	1123	C	N1-C2-O2	5.25	122.05	118.90
1	2	168	C	N3-C2-O2	-5.23	118.24	121.90
1	2	1865	C	C6-N1-C1'	-5.23	114.53	120.80
1	2	570	C	N3-C2-O2	-5.21	118.25	121.90
1	2	466	G	N3-C4-N9	5.20	129.12	126.00
1	2	856	C	C6-N1-C2	-5.19	118.22	120.30
13	x	230	LEU	CA-CB-CG	5.18	127.22	115.30
1	2	1366	G	N1-C6-O6	-5.18	116.80	119.90
1	2	1683	C	N3-C2-O2	-5.18	118.28	121.90
1	2	143	U	P-O3'-C3'	5.17	125.91	119.70
1	2	470	G	O4'-C1'-N9	5.17	112.34	108.20
13	x	152	LEU	CA-CB-CG	5.16	127.17	115.30
1	2	877	C	C2-N1-C1'	5.16	124.47	118.80
15	w	326	MET	CA-CB-CG	5.13	122.02	113.30
1	2	1314	U	C2-N1-C1'	5.12	123.85	117.70
1	2	216	C	N1-C2-O2	5.12	121.97	118.90
10	G	106	LEU	CA-CB-CG	5.12	127.06	115.30
1	2	824	C	N1-C2-O2	5.10	121.96	118.90
4	B	135	LEU	CA-CB-CG	5.08	126.97	115.30
1	2	1698	C	N1-C2-O2	5.07	121.94	118.90
1	2	1165	G	O4'-C1'-N9	5.07	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1501	C	N1-C2-O2	5.05	121.93	118.90
1	2	130	G	N3-C4-C5	-5.04	126.08	128.60
1	2	659	G	C8-N9-C1'	-5.04	120.44	127.00
1	2	216	C	N3-C2-O2	-5.04	118.37	121.90
1	2	1218	C	C6-N1-C2	-5.03	118.29	120.30
1	2	1590	C	C5-C6-N1	5.03	123.52	121.00
1	2	750	C	N1-C2-O2	5.02	121.91	118.90
1	2	1453	C	C6-N1-C1'	-5.02	114.77	120.80
1	2	4	C	C6-N1-C1'	-5.02	114.78	120.80
1	2	1374	C	N1-C2-O2	5.01	121.91	118.90
1	2	119	U	N1-C2-O2	5.01	126.31	122.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	I	66	SER	Peptide
30	K	378	VAL	Peptide
21	Q	42	ILE	Peptide
18	t	255	GLN	Peptide
17	u	345	MET	Peptide
17	u	348	ASP	Peptide
17	u	680	ALA	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	R	79/135 (58%)	77 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	b	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
4	B	211/264 (80%)	202 (96%)	9 (4%)	0	100	100
5	c	59/69 (86%)	56 (95%)	3 (5%)	0	100	100
6	E	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
7	e	18/59 (30%)	18 (100%)	0	0	100	100
8	F	187/204 (92%)	178 (95%)	8 (4%)	1 (0%)	29	68
9	H	184/194 (95%)	174 (95%)	10 (5%)	0	100	100
10	G	228/249 (92%)	222 (97%)	6 (3%)	0	100	100
11	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
12	Y	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
13	x	173/252 (69%)	165 (95%)	8 (5%)	0	100	100
14	X	139/143 (97%)	138 (99%)	1 (1%)	0	100	100
15	w	321/437 (74%)	310 (97%)	11 (3%)	0	100	100
16	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
17	u	630/804 (78%)	601 (95%)	29 (5%)	0	100	100
18	t	53/475 (11%)	43 (81%)	10 (19%)	0	100	100
19	T	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
20	S	125/152 (82%)	117 (94%)	8 (6%)	0	100	100
21	Q	123/146 (84%)	118 (96%)	5 (4%)	0	100	100
22	P	117/145 (81%)	113 (97%)	4 (3%)	0	100	100
23	O	133/151 (88%)	124 (93%)	9 (7%)	0	100	100
24	N	147/151 (97%)	147 (100%)	0	0	100	100
25	L	149/158 (94%)	142 (95%)	7 (5%)	0	100	100
26	J	178/194 (92%)	170 (96%)	8 (4%)	0	100	100
27	I	203/208 (98%)	196 (97%)	7 (3%)	0	100	100
28	r	116/125 (93%)	106 (91%)	10 (9%)	0	100	100
29	q	231/281 (82%)	214 (93%)	17 (7%)	0	100	100
30	K	1000/1297 (77%)	955 (96%)	45 (4%)	0	100	100
31	M	102/132 (77%)	101 (99%)	1 (1%)	0	100	100
32	f	53/156 (34%)	47 (89%)	6 (11%)	0	100	100
33	z	78/230 (34%)	75 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5838/7691 (76%)	5584 (96%)	253 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	163	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	R	72/122 (59%)	71 (99%)	1 (1%)	67 88
3	b	74/76 (97%)	74 (100%)	0	100 100
4	B	194/231 (84%)	194 (100%)	0	100 100
5	c	52/62 (84%)	52 (100%)	0	100 100
6	E	224/225 (100%)	224 (100%)	0	100 100
7	e	18/48 (38%)	18 (100%)	0	100 100
8	F	159/170 (94%)	159 (100%)	0	100 100
9	H	167/174 (96%)	166 (99%)	1 (1%)	86 95
10	G	200/218 (92%)	199 (100%)	1 (0%)	88 96
11	Z	64/103 (62%)	64 (100%)	0	100 100
12	Y	108/115 (94%)	108 (100%)	0	100 100
13	x	148/208 (71%)	147 (99%)	1 (1%)	84 94
14	X	113/115 (98%)	113 (100%)	0	100 100
15	w	262/370 (71%)	260 (99%)	2 (1%)	81 93
16	W	112/113 (99%)	112 (100%)	0	100 100
17	u	561/705 (80%)	558 (100%)	3 (0%)	88 96
18	t	59/434 (14%)	59 (100%)	0	100 100
19	T	114/115 (99%)	114 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	S	111/132 (84%)	111 (100%)	0	100 100
21	Q	106/121 (88%)	104 (98%)	2 (2%)	57 84
22	P	111/130 (85%)	111 (100%)	0	100 100
23	O	105/119 (88%)	105 (100%)	0	100 100
24	N	130/131 (99%)	129 (99%)	1 (1%)	81 93
25	L	135/142 (95%)	133 (98%)	2 (2%)	65 87
26	J	160/168 (95%)	160 (100%)	0	100 100
27	I	178/180 (99%)	178 (100%)	0	100 100
28	r	105/112 (94%)	103 (98%)	2 (2%)	57 84
29	q	198/240 (82%)	158 (80%)	40 (20%)	1 6
30	K	871/1094 (80%)	866 (99%)	5 (1%)	86 95
31	M	91/108 (84%)	91 (100%)	0	100 100
32	f	51/140 (36%)	51 (100%)	0	100 100
33	z	72/185 (39%)	72 (100%)	0	100 100
All	All	5125/6606 (78%)	5064 (99%)	61 (1%)	72 90

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	11	LYS
9	H	114	GLN
10	G	221	LYS
13	x	77	LYS
15	w	83	ARG
15	w	88	ARG
17	u	93	ARG
17	u	351	ARG
17	u	499	ARG
21	Q	117	ARG
21	Q	126	ARG
24	N	104	ARG
25	L	30	LYS
25	L	69	ARG
28	r	19	ARG
28	r	24	ARG
29	q	15	GLU
29	q	24	ARG

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Mol	Chain	Res	Type
29	q	25	LYS
29	q	28	ARG
29	q	32	MET
29	q	36	GLN
29	q	38	ARG
29	q	47	LEU
29	q	48	TYR
29	q	49	LEU
29	q	55	CYS
29	q	57	LEU
29	q	59	ASP
29	q	60	ILE
29	q	66	LEU
29	q	69	SER
29	q	73	ASP
29	q	81	LEU
29	q	82	ASP
29	q	83	ILE
29	q	87	MET
29	q	92	VAL
29	q	96	ILE
29	q	102	LEU
29	q	107	GLN
29	q	119	CYS
29	q	129	CYS
29	q	130	ASN
29	q	140	LYS
29	q	141	ARG
29	q	151	SER
29	q	153	LEU
29	q	155	ARG
29	q	163	LEU
29	q	166	GLU
29	q	172	GLU
29	q	176	THR
29	q	183	PHE
29	q	198	LYS
29	q	202	LEU
30	K	186	LYS
30	K	192	LYS
30	K	294	LYS
30	K	771	LYS

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Mol	Chain	Res	Type
30	K	845	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
9	H	25	GLN
9	H	114	GLN
10	G	197	GLN
15	w	251	ASN
17	u	762	GLN
29	q	36	GLN
29	q	132	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1557/1873 (83%)	350 (22%)	26 (1%)

All (350) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	26	U
1	2	33	G
1	2	41	G
1	2	46	A
1	2	54	A
1	2	55	U
1	2	56	G
1	2	62	G
1	2	64	A
1	2	65	C
1	2	67	C
1	2	68	A
1	2	69	C
1	2	70	G
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G

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Mol	Chain	Res	Type
1	2	76	U
1	2	77	A
1	2	79	A
1	2	92	A
1	2	100	U
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	116	U
1	2	126	G
1	2	128	U
1	2	130	G
1	2	143	U
1	2	144	U
1	2	155	G
1	2	160	U
1	2	163	U
1	2	168	C
1	2	172	U
1	2	175	A
1	2	181	A
1	2	184	G
1	2	291	G
1	2	292	A
1	2	295	C
1	2	302	A
1	2	309	G
1	2	310	C
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C
1	2	333	G
1	2	335	G
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	368	U
1	2	369	C
1	2	370	G

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Mol	Chain	Res	Type
1	2	377	G
1	2	383	G
1	2	385	G
1	2	386	C
1	2	399	C
1	2	400	C
1	2	407	G
1	2	409	C
1	2	413	G
1	2	418	A
1	2	429	C
1	2	436	G
1	2	438	G
1	2	441	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	487	U
1	2	492	C
1	2	493	A
1	2	496	C
1	2	516	A
1	2	525	A
1	2	544	G
1	2	546	G
1	2	547	G
1	2	548	C
1	2	554	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	563	G
1	2	564	A
1	2	570	C

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Mol	Chain	Res	Type
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	595	U
1	2	600	G
1	2	601	G
1	2	603	C
1	2	604	A
1	2	605	A
1	2	607	U
1	2	608	C
1	2	631	U
1	2	637	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	658	U
1	2	660	C
1	2	664	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	678	U
1	2	683	G
1	2	684	G
1	2	687	C
1	2	688	U
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	794	A
1	2	797	C
1	2	798	G
1	2	799	U

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Mol	Chain	Res	Type
1	2	800	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	844	U
1	2	847	A
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	880	G
1	2	881	G
1	2	886	A
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	896	U
1	2	898	U
1	2	903	A
1	2	908	A
1	2	913	A
1	2	914	U
1	2	920	A
1	2	927	C
1	2	930	C
1	2	933	G
1	2	959	G
1	2	963	A
1	2	970	G
1	2	971	G
1	2	981	A
1	2	990	A
1	2	992	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1039	C

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Mol	Chain	Res	Type
1	2	1041	G
1	2	1044	G
1	2	1045	U
1	2	1049	A
1	2	1083	A
1	2	1085	C
1	2	1089	G
1	2	1096	G
1	2	1099	G
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1120	U
1	2	1121	G
1	2	1123	C
1	2	1130	G
1	2	1138	C
1	2	1140	G
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1165	G
1	2	1170	A
1	2	1171	G
1	2	1172	U
1	2	1195	A
1	2	1200	A
1	2	1202	U
1	2	1206	G
1	2	1211	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1238	U
1	2	1242	U
1	2	1243	U
1	2	1265	A

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Mol	Chain	Res	Type
1	2	1272	C
1	2	1273	C
1	2	1274	G
1	2	1275	G
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1296	U
1	2	1299	A
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1305	C
1	2	1307	U
1	2	1308	U
1	2	1309	C
1	2	1312	G
1	2	1313	A
1	2	1315	U
1	2	1317	C
1	2	1322	G
1	2	1323	U
1	2	1325	G
1	2	1327	G
1	2	1335	G
1	2	1364	U
1	2	1371	U
1	2	1372	U
1	2	1376	A
1	2	1383	A
1	2	1387	G
1	2	1388	A
1	2	1389	C
1	2	1396	A
1	2	1397	U
1	2	1398	G
1	2	1445	U
1	2	1446	A
1	2	1447	G
1	2	1454	A
1	2	1462	U

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Mol	Chain	Res	Type
1	2	1463	U
1	2	1465	A
1	2	1476	A
1	2	1477	U
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1491	G
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1503	C
1	2	1512	C
1	2	1519	U
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1551	U
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1570	G
1	2	1571	G
1	2	1580	A
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1588	A
1	2	1601	A
1	2	1606	G
1	2	1617	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1637	A
1	2	1639	G7M
1	2	1640	A
1	2	1641	A
1	2	1647	A
1	2	1648	G
1	2	1654	G
1	2	1660	C

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Mol	Chain	Res	Type
1	2	1661	A
1	2	1662	U
1	2	1663	A
1	2	1664	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1686	G
1	2	1689	C
1	2	1694	U
1	2	1704	C
1	2	1705	C
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1727	G
1	2	1728	U
1	2	1729	U
1	2	1744	G
1	2	1756	C
1	2	1761	U
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1800	A
1	2	1801	A
1	2	1805	G
1	2	1806	A
1	2	1826	G
1	2	1829	G
1	2	1836	G
1	2	1839	U
1	2	1841	C
1	2	1861	G
1	2	1863	A
1	2	1864	U
1	2	1872	G

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	102	A

Continued on next page...

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Mol	Chain	Res	Type
1	2	114	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	417	C
1	2	440	G
1	2	465	A
1	2	604	A
1	2	636	C
1	2	750	C
1	2	958	G
1	2	980	A
1	2	1231	C
1	2	1264	C
1	2	1295	A
1	2	1304	U
1	2	1386	A
1	2	1497	G
1	2	1511	U
1	2	1534	C
1	2	1565	C
1	2	1693	G
1	2	1726	G

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

1 non-standard protein/DNA/RNA residue is 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	G7M	2	1639	1	20,26,27	5.84	13 (65%)	17,39,42	1.54	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	2	1639	1	-	0/3/25/26	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	G7M	C2'-C1'	-17.01	1.27	1.53
1	2	1639	G7M	C3'-C4'	-9.98	1.27	1.53
1	2	1639	G7M	O4'-C1'	9.11	1.53	1.41
1	2	1639	G7M	C2-N2	6.46	1.49	1.34
1	2	1639	G7M	C2-N3	5.66	1.47	1.33
1	2	1639	G7M	C2'-C3'	5.31	1.67	1.53
1	2	1639	G7M	O4'-C4'	5.14	1.56	1.45
1	2	1639	G7M	C4-N3	5.02	1.49	1.37
1	2	1639	G7M	C6-N1	4.27	1.44	1.37
1	2	1639	G7M	C5-C6	3.60	1.54	1.45
1	2	1639	G7M	C2-N1	2.93	1.44	1.37
1	2	1639	G7M	O3'-C3'	2.33	1.48	1.43
1	2	1639	G7M	O6-C6	-2.21	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1639	G7M	O4'-C1'-C2'	-2.88	102.71	106.93
1	2	1639	G7M	C2-N1-C6	-2.88	119.80	125.10
1	2	1639	G7M	C3'-C2'-C1'	2.65	104.97	100.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	SAH	q	301	-	24,28,28	0.68	0	25,40,40	0.89	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SAH	q	301	-	-	6/11/31/31	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	q	301	SAH	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

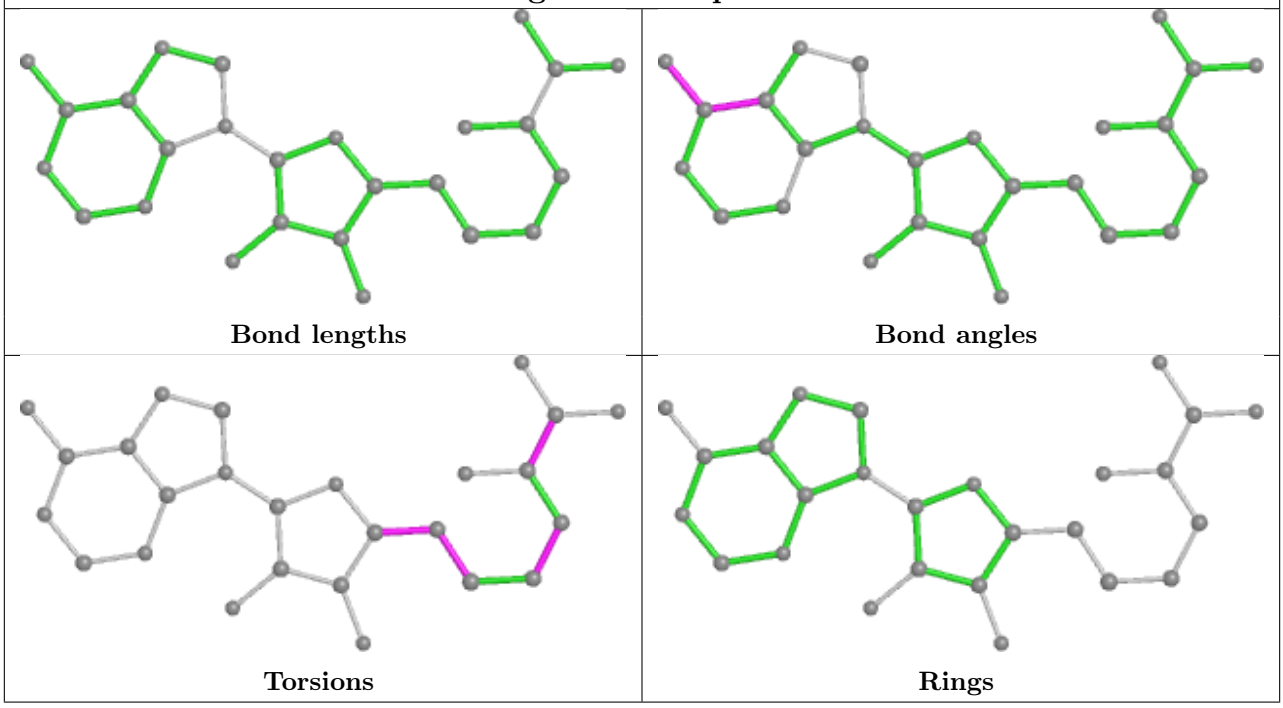
Mol	Chain	Res	Type	Atoms
34	q	301	SAH	CA-CB-CG-SD
34	q	301	SAH	O4'-C4'-C5'-SD
34	q	301	SAH	C3'-C4'-C5'-SD
34	q	301	SAH	OXT-C-CA-N
34	q	301	SAH	O-C-CA-N
34	q	301	SAH	C4'-C5'-SD-CG

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SAH q 301



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.

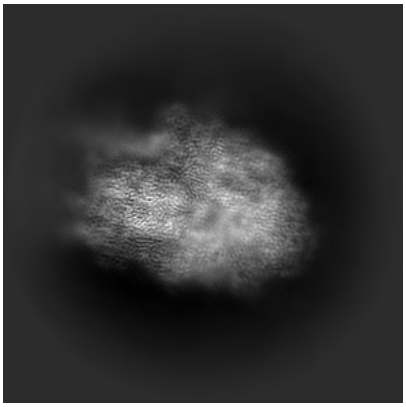
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32801. These allow visual inspection of the internal detail of the map and identification of artifacts.

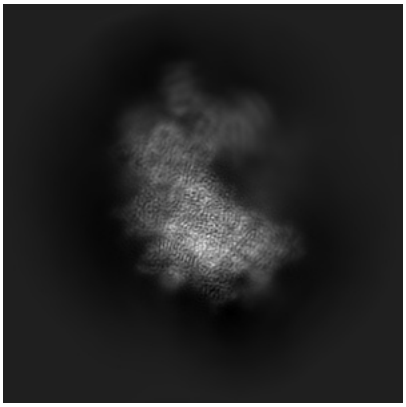
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

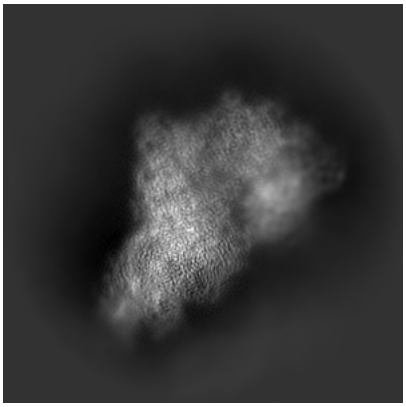
6.1.1 Primary map



X



Y

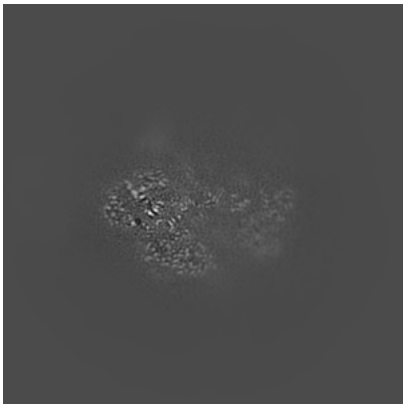


Z

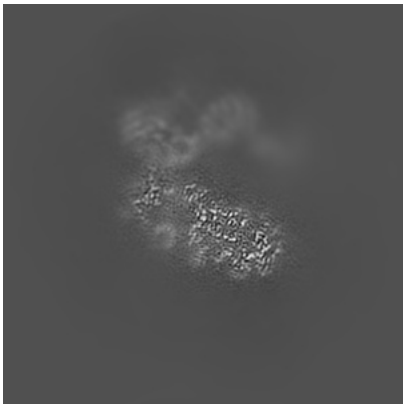
The images above show the map projected in three orthogonal directions.

6.2 Central slices

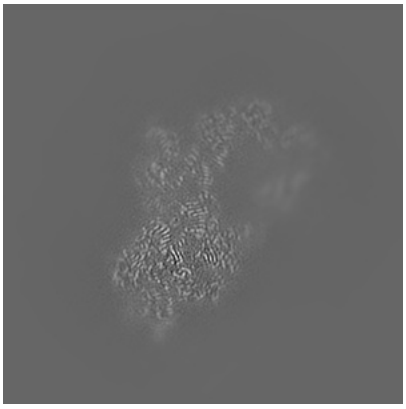
6.2.1 Primary map



X Index: 180



Y Index: 180



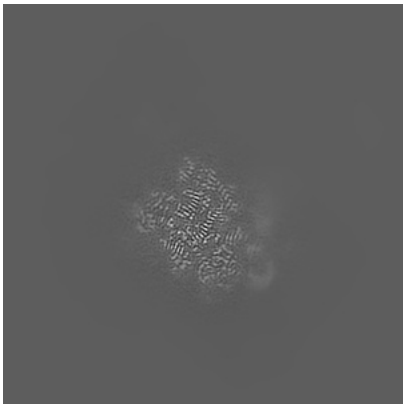
Z Index: 180

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

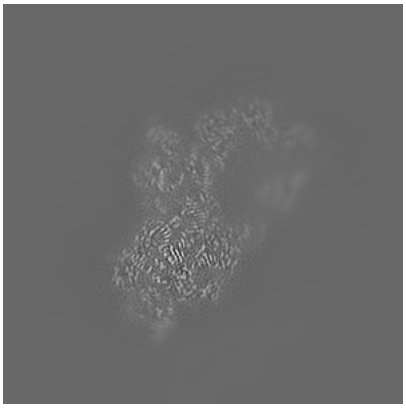
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 159



Y Index: 134

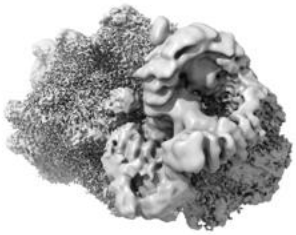


Z Index: 181

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

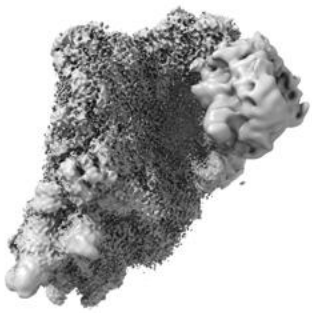
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

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

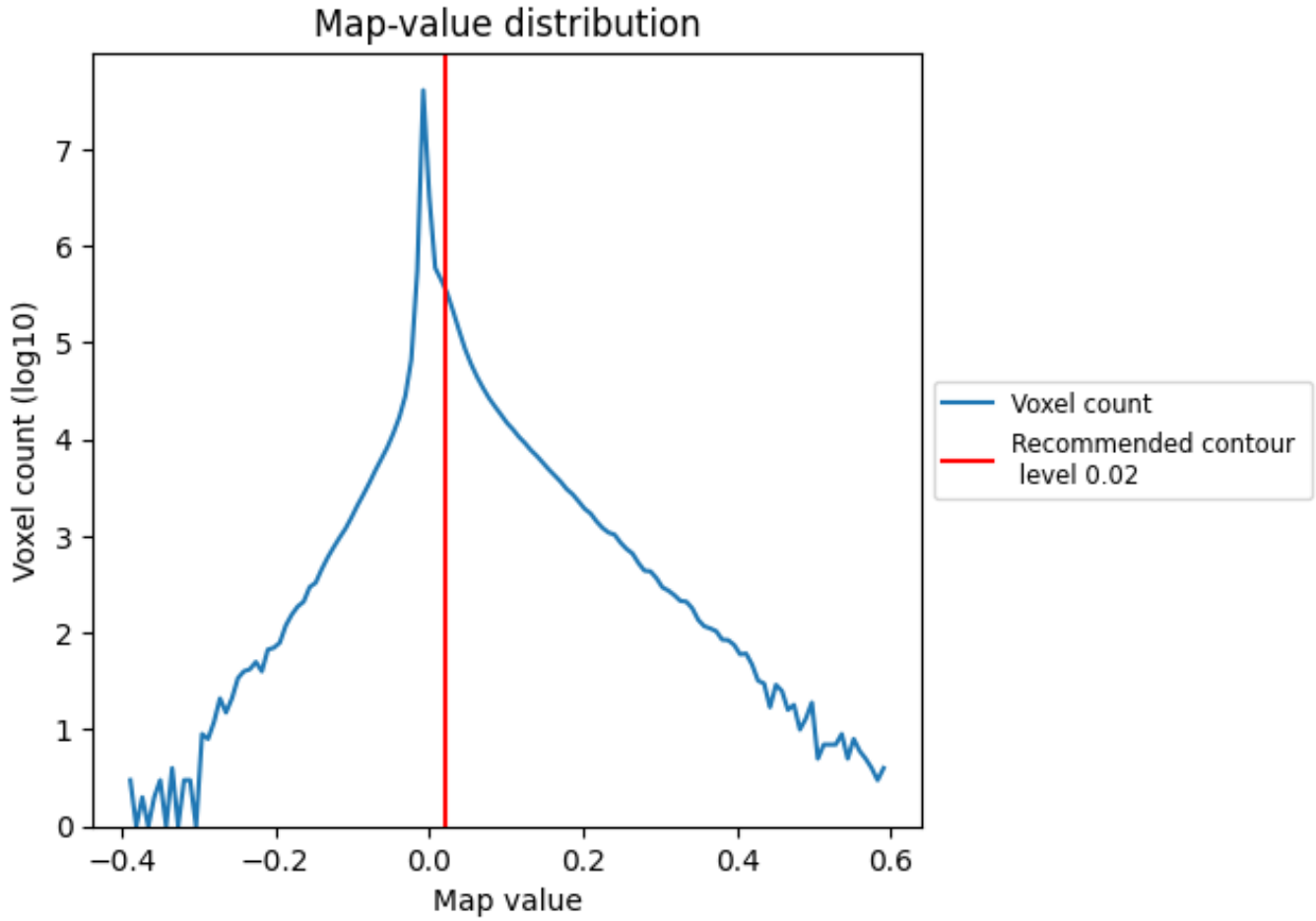
6.5 Mask visualisation (i)

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

7 Map analysis

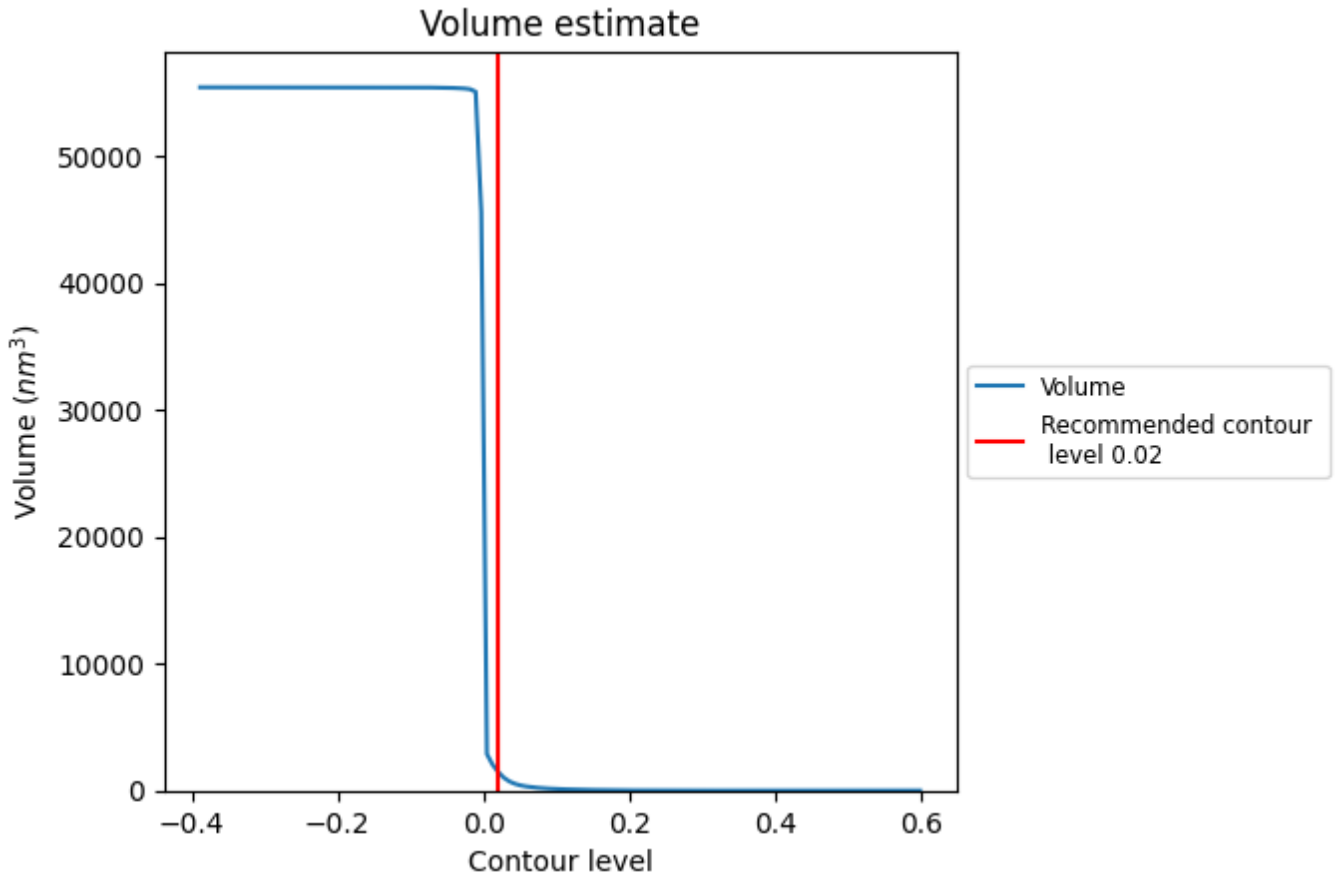
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

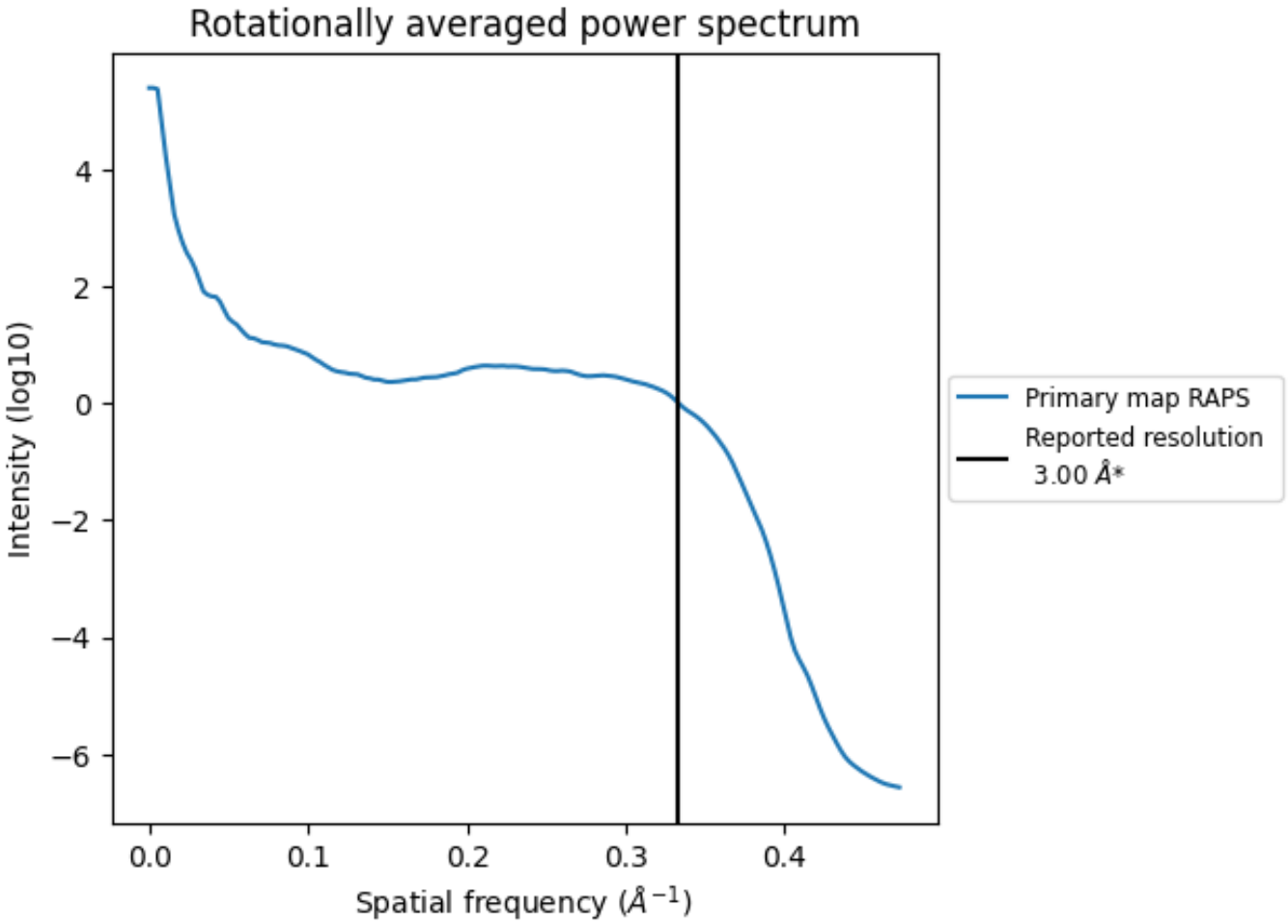
7.2 Volume estimate



The volume at the recommended contour level is 1484 nm^3; this corresponds to an approximate mass of 1340 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)

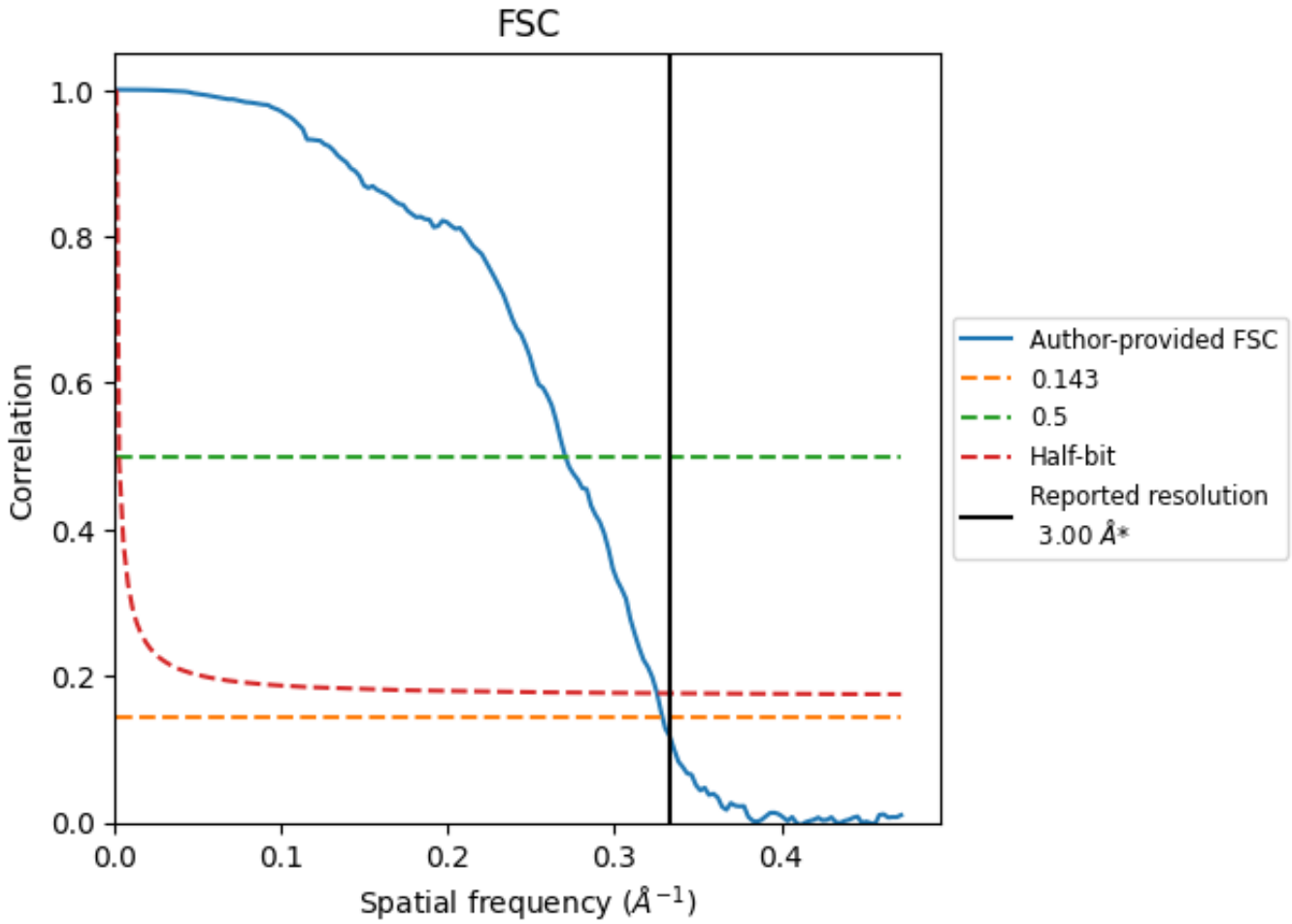


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

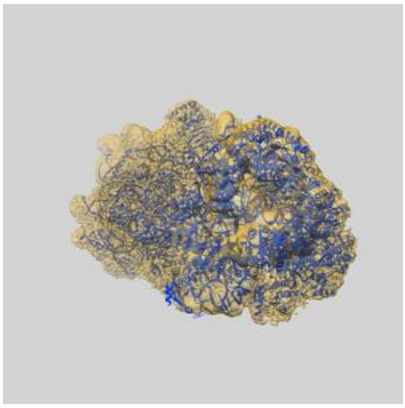
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.70	3.07
Unmasked-calculated*	-	-	-

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

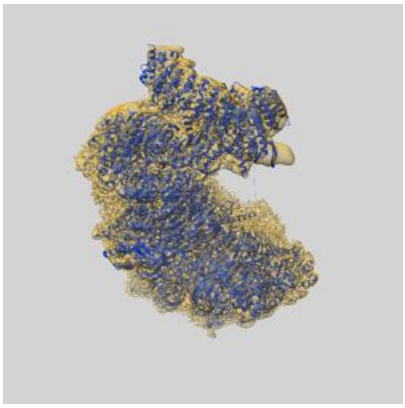
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32801 and PDB model 7WTU. Per-residue inclusion information can be found in section 3 on page 10.

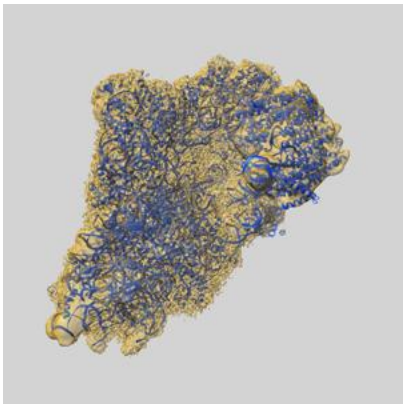
9.1 Map-model overlay



X



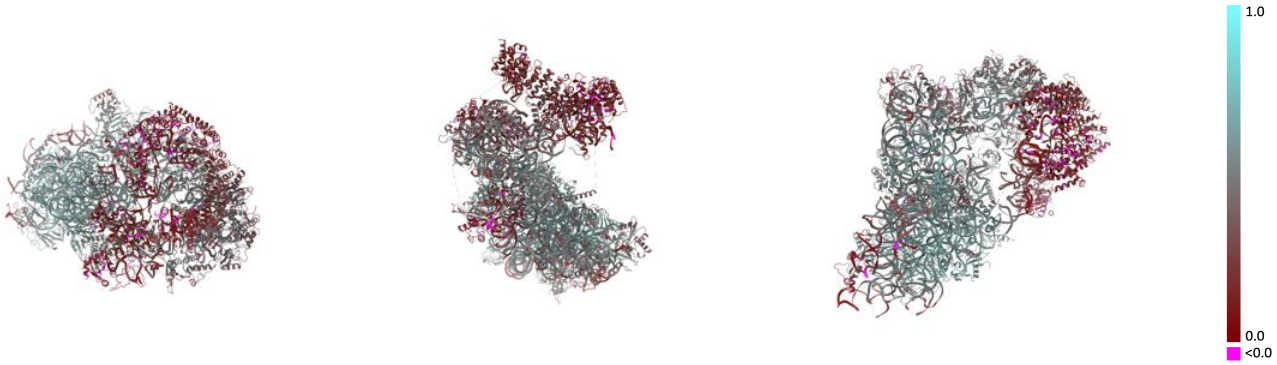
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

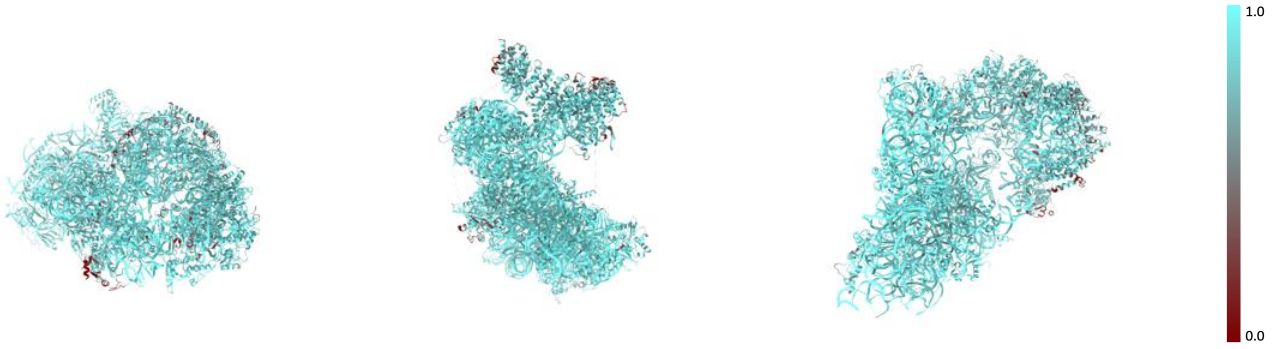
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

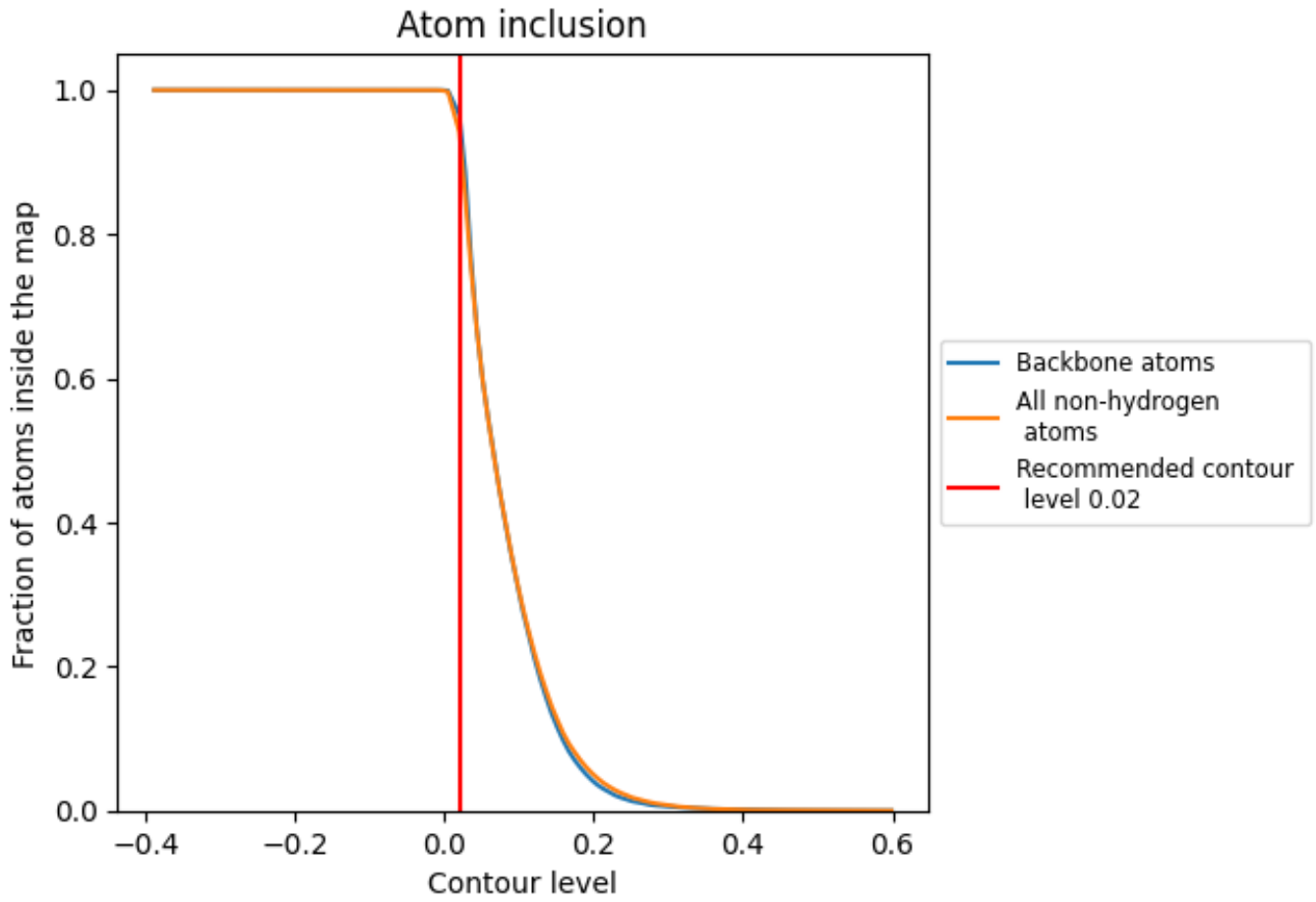
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 97% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9420	0.4300
2	0.9864	0.4770
B	0.9205	0.4390
E	0.9877	0.6060
F	0.9456	0.4630
G	0.9661	0.4940
H	0.9402	0.4160
I	0.9415	0.4920
J	0.9847	0.5730
K	0.8279	0.1910
L	0.9581	0.5510
M	0.4630	0.1300
N	0.9803	0.5140
O	0.9276	0.4410
P	0.9570	0.4360
Q	0.9278	0.4310
R	0.9164	0.1710
S	0.9225	0.4180
T	0.9203	0.4490
W	0.9941	0.5630
X	0.9813	0.5220
Y	0.9929	0.5910
Z	0.8717	0.3640
b	0.9650	0.5120
c	0.9249	0.4370
e	0.9881	0.5320
f	0.7522	0.1230
q	0.9044	0.3080
r	0.6380	0.1420
t	0.8611	0.2990
u	0.9818	0.5260
w	0.9115	0.2270
x	0.9754	0.4880
z	0.6834	0.2150