



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 11:07 PM UTC

PDB ID : 9IGU / pdb\_00009igu  
EMDB ID : EMD-52858  
Title : Assembly intermediate of human mitochondrial ribosome small subunit bound to METTL15 and RBFA (Inward conformation) (State M2)  
Authors : Khawaja, A.; Singh, V.; Shiriaev, D.I.; Rorbach, J.  
Deposited on : 2025-02-20  
Resolution : 3.64 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](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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

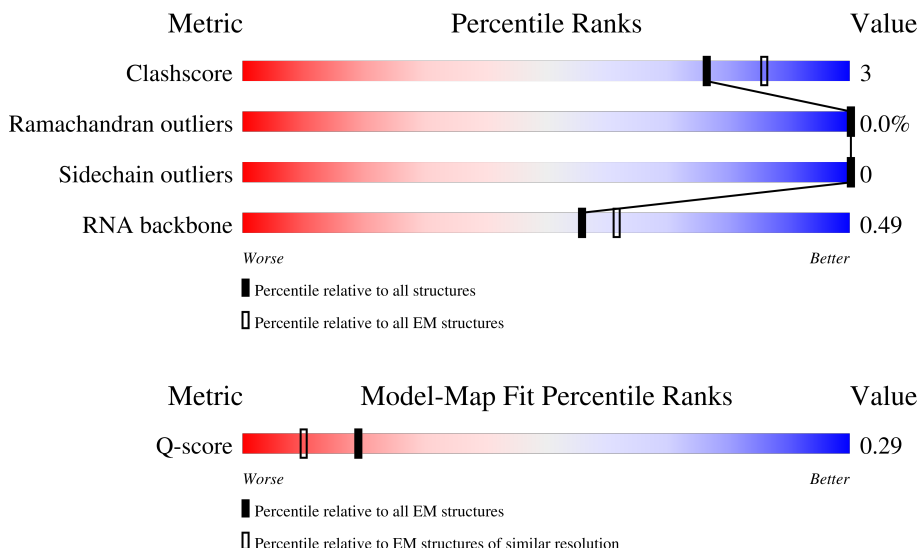
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.








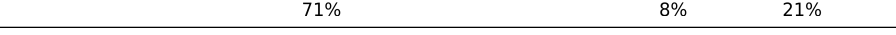

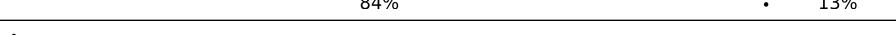
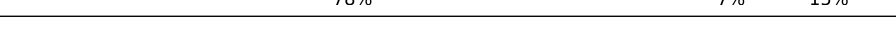
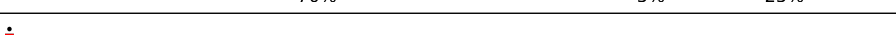
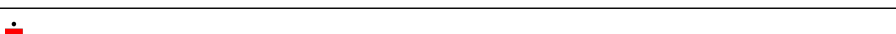

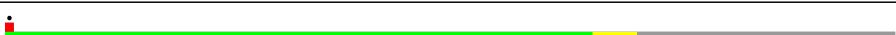







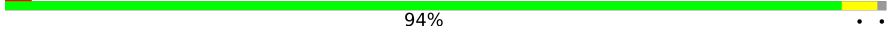




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11633 ( 3.14 - 4.14 )

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	B	296	
2	C	167	
3	D	430	

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Mol	Chain	Length	Quality of chain
4	E	125	
5	F	242	
6	G	396	
7	I	194	
8	J	138	
9	K	128	
10	L	257	
11	M	137	
12	N	130	
13	O	258	
14	P	142	
15	Q	87	
16	R	360	
17	S	190	
18	T	173	
19	U	205	
20	V	414	
21	W	187	
22	X	398	
23	Y	395	
24	Z	106	
25	0	218	
26	1	323	
27	3	199	
28	4	689	

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Mol	Chain	Length	Quality of chain
29	b	407	<div><div>5%</div><div>62%</div><div>11%</div><div>27%</div></div>
30	A	954	<div><div>67%</div><div>25%</div><div>8%</div></div>
31	H	201	<div><div>7%</div><div>65%</div><div>31%</div></div>
32	a	302	<div><div>43%</div><div>9%</div><div>48%</div></div>

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 128481 atoms, of which 59520 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	225	Total	C	H	N	O	S	0	0
			3644	1164	1816	331	323	10		

- Molecule 2 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	132	Total	C	H	N	O	S	0	0
			2171	699	1088	195	185	4		

- Molecule 3 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	321	Total	C	H	N	O	S	0	0
			5179	1614	2609	482	461	13		

- Molecule 4 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	115	Total	C	H	N	O	S	0	0
			1839	574	929	165	167	4		

- Molecule 5 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	205	Total	C	H	N	O	S	0	0
			3421	1076	1736	304	294	11		

- Molecule 6 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	313	Total	C	H	N	O	S	0	0
			5136	1637	2560	456	469	14		

- Molecule 7 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	137	Total	C	H	N	O	S	0	0
			2080	642	1060	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 8 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	108	Total	C	H	N	O	S	0	0
			1726	521	887	169	143	6		

- Molecule 9 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	101	Total	C	H	N	O	S	0	0
			1747	537	885	179	141	5		

- Molecule 10 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	174	Total	C	H	N	O	S	0	0
			2993	925	1540	270	251	7		

- Molecule 11 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	119	Total	C	H	N	O	S	0	0
			1908	594	966	185	157	6		

- Molecule 12 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	110	Total	C	H	N	O	S	0	0
			1796	562	928	156	147	3		

- Molecule 13 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	194	Total	C	H	N	O	S	0	0
			3164	1019	1565	295	278	7		

- Molecule 14 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	97	Total	C	H	N	O	S	0	0
			1589	501	808	134	138	8		

- Molecule 15 is a protein called MRPS21 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	87	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP A0A2J8VEN6

- Molecule 16 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	295	Total	C	H	N	O	S	0	0
			4837	1533	2428	413	455	8		

- Molecule 17 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	135	Total	C	H	N	O	S	0	0
			2226	716	1115	198	196	1		

- Molecule 18 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

- Molecule 19 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	176	Total	C	H	N	O	S	0	0
			2987	916	1499	301	267	4		

- Molecule 20 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	362	Total	C	H	N	O	S	0	0
			5929	1904	2960	495	558	12		

- Molecule 21 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	W	100	Total	C	H	N	O	S	0	0
			1591	498	802	141	146	4		

- Molecule 22 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	X	352	Total	C	H	N	O	S	0	0
			5693	1822	2844	499	517	11		

- Molecule 23 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	121	Total	C	H	N	O	S	0	0
			1993	662	970	168	191	2		

- Molecule 24 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	88	Total	C	H	N	O	S	0	0
			1495	476	750	133	132	4		

- Molecule 25 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	0	215	Total	C	H	N	O	S	0	0
			3583	1130	1796	339	313	5		

- Molecule 26 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	276	Total	C	H	N	O	S	0	0
			4507	1419	2269	381	427	11		

- Molecule 27 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	3	70	Total	C	H	N	O	S	0	0
			1324	401	699	134	89	1		

- Molecule 28 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	4	588	Total	C	H	N	O	S	0	0
			9534	3053	4766	808	879	28		

- Molecule 29 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	b	296	Total	C	H	N	O	S	0	0
			4680	1464	2367	410	426	13		

- Molecule 30 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	A	949	Total	C	H	N	O	P	0	0
			30398	9042	10240	3633	6534	949		

- Molecule 31 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	H	139	Total	C	H	N	O	S	0	0
			2317	739	1173	193	209	3		

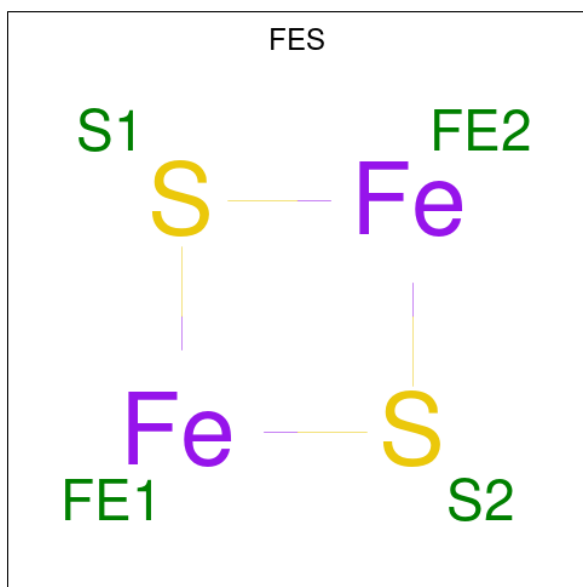
- Molecule 32 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	a	158	Total	C	H	N	O	S	0	0
			2515	783	1263	221	241	7		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	G	1	Total	Mg	0
			1	1	
33	A	30	Total	Mg	0
			30	30	

- Molecule 34 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).

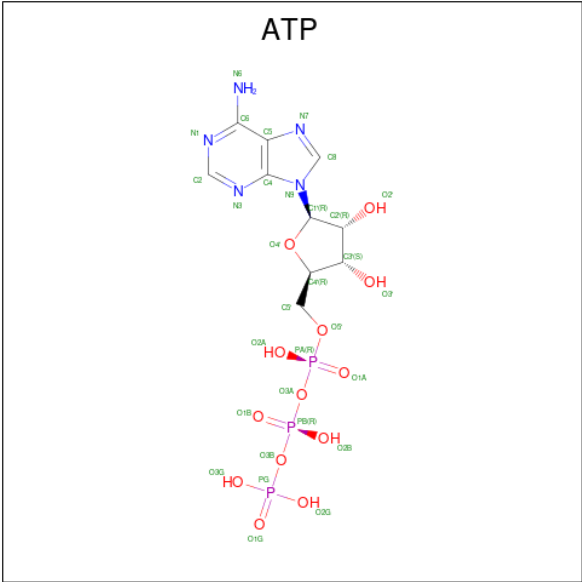


Mol	Chain	Residues	Atoms			AltConf
34	M	1	Total	Fe	S	0
			4	2	2	
34	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

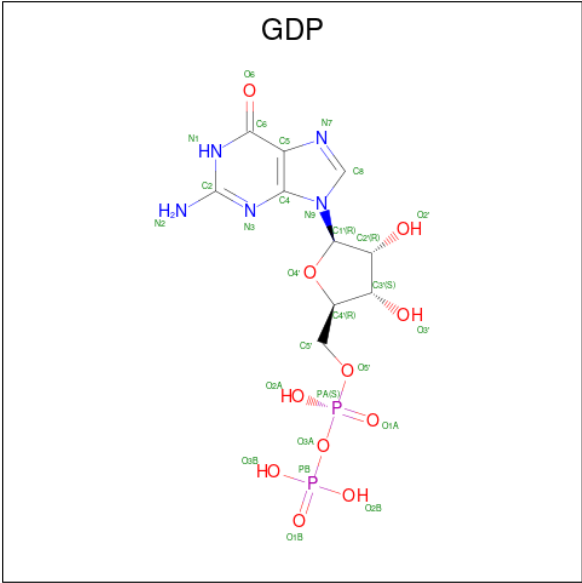
Mol	Chain	Residues	Atoms		AltConf
35	O	1	Total	Zn	0
			1	1	

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



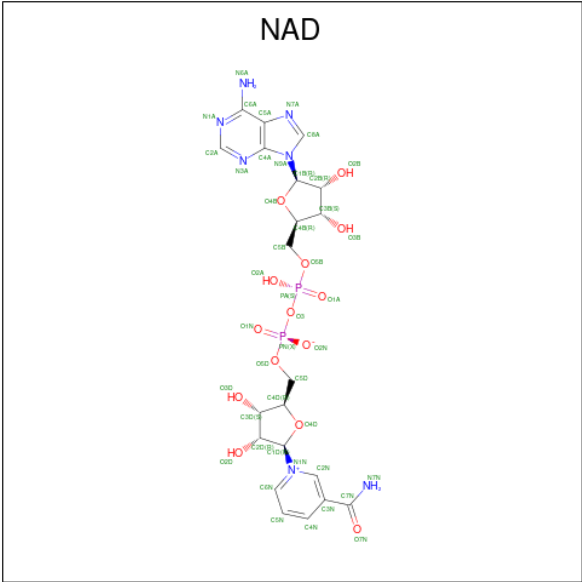
Mol	Chain	Residues	Atoms						AltConf
36	X	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 37 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



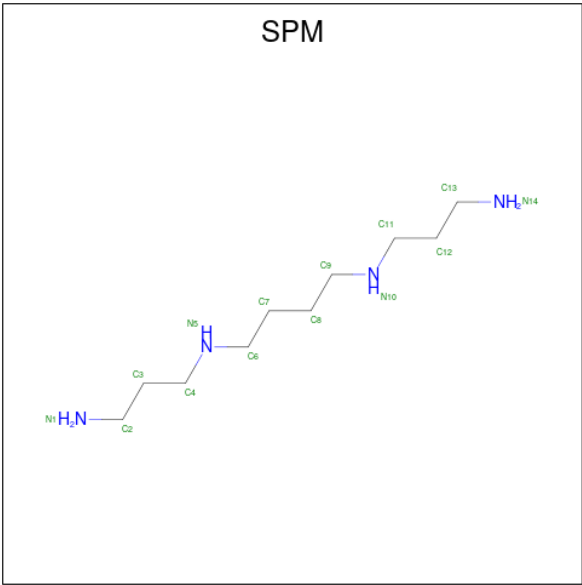
Mol	Chain	Residues	Atoms						AltConf
37	X	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

- Molecule 38 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						AltConf
38	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 39 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			AltConf
39	A	1	Total	C	N	0
			14	10	4	

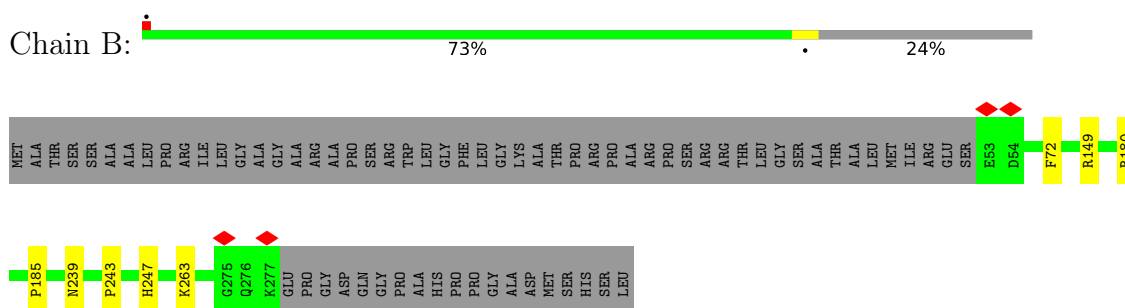
- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	G	1	Total 1	O 1	0
40	K	1	Total 1	O 1	0
40	T	1	Total 1	O 1	0
40	0	1	Total 1	O 1	0
40	b	1	Total 1	O 1	0

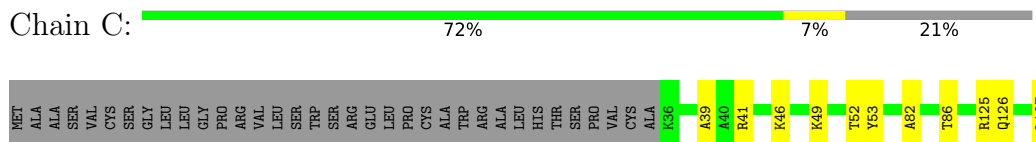
### 3 Residue-property plots [i](#)

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.

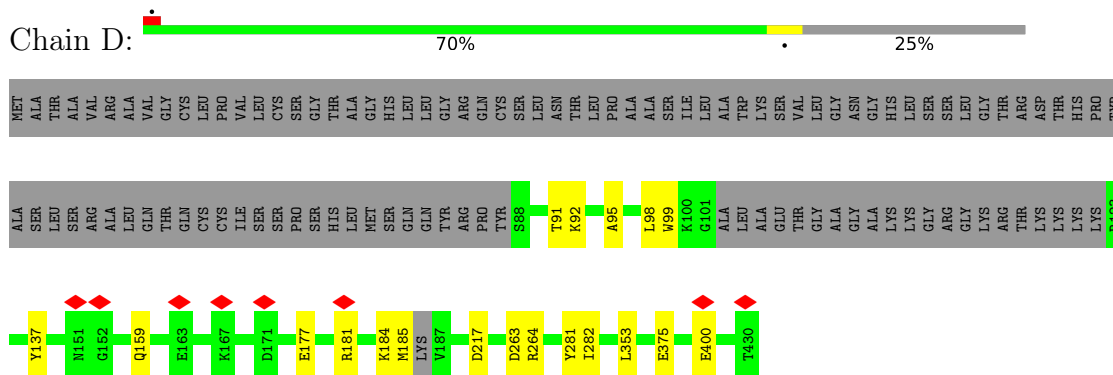
- Molecule 1: 28S ribosomal protein S2, mitochondrial



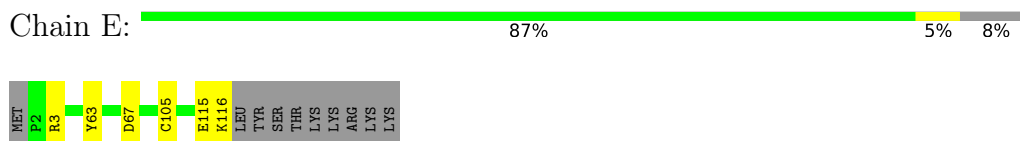
- Molecule 2: 28S ribosomal protein S24, mitochondrial



- Molecule 3: 28S ribosomal protein S5, mitochondrial



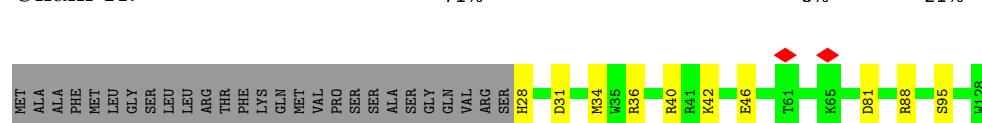
- Molecule 4: 28S ribosomal protein S6, mitochondrial



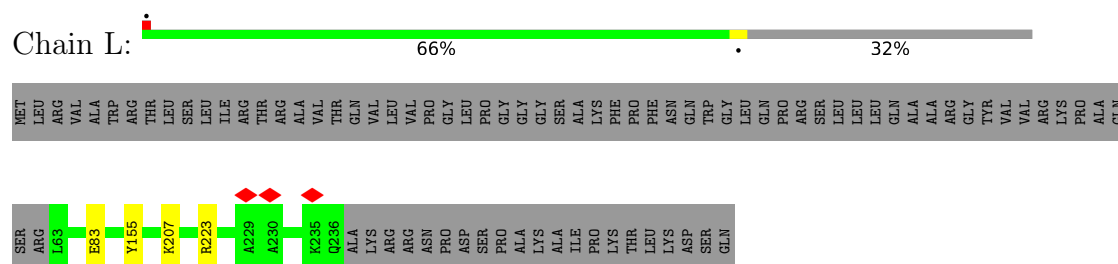
- Chain F:



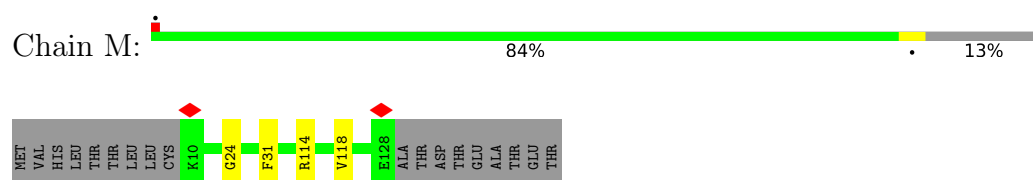
Chain K:



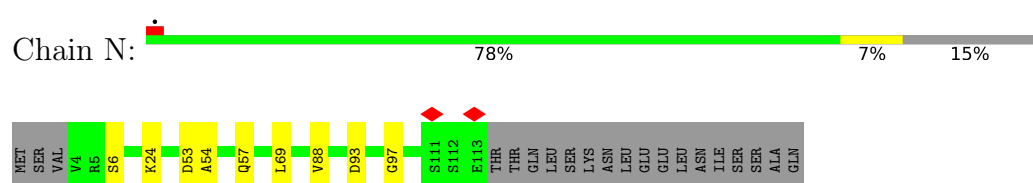
- Molecule 10: 28S ribosomal protein S15, mitochondrial



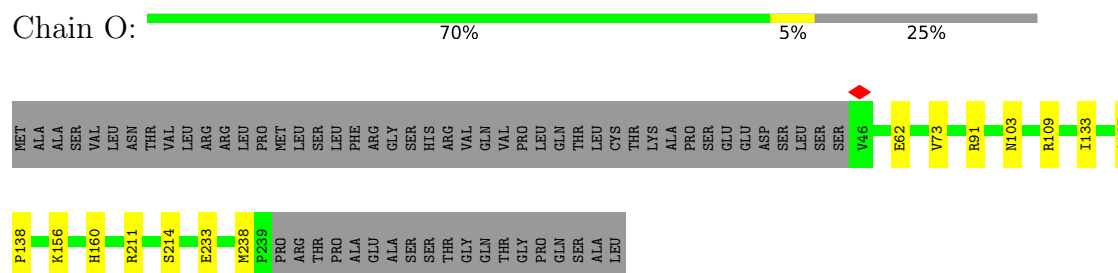
- Molecule 11: 28S ribosomal protein S16, mitochondrial



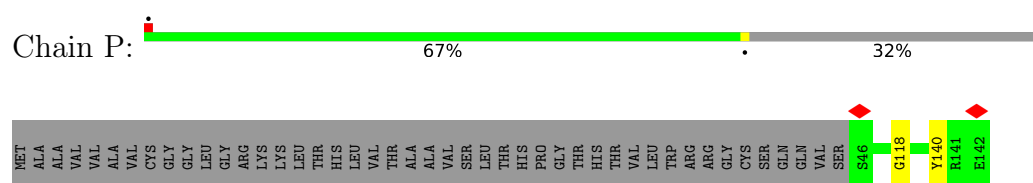
- Molecule 12: 28S ribosomal protein S17, mitochondrial



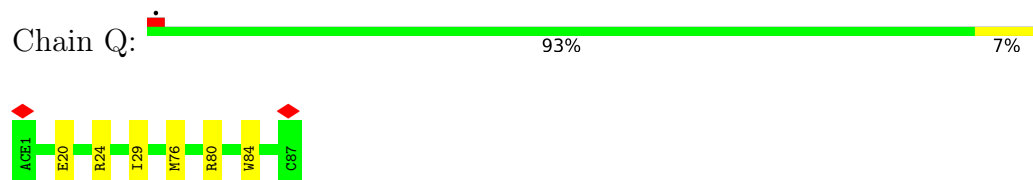
- Molecule 13: 28S ribosomal protein S18b, mitochondrial




- Molecule 14: 28S ribosomal protein S18c, mitochondrial



- Molecule 15: MRPS21 isoform 1



- Molecule 16: 28S ribosomal protein S22, mitochondrial

Chain R:  79% 18%

MET ALA PRO LEU GLY THR THR VAL LEU LEU TRP SER LEU LEU ARG SER PRO PRO GLY VAL GLU ARG VAL CYS PHE ARG ALA ARG ILE GLN PRO TRP HIS GLY GLY LEU LEU GLN PRO LEU LEU PRO CYS SER PHE MET GLY LEU PRO ARG ARG PHE SER ALA ALA SER

GLY SER PRO E64 E73 E97 S162 I165 I208 N214 D260 R263 A317 A321 S357 A358 ALA SER

- Molecule 17: 28S ribosomal protein S23, mitochondrial

Chain S:  66% 5% 29%

MET A2 E7 R21 E27 K28 R42 Q47 Q61 D62 T63 W64 E116 G136 GLU ALA ARG THR GLN HIS GLY GLY SER HIS VAL SER ARG LYS SER GLU LEU HIS LEU SER VAL ARG PRO GLN THR ALA LEU GLU ASN GLU THR GLN LYS VAL VAL PRO GLN ASP


GLN HIS LEU GLU ALA PRO ASP GLN SER LYS GLY LEU LEU PRO

- Molecule 18: 28S ribosomal protein S25, mitochondrial

Chain T:  93% . .


MET P2 R11 I52 P63 C139 I140 L155 R160 A169 ASP ALA GLN ASP

- Molecule 19: 28S ribosomal protein S26, mitochondrial

Chain U:  82% . 14%

MET LEU ARG ALA LEU SER VAL ARG LEU GLY ALA THR PRO CYS ARG PRO ARG ALA PRO LEU VAL LEU PRO ALA ARG GLY R27 K38 V42 R64 R80 E84 L137 R141 R202 ARG ASP SER

- Molecule 20: 28S ribosomal protein S27, mitochondrial

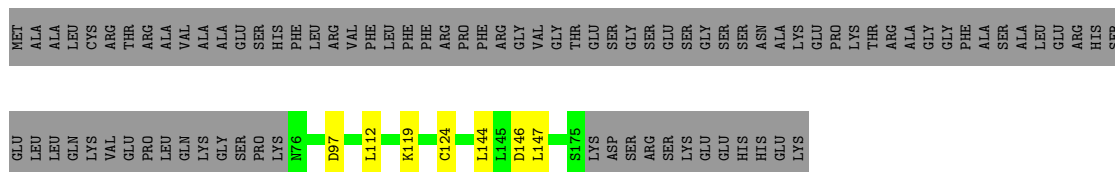
Chain V:  82% 6% 13%

MET ALA ALA SER ILE VAL ARG ARG GLY MET LEU LEU ALA ARG GLN GLN VAL LEU LEU PRO GLN SER PRO PRO GLY LYS TYR L29 H38 K39 V40 E41 A42 R43 E44 H47 L70 R74 D77 N78 H97 Y103 L104 R105 D123 I137 F138 P139 F151

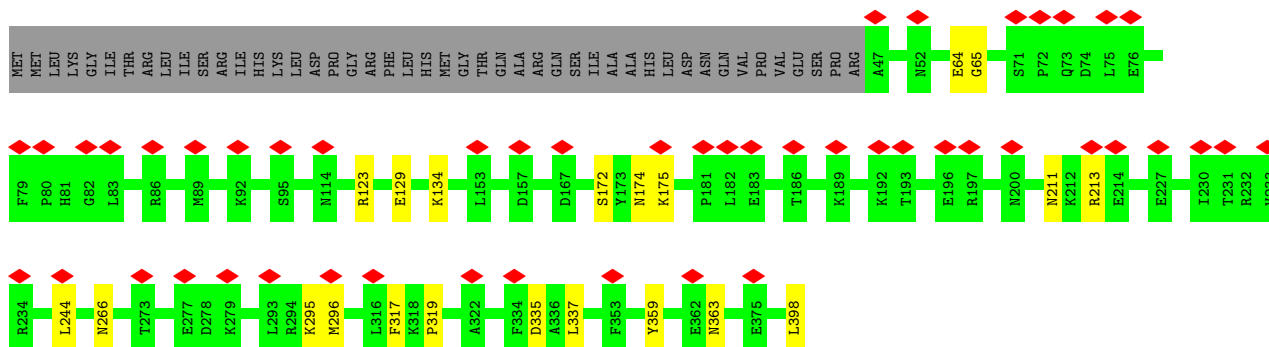
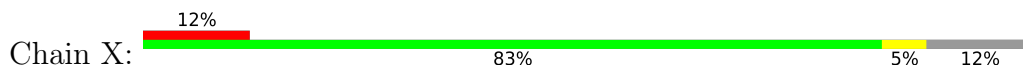
I152 K153 K154 E155 A293 ASP GLY ALA SER MET GLU GLU GLN GLN ASN ASP GLU ASP GLN SER E311 W382 L386 L389 K401 Y404 A405 A406 Q407 LYS ALA ALA LYS ALA SER ALA

- Molecule 21: 28S ribosomal protein S28, mitochondrial

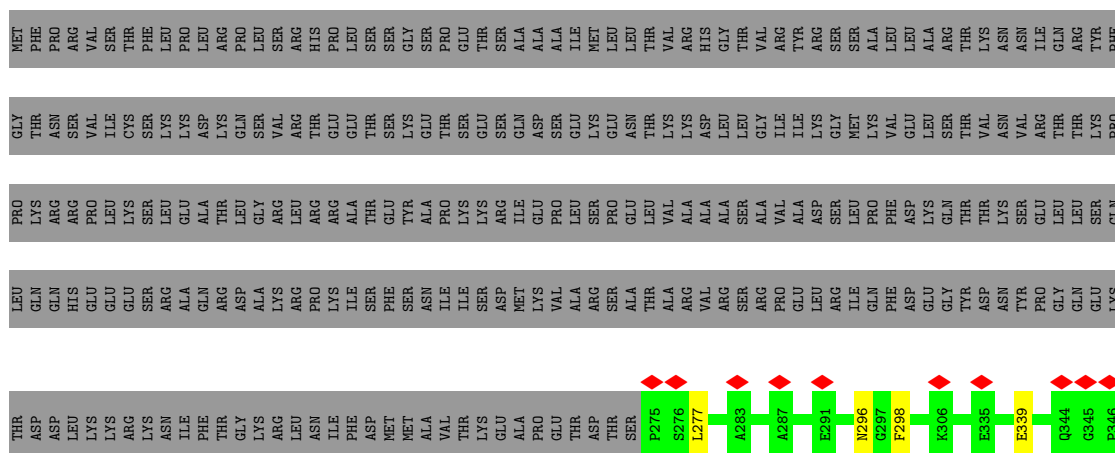
Chain W:  50% . 47%



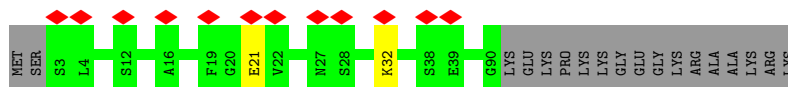
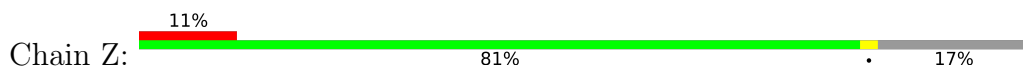
- Molecule 22: 28S ribosomal protein S29, mitochondrial



- Molecule 23: 28S ribosomal protein S31, mitochondrial

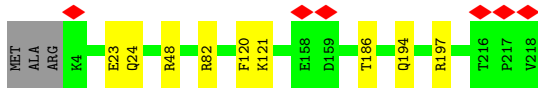


- Molecule 24: 28S ribosomal protein S33, mitochondrial



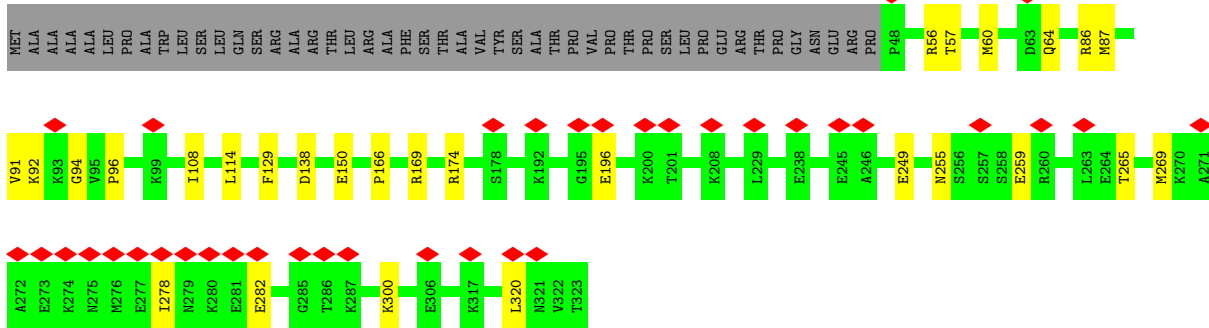
- Molecule 25: 28S ribosomal protein S34, mitochondrial

94%



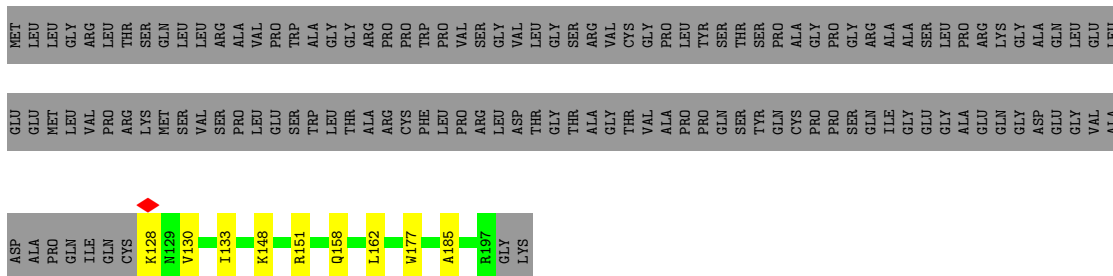
- Molecule 26: 28S ribosomal protein S35, mitochondrial

77%



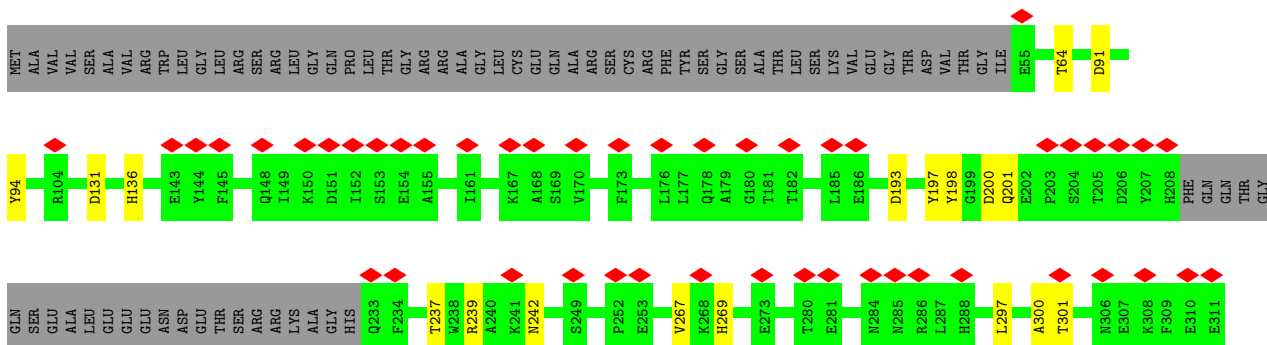
- Molecule 27: Aurora kinase A-interacting protein

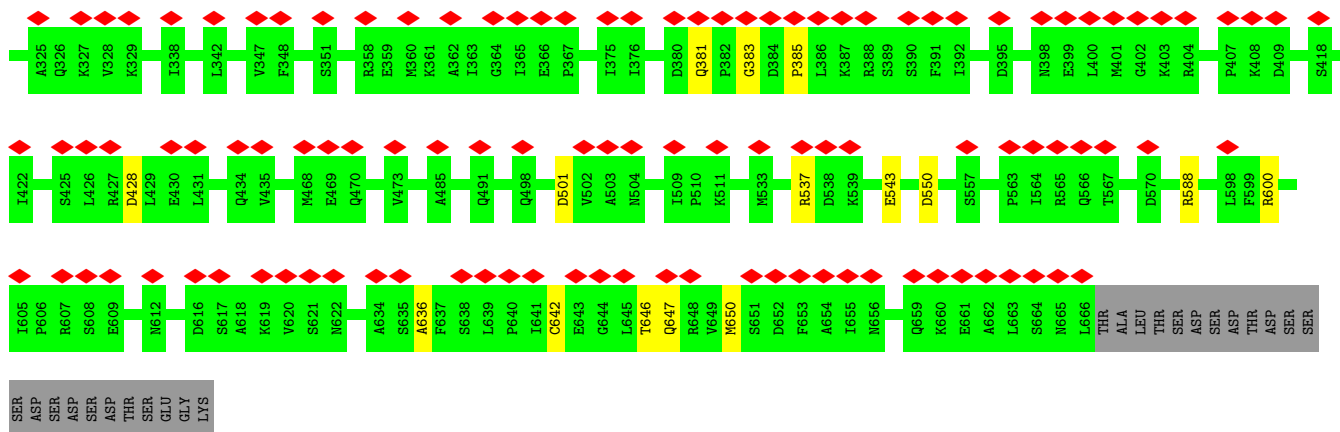
31%



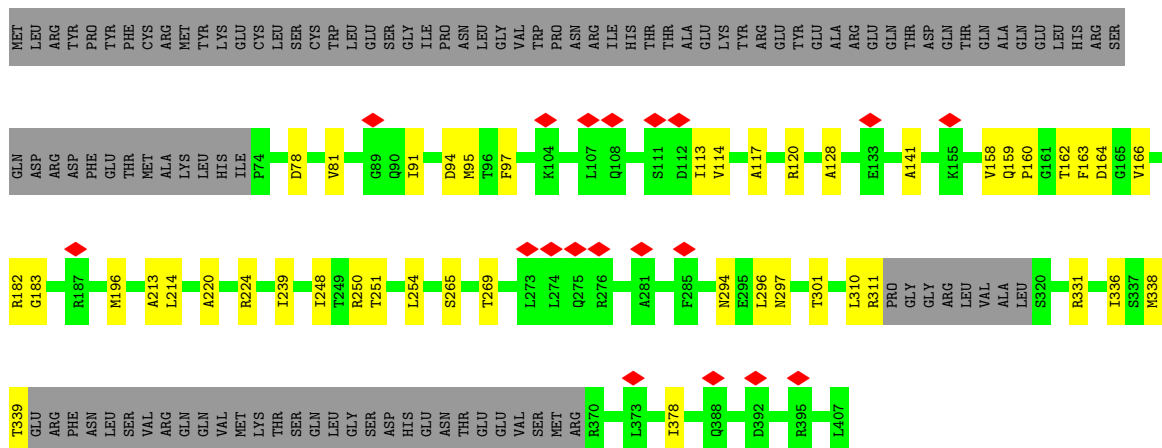
- Molecule 28: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

23%

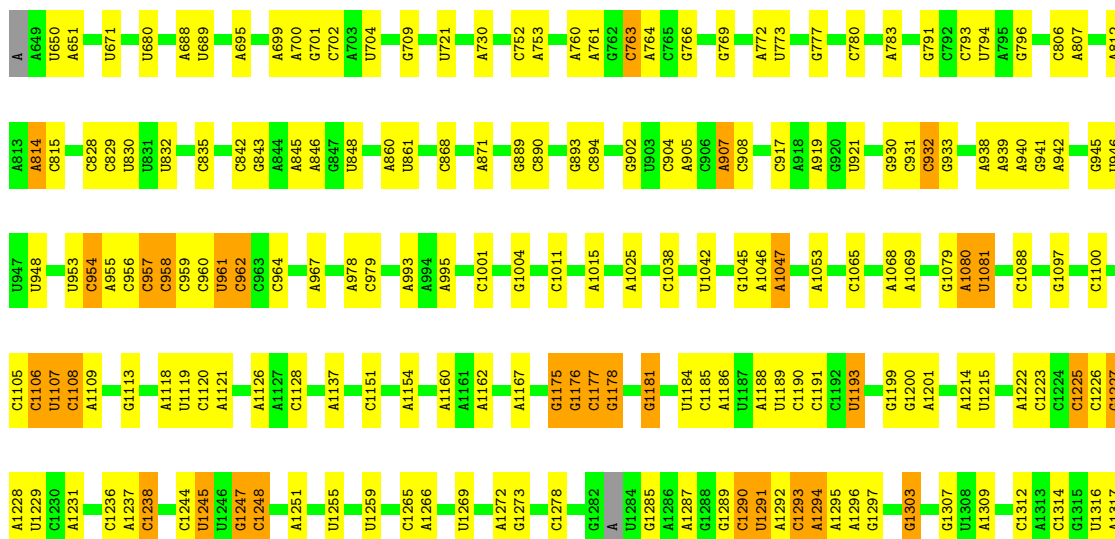




• Molecule 29: 12S rRNA N4-methylcytidine (m4C) methyltransferase



• Molecule 30: 12S mitochondrial rRNA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10529	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5F0, FES, 5MC, ATP, GDP, NAD, SPM, B8T, ZN, MA6, 5MU, ACE, MG

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	B	0.11	0/1871	0.23	0/2531
2	C	0.12	0/1113	0.24	0/1505
3	D	0.11	0/2620	0.23	0/3511
4	E	0.11	0/926	0.25	0/1252
5	F	0.11	0/1723	0.24	0/2313
6	G	0.14	0/2631	0.25	0/3527
7	I	0.11	0/1030	0.23	0/1386
8	J	0.12	0/855	0.23	0/1148
9	K	0.12	0/880	0.24	0/1182
10	L	0.11	0/1477	0.21	0/1974
11	M	0.12	0/963	0.24	0/1295
12	N	0.11	0/886	0.22	0/1199
13	O	0.13	0/1655	0.24	0/2254
14	P	0.14	0/798	0.27	0/1070
15	Q	0.12	0/754	0.25	0/1003
16	R	0.11	0/2456	0.22	0/3317
17	S	0.11	0/1138	0.21	0/1533
18	T	0.12	0/1402	0.23	0/1883
19	U	0.10	0/1510	0.22	0/2025
20	V	0.10	0/3030	0.23	0/4093
21	W	0.10	0/801	0.23	0/1079
22	X	0.11	0/2921	0.24	0/3954
23	Y	0.12	0/1054	0.24	0/1421
24	Z	0.12	0/762	0.23	0/1019
25	0	0.10	0/1834	0.23	0/2484
26	1	0.11	0/2285	0.23	0/3090
27	3	0.12	0/636	0.25	0/839
28	4	0.09	0/4877	0.22	0/6598
29	b	0.10	0/2353	0.26	0/3171
30	A	0.13	0/22421	0.22	2/34898 (0.0%)
31	H	0.11	0/1170	0.24	0/1587
32	a	0.10	0/1267	0.30	0/1705

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.12	0/72099	0.23	2/101846 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	I	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1379	A	C5'-C4'-C3'	5.88	124.81	116.00
30	A	1379	A	C5'-C4'-O4'	5.34	117.81	109.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	I	183	HIS	Mainchain
7	I	184	5F0	Mainchain
7	I	185	GLY	Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1828	1816	1815	5	0
2	C	1083	1088	1088	7	0
3	D	2570	2609	2609	12	0
4	E	910	929	929	4	0
5	F	1685	1736	1736	16	0
6	G	2576	2560	2560	18	0
7	I	1020	1060	1053	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	839	887	887	7	0
9	K	862	885	885	7	0
10	L	1453	1540	1540	5	0
11	M	942	966	966	2	0
12	N	868	928	928	5	0
13	O	1599	1565	1565	9	0
14	P	781	808	808	2	0
15	Q	744	758	758	6	0
16	R	2409	2428	2428	6	0
17	S	1111	1115	1115	8	0
18	T	1371	1396	1396	6	0
19	U	1488	1499	1499	5	0
20	V	2969	2960	2961	18	0
21	W	789	802	802	4	0
22	X	2849	2844	2844	14	0
23	Y	1023	970	970	4	0
24	Z	745	750	750	2	0
25	0	1787	1796	1796	6	0
26	1	2238	2269	2269	23	0
27	3	625	699	699	5	0
28	4	4768	4766	4766	22	0
29	b	2313	2367	2366	30	0
30	A	20158	10240	10243	121	0
31	H	1144	1173	1172	7	0
32	a	1252	1263	1261	30	0
33	A	30	0	0	0	0
33	G	1	0	0	0	0
34	M	4	0	0	0	0
34	P	4	0	0	1	0
35	O	1	0	0	0	0
36	X	31	12	12	0	0
37	X	28	10	12	1	0
38	A	44	26	26	0	0
39	A	14	0	26	3	0
40	0	1	0	0	1	0
40	G	1	0	0	1	0
40	K	1	0	0	0	0
40	T	1	0	0	0	0
40	b	1	0	0	0	0
All	All	68961	59520	59540	367	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 (367) 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)
20:V:103:TYR:OH	30:A:1524:A:O2'	2.01	0.76
20:V:404:TYR:OH	30:A:1521:U:O5'	2.03	0.76
6:G:388:ARG:NH1	30:A:1430:A:O5'	2.18	0.76
5:F:50:TYR:O	5:F:66:ARG:NH2	2.21	0.74
32:a:298:GLY:O	32:a:301:VAL:HG22	1.88	0.73
24:Z:32:LYS:NZ	30:A:1400:U:OP1	2.16	0.71
5:F:155:MET:O	32:a:196:LEU:HD11	1.91	0.70
17:S:42:ARG:NH2	17:S:47:GLN:OE1	2.25	0.70
6:G:196:GLY:O	6:G:248:VAL:N	2.27	0.68
10:L:83:GLU:N	10:L:83:GLU:OE1	2.27	0.67
17:S:27:GLU:OE2	17:S:28:LYS:N	2.28	0.67
32:a:135:ALA:O	32:a:137:ARG:NH1	2.28	0.67
5:F:119:LYS:NZ	22:X:398:LEU:OXT	2.28	0.66
7:I:98:GLN:NE2	30:A:1004:G:O2'	2.29	0.66
30:A:1550:A:O2'	30:A:1551:G:OP1	2.11	0.66
32:a:187:ASN:O	32:a:191:ALA:N	2.30	0.65
32:a:143:THR:HG22	32:a:144:LEU:H	1.61	0.65
30:A:843:G:N2	30:A:846:A:OP2	2.30	0.65
25:0:82:ARG:NH1	40:0:301:HOH:O	2.29	0.64
29:b:94:ASP:OD1	29:b:95:MET:N	2.31	0.64
30:A:1175:G:N2	30:A:1481:C:O2'	2.32	0.63
8:J:98:GLU:N	8:J:98:GLU:OE1	2.31	0.63
30:A:1569:G:O2'	30:A:1570:G:O4'	2.17	0.63
20:V:43:ARG:NH2	20:V:77:ASP:OD2	2.32	0.62
30:A:1401:G:N1	30:A:1404:A:OP2	2.32	0.62
27:3:128:LYS:NZ	30:A:1107:U:O4	2.27	0.62
9:K:40:ARG:NH1	9:K:81:ASP:OD1	2.33	0.62
29:b:120:ARG:NH1	29:b:196:MET:SD	2.73	0.62
9:K:88:ARG:NH2	30:A:1231:A:OP1	2.33	0.61
3:D:281:TYR:OH	17:S:21:ARG:NH1	2.33	0.61
13:O:211:ARG:O	13:O:214:SER:OG	2.15	0.61
29:b:297:ASN:O	29:b:301:THR:OG1	2.18	0.61
30:A:905:A:O2'	30:A:907:A:OP1	2.19	0.61
28:4:239:ARG:O	28:4:242:ASN:ND2	2.34	0.61
16:R:317:ALA:O	16:R:321:ALA:N	2.33	0.60
30:A:1583:MA6:H93	30:A:1584:MA6:C2	2.31	0.60
25:0:23:GLU:OE1	25:0:24:GLN:NE2	2.35	0.60
20:V:97:HIS:O	20:V:97:HIS:ND1	2.35	0.60
22:X:295:LYS:NZ	37:X:502:GDP:H5''	2.17	0.60
26:1:150:GLU:OE1	26:1:174:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:4:550:ASP:OD1	28:4:588:ARG:NH2	2.34	0.59
5:F:156:ILE:HD12	5:F:230:ALA:HB3	1.84	0.59
20:V:74:ARG:O	20:V:78:ASN:ND2	2.35	0.59
8:J:117:ASP:OD2	30:A:894:C:N4	2.35	0.59
22:X:317:PHE:N	30:A:1374:A:O2'	2.35	0.59
30:A:946:U:OP2	39:A:1732:SPM:N10	2.35	0.59
15:Q:80:ARG:O	30:A:1293:C:N4	2.36	0.59
27:3:148:LYS:O	27:3:151:ARG:NH1	2.35	0.59
30:A:1245:U:N3	30:A:1342:C:OP1	2.35	0.59
30:A:1563:U:O2'	30:A:1564:A:OP2	2.19	0.59
32:a:239:ILE:HG23	32:a:239:ILE:O	2.03	0.58
30:A:1309:A:O2'	31:H:137:ARG:NH2	2.36	0.58
31:H:71:ILE:O	31:H:150:GLY:N	2.37	0.58
1:B:72:PHE:O	1:B:263:LYS:NZ	2.37	0.58
16:R:260:ASP:OD1	16:R:263:ARG:NH2	2.34	0.58
26:1:265:THR:HG22	26:1:269:MET:HE3	1.85	0.58
1:B:180:ARG:NH1	1:B:185:PRO:O	2.37	0.57
16:R:208:ILE:O	16:R:214:ASN:ND2	2.38	0.57
26:1:64:GLN:N	26:1:64:GLN:OE1	2.34	0.57
7:I:193:LYS:NZ	30:A:1587:U:OP1	2.36	0.57
29:b:97:PHE:CD2	29:b:128:ALA:HB2	2.39	0.57
29:b:166:VAL:HG21	29:b:310:LEU:HD13	1.86	0.57
3:D:95:ALA:HB1	3:D:98:LEU:HD13	1.87	0.56
17:S:61:GLN:N	17:S:61:GLN:OE1	2.36	0.56
29:b:158:VAL:HG13	29:b:158:VAL:O	2.05	0.56
30:A:1598:G:O2'	30:A:1599:A:O4'	2.23	0.56
26:1:269:MET:HE2	26:1:320:LEU:CD1	2.36	0.56
7:I:146:HIS:ND1	7:I:171:GLU:OE1	2.37	0.56
9:K:36:ARG:NH1	30:A:1237:A:OP1	2.39	0.56
7:I:89:LYS:NZ	30:A:1004:G:OP1	2.39	0.56
5:F:136:THR:HG22	5:F:136:THR:O	2.05	0.55
30:A:1484:C:O2'	30:A:1485:G:N2	2.37	0.55
2:C:126:GLN:OE1	2:C:126:GLN:N	2.38	0.55
30:A:942:A:N6	30:A:1047:A:OP2	2.32	0.55
30:A:917:C:O2'	30:A:921:U:OP1	2.23	0.55
6:G:289:GLY:N	6:G:325:LYS:O	2.38	0.55
2:C:49:LYS:N	2:C:167:LEU:OXT	2.39	0.54
22:X:211:ASN:OD1	22:X:213:ARG:O	2.24	0.54
8:J:78:ARG:NH2	8:J:117:ASP:OD2	2.41	0.54
13:O:233:GLU:N	13:O:233:GLU:OE1	2.40	0.54
29:b:128:ALA:HB1	29:b:141:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:192:GLU:OE1	32:a:196:LEU:HD22	2.08	0.54
2:C:46:LYS:HD2	2:C:46:LYS:O	2.08	0.54
28:4:200:ASP:O	28:4:239:ARG:NH2	2.41	0.54
1:B:243:PRO:O	1:B:247:HIS:ND1	2.37	0.53
29:b:128:ALA:HB1	29:b:141:ALA:CB	2.38	0.53
8:J:48:LYS:NZ	30:A:1162:A:OP1	2.38	0.53
19:U:80:ARG:O	19:U:84:GLU:N	2.39	0.53
12:N:24:LYS:NZ	12:N:54:ALA:O	2.40	0.53
13:O:156:LYS:O	13:O:160:HIS:ND1	2.40	0.53
30:A:1407:U:HO2'	30:A:1446:A:HO2'	1.55	0.53
30:A:1482:A:O2'	30:A:1485:G:N2	2.41	0.53
23:Y:339:GLU:OE1	23:Y:339:GLU:N	2.37	0.53
17:S:62:ASP:OD2	17:S:64:TRP:NE1	2.42	0.53
19:U:64:ARG:NH2	30:A:845:A:OP1	2.38	0.52
28:4:297:LEU:O	28:4:301:THR:N	2.41	0.52
20:V:151:PHE:O	20:V:155:GLU:N	2.42	0.52
28:4:600:ARG:NH2	28:4:636:ALA:O	2.42	0.52
5:F:168:TYR:O	5:F:170:VAL:HG13	2.09	0.52
28:4:131:ASP:OD2	28:4:136:HIS:ND1	2.37	0.51
30:A:1464:G:H21	30:A:1466:C:H41	1.59	0.51
32:a:232:THR:HB	32:a:239:ILE:HG21	1.92	0.51
28:4:267:VAL:HG22	28:4:300:ALA:HB2	1.92	0.51
30:A:760:A:N1	30:A:780:C:O2'	2.42	0.51
30:A:1566:C:N4	30:A:1570:G:OP2	2.44	0.51
5:F:35:SER:N	30:A:1430:A:OP2	2.44	0.51
26:1:249:GLU:OE1	26:1:249:GLU:N	2.34	0.51
20:V:40:TRP:O	20:V:43:ARG:NH1	2.43	0.51
18:T:11:ARG:NH2	30:A:932:C:N3	2.58	0.51
22:X:359:TYR:O	22:X:363:ASN:ND2	2.44	0.51
26:1:255:ASN:N	26:1:259:GLU:OE1	2.38	0.51
29:b:94:ASP:O	29:b:117:ALA:HB1	2.11	0.51
30:A:1272:A:N6	30:A:1320:G:O2'	2.44	0.51
5:F:170:VAL:HG21	5:F:239:TYR:CD2	2.45	0.50
13:O:73:VAL:O	13:O:109:ARG:NH2	2.44	0.50
28:4:237:THR:O	28:4:237:THR:HG22	2.11	0.50
30:A:1391:U:H3'	30:A:1392:A:C5'	2.41	0.50
15:Q:24:ARG:NH2	32:a:118:TYR:O	2.45	0.50
30:A:1214:A:O2'	30:A:1238:C:O2'	2.27	0.50
4:E:3:ARG:NH2	4:E:67:ASP:OD2	2.41	0.50
2:C:39:ALA:O	2:C:41:ARG:NH1	2.42	0.50
32:a:198:ALA:O	32:a:199:VAL:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:380:LYS:NZ	30:A:1452:U:OP2	2.40	0.50
26:1:282:GLU:N	26:1:282:GLU:OE1	2.45	0.50
29:b:338:MET:N	29:b:338:MET:SD	2.84	0.50
6:G:120:ARG:NH2	30:A:1307:G:O2'	2.45	0.50
18:T:155:LEU:O	18:T:160:ARG:NH1	2.44	0.50
26:1:269:MET:HE2	26:1:320:LEU:HD13	1.93	0.50
30:A:948:U:OP2	30:A:1045:G:N1	2.43	0.49
30:A:1106:C:O2'	30:A:1108:C:OP2	2.30	0.49
3:D:91:THR:HG23	3:D:92:LYS:N	2.27	0.49
32:a:190:LEU:HD12	32:a:193:LEU:HD21	1.93	0.49
10:L:207:LYS:CD	30:A:763:C:H42	2.25	0.49
30:A:1386:U:H3'	30:A:1387:A:C5'	2.43	0.49
6:G:110:TYR:OH	26:1:114:LEU:O	2.27	0.49
22:X:64:GLU:OE1	22:X:65:GLY:N	2.46	0.49
28:4:198:TYR:O	28:4:201:GLN:HG2	2.13	0.49
7:I:133:ILE:HD13	7:I:164:GLY:O	2.12	0.49
28:4:647:GLN:HA	28:4:650:MET:HE3	1.95	0.49
20:V:404:TYR:HH	30:A:1521:U:C5'	2.24	0.49
21:W:146:ASP:OD1	21:W:147:LEU:N	2.45	0.49
30:A:812:A:O2'	30:A:814:A:N1	2.42	0.49
3:D:375:GLU:OE1	3:D:375:GLU:N	2.38	0.49
8:J:103:GLN:N	8:J:103:GLN:OE1	2.46	0.49
27:3:130:VAL:HG13	27:3:133:ILE:HB	1.95	0.49
30:A:1550:A:O2'	30:A:1551:G:P	2.70	0.49
32:a:130:THR:OG1	32:a:137:ARG:NH2	2.46	0.48
22:X:319:PRO:HA	30:A:1375:C:H4'	1.95	0.48
32:a:45:LEU:HD23	32:a:46:LYS:N	2.28	0.48
32:a:143:THR:HG22	32:a:144:LEU:N	2.27	0.48
1:B:239:ASN:OD1	21:W:119:LYS:NZ	2.46	0.48
30:A:1199:G:O2'	30:A:1423:A:N6	2.46	0.48
4:E:105:CYS:HB2	34:P:201:FES:S1	2.49	0.48
6:G:320:VAL:HG23	6:G:322:ARG:HG2	1.95	0.48
16:R:73:GLU:OE1	16:R:73:GLU:N	2.44	0.48
30:A:1289:G:H5'	30:A:1290:C:OP1	2.14	0.48
13:O:62:GLU:OE1	13:O:62:GLU:N	2.40	0.48
19:U:137:LEU:O	19:U:141:ARG:N	2.40	0.48
21:W:112:LEU:N	21:W:124:CYS:O	2.43	0.48
30:A:1563:U:O2'	30:A:1570:G:OP1	2.32	0.48
3:D:184:LYS:O	3:D:185:MET:C	2.57	0.48
18:T:139:CYS:SG	18:T:140:ILE:N	2.87	0.48
28:4:197:TYR:O	28:4:269:HIS:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:1519:A:H2'	30:A:1520:U:O4'	2.14	0.48
25:O:48:ARG:NH1	30:A:701:G:O6	2.47	0.47
25:O:120:PHE:CD2	25:O:121:LYS:HG2	2.48	0.47
6:G:389:ARG:HB2	30:A:1433:A:H5''	1.96	0.47
20:V:70:LEU:HD22	20:V:389:LEU:HB3	1.96	0.47
30:A:1080:A:H2'	30:A:1081:U:C5'	2.44	0.47
32:a:142:THR:HG22	32:a:143:THR:N	2.29	0.47
32:a:255:LYS:O	32:a:256:ASP:C	2.56	0.47
4:E:63:TYR:OH	14:P:118:GLY:O	2.25	0.47
11:M:114:ARG:O	11:M:118:VAL:HG23	2.13	0.47
22:X:244:LEU:HD13	22:X:296:MET:HE2	1.96	0.47
30:A:1214:A:HO2'	30:A:1238:C:HO2'	1.57	0.47
6:G:276:ARG:NH1	40:G:2001:HOH:O	2.38	0.47
8:J:99:GLY:O	8:J:127:ARG:NH2	2.42	0.47
28:4:64:THR:O	31:H:64:THR:OG1	2.31	0.47
30:A:702:C:OP1	30:A:848:U:O2'	2.32	0.47
7:I:182:PRO:HB2	7:I:184:5F0:O	2.14	0.47
26:1:278:ILE:O	26:1:278:ILE:HG13	2.14	0.47
29:b:163:PHE:HB2	29:b:166:VAL:HG22	1.96	0.47
30:A:1293:C:H4'	30:A:1294:A:OP2	2.15	0.47
20:V:137:ILE:HG22	20:V:139:PRO:HD3	1.96	0.47
2:C:125:ARG:HD2	28:4:94:TYR:CD1	2.50	0.47
10:L:155:TYR:OH	30:A:1038:C:O2'	2.30	0.47
17:S:115:GLU:OE1	17:S:115:GLU:N	2.43	0.47
26:1:56:ARG:NH2	28:4:91:ASP:OD2	2.47	0.47
26:1:166:PRO:O	26:1:169:ARG:NH1	2.48	0.47
29:b:378:ILE:HG22	29:b:378:ILE:O	2.15	0.47
30:A:1558:A:H1'	30:A:1559:G:P	2.55	0.47
30:A:957:C:C6	30:A:958:C:H2'	2.50	0.47
30:A:1316:U:H2'	30:A:1317:A:O4'	2.15	0.47
30:A:1489:G:H2'	30:A:1490:U:O4'	2.15	0.46
3:D:400:GLU:OE1	3:D:400:GLU:N	2.40	0.46
20:V:406:ALA:O	20:V:407:GLN:C	2.58	0.46
26:1:138:ASP:OD1	26:1:138:ASP:N	2.45	0.46
29:b:296:LEU:HB2	32:a:232:THR:HG23	1.96	0.46
29:b:239:ILE:HD12	29:b:254:LEU:HD11	1.97	0.46
26:1:87:MET:HE1	26:1:108:ILE:HD12	1.97	0.46
30:A:1487:C:N4	30:A:1565:A:N1	2.64	0.46
26:1:86:ARG:NH1	26:1:96:PRO:O	2.49	0.46
5:F:88:ASP:OD2	5:F:146:HIS:NE2	2.49	0.46
10:L:207:LYS:HD2	30:A:763:C:H42	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:97:ASP:N	21:W:144:LEU:O	2.49	0.46
29:b:91:ILE:HD12	29:b:162:THR:HB	1.98	0.46
30:A:1478:A:N3	30:A:1478:A:H2'	2.31	0.46
31:H:52:VAL:HG12	31:H:52:VAL:O	2.16	0.45
28:4:646:THR:HG22	28:4:650:MET:HE2	1.98	0.45
30:A:1327:G:N2	31:H:127:TYR:OH	2.45	0.45
30:A:1460:C:H3'	30:A:1461:A:H5''	1.97	0.45
20:V:123:ASP:OD1	20:V:123:ASP:N	2.49	0.45
11:M:24:GLY:N	11:M:31:PHE:O	2.49	0.45
12:N:53:ASP:OD2	12:N:57:GLN:N	2.49	0.45
5:F:198:ARG:NH2	30:A:1383:A:N7	2.64	0.45
28:4:501:ASP:OD1	28:4:537:ARG:NH2	2.48	0.45
29:b:294:ASN:OD1	32:a:232:THR:HG21	2.17	0.45
30:A:1512:A:O2'	30:A:1536:A:N1	2.41	0.45
30:A:1566:C:H1'	30:A:1568:U:H2'	1.99	0.45
32:a:144:LEU:H	32:a:144:LEU:HD23	1.82	0.45
2:C:52:THR:HG22	2:C:53:TYR:N	2.32	0.45
17:S:62:ASP:OD1	17:S:62:ASP:N	2.49	0.45
29:b:91:ILE:HG22	29:b:163:PHE:HD1	1.81	0.45
30:A:769:G:N2	30:A:772:A:OP2	2.49	0.45
23:Y:360:LYS:NZ	24:Z:21:GLU:OE1	2.43	0.45
29:b:164:ASP:OD1	29:b:311:ARG:NH2	2.50	0.45
20:V:382:TRP:O	20:V:386:LEU:N	2.50	0.45
22:X:123:ARG:NH2	22:X:337:LEU:O	2.49	0.45
3:D:177:GLU:O	3:D:181:ARG:N	2.45	0.44
3:D:137:TYR:O	3:D:159:GLN:NE2	2.49	0.44
30:A:1178:G:H22	32:a:134:SER:HB3	1.82	0.44
9:K:31:ASP:N	9:K:31:ASP:OD1	2.49	0.44
6:G:377:ARG:NE	30:A:1454:G:N7	2.65	0.44
12:N:93:ASP:O	12:N:97:GLY:N	2.41	0.44
30:A:945:G:N7	39:A:1732:SPM:H62	2.33	0.44
30:A:1225:C:N4	30:A:1448:U:O2'	2.50	0.44
6:G:325:LYS:O	6:G:325:LYS:HD3	2.18	0.44
30:A:961:U:H1'	30:A:962:C:OP1	2.17	0.44
6:G:384:GLN:HB3	6:G:389:ARG:O	2.17	0.44
9:K:34:MET:HE3	9:K:95:SER:HB3	1.99	0.44
19:U:42:VAL:HG13	19:U:42:VAL:O	2.17	0.44
30:A:1176:G:N2	30:A:1482:A:OP1	2.47	0.44
30:A:1583:MA6:H93	30:A:1584:MA6:N1	2.33	0.44
6:G:126:LYS:H	6:G:131:ILE:HD11	1.82	0.44
28:4:267:VAL:HG22	28:4:300:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:4:428:ASP:OD1	28:4:428:ASP:N	2.51	0.44
30:A:1488:5MC:H2'	30:A:1489:G:C8	2.53	0.44
18:T:52:ILE:N	18:T:53:PRO:CD	2.81	0.43
20:V:103:TYR:O	20:V:104:LEU:C	2.60	0.43
29:b:265:SER:O	29:b:269:THR:HG23	2.17	0.43
30:A:945:G:N7	39:A:1732:SPM:H42	2.32	0.43
30:A:1550:A:HO2'	30:A:1551:G:P	2.37	0.43
22:X:172:SER:O	22:X:175:LYS:NZ	2.51	0.43
28:4:642:CYS:O	28:4:646:THR:OG1	2.30	0.43
29:b:331:ARG:HG2	29:b:336:ILE:HA	2.00	0.43
13:O:238:MET:SD	13:O:238:MET:N	2.92	0.43
25:0:186:THR:O	25:0:186:THR:HG22	2.17	0.43
5:F:170:VAL:O	5:F:170:VAL:HG23	2.18	0.43
14:P:140:TYR:CD1	15:Q:29:ILE:HD12	2.54	0.43
15:Q:20:GLU:N	15:Q:20:GLU:OE1	2.51	0.43
29:b:113:ILE:HG12	29:b:114:VAL:H	1.83	0.43
30:A:1181:G:H4'	32:a:182:VAL:HG22	2.00	0.43
30:A:1386:U:H3'	30:A:1387:A:H5''	2.01	0.43
32:a:130:THR:OG1	32:a:137:ARG:NH1	2.50	0.43
20:V:401:LYS:HA	20:V:404:TYR:HB3	2.00	0.43
20:V:105:ARG:NH1	20:V:389:LEU:HD11	2.33	0.43
30:A:1430:A:N1	30:A:1458:A:H5''	2.33	0.43
19:U:38:LYS:NZ	30:A:699:A:OP1	2.45	0.43
30:A:1414:C:H2'	30:A:1415:G:C1'	2.49	0.43
30:A:1191:C:H1'	30:A:1466:C:H42	1.84	0.43
5:F:176:ASP:OD1	5:F:177:ARG:N	2.51	0.43
6:G:315:PHE:HB3	6:G:316:PRO:HD3	1.99	0.43
26:1:265:THR:CG2	26:1:269:MET:HE3	2.48	0.43
29:b:159:GLN:N	29:b:160:PRO:CD	2.82	0.43
30:A:1227:G:O5'	30:A:1228:A:H2'	2.19	0.43
30:A:752:C:O2'	30:A:793:C:N4	2.50	0.42
30:A:1177:C:H2'	30:A:1178:G:H5''	2.01	0.42
3:D:95:ALA:HB3	3:D:99:TRP:CZ2	2.54	0.42
30:A:806:C:OP2	30:A:807:A:N6	2.40	0.42
30:A:1569:G:O3'	30:A:1570:G:H4'	2.19	0.42
30:A:953:U:H4'	30:A:954:C:OP1	2.19	0.42
30:A:1558:A:O2'	30:A:1559:G:OP1	2.29	0.42
10:L:223:ARG:NE	10:L:223:ARG:HA	2.34	0.42
12:N:6:SER:OG	12:N:69:LEU:O	2.33	0.42
30:A:1178:G:C6	30:A:1476:G:H1'	2.53	0.42
26:1:129:PHE:HB2	31:H:155:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:182:ARG:NH2	29:b:196:MET:O	2.53	0.42
29:b:220:ALA:O	29:b:224:ARG:N	2.48	0.42
3:D:282:ILE:HG23	3:D:353:LEU:HB3	2.01	0.42
6:G:388:ARG:O	6:G:390:LYS:NZ	2.48	0.42
9:K:28:HIS:N	30:A:1248:C:O2	2.53	0.42
26:1:269:MET:HE2	26:1:320:LEU:HD12	2.01	0.42
30:A:1560:U:C4	30:A:1561:C:C4	3.07	0.42
4:E:115:GLU:O	4:E:116:LYS:C	2.62	0.42
13:O:137:ALA:HB3	13:O:138:PRO:HD3	2.02	0.42
26:1:91:VAL:O	26:1:94:GLY:N	2.53	0.42
30:A:1290:C:O2'	30:A:1291:U:O5'	2.34	0.42
6:G:320:VAL:O	6:G:321:ASP:OD1	2.38	0.42
6:G:364:MET:HB3	6:G:369:LEU:HB2	2.02	0.42
22:X:174:ASN:OD1	22:X:175:LYS:N	2.53	0.42
30:A:1582:G:H3'	30:A:1583:MA6:H8	2.01	0.42
32:a:176:VAL:O	32:a:176:VAL:HG13	2.20	0.42
5:F:156:ILE:HG22	32:a:196:LEU:HD23	2.02	0.42
28:4:381:GLN:O	28:4:383:GLY:N	2.50	0.42
29:b:213:ALA:O	29:b:214:LEU:C	2.62	0.42
32:a:297:SER:O	32:a:301:VAL:HG13	2.20	0.42
7:I:179:THR:O	7:I:181:ILE:HD12	2.20	0.41
16:R:162:SER:HB3	16:R:165:ILE:HD12	2.01	0.41
18:T:52:ILE:HG12	18:T:53:PRO:HD3	2.02	0.41
22:X:129:GLU:O	22:X:134:LYS:NZ	2.53	0.41
29:b:78:ASP:HA	29:b:81:VAL:HG12	2.02	0.41
32:a:190:LEU:HA	32:a:193:LEU:HD23	2.01	0.41
28:4:543:GLU:OE1	28:4:543:GLU:N	2.41	0.41
29:b:248:ILE:HG22	29:b:250:ARG:H	1.83	0.41
30:A:1272:A:N1	30:A:1303:G:O2'	2.49	0.41
30:A:1293:C:O2'	30:A:1294:A:OP1	2.34	0.41
5:F:155:MET:HG3	32:a:196:LEU:O	2.21	0.41
6:G:391:PHE:O	6:G:392:THR:C	2.63	0.41
8:J:107:ILE:N	8:J:131:ASP:OD2	2.41	0.41
9:K:42:LYS:O	9:K:46:GLU:OE1	2.37	0.41
3:D:263:ASP:OD1	3:D:264:ARG:N	2.54	0.41
7:I:153:GLY:O	7:I:158:ARG:NH1	2.51	0.41
29:b:269:THR:O	30:A:1559:G:N2	2.52	0.41
31:H:159:TYR:O	31:H:163:ASN:ND2	2.54	0.41
32:a:232:THR:CB	32:a:239:ILE:HG21	2.49	0.41
1:B:149:ARG:NH2	15:Q:84:TRP:O	2.50	0.41
2:C:82:ALA:O	2:C:86:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:1489:G:H2'	30:A:1490:U:H5''	2.02	0.41
13:O:133:ILE:HD11	16:R:97:GLU:OE2	2.21	0.41
30:A:1558:A:H1'	30:A:1559:G:OP1	2.20	0.41
5:F:224:HIS:O	5:F:228:LYS:N	2.53	0.41
25:O:194:GLN:O	25:O:197:ARG:NH2	2.54	0.41
26:1:57:THR:HA	26:1:60:MET:HE3	2.03	0.41
29:b:338:MET:O	29:b:339:THR:C	2.64	0.41
27:3:158:GLN:O	27:3:162:LEU:HD23	2.21	0.41
3:D:217:ASP:OD1	3:D:217:ASP:N	2.54	0.41
13:O:91:ARG:NH1	13:O:103:ASN:O	2.54	0.41
15:Q:76:MET:O	15:Q:76:MET:SD	2.79	0.41
17:S:7:GLU:OE1	17:S:7:GLU:N	2.48	0.41
18:T:52:ILE:CG1	18:T:53:PRO:HD3	2.51	0.41
20:V:404:TYR:OH	30:A:1521:U:O3'	2.39	0.41
26:1:91:VAL:HG12	26:1:92:LYS:N	2.36	0.41
26:1:196:GLU:OE1	26:1:196:GLU:N	2.44	0.41
30:A:958:C:O2'	30:A:959:C:OP2	2.38	0.41
30:A:1079:G:H2'	30:A:1080:A:O4'	2.21	0.41
30:A:1265:C:H2'	30:A:1266:A:H8	1.86	0.41
23:Y:296:ASN:OD1	23:Y:298:PHE:N	2.49	0.41
27:3:177:TRP:CZ2	27:3:185:ALA:HB2	2.55	0.41
30:A:702:C:O2'	30:A:842:C:O2	2.39	0.41
30:A:1053:A:N1	30:A:1100:C:O2'	2.44	0.41
30:A:1080:A:H2'	30:A:1081:U:H5''	2.03	0.41
30:A:1193:U:O2	30:A:1462:G:N1	2.53	0.41
23:Y:277:LEU:HB3	28:4:193:ASP:HB3	2.03	0.40
30:A:700:A:N1	30:A:709:G:O2'	2.51	0.40
30:A:954:C:O2'	30:A:1042:U:O2	2.40	0.40
30:A:1177:C:N3	30:A:1477:U:O4'	2.54	0.40
30:A:1389:G:H1'	30:A:1417:A:N6	2.37	0.40
32:a:192:GLU:OE1	32:a:196:LEU:HB2	2.22	0.40
12:N:88:VAL:O	12:N:88:VAL:HG13	2.22	0.40
5:F:234:ARG:O	5:F:235:ALA:HB3	2.21	0.40
22:X:335:ASP:OD1	26:1:300:LYS:NZ	2.54	0.40
29:b:183:GLY:C	29:b:251:THR:HG21	2.47	0.40
30:A:1247:G:H4'	30:A:1248:C:OP2	2.22	0.40
20:V:154:LYS:O	20:V:154:LYS:HG3	2.22	0.40
22:X:266:ASN:OD1	22:X:266:ASN:N	2.55	0.40
30:A:1080:A:H2'	30:A:1081:U:H5'	2.04	0.40
32:a:130:THR:HG23	32:a:131:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	223/296 (75%)	218 (98%)	5 (2%)	0	100	100
2	C	130/167 (78%)	123 (95%)	7 (5%)	0	100	100
3	D	315/430 (73%)	303 (96%)	12 (4%)	0	100	100
4	E	113/125 (90%)	111 (98%)	2 (2%)	0	100	100
5	F	203/242 (84%)	199 (98%)	4 (2%)	0	100	100
6	G	309/396 (78%)	296 (96%)	13 (4%)	0	100	100
7	I	134/194 (69%)	129 (96%)	5 (4%)	0	100	100
8	J	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
9	K	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
10	L	172/257 (67%)	166 (96%)	6 (4%)	0	100	100
11	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
12	N	108/130 (83%)	103 (95%)	5 (5%)	0	100	100
13	O	192/258 (74%)	185 (96%)	7 (4%)	0	100	100
14	P	95/142 (67%)	92 (97%)	3 (3%)	0	100	100
15	Q	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
16	R	293/360 (81%)	285 (97%)	8 (3%)	0	100	100
17	S	133/190 (70%)	126 (95%)	7 (5%)	0	100	100
18	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
19	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
20	V	358/414 (86%)	349 (98%)	9 (2%)	0	100	100
21	W	98/187 (52%)	92 (94%)	6 (6%)	0	100	100
22	X	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
23	Y	119/395 (30%)	118 (99%)	1 (1%)	0	100	100
24	Z	86/106 (81%)	84 (98%)	2 (2%)	0	100	100
25	0	213/218 (98%)	208 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	1	274/323 (85%)	265 (97%)	9 (3%)	0	100	100
27	3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
28	4	584/689 (85%)	571 (98%)	12 (2%)	1 (0%)	43	71
29	b	290/407 (71%)	264 (91%)	26 (9%)	0	100	100
31	H	137/201 (68%)	134 (98%)	3 (2%)	0	100	100
32	a	150/302 (50%)	141 (94%)	9 (6%)	0	100	100
All	All	5894/7894 (75%)	5707 (97%)	186 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	4	385	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	198/249 (80%)	198 (100%)	0	100	100
2	C	115/143 (80%)	115 (100%)	0	100	100
3	D	272/357 (76%)	272 (100%)	0	100	100
4	E	97/107 (91%)	97 (100%)	0	100	100
5	F	182/209 (87%)	182 (100%)	0	100	100
6	G	272/342 (80%)	272 (100%)	0	100	100
7	I	104/146 (71%)	104 (100%)	0	100	100
8	J	93/118 (79%)	93 (100%)	0	100	100
9	K	91/113 (80%)	91 (100%)	0	100	100
10	L	158/226 (70%)	158 (100%)	0	100	100
11	M	97/113 (86%)	97 (100%)	0	100	100
12	N	96/115 (84%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	O	175/230 (76%)	175 (100%)	0	100	100
14	P	88/123 (72%)	88 (100%)	0	100	100
15	Q	78/78 (100%)	78 (100%)	0	100	100
16	R	264/318 (83%)	264 (100%)	0	100	100
17	S	116/164 (71%)	116 (100%)	0	100	100
18	T	153/157 (98%)	153 (100%)	0	100	100
19	U	152/174 (87%)	152 (100%)	0	100	100
20	V	325/364 (89%)	325 (100%)	0	100	100
21	W	87/158 (55%)	87 (100%)	0	100	100
22	X	311/351 (89%)	311 (100%)	0	100	100
23	Y	112/357 (31%)	112 (100%)	0	100	100
24	Z	81/95 (85%)	81 (100%)	0	100	100
25	0	188/190 (99%)	188 (100%)	0	100	100
26	1	254/291 (87%)	254 (100%)	0	100	100
27	3	65/166 (39%)	65 (100%)	0	100	100
28	4	526/609 (86%)	526 (100%)	0	100	100
29	b	249/350 (71%)	249 (100%)	0	100	100
31	H	129/180 (72%)	129 (100%)	0	100	100
32	a	138/260 (53%)	138 (100%)	0	100	100
All	All	5266/6853 (77%)	5266 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	115	ASN
2	C	130	HIS
3	D	288	HIS
5	F	151	ASN
5	F	238	HIS
6	G	82	ASN
6	G	90	ASN
6	G	175	HIS
7	I	98	GLN

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Mol	Chain	Res	Type
9	K	68	GLN
11	M	82	HIS
13	O	80	ASN
13	O	111	HIS
13	O	147	HIS
16	R	356	HIS
18	T	37	HIS
18	T	146	GLN
19	U	109	ASN
20	V	145	ASN
20	V	188	HIS
20	V	316	GLN
22	X	110	HIS
22	X	190	ASN
22	X	205	GLN
24	Z	75	HIS
25	0	145	HIS
26	1	102	ASN
27	3	139	ASN
28	4	374	HIS
28	4	504	ASN
28	4	577	ASN
31	H	83	HIS
31	H	163	ASN
32	a	165	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	A	945/954 (99%)	230 (24%)	10 (1%)

All (230) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	A	650	U
30	A	651	A
30	A	671	U
30	A	680	U
30	A	688	A
30	A	689	U
30	A	695	A

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Mol	Chain	Res	Type
30	A	704	U
30	A	721	U
30	A	730	A
30	A	753	A
30	A	761	A
30	A	763	C
30	A	764	A
30	A	766	G
30	A	773	U
30	A	777	G
30	A	783	A
30	A	791	G
30	A	794	U
30	A	796	G
30	A	814	A
30	A	815	C
30	A	828	C
30	A	829	C
30	A	830	U
30	A	832	U
30	A	835	C
30	A	860	A
30	A	861	U
30	A	868	C
30	A	871	A
30	A	889	G
30	A	890	C
30	A	893	G
30	A	902	G
30	A	904	C
30	A	907	A
30	A	908	C
30	A	919	A
30	A	930	G
30	A	931	C
30	A	932	C
30	A	933	G
30	A	938	A
30	A	939	A
30	A	940	A
30	A	941	G
30	A	954	C

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Mol	Chain	Res	Type
30	A	955	A
30	A	957	C
30	A	958	C
30	A	960	C
30	A	961	U
30	A	962	C
30	A	964	C
30	A	967	A
30	A	978	A
30	A	979	C
30	A	993	A
30	A	995	A
30	A	1001	C
30	A	1011	C
30	A	1015	A
30	A	1025	A
30	A	1047	A
30	A	1065	C
30	A	1068	A
30	A	1069	A
30	A	1080	A
30	A	1081	U
30	A	1088	C
30	A	1097	G
30	A	1105	C
30	A	1106	C
30	A	1107	U
30	A	1108	C
30	A	1109	A
30	A	1113	G
30	A	1118	A
30	A	1119	U
30	A	1120	C
30	A	1121	A
30	A	1126	A
30	A	1128	C
30	A	1137	A
30	A	1151	C
30	A	1154	A
30	A	1160	A
30	A	1167	A
30	A	1175	G

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Mol	Chain	Res	Type
30	A	1176	G
30	A	1177	C
30	A	1178	G
30	A	1181	G
30	A	1184	U
30	A	1185	C
30	A	1186	A
30	A	1188	A
30	A	1189	U
30	A	1190	C
30	A	1193	U
30	A	1200	G
30	A	1201	A
30	A	1215	U
30	A	1222	A
30	A	1223	C
30	A	1225	C
30	A	1226	C
30	A	1227	G
30	A	1229	U
30	A	1236	C
30	A	1238	C
30	A	1244	C
30	A	1245	U
30	A	1247	G
30	A	1248	C
30	A	1251	A
30	A	1255	U
30	A	1259	U
30	A	1269	U
30	A	1273	G
30	A	1278	C
30	A	1285	G
30	A	1287	A
30	A	1290	C
30	A	1291	U
30	A	1292	A
30	A	1293	C
30	A	1294	A
30	A	1295	A
30	A	1296	A
30	A	1297	G

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Mol	Chain	Res	Type
30	A	1303	G
30	A	1312	C
30	A	1314	C
30	A	1318	A
30	A	1326	A
30	A	1327	G
30	A	1331	A
30	A	1332	A
30	A	1341	C
30	A	1342	C
30	A	1343	A
30	A	1345	G
30	A	1352	C
30	A	1354	A
30	A	1356	A
30	A	1367	A
30	A	1371	U
30	A	1378	C
30	A	1379	A
30	A	1381	A
30	A	1383	A
30	A	1385	C
30	A	1386	U
30	A	1387	A
30	A	1390	A
30	A	1392	A
30	A	1399	A
30	A	1405	C
30	A	1406	U
30	A	1407	U
30	A	1408	A
30	A	1410	G
30	A	1415	G
30	A	1417	A
30	A	1420	U
30	A	1421	G
30	A	1422	G
30	A	1427	A
30	A	1430	A
30	A	1438	G
30	A	1442	G
30	A	1443	U

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Mol	Chain	Res	Type
30	A	1444	A
30	A	1447	G
30	A	1457	G
30	A	1461	A
30	A	1464	G
30	A	1476	G
30	A	1477	U
30	A	1478	A
30	A	1479	C
30	A	1480	A
30	A	1481	C
30	A	1482	A
30	A	1483	C
30	A	1484	C
30	A	1486	B8T
30	A	1488	5MC
30	A	1489	G
30	A	1490	U
30	A	1491	C
30	A	1493	C
30	A	1507	A
30	A	1512	A
30	A	1513	A
30	A	1519	A
30	A	1521	U
30	A	1523	A
30	A	1524	A
30	A	1525	C
30	A	1526	U
30	A	1527	A
30	A	1532	C
30	A	1533	C
30	A	1537	C
30	A	1539	C
30	A	1546	A
30	A	1547	U
30	A	1551	G
30	A	1558	A
30	A	1559	G
30	A	1560	U
30	A	1562	G
30	A	1564	A

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Mol	Chain	Res	Type
30	A	1565	A
30	A	1566	C
30	A	1567	A
30	A	1568	U
30	A	1569	G
30	A	1570	G
30	A	1571	U
30	A	1572	A
30	A	1584	MA6
30	A	1590	A
30	A	1594	G
30	A	1595	G
30	A	1598	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	A	956	C
30	A	961	U
30	A	1046	A
30	A	1293	C
30	A	1478	A
30	A	1488	5MC
30	A	1550	A
30	A	1558	A
30	A	1566	C
30	A	1567	A

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

6 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
30	B8T	A	1486	-	19,22,23	3.37	8 (42%)	25,31,34	0.91	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	5F0	I	184	7	8,8,9	0.53	0	8,9,11	1.08	1 (12%)
30	5MC	A	1488	30	19,22,23	0.46	0	26,32,35	0.74	0
30	MA6	A	1583	30	23,26,27	1.33	3 (13%)	33,38,41	3.10	11 (33%)
30	MA6	A	1584	30	23,26,27	1.35	4 (17%)	33,38,41	3.11	12 (36%)
30	5MU	A	1076	30	19,22,23	0.38	0	27,32,35	0.47	0

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
30	B8T	A	1486	-	-	3/7/27/28	0/2/2/2
7	5F0	I	184	7	-	0/9/9/10	-
30	5MC	A	1488	30	-	1/7/25/26	0/2/2/2
30	MA6	A	1583	30	-	3/11/29/30	0/3/3/3
30	MA6	A	1584	30	-	3/11/29/30	0/3/3/3
30	5MU	A	1076	30	-	0/7/25/26	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	1486	B8T	C4-N3	8.02	1.46	1.32
30	A	1486	B8T	C2-N3	6.13	1.48	1.36
30	A	1486	B8T	C6-C5	5.93	1.48	1.35
30	A	1486	B8T	C4-N4	4.87	1.46	1.36
30	A	1486	B8T	C2-N1	4.65	1.49	1.40
30	A	1584	MA6	C6-N6	3.55	1.46	1.36
30	A	1583	MA6	C6-N6	3.50	1.46	1.36
30	A	1486	B8T	C6-N1	3.44	1.46	1.38
30	A	1486	B8T	C5-C4	3.30	1.48	1.41
30	A	1486	B8T	O2-C2	-2.92	1.18	1.23
30	A	1584	MA6	C5-C4	-2.82	1.34	1.39
30	A	1583	MA6	C5-C4	-2.76	1.34	1.39
30	A	1583	MA6	C5-N7	-2.49	1.34	1.39
30	A	1584	MA6	C5-N7	-2.47	1.34	1.39
30	A	1584	MA6	C8-N9	-2.04	1.34	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1583	MA6	N1-C6-N6	-11.17	103.25	116.86
30	A	1584	MA6	N1-C6-N6	-11.16	103.25	116.86
30	A	1584	MA6	C5-C6-N6	7.07	136.52	125.33
30	A	1583	MA6	C5-C6-N6	6.99	136.39	125.33
30	A	1583	MA6	N1-C2-N3	-5.58	120.14	128.58
30	A	1584	MA6	N1-C2-N3	-5.55	120.19	128.58
30	A	1583	MA6	C5-C4-N3	-5.03	119.78	126.72
30	A	1584	MA6	C5-C4-N3	-4.97	119.87	126.72
30	A	1584	MA6	N9-C8-N7	-4.16	108.03	113.94
30	A	1583	MA6	N9-C8-N7	-3.99	108.28	113.94
30	A	1584	MA6	C4-C5-C6	3.91	119.96	115.91
30	A	1583	MA6	C4-C5-C6	3.79	119.83	115.91
30	A	1583	MA6	C2-N3-C4	3.41	120.17	111.83
30	A	1584	MA6	C2-N3-C4	3.35	120.00	111.83
30	A	1584	MA6	C2-N1-C6	3.24	119.75	111.83
30	A	1583	MA6	C2-N1-C6	3.23	119.72	111.83
30	A	1583	MA6	N3-C4-N9	2.99	132.25	127.17
30	A	1584	MA6	N3-C4-N9	2.96	132.20	127.17
30	A	1584	MA6	C5-N7-C8	2.88	107.97	103.45
30	A	1583	MA6	C5-N7-C8	2.79	107.84	103.45
7	I	184	5F0	O-C-CB	-2.72	117.45	125.38
30	A	1486	B8T	C6-C5-C4	2.62	120.15	117.00
30	A	1584	MA6	C4-C5-N7	-2.24	108.03	110.58
30	A	1584	MA6	C4-N9-C8	2.19	108.04	105.74
30	A	1583	MA6	C4-C5-N7	-2.14	108.14	110.58

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	1583	MA6	O4'-C4'-C5'-O5'
30	A	1584	MA6	O4'-C4'-C5'-O5'
30	A	1583	MA6	C3'-C4'-C5'-O5'
30	A	1584	MA6	C3'-C4'-C5'-O5'
30	A	1486	B8T	C4'-C5'-O5'-P
30	A	1486	B8T	C2'-C1'-N1-C6
30	A	1583	MA6	C4'-C5'-O5'-P
30	A	1488	5MC	O4'-C4'-C5'-O5'
30	A	1584	MA6	C4'-C5'-O5'-P
30	A	1486	B8T	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	184	5F0	1	0
30	A	1488	5MC	1	0
30	A	1583	MA6	3	0
30	A	1584	MA6	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 32 are monoatomic - leaving 6 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	$\# Z  > 2$
36	ATP	X	501	-	32,33,33	0.34	0	48,52,52	0.63	1 (2%)
34	FES	M	201	-	0,4,4	-	-	-		
37	GDP	X	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	6 (13%)
38	NAD	A	1731	33	46,48,48	1.20	3 (6%)	64,73,73	0.77	2 (3%)
39	SPM	A	1732	-	13,13,13	0.35	0	12,12,12	0.98	0
34	FES	P	201	4,14	0,4,4	-	-	-		

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
36	ATP	X	501	-	-	5/22/38/38	0/3/3/3
34	FES	P	201	4,14	-	-	0/1/1/1
37	GDP	X	502	-	-	0/16/32/32	0/3/3/3
38	NAD	A	1731	33	-	4/30/62/62	0/5/5/5
39	SPM	A	1732	-	-	0/11/11/11	-
34	FES	M	201	-	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A	1731	NAD	PA-O3	5.32	1.65	1.59
38	A	1731	NAD	PN-O3	3.59	1.63	1.59
37	X	502	GDP	C5-C4	3.08	1.47	1.38
37	X	502	GDP	C6-N1	-2.45	1.34	1.38
38	A	1731	NAD	O4D-C1D	-2.39	1.37	1.40
37	X	502	GDP	C5-N7	-2.07	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	X	502	GDP	C5-C4-N3	-5.93	118.95	128.39
37	X	502	GDP	C2-N3-C4	5.05	121.00	112.30
37	X	502	GDP	N9-C4-N3	4.43	134.81	125.95
37	X	502	GDP	C6-C5-N7	3.47	136.60	130.29
37	X	502	GDP	C4-C5-N7	-2.59	106.56	110.67
38	A	1731	NAD	O2A-PA-O1A	2.30	123.16	112.44
38	A	1731	NAD	O3-PA-O1A	-2.15	104.25	110.70
37	X	502	GDP	O6-C6-C5	-2.02	121.20	126.53
36	X	501	ATP	O3'-C3'-C2'	-2.01	105.37	111.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	A	1731	NAD	C5B-O5B-PA-O1A
38	A	1731	NAD	O4B-C4B-C5B-O5B
38	A	1731	NAD	C3B-C4B-C5B-O5B
36	X	501	ATP	C3'-C4'-C5'-O5'
36	X	501	ATP	PB-O3A-PA-O2A
36	X	501	ATP	C4'-C5'-O5'-PA
36	X	501	ATP	PB-O3A-PA-O1A
38	A	1731	NAD	PA-O3-PN-O2N
36	X	501	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 5 short contacts:

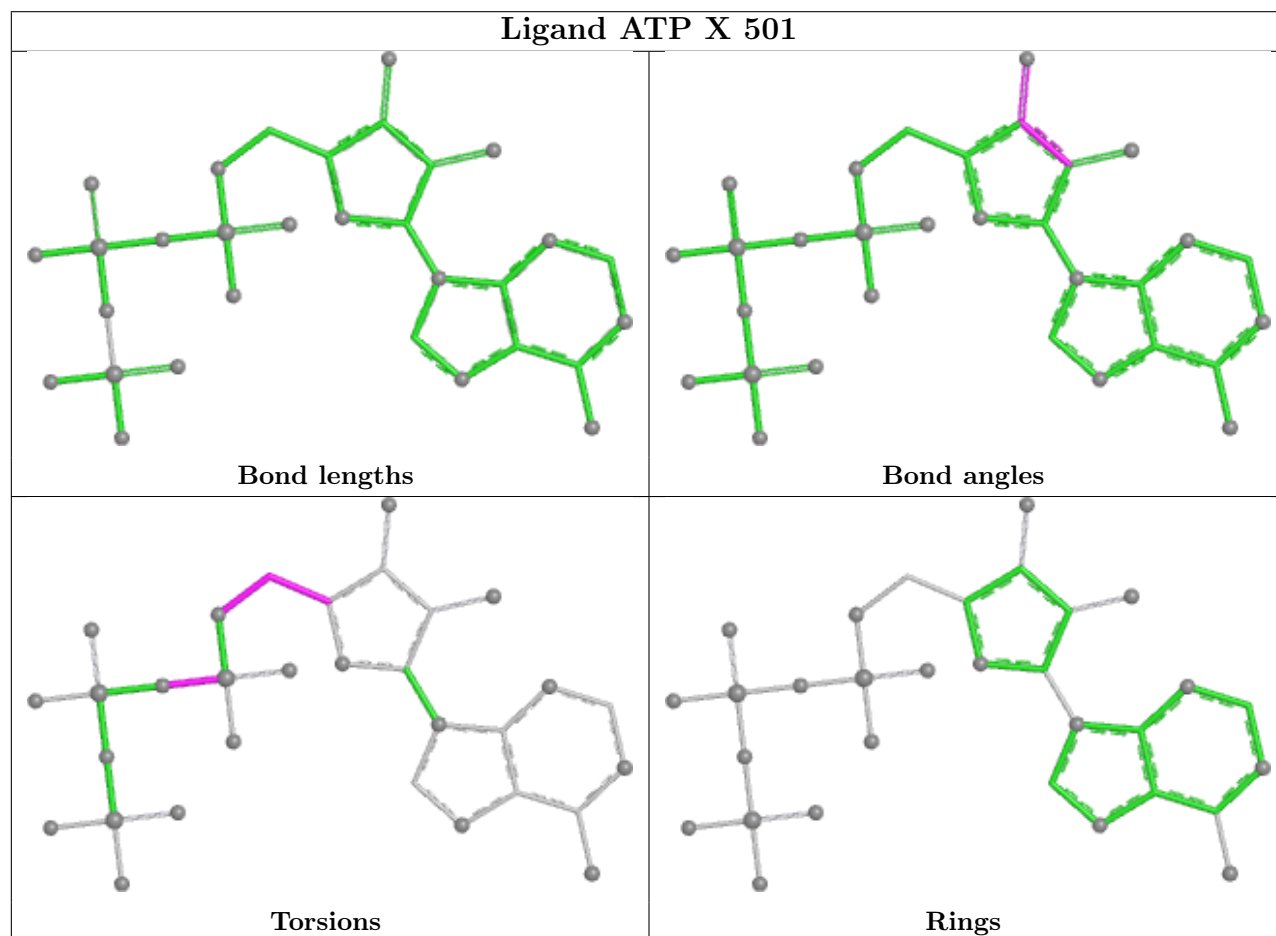
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	X	502	GDP	1	0
39	A	1732	SPM	3	0

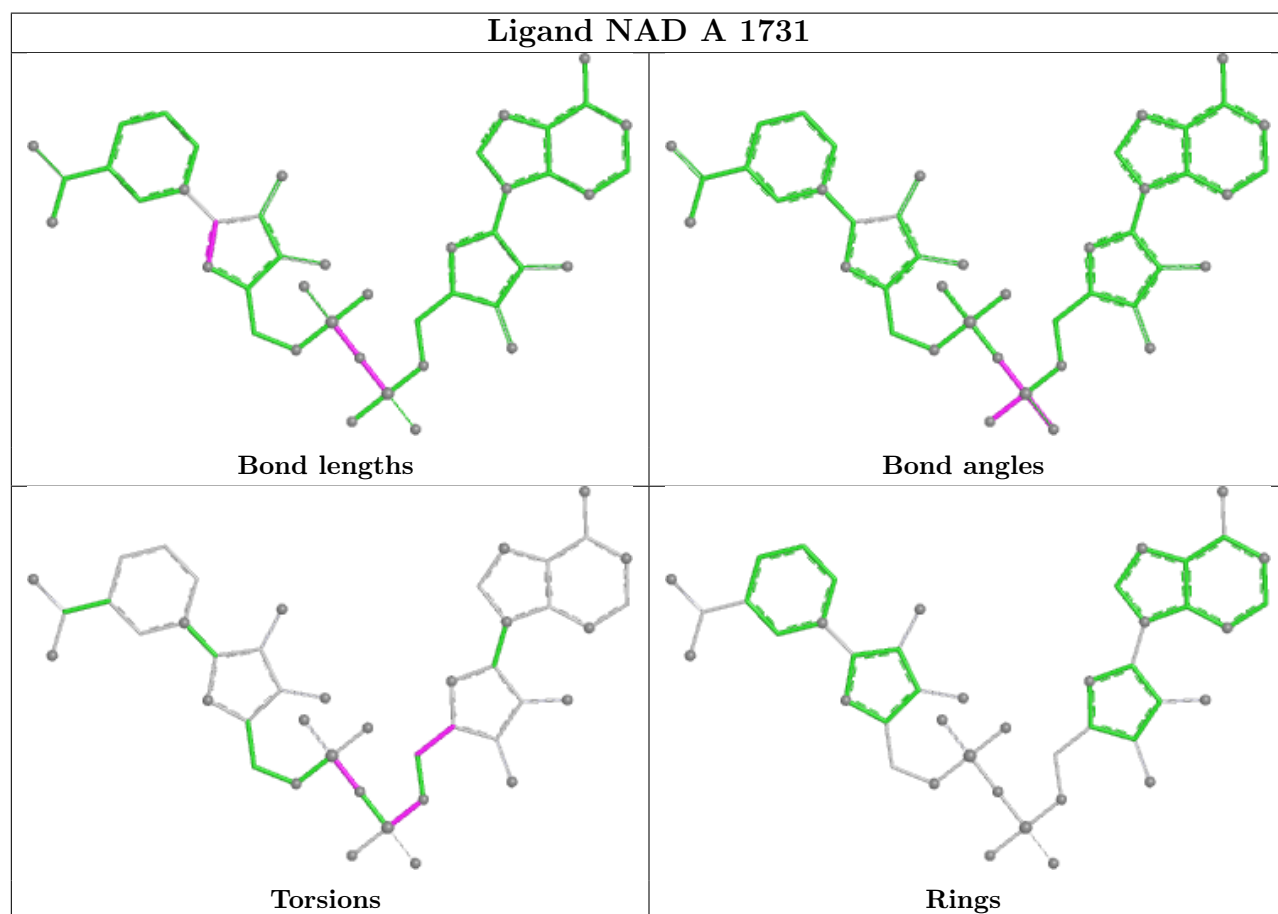
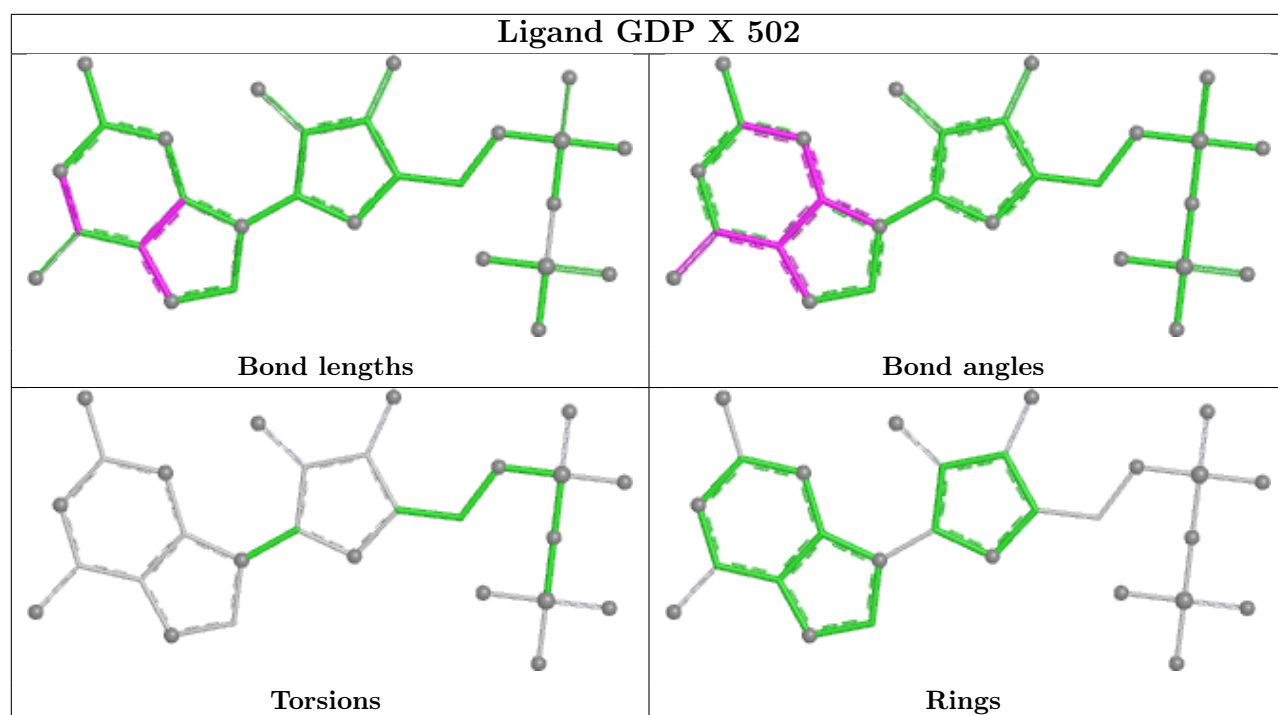
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	P	201	FES	1	0

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 than 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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1486:B8T	O3'	1487:C	P	3.78
1	A	1485:G	O3'	1486:B8T	P	3.32

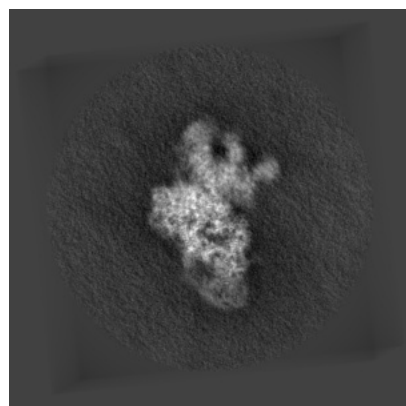
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52858. These allow visual inspection of the internal detail of the map and identification of artifacts.

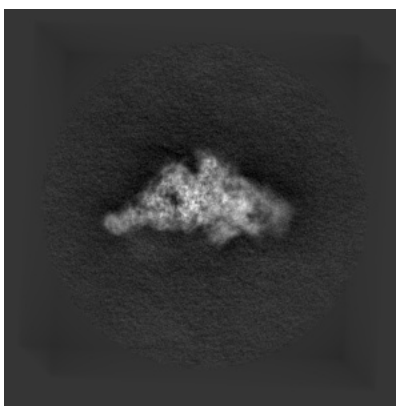
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

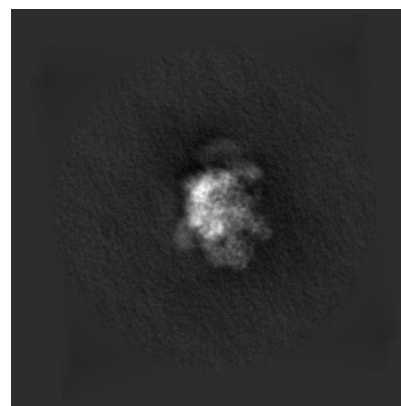
#### 6.1.1 Primary map



X

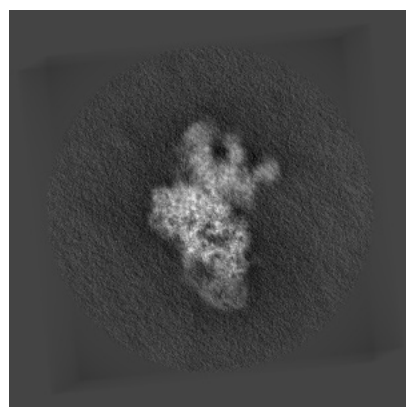


Y

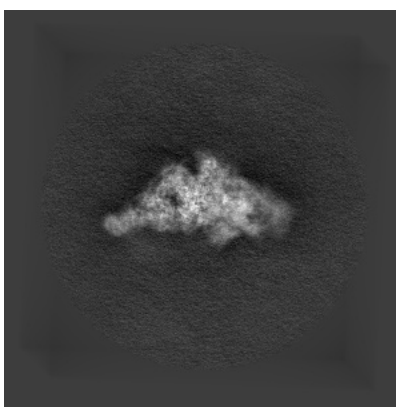


Z

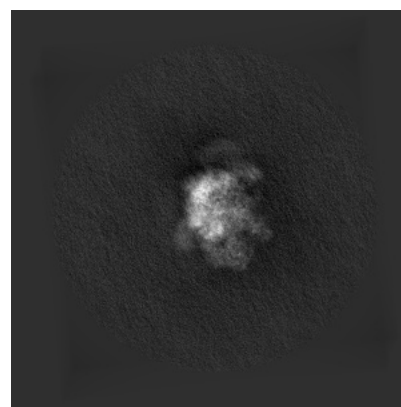
#### 6.1.2 Raw map



X



Y

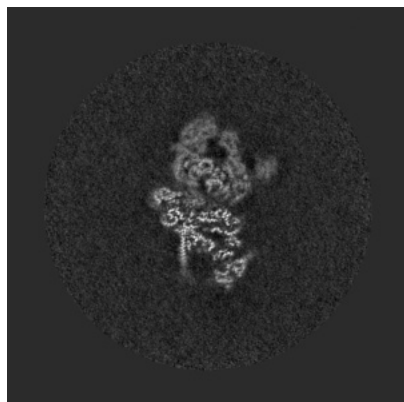


Z

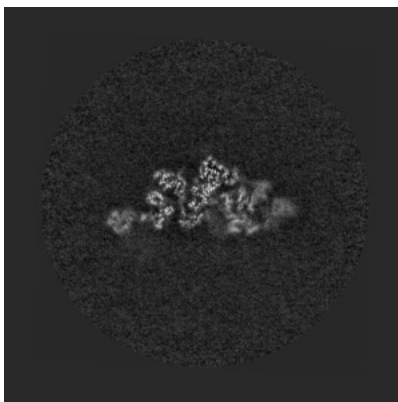
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

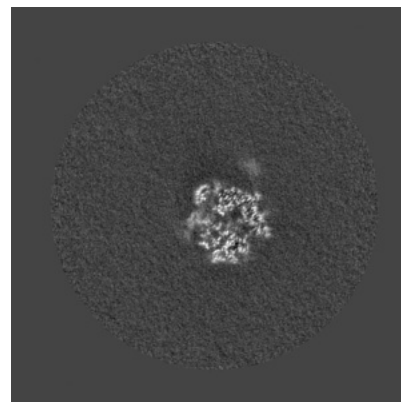
### 6.2.1 Primary map



X Index: 300

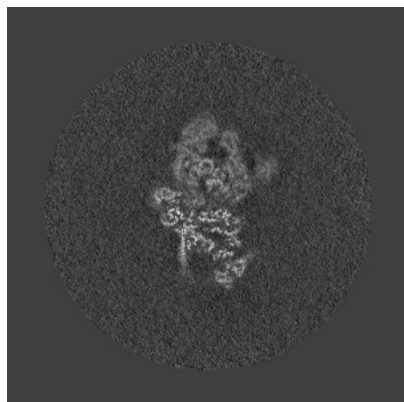


Y Index: 300

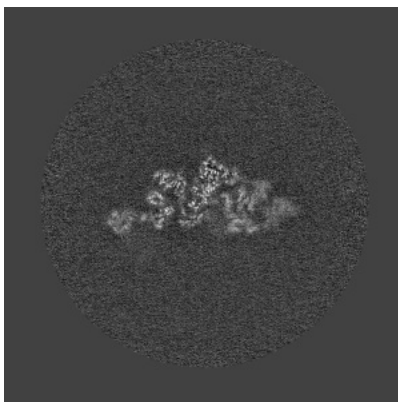


Z Index: 300

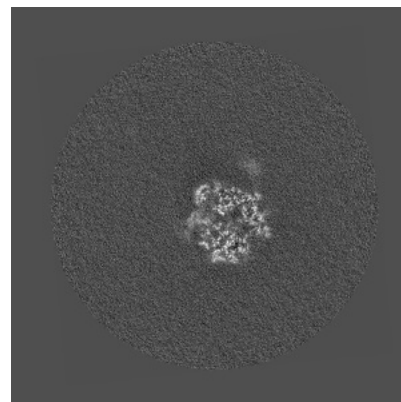
### 6.2.2 Raw map



X Index: 300



Y Index: 300

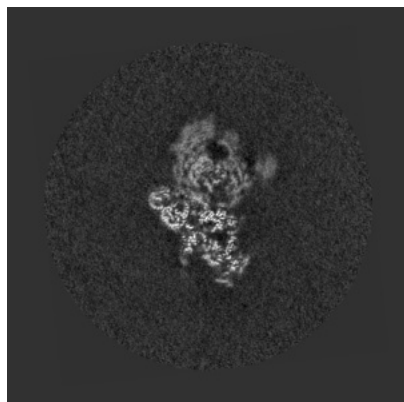


Z Index: 300

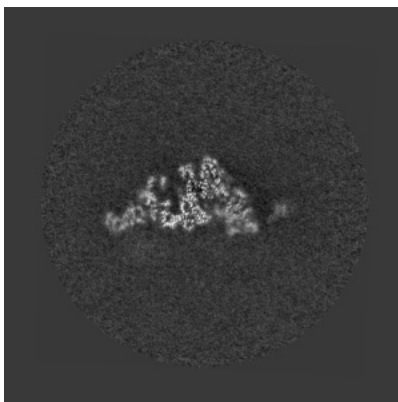
The images above show central slices of the map in three orthogonal directions.

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

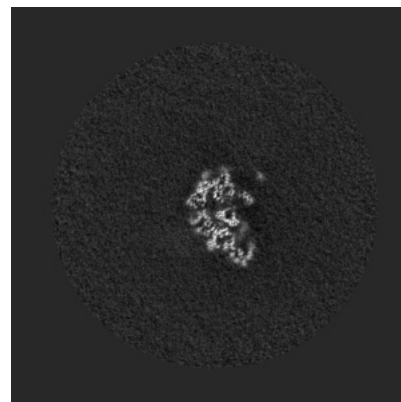
### 6.3.1 Primary map



X Index: 305

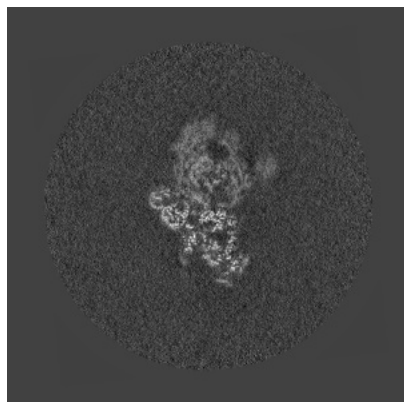


Y Index: 312

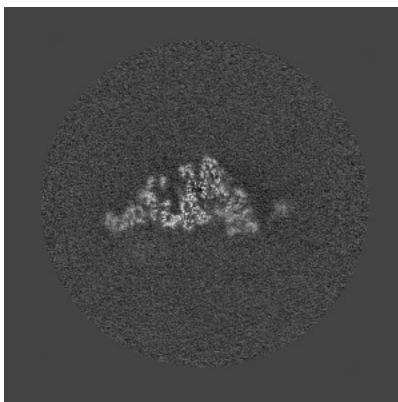


Z Index: 273

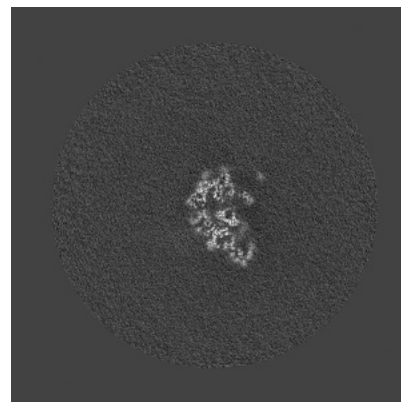
### 6.3.2 Raw map



X Index: 305



Y Index: 312

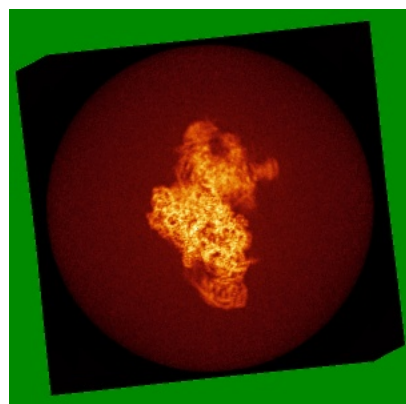


Z Index: 273

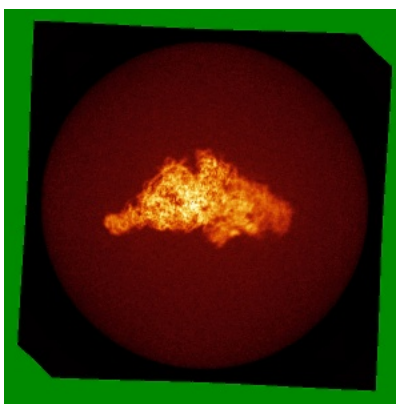
The images above show the largest variance slices of the map in three orthogonal directions.

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

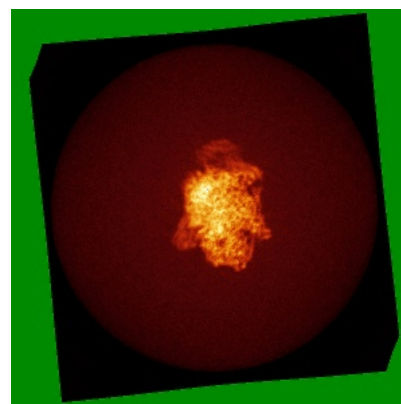
### 6.4.1 Primary map



X

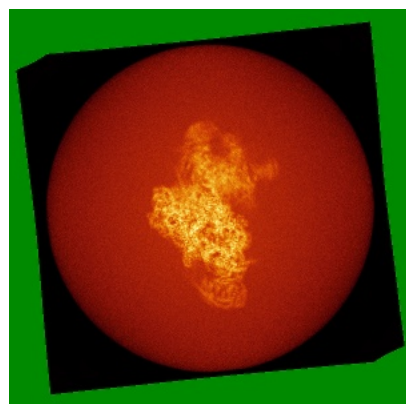


Y

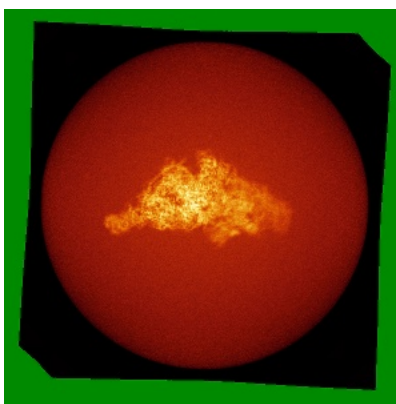


Z

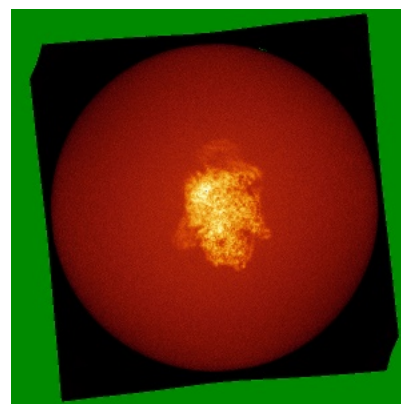
### 6.4.2 Raw map



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.

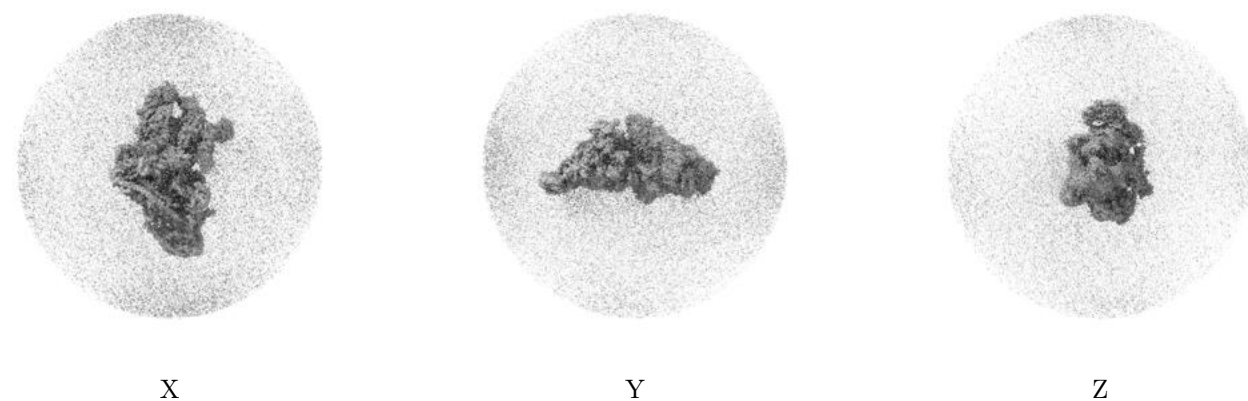
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

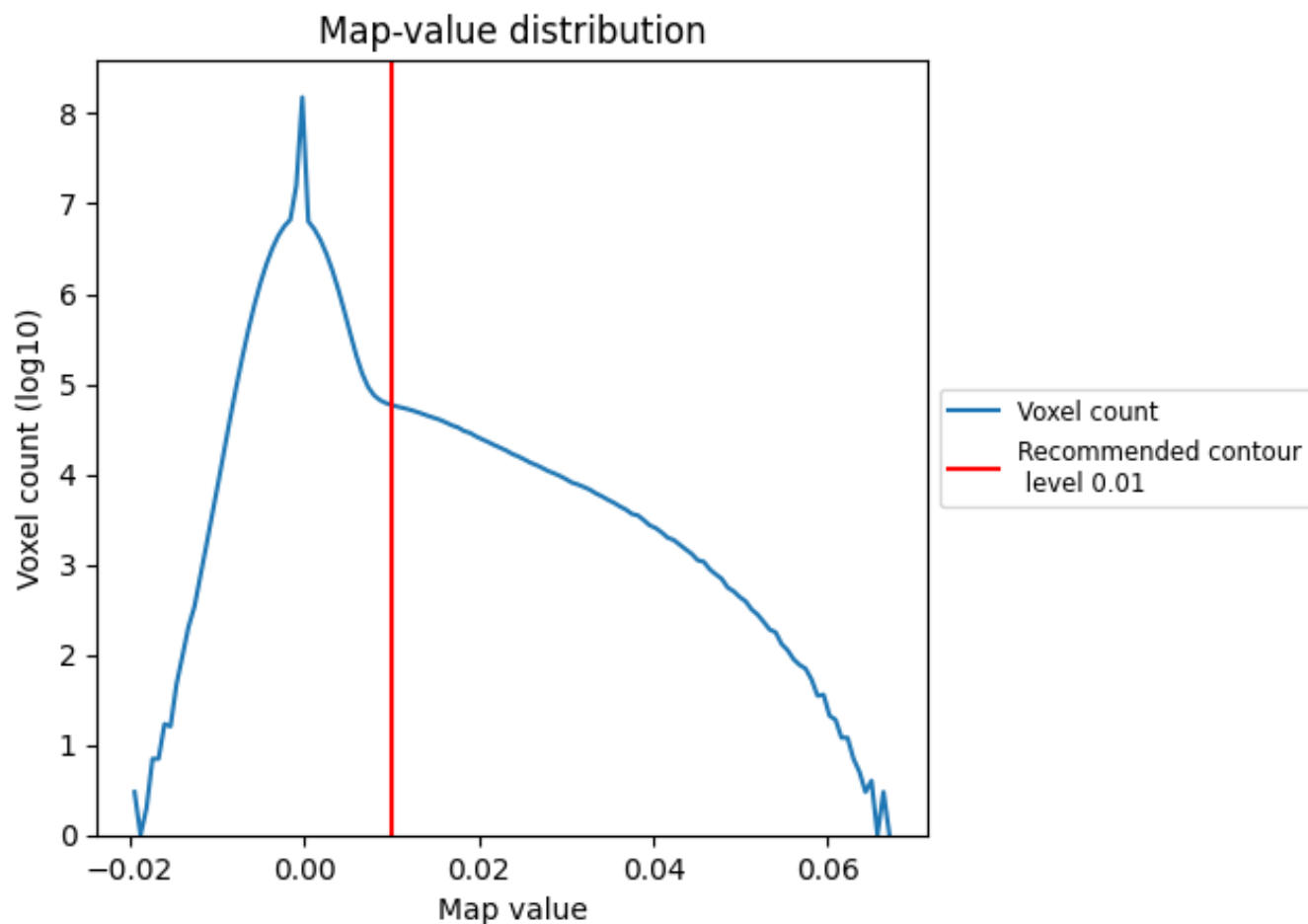
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

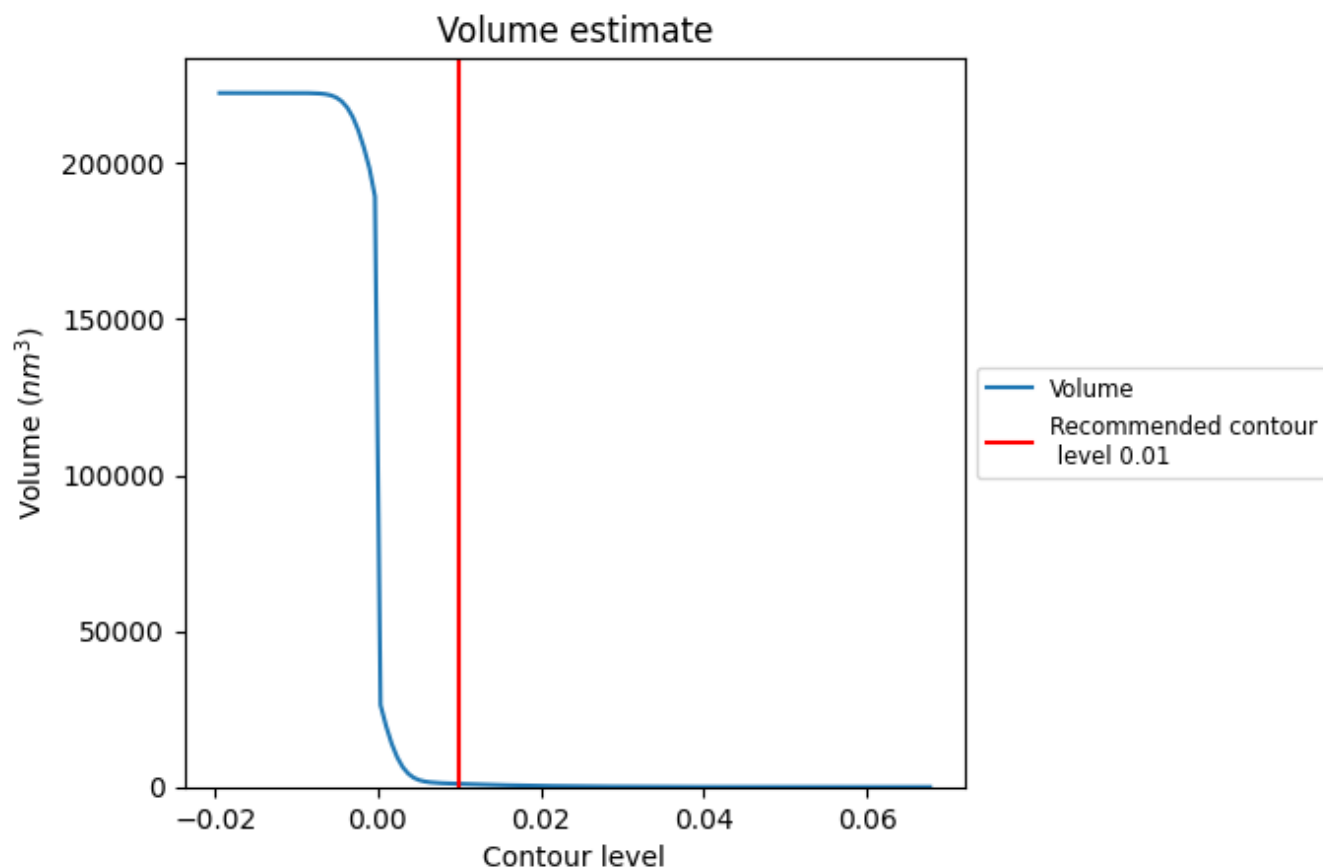
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

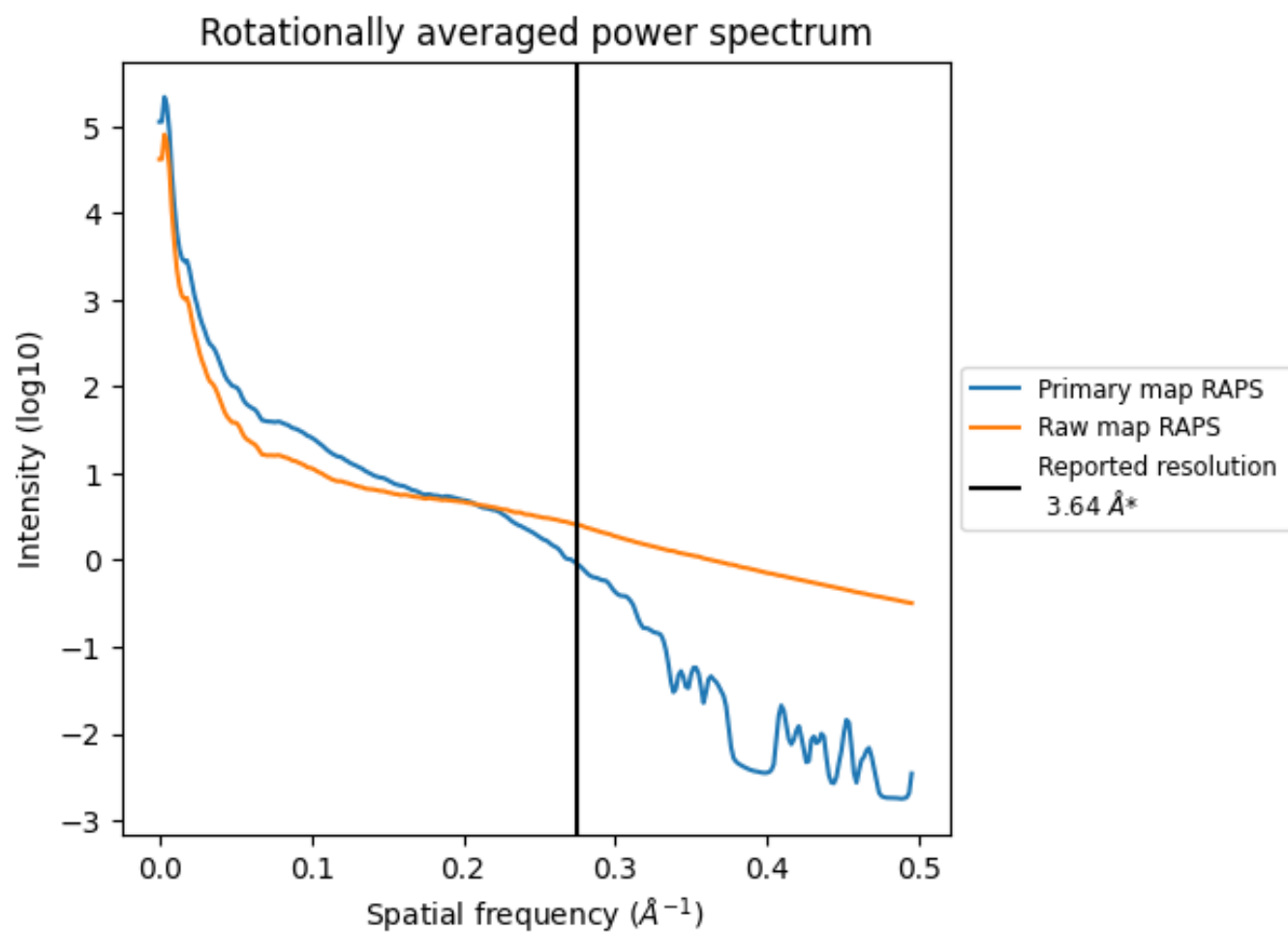
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 997  $\text{nm}^3$ ; this corresponds to an approximate mass of 901 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 ⓘ

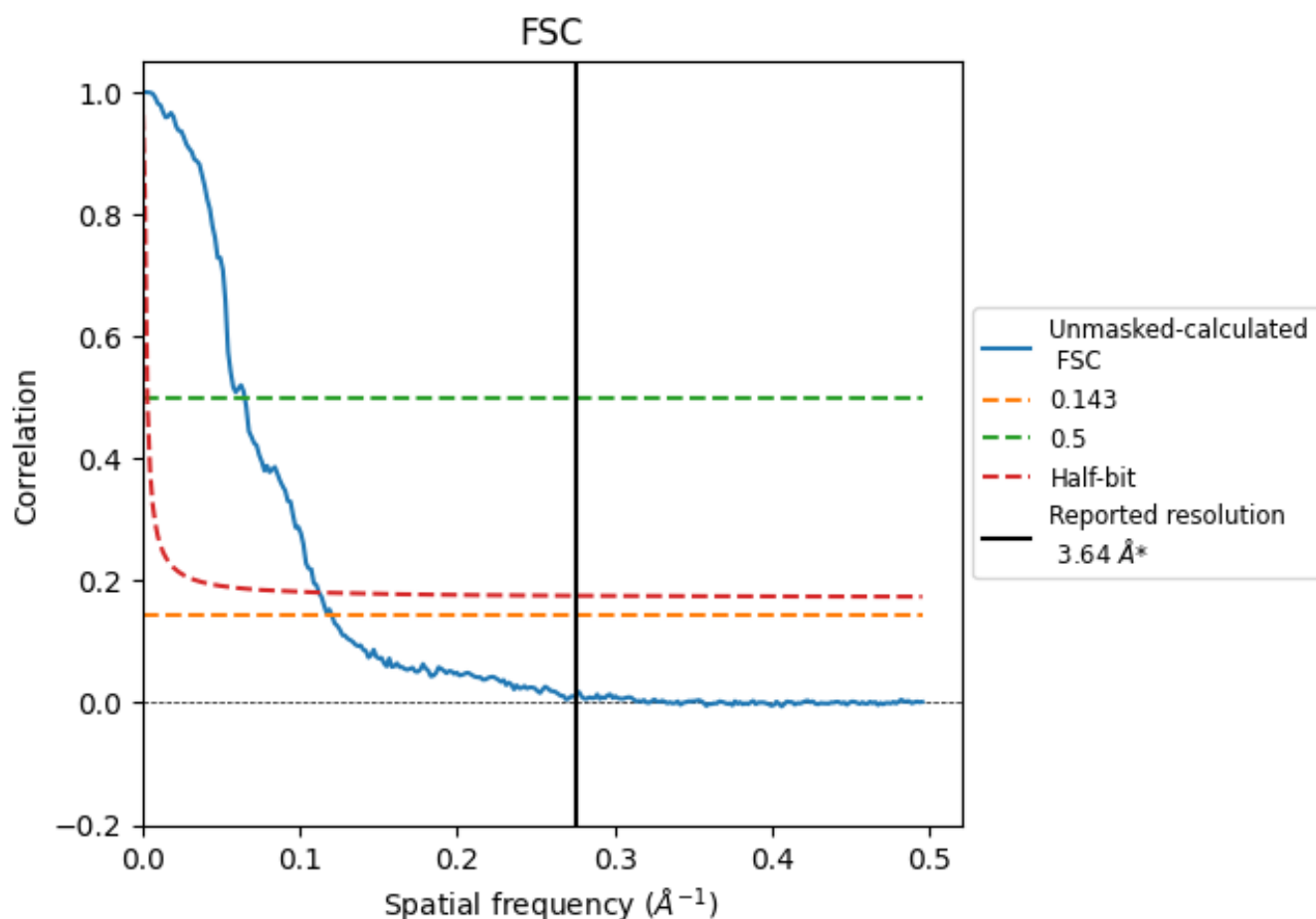


\*Reported resolution corresponds to spatial frequency of 0.275 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

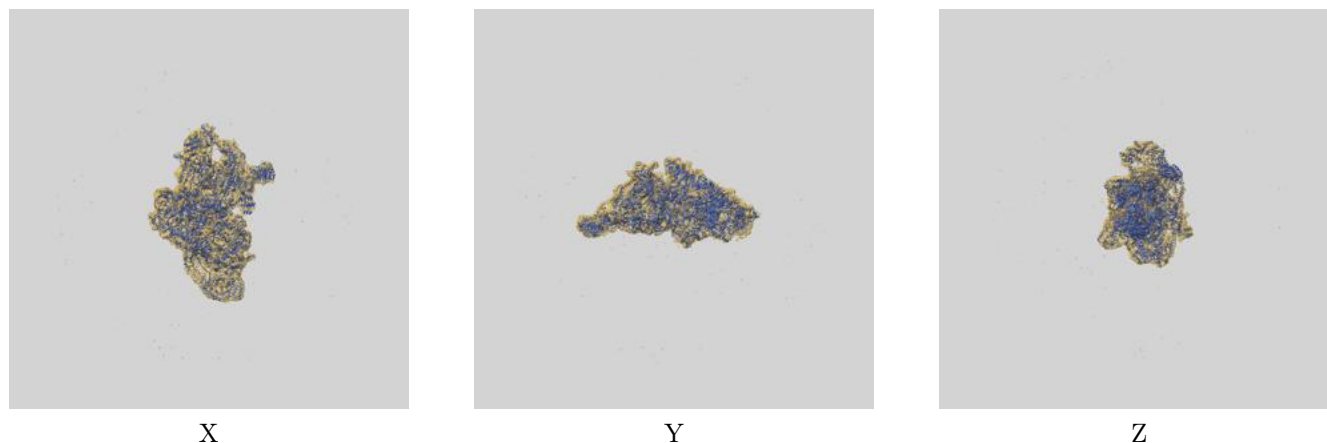
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.31	15.38	8.91

\*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 8.31 differs from the reported value 3.64 by more than 10 %

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

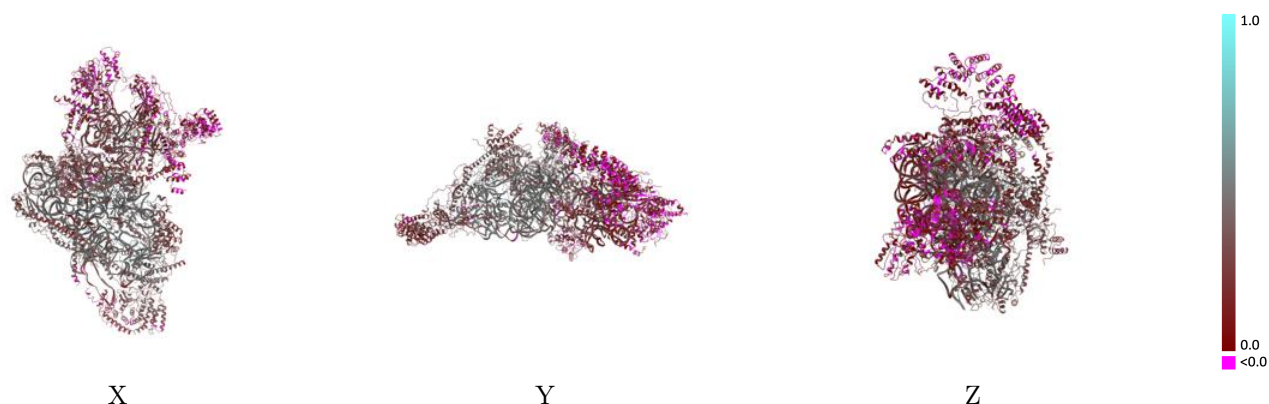
This section contains information regarding the fit between EMDB map EMD-52858 and PDB model 9IGU. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



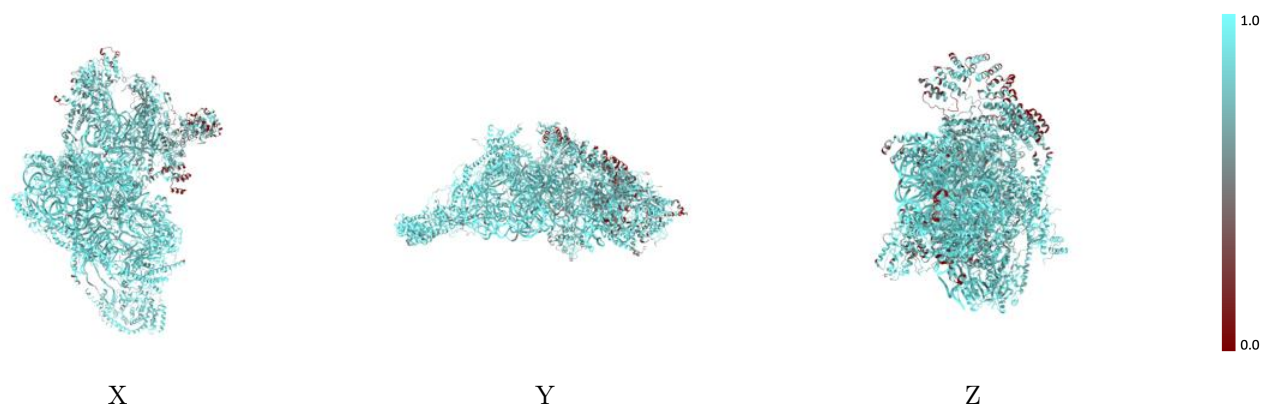
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



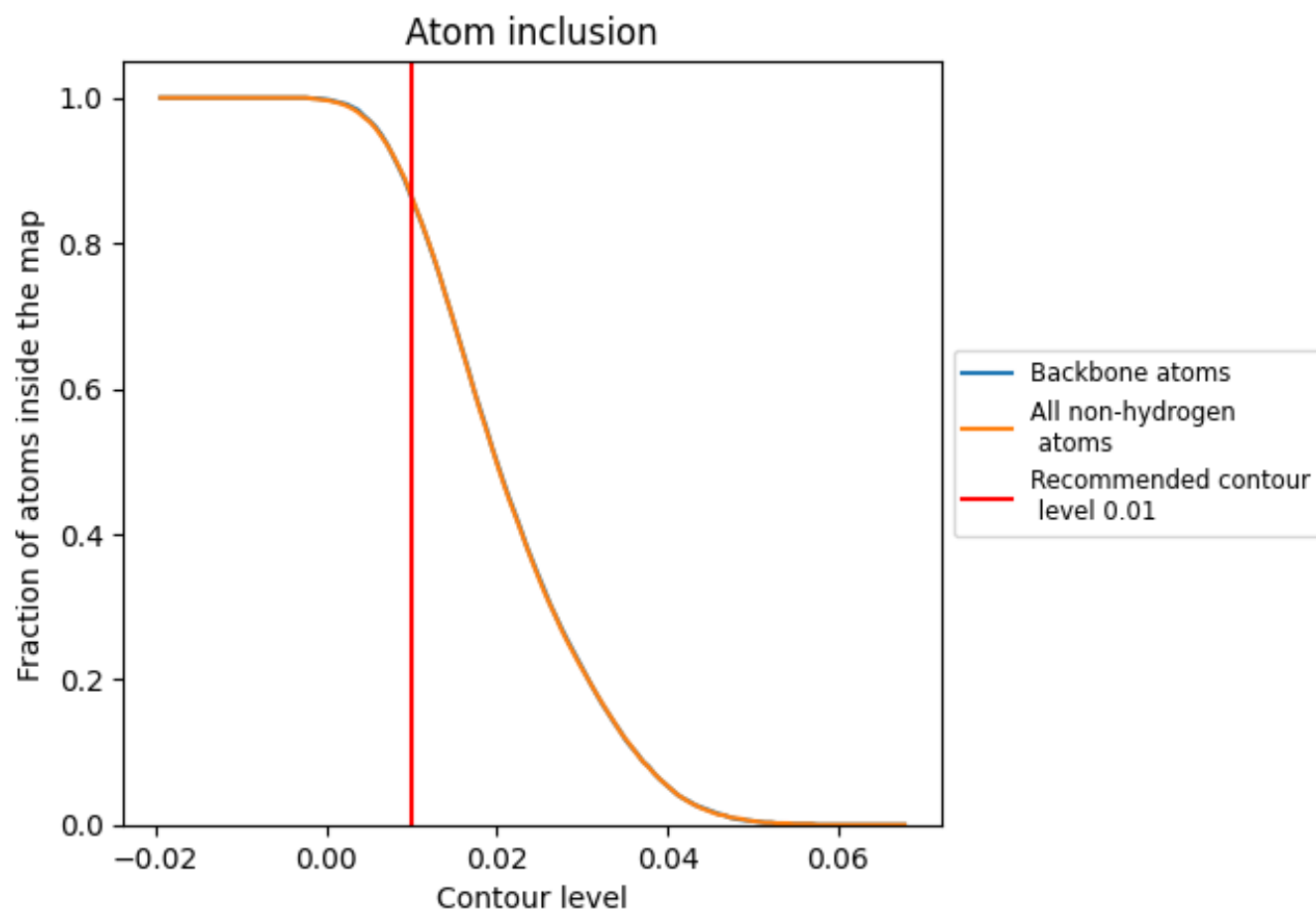
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).



































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.2900
0	 0.8820	 0.3240
1	 0.7360	 0.1220
3	 0.8610	 0.3590
4	 0.6280	 0.0850
A	 0.9690	 0.3730
B	 0.8830	 0.3460
C	 0.8510	 0.2850
D	 0.8630	 0.3720
E	 0.8860	 0.3530
F	 0.7280	 0.1160
G	 0.8330	 0.1990
H	 0.7670	 0.1900
I	 0.9050	 0.3590
J	 0.9070	 0.4350
K	 0.8800	 0.2540
L	 0.8870	 0.3860
M	 0.9270	 0.4270
N	 0.9250	 0.4430
O	 0.9360	 0.4070
P	 0.8860	 0.3790
Q	 0.8750	 0.3550
R	 0.9090	 0.3730
S	 0.8920	 0.3290
T	 0.9140	 0.4270
U	 0.8870	 0.3400
V	 0.8770	 0.1920
W	 0.9050	 0.3550
X	 0.7740	 0.0790
Y	 0.7190	 0.1220
Z	 0.7700	 0.2040
a	 0.7690	 0.2390
b	 0.8190	 0.1290

