



## Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 02:35 pm BST

PDB ID : 9ROT / pdb\_00009rot  
EMDB ID : EMD-54130  
Title : Assembly intermediate of human mitochondrial ribosome small subunit bound to METTL15, RBFA, and mtIF2 (State M2.1)  
Authors : Khawaja, A.; Singh, V.; Shiriaev, D.I.; Rorbach, J.  
Deposited on : 2025-06-22  
Resolution : 4.30 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:

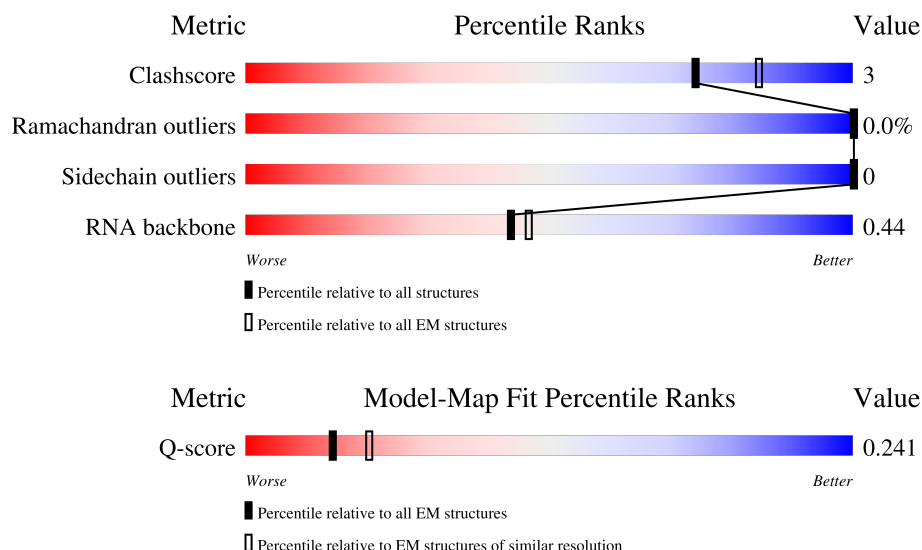
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 4.30 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.





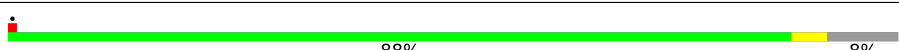
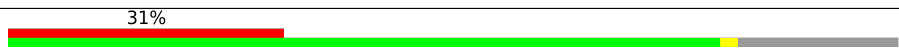

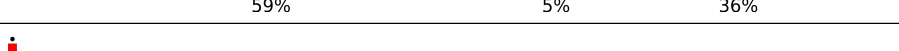
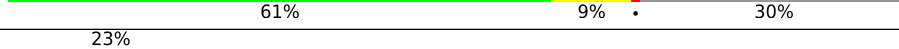





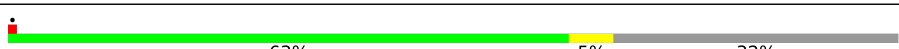

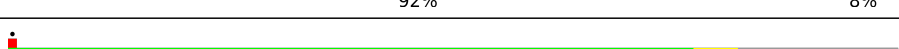
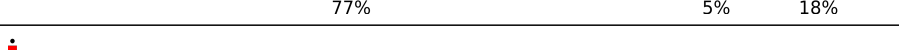

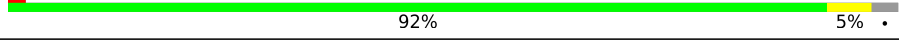






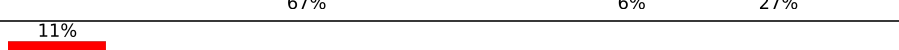
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4585 ( 3.80 - 4.80 )

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	0	218	
2	1	323	
3	3	199	

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Mol	Chain	Length	Quality of chain
4	B	296	
5	C	167	
6	E	125	
7	F	242	
8	H	201	
9	I	194	
10	K	128	
11	L	257	
12	M	137	
13	N	130	
14	O	258	
15	P	142	
16	Q	87	
17	R	360	
18	S	190	
19	T	173	
20	U	205	
21	W	187	
22	X	398	
23	Y	395	
24	Z	106	
25	D	430	
26	G	396	
27	J	138	
28	V	414	

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Mol	Chain	Length	Quality of chain
29	4	689	
30	b	407	
31	A	954	
32	7	727	
33	a	343	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	FES	T	201	-	-	X	-

## 2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 131983 atoms, of which 61276 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 S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	214	Total	C	H	N	O	S	0	0
			3562	1124	1784	337	312	5		

- Molecule 2 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	261	Total	C	H	N	O	S	0	0
			4265	1346	2148	362	399	10		

- Molecule 3 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	3	69	Total	C	H	N	O	S	0	0
			1302	395	686	132	88	1		

- Molecule 4 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B	225	Total	C	H	N	O	S	0	0
			3643	1164	1815	331	323	10		

- Molecule 5 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	C	121	Total	C	H	N	O	S	0	0
			1979	646	985	172	172	4		

- Molecule 6 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 7 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	199	Total	C	H	N	O	S	0	0
			3320	1043	1686	293	287	11		

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	129	Total	C	H	N	O	S	0	0
			2153	688	1089	179	194	3		

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	136	Total	C	H	N	O	S	0	0
			2060	636	1049	191	180	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 10 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 11 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 12 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	119	Total	C	H	N	O	S	0	0
			1907	594	965	185	157	6		

- Molecule 13 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 14 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	O	194	Total	C	H	N	O	S	0	0
			3165	1019	1566	295	278	7		

- Molecule 15 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	97	Total	C	H	N	O	S	0	0
			1588	501	807	134	138	8		

- Molecule 16 is a protein called Small ribosomal subunit protein bS21m.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 17 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 18 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 19 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	168	Total	C	H	N	O	S	0	0
			2764	877	1393	239	244	11		

- Molecule 20 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- 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	118	Total	C	H	N	O	S	0	0
			1949	648	947	165	187	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	94	Total	C	H	N	O	S	0	0
			1612	510	815	143	140	4		

- Molecule 25 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	D	313	Total	C	H	N	O	S	0	0
			5043	1574	2545	469	443	12		

- Molecule 26 is a protein called 28S ribosomal protein S9, mitochondrial.



Mol	Chain	Residues	Atoms						AltConf	Trace
26	G	304	Total	C	H	N	O	S	0	0
			4996	1592	2488	445	457	14		

- Molecule 27 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	J	103	Total	C	H	N	O	S	0	0
			1624	493	830	157	138	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	V	355	Total	C	H	N	O	S	0	0
			5814	1866	2907	485	544	12		

- Molecule 29 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	543	Total	C	H	N	O	S	0	0
			8822	2830	4411	749	806	26		

- Molecule 30 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	b	290	Total	C	H	N	O	S	0	0
			4579	1434	2318	400	415	12		

- Molecule 31 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	A	949	Total	C	H	N	O	P	0	0
			30389	9038	10235	3633	6534	949		

- Molecule 32 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	7	455	Total	C	H	N	O	S	0	0
			7049	2202	3548	612	675	12		

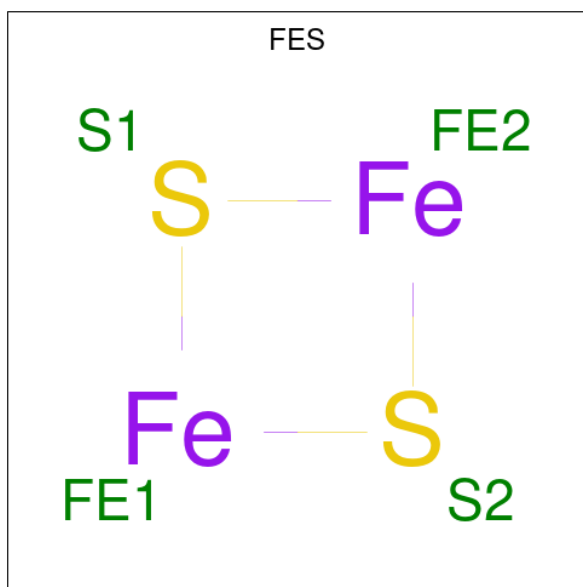
- Molecule 33 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	a	62	Total	C	H	N	O	S	0	0
			955	300	473	81	99	2		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

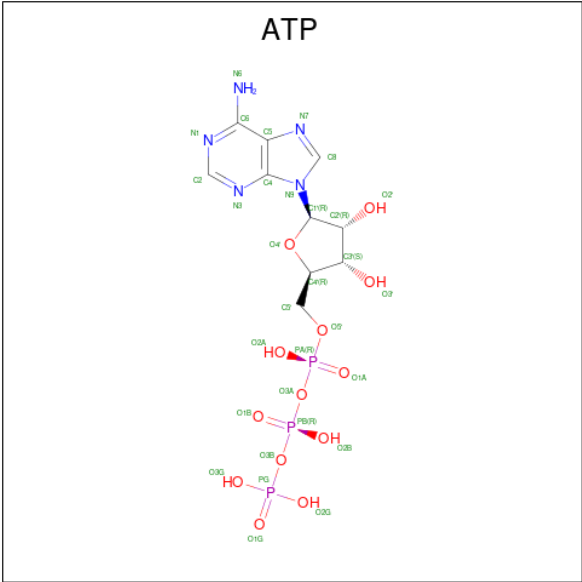
Mol	Chain	Residues	Atoms		AltConf
34	O	1	Total	Zn	0
			1	1	

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



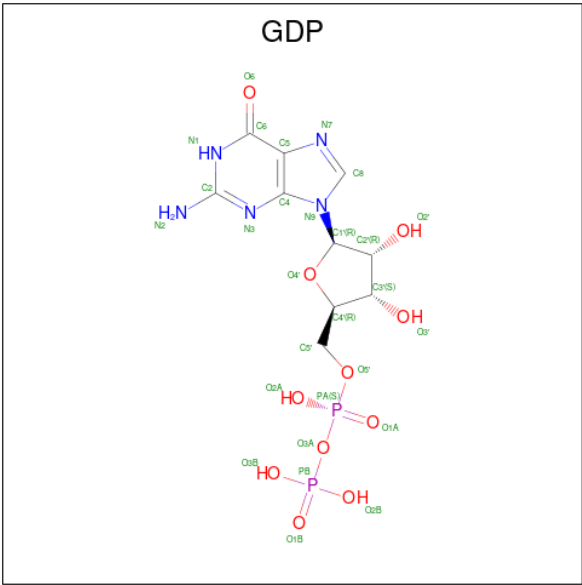
Mol	Chain	Residues	Atoms			AltConf
35	P	1	Total	Fe	S	0
			4	2	2	
35	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

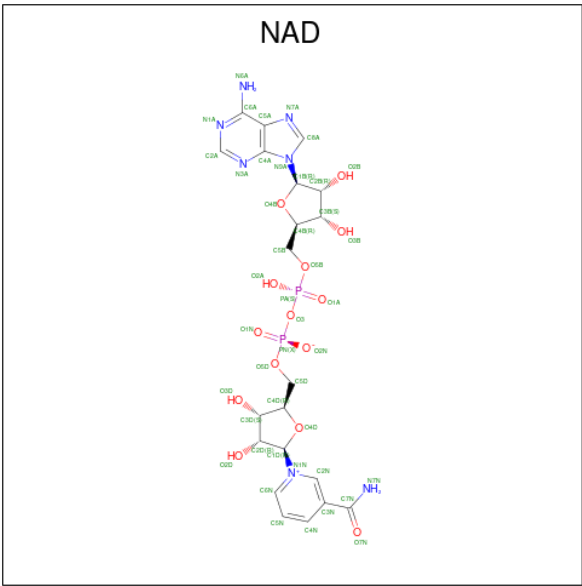
- Molecule 37 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms						AltConf
37	X	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	
37	7	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

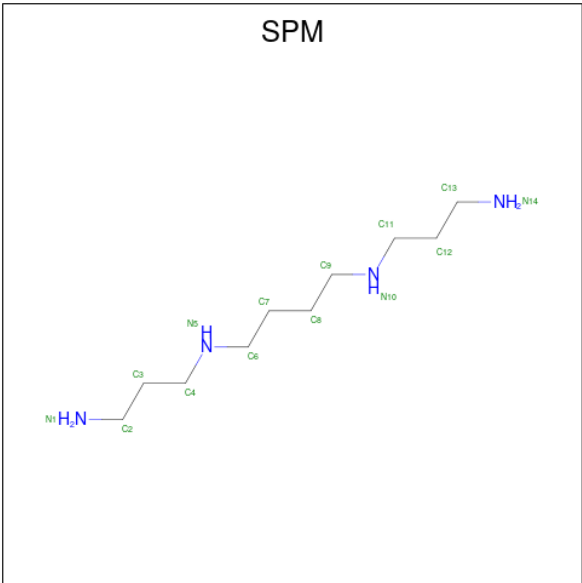
- Molecule 38 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:

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
			Total	C	H	N	O	
38	A	1	70	21	26	7	14	2

- Molecule 39 is SPERMINE (CCD ID: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).



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

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
40	A	11	Total	Mg	0
			11	11	

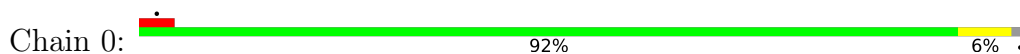
- Molecule 41 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
41	A	8	Total	K	0
			8	8	
41	a	1	Total	K	0
			1	1	

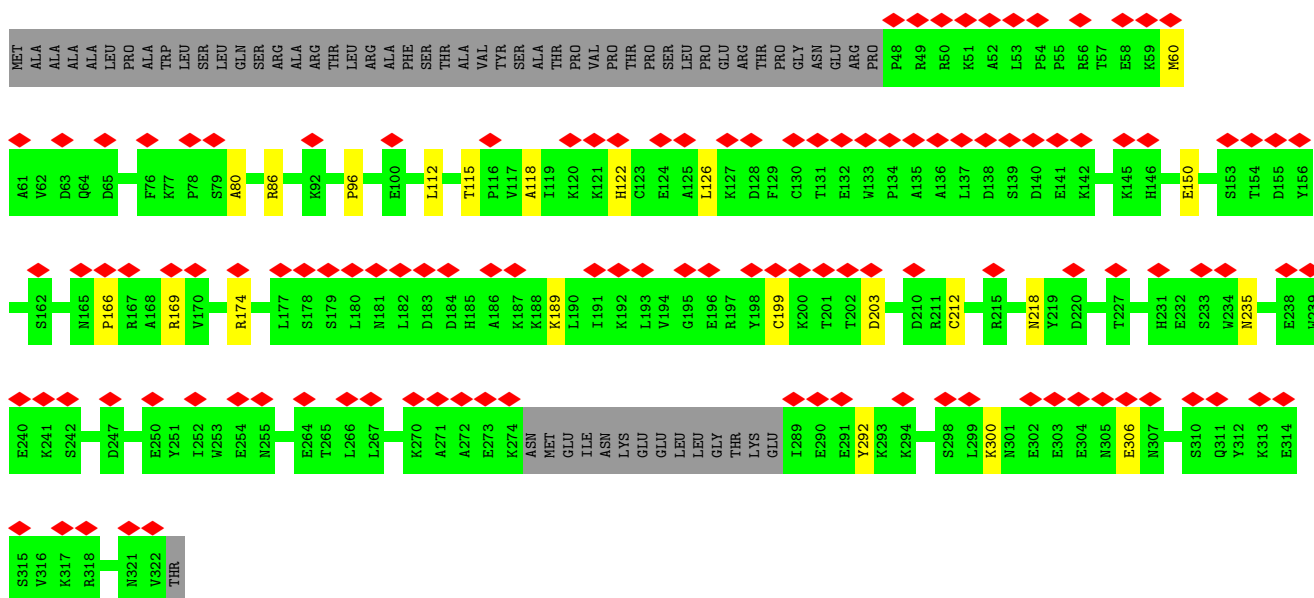
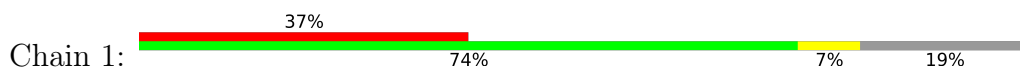
### 3 Residue-property plots

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

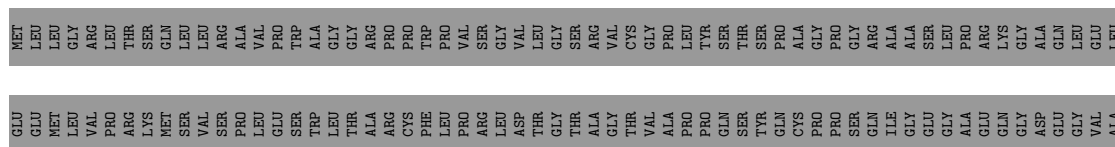
- Molecule 1: 28S ribosomal protein S34, mitochondrial



- Molecule 2: 28S ribosomal protein S35, mitochondrial



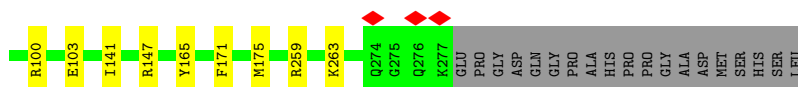
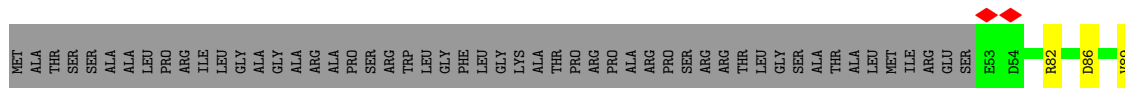
- Molecule 3: Aurora kinase A-interacting protein





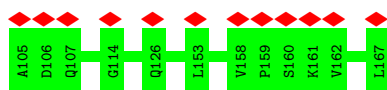
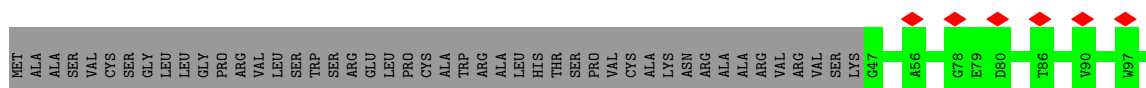
- Molecule 4: 28S ribosomal protein S2, mitochondrial

Chain B: 72% 24%



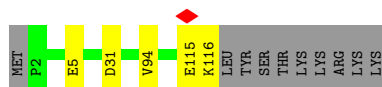
- Molecule 5: 28S ribosomal protein S24, mitochondrial

Chain C: 11% 72% 28%



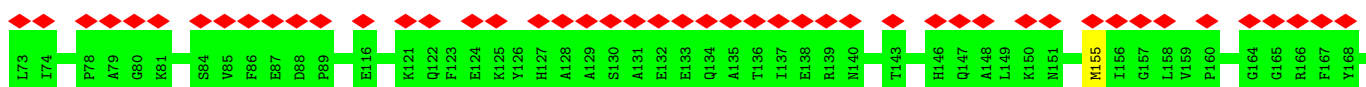
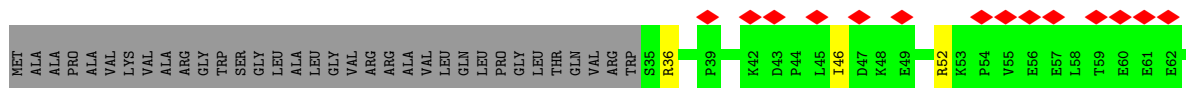
- Molecule 6: 28S ribosomal protein S6, mitochondrial

Chain E: 88% 8%

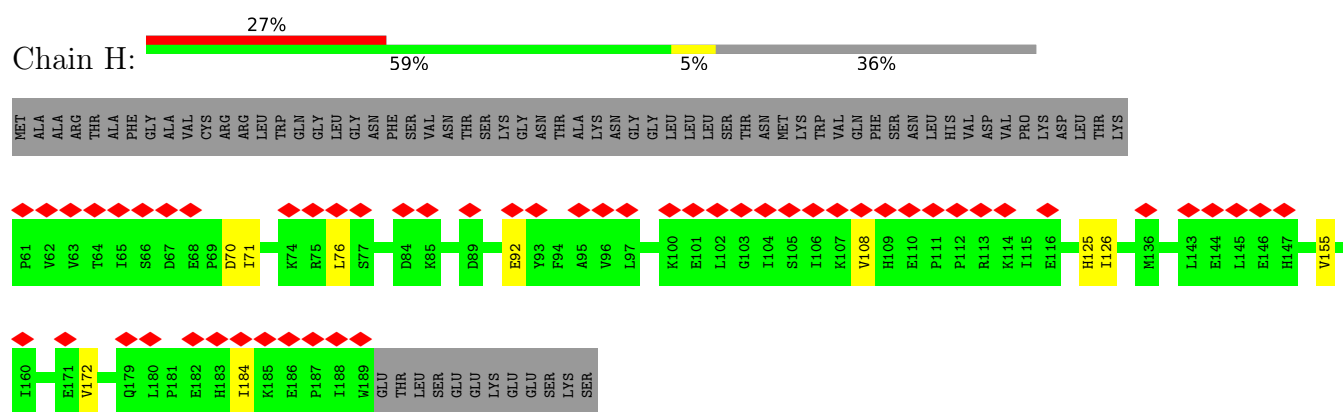


- Molecule 7: 28S ribosomal protein S7, mitochondrial

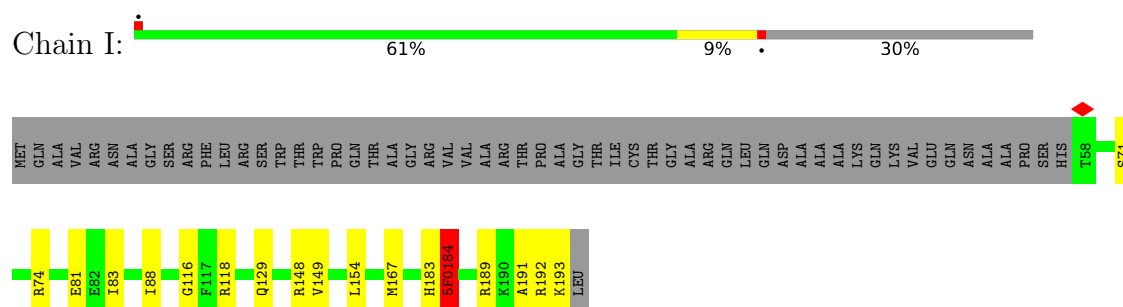
Chain F: 31% 80% 18%



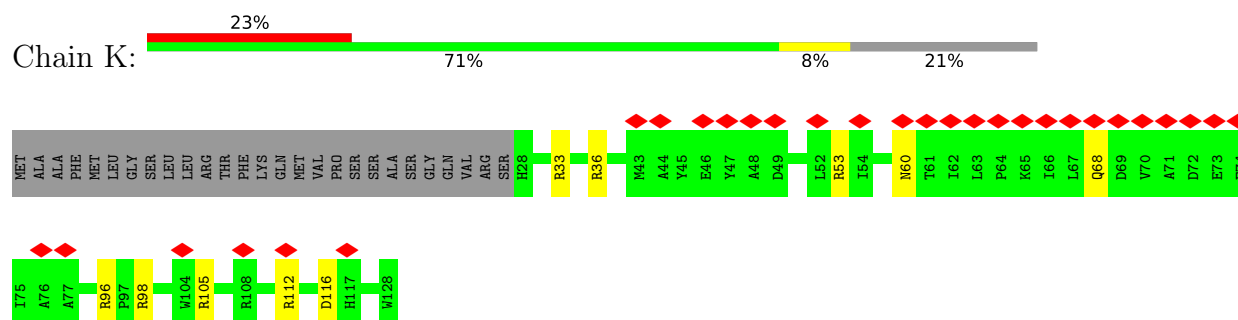
- Molecule 8: 28S ribosomal protein S10, mitochondrial



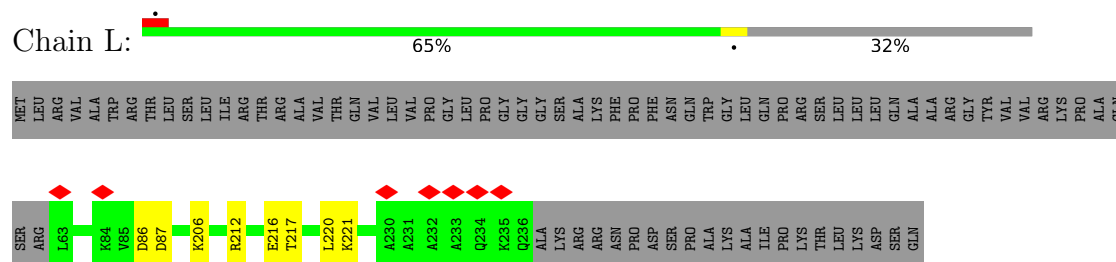
- Molecule 9: 28S ribosomal protein S11, mitochondrial



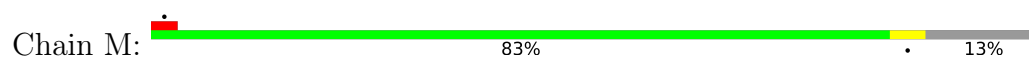
- Molecule 10: 28S ribosomal protein S14, mitochondrial



- Molecule 11: 28S ribosomal protein S15, mitochondrial



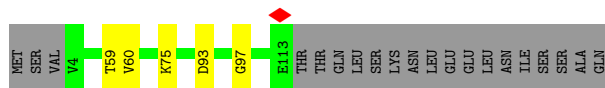
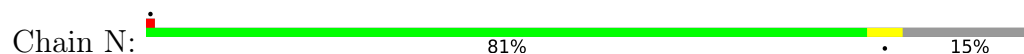
- Molecule 12: 28S ribosomal protein S16, mitochondrial



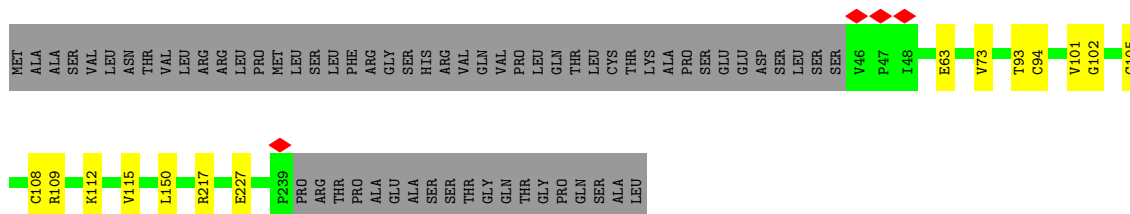




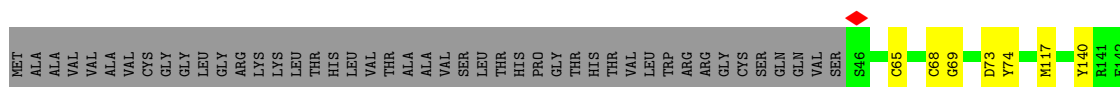
- Molecule 13: 28S ribosomal protein S17, mitochondrial



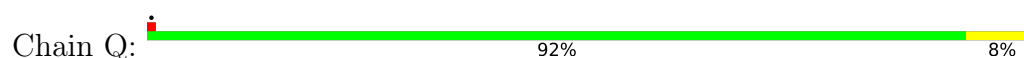
- Molecule 14: 28S ribosomal protein S18b, mitochondrial



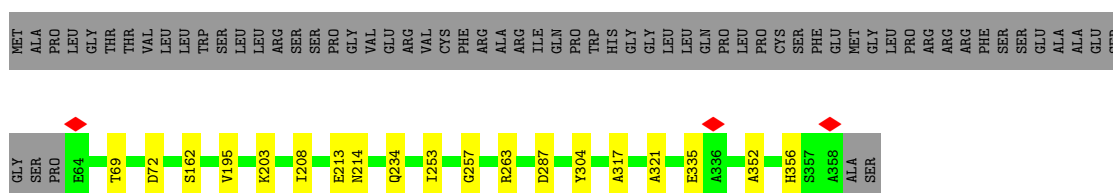
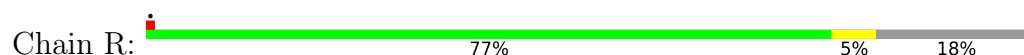
- Molecule 15: 28S ribosomal protein S18c, mitochondrial



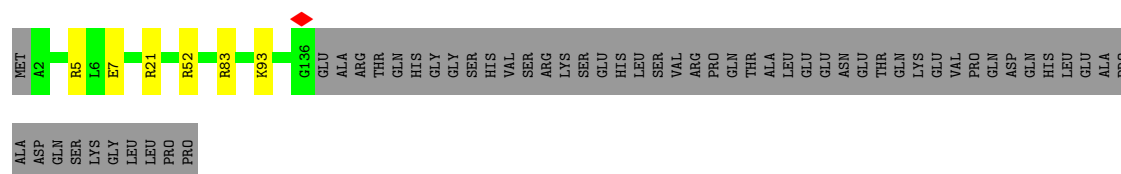
- Molecule 16: Small ribosomal subunit protein bS21m



- Molecule 17: 28S ribosomal protein S22, mitochondrial



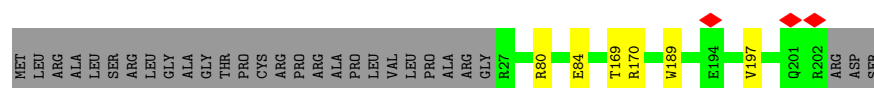
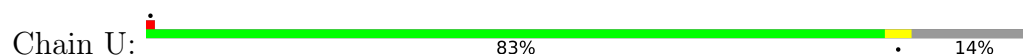
- Molecule 18: 28S ribosomal protein S23, mitochondrial



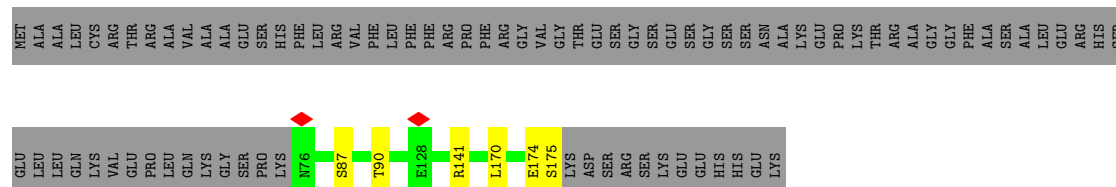
- Molecule 19: 28S ribosomal protein S25, mitochondrial



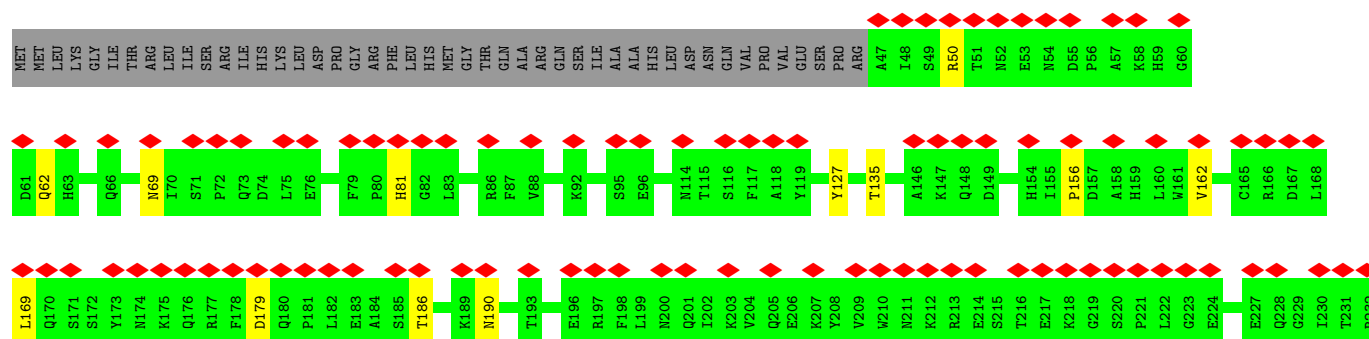
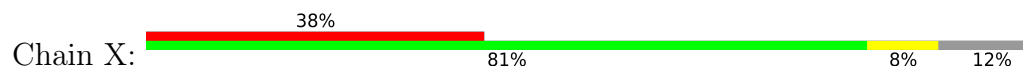
- Molecule 20: 28S ribosomal protein S26, mitochondrial

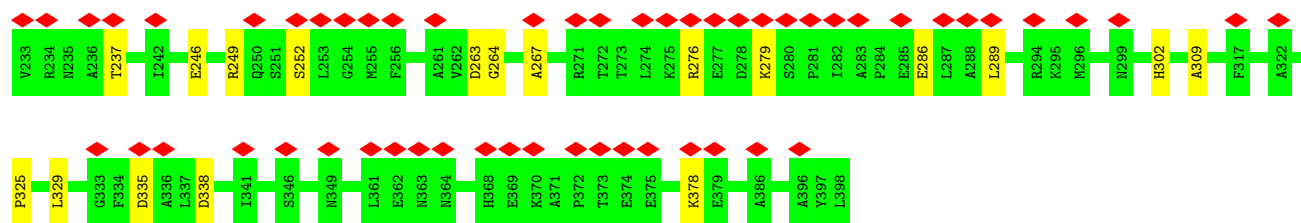


- Molecule 21: 28S ribosomal protein S28, mitochondrial

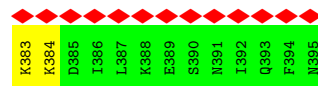
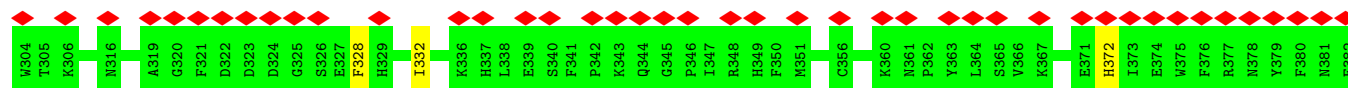
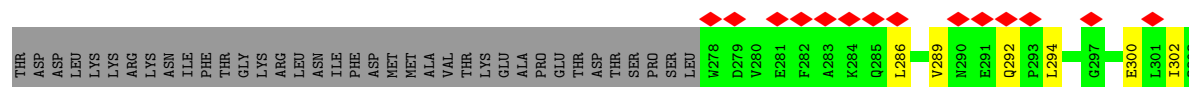
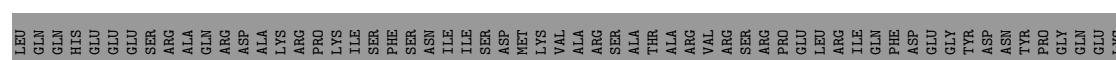
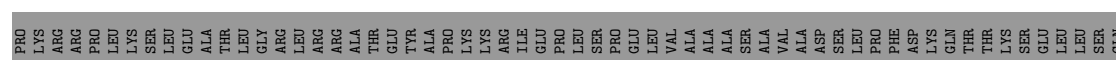
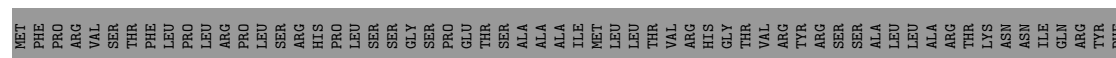


- Molecule 22: 28S ribosomal protein S29, mitochondrial

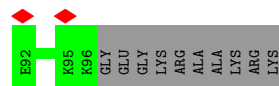
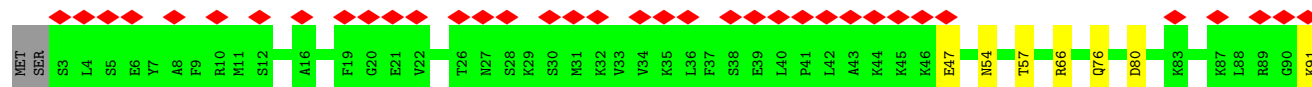
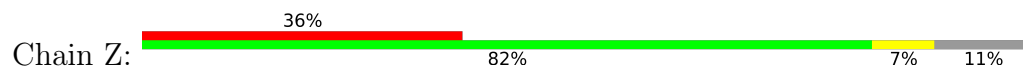




• Molecule 23: 28S ribosomal protein S31, mitochondrial

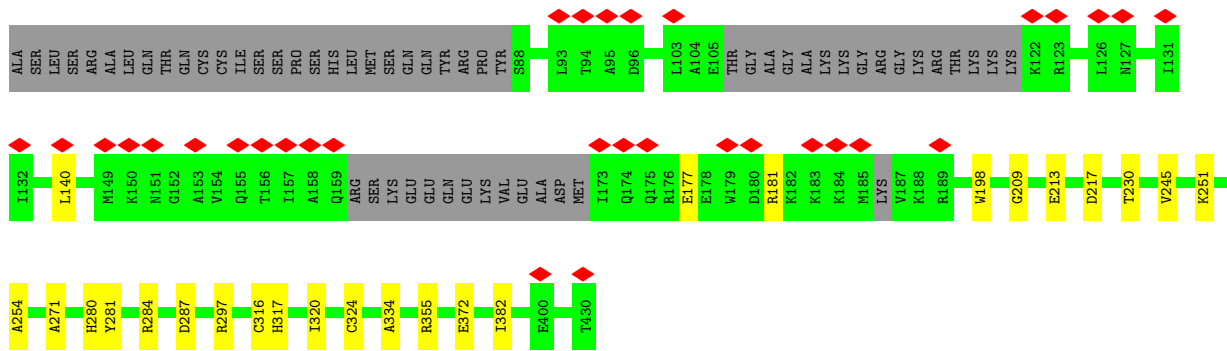


• Molecule 24: 28S ribosomal protein S33, mitochondrial

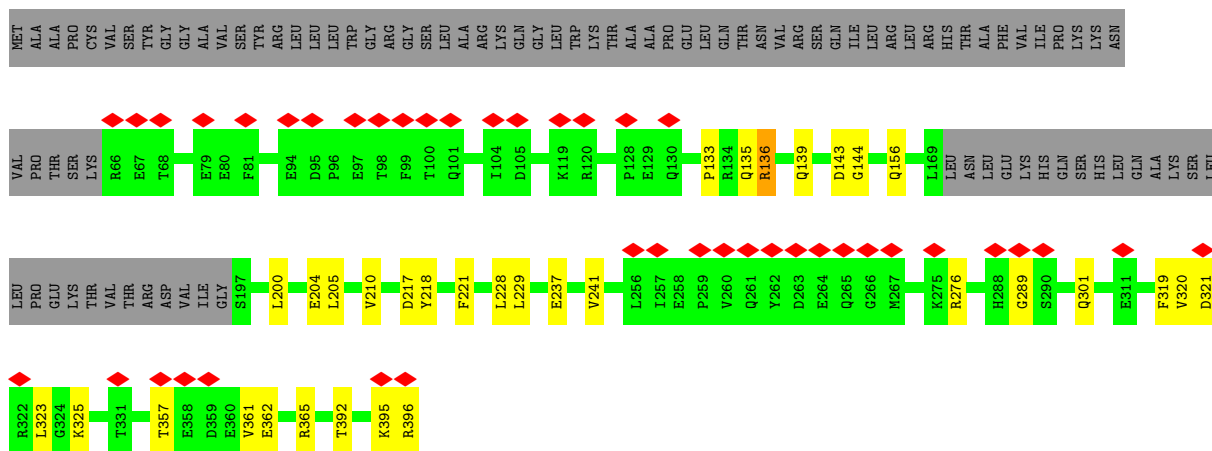


• Molecule 25: 28S ribosomal protein S5, mitochondrial

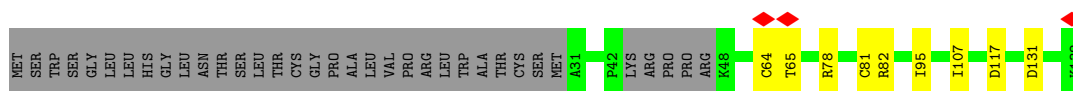




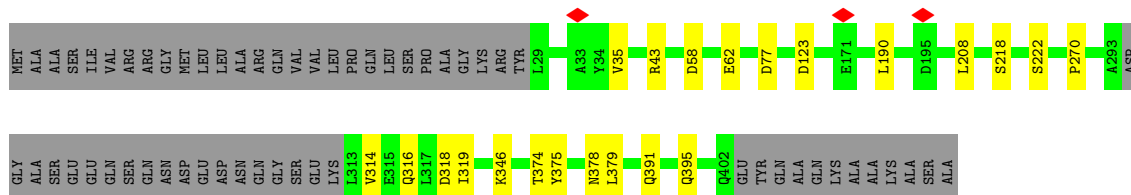
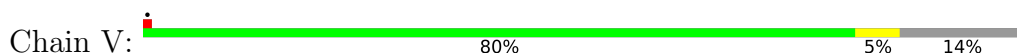
- Molecule 26: 28S ribosomal protein S9, mitochondrial



- Molecule 27: 28S ribosomal protein S12, mitochondrial

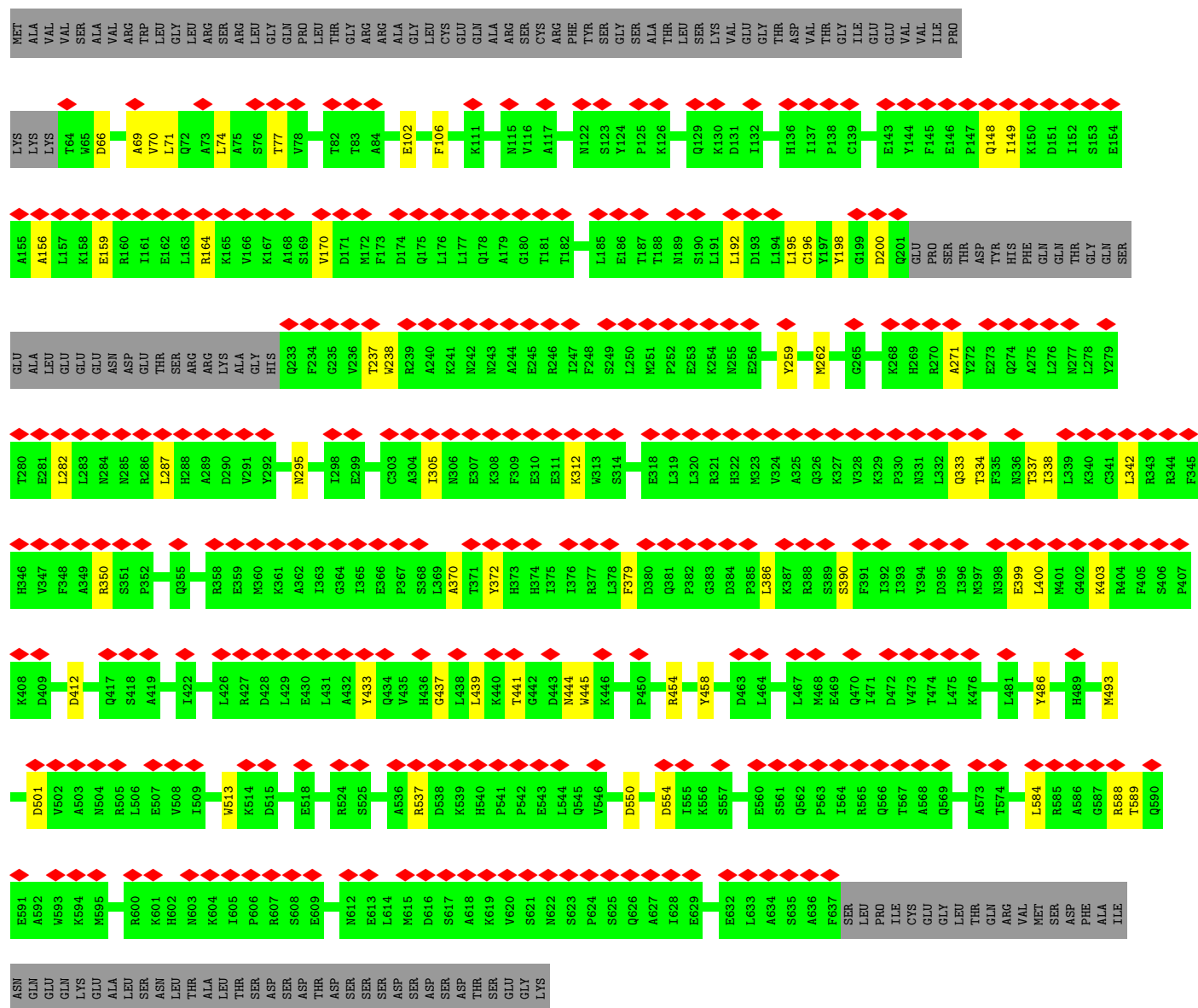


- Molecule 28: 28S ribosomal protein S27, mitochondrial

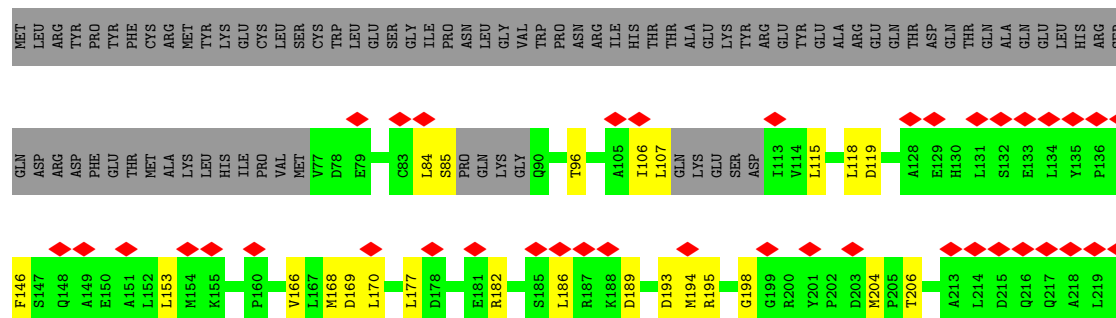


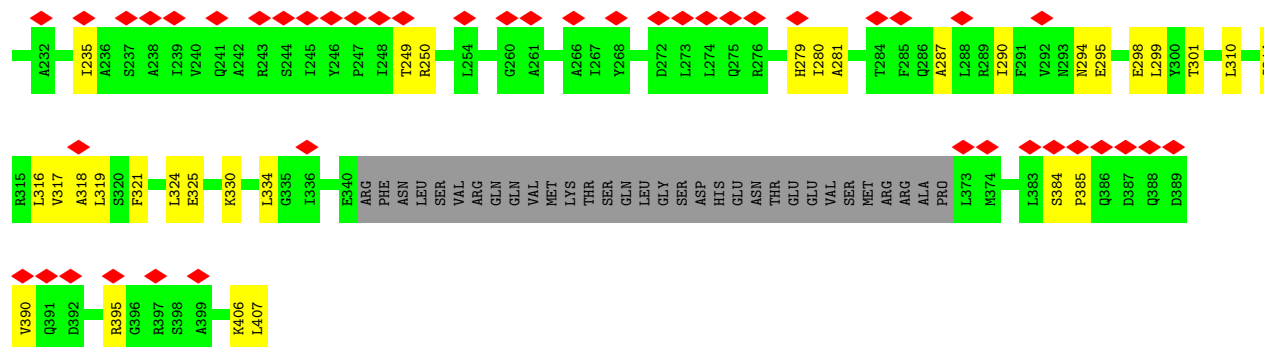
- Molecule 29: Pentatricopeptide repeat domain-containing protein 3, mitochondrial





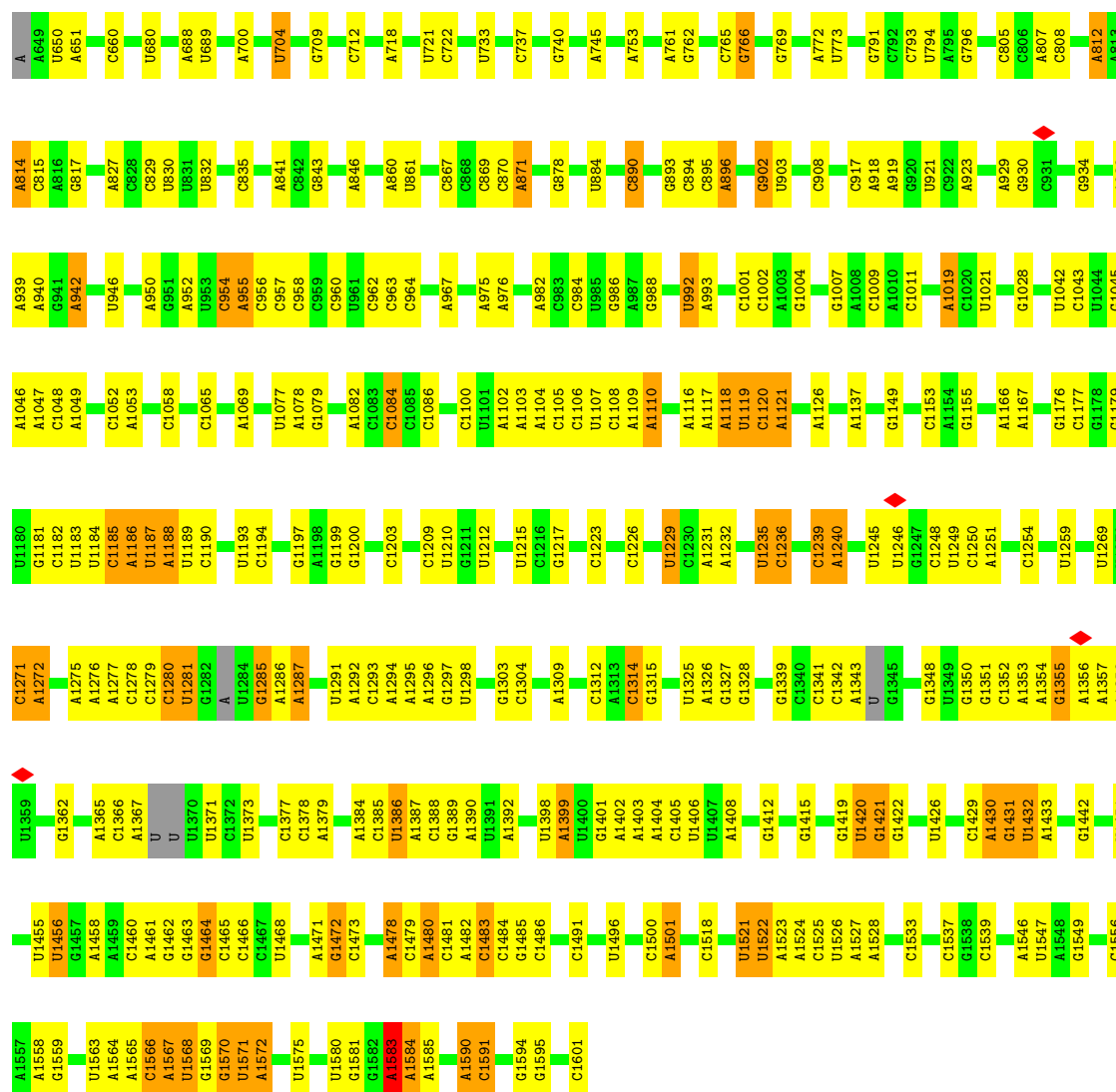
- Molecule 30: 12S rRNA N4-methylcytidine (m4C) methyltransferase





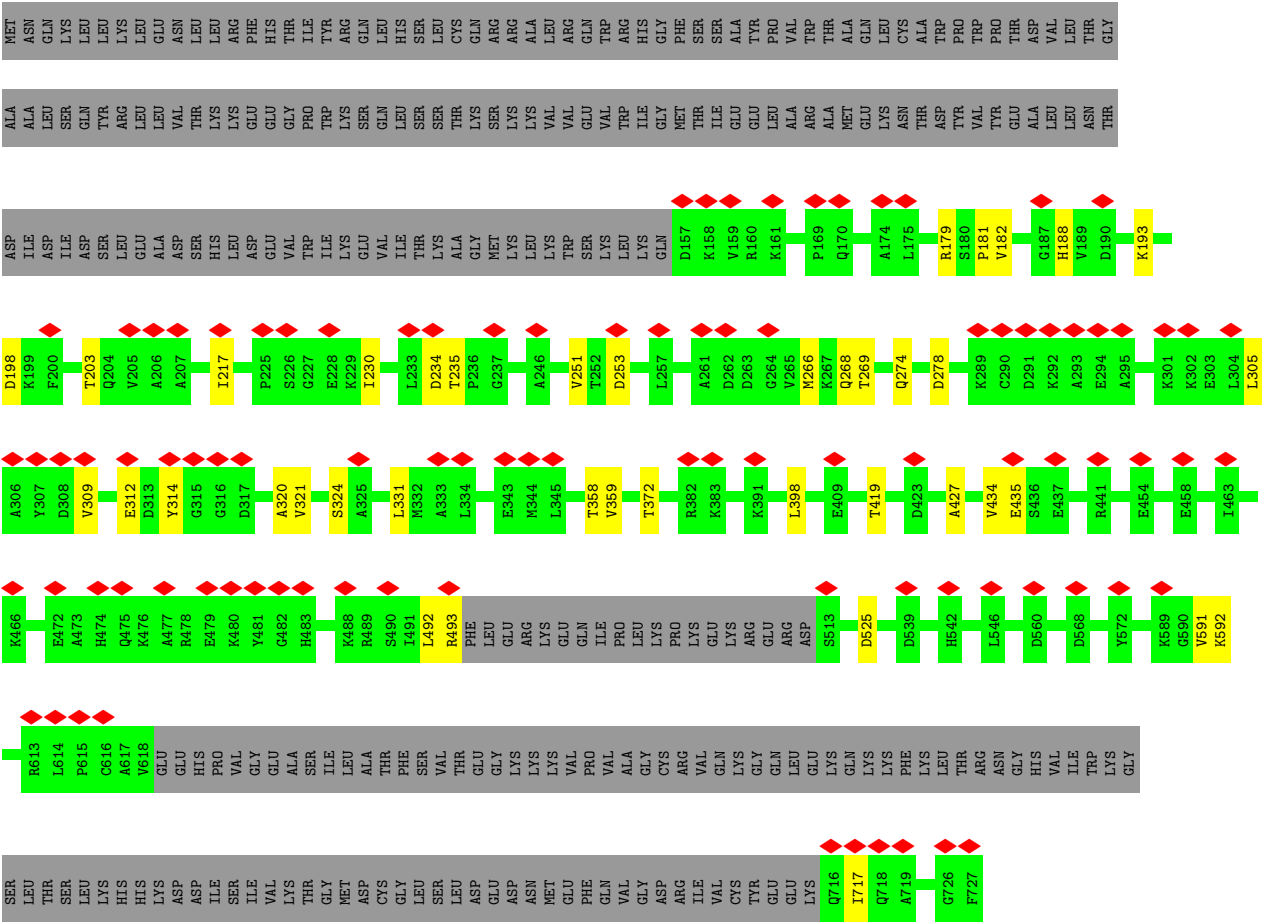
• Molecule 31: 12S mitochondrial rRNA

Chain A: 64% 29% 6% •

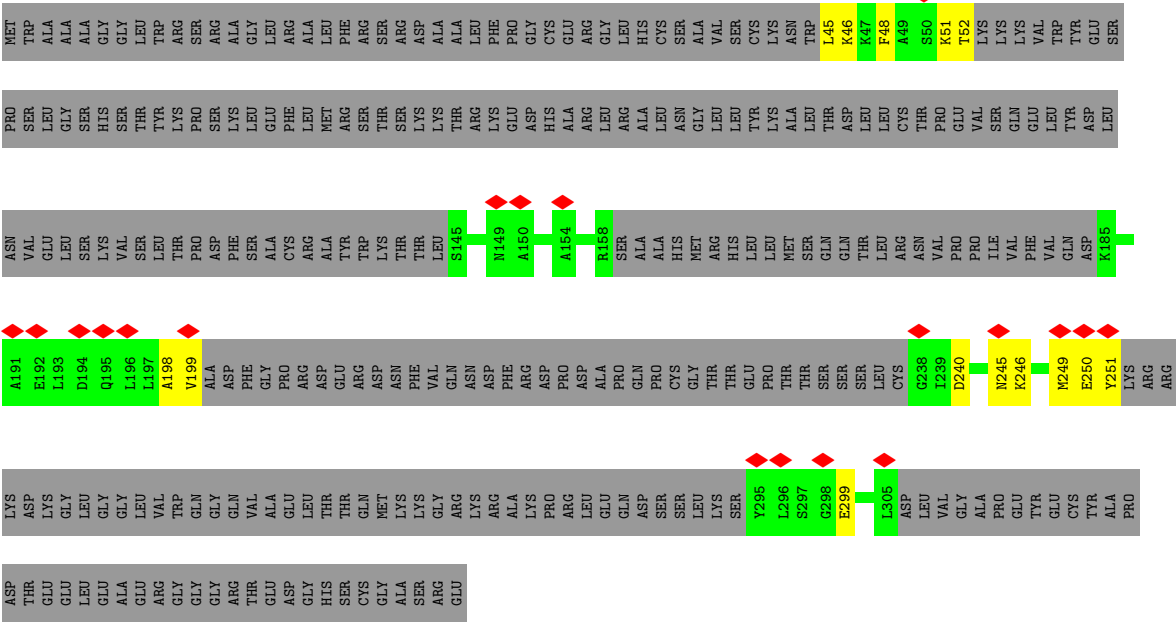


• Molecule 32: Translation initiation factor IF-2, mitochondrial

Chain 7: 13% 57% 6% 37%



● Molecule 33: Putative ribosome-binding factor A, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3598	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	0.062	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.011	Depositor
Map size ( $\text{\AA}$ )	495.0, 495.0, 495.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.825, 0.825, 0.825	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.08	0/1825	0.22	0/2473
2	1	0.09	0/2163	0.22	0/2927
3	3	0.08	0/627	0.22	0/828
4	B	0.09	0/1871	0.21	0/2531
5	C	0.08	0/1024	0.20	0/1388
6	E	0.09	0/926	0.22	0/1252
7	F	0.07	0/1670	0.21	0/2241
8	H	0.08	0/1088	0.20	0/1474
9	I	0.09	0/1021	0.22	0/1375
10	K	0.08	0/880	0.22	0/1182
11	L	0.08	0/1477	0.21	0/1974
12	M	0.09	0/963	0.22	0/1295
13	N	0.08	0/886	0.19	0/1199
14	O	0.10	0/1655	0.23	0/2254
15	P	0.08	0/798	0.22	0/1070
16	Q	0.09	0/754	0.21	0/1003
17	R	0.09	0/2456	0.19	0/3317
18	S	0.08	0/1138	0.18	0/1533
19	T	0.10	0/1402	0.21	0/1883
20	U	0.08	0/1510	0.19	0/2025
21	W	0.09	0/801	0.23	0/1079
22	X	0.08	0/2921	0.22	0/3954
23	Y	0.09	0/1032	0.22	0/1391
24	Z	0.08	0/815	0.21	0/1087
25	D	0.09	0/2547	0.21	0/3414
26	G	0.09	0/2562	0.24	0/3432
27	J	0.09	0/807	0.23	0/1082
28	V	0.07	0/2967	0.20	0/4009
29	4	0.08	0/4514	0.24	0/6107
30	b	0.09	0/2298	0.26	0/3097
31	A	0.10	0/22486	0.21	0/35000
32	7	0.07	0/3554	0.21	0/4805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	a	0.09	0/482	0.32	0/640
All	All	0.09	0/73920	0.22	0/104321

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
9	I	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	183	HIS	Mainchain
9	I	184	5F0	Mainchain,Peptide

## 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	0	1778	1784	1783	10	0
2	1	2117	2148	2147	14	0
3	3	616	686	686	7	0
4	B	1828	1815	1815	9	0
5	C	994	985	984	0	0
6	E	910	929	929	4	0
7	F	1634	1686	1686	5	0
8	H	1064	1089	1089	8	0
9	I	1011	1049	1042	17	0
10	K	862	885	885	7	0
11	L	1453	1540	1540	5	0
12	M	942	965	965	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	868	928	928	4	0
14	O	1599	1566	1564	8	0
15	P	781	807	807	5	0
16	Q	744	758	758	6	0
17	R	2409	2428	2428	11	0
18	S	1111	1115	1115	5	0
19	T	1371	1393	1396	10	0
20	U	1488	1499	1499	4	0
21	W	789	802	802	3	0
22	X	2849	2844	2844	22	0
23	Y	1002	947	946	8	0
24	Z	797	815	815	5	0
25	D	2498	2545	2545	18	0
26	G	2508	2488	2488	20	0
27	J	794	830	833	8	0
28	V	2907	2907	2906	13	0
29	4	4411	4411	4410	40	0
30	b	2261	2318	2315	44	0
31	A	20154	10235	10247	101	0
32	7	3501	3548	3548	23	0
33	a	482	473	470	9	0
34	O	1	0	0	0	0
35	P	4	0	0	1	0
35	T	4	0	0	4	0
36	X	31	12	12	1	0
37	7	28	10	12	1	0
37	X	28	10	12	0	0
38	A	44	26	26	0	0
39	A	14	0	26	1	0
40	A	11	0	0	0	0
41	A	8	0	0	0	0
41	a	1	0	0	0	0
All	All	70707	61276	61303	393	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 (393) 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)
19:T:141:CYS:SG	35:T:201:FES:S2	2.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:149:CYS:SG	35:T:201:FES:FE1	1.66	0.86
32:7:198:ASP:OD1	32:7:203:THR:OG1	1.97	0.82
31:A:1366:C:OP1	31:A:1388:C:O2'	2.06	0.74
23:Y:286:LEU:O	23:Y:289:VAL:HG22	1.90	0.70
2:1:189:LYS:NZ	2:1:235:ASN:O	2.23	0.70
30:b:298:GLU:O	30:b:301:THR:OG1	2.08	0.70
29:4:441:THR:OG1	29:4:444:ASN:OD1	2.08	0.69
9:I:184:5F0:O	31:A:976:A:H2	1.75	0.69
9:I:189:ARG:HH22	31:A:1086:C:P	2.15	0.69
18:S:7:GLU:N	18:S:7:GLU:OE1	2.25	0.69
15:P:65:CYS:N	15:P:68:CYS:SG	2.66	0.69
7:F:52:ARG:NH2	26:G:319:PHE:O	2.26	0.68
31:A:843:G:N2	31:A:846:A:OP2	2.26	0.68
27:J:81:CYS:SG	27:J:82:ARG:N	2.66	0.68
13:N:75:LYS:NZ	31:A:766:G:OP2	2.28	0.66
28:V:190:LEU:HD11	28:V:208:LEU:HD11	1.78	0.66
33:a:245:ASN:OD1	33:a:246:LYS:N	2.29	0.66
31:A:1455:U:O2'	31:A:1456:U:O5'	2.14	0.66
30:b:310:LEU:O	30:b:406:LYS:NZ	2.25	0.66
19:T:149:CYS:SG	35:T:201:FES:S1	2.95	0.65
31:A:1229:U:O2'	31:A:1442:G:O4'	2.13	0.65
31:A:1053:A:N1	31:A:1100:C:O2'	2.29	0.64
19:T:37:HIS:NE2	31:A:955:A:N7	2.45	0.64
31:A:1183:U:O2	31:A:1472:G:N2	2.25	0.64
23:Y:292:GLN:OE1	29:4:454:ARG:NH2	2.30	0.64
22:X:135:THR:N	36:X:501:ATP:O2B	2.30	0.63
26:G:301:GLN:N	26:G:301:GLN:OE1	2.32	0.63
19:T:132:ARG:NH1	19:T:136:LEU:O	2.30	0.63
31:A:700:A:N1	31:A:709:G:O2'	2.32	0.63
25:D:217:ASP:OD2	25:D:251:LYS:NZ	2.32	0.62
32:7:274:GLN:NE2	32:7:278:ASP:OD2	2.33	0.62
24:Z:66:ARG:NH2	24:Z:80:ASP:OD2	2.33	0.61
31:A:942:A:N6	31:A:1047:A:OP2	2.32	0.61
28:V:218:SER:O	28:V:222:SER:OG	2.18	0.61
26:G:136:ARG:NH2	26:G:210:VAL:O	2.31	0.61
9:I:83:ILE:O	9:I:148:ARG:NH2	2.33	0.61
18:S:83:ARG:NH1	18:S:93:LYS:O	2.34	0.61
17:R:317:ALA:O	17:R:321:ALA:N	2.34	0.61
26:G:229:LEU:HD21	26:G:241:VAL:HG11	1.82	0.60
20:U:80:ARG:O	20:U:84:GLU:N	2.34	0.60
10:K:112:ARG:NH1	10:K:116:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:7:266:MET:N	32:7:269:THR:OG1	2.33	0.60
32:7:193:LYS:NZ	37:7:801:GDP:O2B	2.35	0.60
1:0:9:ARG:NH2	31:A:805:C:O2	2.35	0.60
22:X:62:GLN:N	22:X:62:GLN:OE1	2.34	0.60
30:b:106:ILE:HB	30:b:115:LEU:HD11	1.82	0.59
29:4:433:TYR:O	29:4:437:GLY:N	2.34	0.59
1:0:53:ARG:NH1	31:A:704:U:OP1	2.35	0.59
9:I:192:ARG:O	31:A:1084:C:H5'	2.02	0.59
2:1:292:TYR:OH	22:X:338:ASP:OD1	2.21	0.59
15:P:73:ASP:OD1	15:P:74:TYR:N	2.36	0.59
31:A:917:C:O2'	31:A:921:U:OP1	2.19	0.59
27:J:117:ASP:OD1	31:A:895:C:N4	2.36	0.59
2:1:166:PRO:O	2:1:169:ARG:NH1	2.36	0.59
30:b:195:ARG:NH1	30:b:204:MET:O	2.36	0.58
9:I:184:5F0:O	31:A:976:A:C2	2.55	0.58
2:1:150:GLU:OE1	2:1:174:ARG:NH2	2.37	0.58
28:V:43:ARG:NE	28:V:77:ASP:OD1	2.36	0.58
29:4:584:LEU:HD23	29:4:589:THR:OG1	2.04	0.58
27:J:107:ILE:N	27:J:131:ASP:OD2	2.32	0.57
3:3:137:LYS:NZ	31:A:1575:U:OP2	2.26	0.57
17:R:263:ARG:NH2	17:R:287:ASP:OD1	2.37	0.57
27:J:82:ARG:NH1	31:A:1496:U:OP1	2.36	0.57
29:4:295:ASN:OD1	29:4:334:THR:OG1	2.15	0.57
30:b:182:ARG:NH2	30:b:195:ARG:O	2.35	0.57
1:0:63:ARG:NH2	1:0:110:ASP:OD2	2.38	0.57
4:B:141:ILE:HG23	4:B:165:TYR:CE2	2.40	0.57
31:A:1272:A:H61	31:A:1303:G:C2'	2.18	0.57
8:H:70:ASP:OD1	8:H:71:ILE:N	2.37	0.56
26:G:139:GLN:OE1	26:G:156:GLN:NE2	2.38	0.56
26:G:392:THR:HG21	31:A:1362:G:OP1	2.05	0.56
30:b:334:LEU:O	30:b:334:LEU:HG	2.05	0.56
32:7:427:ALA:N	32:7:525:ASP:OD2	2.38	0.56
9:I:71:SER:O	9:I:74:ARG:NH1	2.38	0.56
10:K:96:ARG:NH1	10:K:98:ARG:O	2.38	0.56
16:Q:62:ARG:NH1	31:A:1019:A:O4'	2.38	0.56
2:1:126:LEU:HD12	8:H:155:VAL:CG2	2.36	0.56
30:b:330:LYS:O	30:b:334:LEU:HD23	2.04	0.56
25:D:209:GLY:N	25:D:213:GLU:O	2.39	0.56
17:R:352:ALA:O	17:R:356:HIS:ND1	2.39	0.56
29:4:192:LEU:O	29:4:196:CYS:N	2.38	0.56
8:H:126:ILE:HD11	31:A:1217:G:H21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D:297:ARG:NH1	31:A:1121:A:OP2	2.38	0.56
26:G:200:LEU:O	26:G:218:TYR:OH	2.24	0.55
30:b:222:ILE:O	30:b:287:ALA:HB1	2.06	0.55
15:P:140:TYR:OH	16:Q:33:ASP:OD1	2.15	0.55
29:4:350:ARG:NH2	29:4:379:PHE:O	2.39	0.55
12:M:26:CYS:SG	19:T:149:CYS:SG	2.97	0.55
27:J:65:THR:O	27:J:65:THR:HG22	2.05	0.55
18:S:21:ARG:NH1	25:D:281:TYR:OH	2.40	0.55
11:L:86:ASP:OD1	11:L:87:ASP:N	2.40	0.54
30:b:145:GLN:OE1	30:b:145:GLN:N	2.39	0.54
9:I:189:ARG:NH2	31:A:1086:C:OP1	2.41	0.54
31:A:1235:U:H3'	31:A:1236:C:H5''	1.89	0.54
31:A:689:U:OP1	31:A:827:A:O2'	2.26	0.54
31:A:934:G:O2'	31:A:940:A:N1	2.36	0.54
26:G:135:GLN:O	26:G:136:ARG:C	2.50	0.54
30:b:170:LEU:HD21	30:b:299:LEU:HD13	1.89	0.54
9:I:189:ARG:NH2	31:A:1086:C:P	2.81	0.53
1:O:110:ASP:OD1	1:O:110:ASP:N	2.42	0.53
7:F:198:ARG:NH1	31:A:1384:A:OP2	2.41	0.53
22:X:279:LYS:NZ	31:A:1412:G:OP1	2.41	0.53
29:4:282:LEU:HD12	29:4:287:LEU:HB2	1.91	0.53
7:F:155:MET:SD	7:F:179:ARG:NH1	2.82	0.53
25:D:254:ALA:O	25:D:280:HIS:N	2.37	0.53
25:D:245:VAL:HG22	25:D:271:ALA:HB1	1.90	0.53
28:V:270:PRO:O	28:V:346:LYS:NZ	2.41	0.53
30:b:169:ASP:HB3	30:b:319:LEU:HD13	1.90	0.53
30:b:189:ASP:OD1	30:b:250:ARG:NH2	2.42	0.52
31:A:1110:A:O2'	39:A:1702:SPM:H132	2.09	0.52
31:A:1483:C:N4	31:A:1567:A:O2'	2.43	0.52
3:3:187:GLU:O	11:L:212:ARG:NH2	2.42	0.52
25:D:316:CYS:SG	25:D:317:HIS:N	2.82	0.52
29:4:238:TRP:HZ2	29:4:262:MET:HE3	1.74	0.52
22:X:186:THR:O	22:X:190:ASN:ND2	2.43	0.52
16:Q:59:ARG:NH1	31:A:1021:U:O4	2.43	0.52
14:O:63:GLU:OE1	14:O:112:LYS:NZ	2.36	0.52
2:1:300:LYS:NZ	22:X:335:ASP:OD1	2.41	0.51
31:A:1102:A:OP2	31:A:1104:A:N6	2.40	0.51
14:O:73:VAL:O	14:O:109:ARG:NH2	2.42	0.51
13:N:59:THR:HG22	13:N:60:VAL:H	1.76	0.51
17:R:195:VAL:O	19:T:137:ARG:NH1	2.39	0.51
25:D:320:ILE:HG22	25:D:324:CYS:SG	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:208:ILE:O	17:R:214:ASN:ND2	2.41	0.51
31:A:1185:C:H4'	31:A:1186:A:OP2	2.11	0.51
26:G:217:ASP:OD1	26:G:218:TYR:N	2.43	0.51
32:7:251:VAL:HG22	32:7:358:THR:HG21	1.92	0.51
17:R:203:LYS:O	17:R:234:GLN:NE2	2.38	0.51
29:4:66:ASP:OD1	29:4:69:ALA:N	2.44	0.51
4:B:141:ILE:HG23	4:B:165:TYR:HE2	1.76	0.50
31:A:1567:A:H5'	31:A:1568:U:OP2	2.12	0.50
26:G:362:GLU:OE2	26:G:365:ARG:NH2	2.43	0.50
29:4:372:TYR:CE2	29:4:400:LEU:HD21	2.46	0.50
31:A:769:G:N2	31:A:772:A:OP2	2.31	0.50
31:A:890:C:O2'	31:A:902:G:N2	2.37	0.50
31:A:1231:A:H2'	31:A:1232:A:H5''	1.93	0.50
31:A:1571:U:H3'	31:A:1572:A:H5'	1.93	0.50
8:H:126:ILE:HG23	31:A:1226:C:H1'	1.92	0.50
1:0:43:ARG:O	1:0:47:GLY:N	2.42	0.50
11:L:217:THR:O	11:L:221:LYS:N	2.45	0.50
26:G:357:THR:O	26:G:361:VAL:HG23	2.12	0.50
31:A:1357:A:O2'	33:a:249:MET:SD	2.66	0.50
1:0:135:MET:SD	1:0:135:MET:N	2.84	0.50
13:N:59:THR:HG22	13:N:60:VAL:N	2.27	0.50
27:J:78:ARG:NH2	27:J:117:ASP:OD2	2.44	0.50
29:4:399:GLU:OE2	29:4:403:LYS:NZ	2.35	0.50
30:b:119:ASP:O	30:b:143:LEU:HD12	2.12	0.50
2:1:118:ALA:O	2:1:122:HIS:N	2.41	0.50
22:X:169:LEU:O	22:X:179:ASP:N	2.45	0.50
32:7:321:VAL:HG13	32:7:321:VAL:O	2.11	0.50
33:a:198:ALA:O	33:a:199:VAL:C	2.55	0.50
29:4:386:LEU:O	29:4:390:SER:N	2.45	0.49
33:a:250:GLU:O	33:a:251:TYR:C	2.56	0.49
12:M:39:ASN:ND2	31:A:841:A:OP1	2.45	0.49
29:4:66:ASP:OD1	29:4:69:ALA:HB2	2.12	0.49
29:4:370:ALA:N	29:4:412:ASP:OD1	2.44	0.49
9:I:192:ARG:NH1	31:A:992:U:O5'	2.44	0.49
29:4:148:GLN:N	29:4:159:GLU:OE2	2.46	0.49
22:X:263:ASP:OD1	22:X:264:GLY:N	2.46	0.49
22:X:325:PRO:O	22:X:329:LEU:N	2.41	0.49
30:b:186:LEU:HD11	30:b:279:HIS:NE2	2.28	0.49
22:X:179:ASP:CG	22:X:237:THR:HG21	2.37	0.49
22:X:378:LYS:HB3	26:G:323:LEU:HD22	1.95	0.49
31:A:1177:C:O2'	31:A:1568:U:O4	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:952:A:N3	31:A:954:C:N4	2.61	0.48
31:A:1272:A:N6	31:A:1304:C:O4'	2.46	0.48
9:I:88:ILE:HD12	9:I:149:VAL:HG13	1.94	0.48
15:P:69:GLY:N	35:P:201:FES:S1	2.86	0.48
31:A:1501:A:N6	31:A:1549:G:N3	2.61	0.48
4:B:103:GLU:OE2	18:S:52:ARG:NH2	2.45	0.48
28:V:374:THR:O	28:V:378:ASN:N	2.45	0.48
2:1:212:CYS:O	2:1:218:ASN:ND2	2.47	0.48
22:X:179:ASP:OD1	22:X:237:THR:HG21	2.13	0.48
30:b:316:LEU:O	30:b:316:LEU:HD23	2.14	0.48
29:4:71:LEU:O	29:4:71:LEU:HD23	2.13	0.48
7:F:36:ARG:NH1	31:A:1314:C:O2	2.46	0.48
10:K:105:ARG:NE	24:Z:47:GLU:OE2	2.47	0.48
22:X:246:GLU:OE2	22:X:249:ARG:NH2	2.47	0.48
3:3:148:LYS:O	3:3:151:ARG:NH1	2.46	0.48
31:A:1583:MA6:OP2	31:A:1583:MA6:H8	2.14	0.48
9:I:192:ARG:O	9:I:193:LYS:C	2.56	0.48
32:7:179:ARG:NH2	32:7:253:ASP:OD2	2.40	0.48
32:7:234:ASP:OD1	32:7:235:THR:N	2.47	0.48
2:1:199:CYS:O	2:1:203:ASP:N	2.47	0.48
30:b:168:MET:N	30:b:317:VAL:O	2.47	0.48
30:b:295:GLU:O	30:b:299:LEU:N	2.47	0.48
31:A:1464:G:N2	31:A:1465:C:N3	2.60	0.47
28:V:375:TYR:CZ	28:V:379:LEU:HD11	2.49	0.47
1:0:77:GLY:N	1:0:97:LEU:O	2.43	0.47
28:V:190:LEU:CD1	28:V:208:LEU:HD11	2.43	0.47
18:S:5:ARG:NH1	31:A:1279:C:O3'	2.46	0.47
28:V:391:GLN:O	28:V:395:GLN:N	2.48	0.47
29:4:333:GLN:O	29:4:337:THR:HG23	2.14	0.47
30:b:290:ILE:O	30:b:294:ASN:N	2.47	0.47
31:A:1309:A:N6	31:A:1315:G:O6	2.48	0.47
3:3:150:THR:HG22	3:3:150:THR:O	2.14	0.47
21:W:87:SER:OG	21:W:90:THR:OG1	2.33	0.47
26:G:205:LEU:HD22	26:G:221:PHE:CZ	2.49	0.47
31:A:1119:U:H2'	31:A:1120:C:H5'	1.96	0.47
32:7:305:LEU:HD21	32:7:314:TYR:CD2	2.49	0.47
30:b:249:THR:HG22	30:b:249:THR:O	2.14	0.47
14:O:217:ARG:NH1	14:O:227:GLU:OE2	2.47	0.47
32:7:434:VAL:HG22	32:7:435:GLU:H	1.79	0.47
30:b:106:ILE:HG21	30:b:115:LEU:HD21	1.97	0.47
3:3:165:LYS:NZ	31:A:1149:G:OP2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D:177:GLU:O	25:D:181:ARG:N	2.47	0.47
25:D:230:THR:OG1	31:A:1287:A:OP1	2.33	0.46
29:4:164:ARG:NH1	29:4:198:TYR:OH	2.45	0.46
30:b:166:VAL:HG22	30:b:310:LEU:HD22	1.97	0.46
31:A:1187:U:H4'	31:A:1188:A:OP1	2.15	0.46
1:O:178:ARG:O	1:O:183:ASP:N	2.48	0.46
23:Y:328:PHE:O	23:Y:332:ILE:HD12	2.15	0.46
31:A:1567:A:C8	31:A:1568:U:H2'	2.50	0.46
4:B:147:ARG:NH2	31:A:1294:A:OP1	2.49	0.46
19:T:141:CYS:SG	19:T:149:CYS:SG	3.14	0.46
22:X:276:ARG:NH2	22:X:286:GLU:OE1	2.49	0.46
30:b:227:GLY:HA3	30:b:287:ALA:HB2	1.97	0.46
31:A:1479:C:H5''	31:A:1480:A:OP2	2.16	0.46
31:A:1581:G:O6	31:A:1585:A:N6	2.48	0.46
2:1:86:ARG:NH1	2:1:96:PRO:O	2.48	0.46
25:D:320:ILE:O	25:D:324:CYS:N	2.44	0.46
30:b:406:LYS:O	30:b:407:LEU:C	2.57	0.46
32:7:188:HIS:ND1	32:7:268:GLN:OE1	2.49	0.46
17:R:69:THR:OG1	17:R:72:ASP:OD1	2.30	0.46
31:A:1398:U:H3	31:A:1408:A:H61	1.63	0.46
31:A:1567:A:H3'	31:A:1568:U:H5''	1.97	0.46
2:1:126:LEU:HD11	29:4:70:VAL:HG13	1.96	0.46
25:D:198:TRP:NE1	33:a:299:GLU:OE1	2.49	0.46
27:J:64:CYS:SG	27:J:95:ILE:HD11	2.56	0.46
9:I:191:ALA:HA	16:Q:44:TYR:CD1	2.51	0.45
6:E:115:GLU:O	6:E:116:LYS:C	2.58	0.45
30:b:170:LEU:CD2	30:b:299:LEU:HD13	2.45	0.45
4:B:100:ARG:NH2	31:A:1116:A:OP2	2.50	0.45
9:I:81:GLU:OE1	9:I:81:GLU:N	2.47	0.45
29:4:305:ILE:O	29:4:312:LYS:NZ	2.45	0.45
4:B:259:ARG:O	4:B:263:LYS:N	2.50	0.45
14:O:101:VAL:HG12	14:O:102:GLY:N	2.31	0.45
26:G:228:LEU:HD11	26:G:237:GLU:HG2	1.99	0.45
29:4:102:GLU:O	29:4:106:PHE:N	2.49	0.45
30:b:107:LEU:HG	30:b:115:LEU:HD12	1.98	0.45
2:1:112:LEU:O	2:1:115:THR:HG23	2.17	0.45
30:b:226:TYR:OH	33:a:240:ASP:OD2	2.34	0.45
31:A:1521:U:H2'	31:A:1522:U:C5	2.52	0.45
25:D:140:LEU:C	25:D:140:LEU:HD12	2.42	0.45
21:W:174:GLU:O	21:W:175:SER:C	2.59	0.45
24:Z:91:LYS:NZ	31:A:1339:G:OP2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:660:C:O4'	31:A:1285:G:N2	2.48	0.44
32:7:312:GLU:OE2	32:7:320:ALA:HB3	2.16	0.44
28:V:318:ASP:OD1	28:V:319:ILE:N	2.51	0.44
30:b:223:LEU:HD13	30:b:235:ILE:HG23	1.99	0.44
32:7:217:ILE:O	32:7:217:ILE:HG23	2.17	0.44
17:R:253:ILE:O	17:R:257:GLY:N	2.51	0.44
29:4:170:VAL:CG2	29:4:195:LEU:HD21	2.47	0.44
30:b:146:PHE:HB3	30:b:298:GLU:HB3	2.00	0.44
31:A:1583:MA6:H93	31:A:1584:MA6:C2	2.48	0.44
23:Y:294:LEU:HD13	23:Y:300:GLU:HA	1.98	0.44
26:G:143:ASP:OD1	26:G:144:GLY:N	2.51	0.44
30:b:310:LEU:HD11	30:b:314:GLY:HA3	2.00	0.44
30:b:321:PHE:N	30:b:325:GLU:OE2	2.42	0.44
32:7:398:LEU:N	32:7:419:THR:OG1	2.51	0.44
14:O:94:CYS:SG	14:O:105:CYS:SG	3.16	0.44
8:H:92:GLU:OE2	8:H:108:VAL:HG11	2.17	0.44
30:b:118:LEU:HD22	30:b:153:LEU:HD11	2.00	0.44
17:R:213:GLU:OE1	17:R:213:GLU:N	2.43	0.44
26:G:320:VAL:HG12	26:G:321:ASP:N	2.33	0.44
31:A:1590:A:O2'	31:A:1591:C:H5''	2.18	0.44
4:B:82:ARG:NE	4:B:86:ASP:OD1	2.51	0.43
30:b:390:VAL:O	30:b:390:VAL:HG22	2.17	0.43
31:A:1420:U:O2'	31:A:1421:G:P	2.76	0.43
22:X:50:ARG:NH2	22:X:69:ASN:HB2	2.33	0.43
25:D:372:GLU:N	25:D:382:ILE:O	2.48	0.43
31:A:1271:C:H5'	31:A:1272:A:OP2	2.18	0.43
7:F:46:ILE:O	7:F:46:ILE:HG22	2.18	0.43
12:M:71:ASP:OD2	17:R:162:SER:OG	2.34	0.43
16:Q:57:TYR:O	16:Q:61:ARG:N	2.43	0.43
20:U:189:TRP:CE3	20:U:197:VAL:HG13	2.54	0.43
22:X:264:GLY:N	22:X:309:ALA:O	2.51	0.43
26:G:200:LEU:HD12	26:G:204:GLU:OE1	2.17	0.43
30:b:96:THR:OG1	30:b:169:ASP:OD1	2.35	0.43
32:7:324:SER:O	32:7:331:LEU:HD21	2.17	0.43
31:A:1569:G:OP2	31:A:1570:G:OP2	2.35	0.43
11:L:216:GLU:O	11:L:220:LEU:N	2.46	0.43
30:b:107:LEU:CD2	30:b:115:LEU:HD12	2.49	0.43
31:A:1184:U:H2'	31:A:1185:C:O4'	2.18	0.43
1:O:84:SER:OG	1:O:138:ASP:OD2	2.34	0.43
29:4:550:ASP:OD1	29:4:588:ARG:NH1	2.51	0.43
30:b:195:ARG:NH2	30:b:198:GLY:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:871:A:N1	31:A:918:A:O2'	2.49	0.43
1:0:101:ARG:NH1	31:A:1528:A:OP1	2.52	0.43
10:K:53:ARG:HH12	23:Y:372:HIS:HA	1.84	0.43
25:D:355:ARG:NH1	31:A:1118:A:O2'	2.52	0.43
31:A:1182:C:H2'	31:A:1183:U:O4'	2.19	0.43
32:7:591:VAL:HG12	32:7:592:LYS:N	2.34	0.43
13:N:93:ASP:O	13:N:97:GLY:N	2.43	0.43
22:X:81:HIS:CE1	22:X:156:PRO:HD3	2.54	0.43
31:A:765:C:H5'	31:A:766:G:OP2	2.19	0.43
33:a:51:LYS:O	33:a:52:THR:C	2.62	0.43
10:K:36:ARG:NH1	31:A:1348:G:OP1	2.52	0.43
26:G:395:LYS:O	26:G:396:ARG:C	2.60	0.43
29:4:238:TRP:HB3	29:4:271:ALA:HB2	2.01	0.43
30:b:84:LEU:O	30:b:85:SER:C	2.62	0.43
31:A:1106:C:O2'	31:A:1108:C:OP2	2.23	0.43
29:4:71:LEU:HD23	29:4:71:LEU:C	2.44	0.43
32:7:717:ILE:HG22	32:7:717:ILE:O	2.19	0.43
25:D:316:CYS:SG	25:D:320:ILE:HB	2.59	0.42
29:4:237:THR:O	29:4:237:THR:HG22	2.18	0.42
29:4:458:TYR:HB3	29:4:486:TYR:CD1	2.54	0.42
31:A:1186:A:O2'	31:A:1187:U:O5'	2.37	0.42
22:X:81:HIS:ND1	22:X:156:PRO:HB3	2.35	0.42
24:Z:54:ASN:ND2	24:Z:57:THR:OG1	2.52	0.42
29:4:74:LEU:O	29:4:77:THR:OG1	2.35	0.42
32:7:359:VAL:HG13	32:7:372:THR:CG2	2.49	0.42
3:3:134:ARG:HH12	31:A:1478:A:H61	1.67	0.42
8:H:184:ILE:O	8:H:184:ILE:HG22	2.20	0.42
14:O:94:CYS:SG	14:O:108:CYS:SG	3.17	0.42
31:A:1430:A:H1'	31:A:1432:U:H3'	2.01	0.42
6:E:5:GLU:N	6:E:94:VAL:O	2.49	0.42
27:J:117:ASP:OD2	31:A:894:C:N4	2.52	0.42
30:b:228:GLU:HG3	30:b:324:LEU:HD11	2.01	0.42
4:B:171:PHE:CE2	4:B:175:MET:HE3	2.55	0.42
22:X:252:SER:O	22:X:302:HIS:NE2	2.53	0.42
30:b:223:LEU:HD13	30:b:235:ILE:CG2	2.50	0.42
32:7:492:LEU:O	32:7:493:ARG:C	2.62	0.42
30:b:280:ILE:O	30:b:281:ALA:HB3	2.20	0.42
8:H:76:LEU:HD11	8:H:172:VAL:CG1	2.50	0.42
19:T:149:CYS:SG	35:T:201:FES:S2	3.18	0.42
28:V:58:ASP:O	28:V:62:GLU:N	2.48	0.42
33:a:48:PHE:CG	33:a:48:PHE:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:306:GLU:OE2	22:X:127:TYR:OH	2.37	0.42
4:B:89:VAL:O	4:B:89:VAL:HG12	2.20	0.42
28:V:123:ASP:OD1	28:V:123:ASP:N	2.52	0.42
29:4:338:ILE:O	29:4:342:LEU:N	2.51	0.42
3:3:147:VAL:O	3:3:151:ARG:N	2.53	0.41
29:4:259:TYR:HB2	29:4:282:LEU:HD13	2.01	0.41
29:4:458:TYR:HB3	29:4:486:TYR:CE1	2.55	0.41
30:b:318:ALA:C	30:b:319:LEU:HD12	2.45	0.41
31:A:1385:C:C5'	31:A:1386:U:H2'	2.50	0.41
31:A:1401:G:H22	31:A:1404:A:H5'	1.84	0.41
2:1:60:MET:HE1	2:1:80:ALA:O	2.19	0.41
24:Z:76:GLN:O	24:Z:80:ASP:N	2.53	0.41
25:D:316:CYS:SG	25:D:334:ALA:HB3	2.60	0.41
6:E:31:ASP:OD1	20:U:170:ARG:NH2	2.47	0.41
9:I:192:ARG:O	9:I:192:ARG:CG	2.69	0.41
31:A:812:A:O2'	31:A:814:A:N1	2.41	0.41
31:A:1210:U:O2	31:A:1355:G:N2	2.50	0.41
31:A:1398:U:C2'	31:A:1399:A:H5'	2.50	0.41
28:V:35:VAL:HG22	28:V:35:VAL:O	2.20	0.41
29:4:195:LEU:HD22	29:4:200:ASP:OD1	2.20	0.41
29:4:439:LEU:O	29:4:445:TRP:N	2.52	0.41
32:7:179:ARG:NH1	32:7:182:VAL:HG23	2.36	0.41
10:K:60:ASN:OD1	10:K:68:GLN:NE2	2.54	0.41
22:X:162:VAL:HG21	22:X:267:ALA:HB1	2.02	0.41
22:X:237:THR:HG23	22:X:289:LEU:CD2	2.50	0.41
23:Y:302:ILE:HG13	29:4:71:LEU:HD22	2.02	0.41
29:4:493:MET:HA	29:4:493:MET:HE2	2.02	0.41
29:4:501:ASP:OD1	29:4:537:ARG:NH1	2.53	0.41
31:A:878:G:O6	31:A:896:A:N6	2.54	0.41
14:O:93:THR:O	14:O:93:THR:HG23	2.20	0.41
20:U:169:THR:HG22	20:U:170:ARG:N	2.36	0.41
29:4:513:TRP:NE1	29:4:554:ASP:OD2	2.50	0.41
31:A:1280:C:H2'	31:A:1281:U:H5'	2.03	0.41
31:A:1500:C:O2'	31:A:1549:G:N1	2.51	0.41
33:a:45:LEU:HG	33:a:46:LYS:N	2.35	0.41
23:Y:302:ILE:CG1	29:4:71:LEU:HD22	2.51	0.41
23:Y:383:LYS:O	23:Y:384:LYS:C	2.64	0.41
30:b:182:ARG:O	30:b:194:MET:N	2.50	0.41
11:L:206:LYS:NZ	31:A:762:G:OP1	2.47	0.41
19:T:42:GLU:OE1	19:T:45:ARG:NH2	2.48	0.41
6:E:94:VAL:HG11	15:P:117:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:125:HIS:CE1	8:H:126:ILE:HD12	2.55	0.41
25:D:284:ARG:NH1	25:D:287:ASP:O	2.53	0.41
26:G:289:GLY:N	26:G:325:LYS:O	2.53	0.41
29:4:149:ILE:HG21	29:4:156:ALA:HB2	2.03	0.41
30:b:193:ASP:OD1	30:b:206:THR:HG22	2.20	0.41
32:7:181:PRO:O	32:7:230:ILE:HG23	2.21	0.41
9:I:116:GLY:O	9:I:118:ARG:NH1	2.49	0.41
10:K:33:ARG:NH2	31:A:1236:C:OP2	2.54	0.41
12:M:52:GLY:HA3	12:M:67:ALA:O	2.21	0.41
14:O:115:VAL:HG13	14:O:150:LEU:HD23	2.02	0.40
31:A:1420:U:HO2'	31:A:1421:G:P	2.44	0.40
31:A:1566:C:C2	31:A:1567:A:N7	2.89	0.40
31:A:1239:C:O2'	31:A:1240:A:O5'	2.36	0.40
17:R:304:TYR:OH	17:R:335:GLU:OE1	2.23	0.40
21:W:141:ARG:NH2	21:W:170:LEU:O	2.55	0.40
28:V:314:VAL:HG12	28:V:316:GLN:H	1.87	0.40
9:I:129:GLN:NE2	9:I:167:MET:SD	2.94	0.40
30:b:384:SER:N	30:b:385:PRO:CD	2.84	0.40
31:A:1388:C:H2'	31:A:1389:G:O4'	2.22	0.40
32:7:309:VAL:HG23	32:7:309:VAL:O	2.20	0.40
9:I:154:LEU:HD12	16:Q:39:ILE:HG21	2.02	0.40
26:G:276:ARG:NH1	31:A:1431:G:H21	2.19	0.40
30:b:177:LEU:HB3	30:b:395:ARG:HE	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	212/218 (97%)	206 (97%)	6 (3%)	0	100	100
2	1	257/323 (80%)	251 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	67/199 (34%)	67 (100%)	0	0	100	100
4	B	223/296 (75%)	218 (98%)	5 (2%)	0	100	100
5	C	119/167 (71%)	118 (99%)	1 (1%)	0	100	100
6	E	113/125 (90%)	110 (97%)	3 (3%)	0	100	100
7	F	197/242 (81%)	193 (98%)	4 (2%)	0	100	100
8	H	127/201 (63%)	123 (97%)	4 (3%)	0	100	100
9	I	133/194 (69%)	126 (95%)	7 (5%)	0	100	100
10	K	99/128 (77%)	94 (95%)	5 (5%)	0	100	100
11	L	172/257 (67%)	168 (98%)	4 (2%)	0	100	100
12	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
13	N	108/130 (83%)	104 (96%)	4 (4%)	0	100	100
14	O	192/258 (74%)	182 (95%)	10 (5%)	0	100	100
15	P	95/142 (67%)	95 (100%)	0	0	100	100
16	Q	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
17	R	293/360 (81%)	285 (97%)	8 (3%)	0	100	100
18	S	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
19	T	166/173 (96%)	163 (98%)	3 (2%)	0	100	100
20	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
21	W	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
22	X	350/398 (88%)	340 (97%)	10 (3%)	0	100	100
23	Y	116/395 (29%)	111 (96%)	5 (4%)	0	100	100
24	Z	92/106 (87%)	91 (99%)	1 (1%)	0	100	100
25	D	305/430 (71%)	294 (96%)	11 (4%)	0	100	100
26	G	300/396 (76%)	283 (94%)	15 (5%)	2 (1%)	18	55
27	J	99/138 (72%)	94 (95%)	5 (5%)	0	100	100
28	V	351/414 (85%)	347 (99%)	4 (1%)	0	100	100
29	4	539/689 (78%)	523 (97%)	16 (3%)	0	100	100
30	b	282/407 (69%)	262 (93%)	20 (7%)	0	100	100
32	7	449/727 (62%)	428 (95%)	21 (5%)	0	100	100
33	a	52/343 (15%)	45 (86%)	7 (14%)	0	100	100
All	All	6115/8662 (71%)	5916 (97%)	197 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	G	136	ARG
26	G	133	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	0	187/190 (98%)	187 (100%)	0	100	100
2	1	240/291 (82%)	240 (100%)	0	100	100
3	3	64/166 (39%)	64 (100%)	0	100	100
4	B	198/249 (80%)	198 (100%)	0	100	100
5	C	106/143 (74%)	106 (100%)	0	100	100
6	E	97/107 (91%)	97 (100%)	0	100	100
7	F	178/209 (85%)	178 (100%)	0	100	100
8	H	119/180 (66%)	119 (100%)	0	100	100
9	I	103/146 (70%)	103 (100%)	0	100	100
10	K	91/113 (80%)	91 (100%)	0	100	100
11	L	158/226 (70%)	158 (100%)	0	100	100
12	M	97/113 (86%)	97 (100%)	0	100	100
13	N	96/115 (84%)	96 (100%)	0	100	100
14	O	175/230 (76%)	175 (100%)	0	100	100
15	P	88/123 (72%)	88 (100%)	0	100	100
16	Q	78/78 (100%)	78 (100%)	0	100	100
17	R	264/318 (83%)	264 (100%)	0	100	100
18	S	116/164 (71%)	116 (100%)	0	100	100
19	T	153/157 (98%)	153 (100%)	0	100	100
20	U	152/174 (87%)	152 (100%)	0	100	100
21	W	87/158 (55%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	X	311/351 (89%)	311 (100%)	0	100	100
23	Y	109/357 (30%)	109 (100%)	0	100	100
24	Z	87/95 (92%)	87 (100%)	0	100	100
25	D	263/357 (74%)	263 (100%)	0	100	100
26	G	264/342 (77%)	264 (100%)	0	100	100
27	J	88/118 (75%)	88 (100%)	0	100	100
28	V	319/364 (88%)	319 (100%)	0	100	100
29	4	484/609 (80%)	484 (100%)	0	100	100
30	b	242/350 (69%)	242 (100%)	0	100	100
32	7	377/621 (61%)	377 (100%)	0	100	100
33	a	50/288 (17%)	50 (100%)	0	100	100
All	All	5441/7502 (72%)	5441 (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 (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	185	HIS
3	3	140	HIS
4	B	167	HIS
5	C	156	GLN
6	E	54	HIS
6	E	58	HIS
7	F	214	HIS
8	H	122	GLN
8	H	130	HIS
9	I	183	HIS
10	K	113	HIS
12	M	61	HIS
12	M	69	ASN
12	M	75	HIS
14	O	98	ASN
14	O	147	HIS
16	Q	85	GLN
19	T	59	ASN
22	X	110	HIS
22	X	235	ASN

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Mol	Chain	Res	Type
22	X	312	GLN
22	X	347	ASN
22	X	363	ASN
24	Z	54	ASN
25	D	288	HIS
25	D	347	GLN
25	D	356	GLN
26	G	308	GLN
26	G	384	GLN
27	J	100	HIS
28	V	87	HIS
28	V	329	GLN
28	V	394	GLN
28	V	395	GLN
29	4	136	HIS
29	4	455	ASN
29	4	540	HIS
29	4	545	GLN
30	b	297	ASN
30	b	393	ASN
32	7	352	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	A	945/954 (99%)	258 (27%)	5 (0%)

All (258) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	A	650	U
31	A	651	A
31	A	680	U
31	A	688	A
31	A	704	U
31	A	712	C
31	A	718	A
31	A	721	U
31	A	722	C
31	A	733	U
31	A	737	C

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Mol	Chain	Res	Type
31	A	740	G
31	A	745	A
31	A	753	A
31	A	761	A
31	A	766	G
31	A	773	U
31	A	791	G
31	A	793	C
31	A	794	U
31	A	796	G
31	A	807	A
31	A	808	C
31	A	812	A
31	A	814	A
31	A	815	C
31	A	817	G
31	A	829	C
31	A	830	U
31	A	832	U
31	A	835	C
31	A	860	A
31	A	861	U
31	A	867	C
31	A	869	C
31	A	870	C
31	A	871	A
31	A	884	U
31	A	890	C
31	A	893	G
31	A	896	A
31	A	902	G
31	A	903	U
31	A	908	C
31	A	919	A
31	A	923	A
31	A	929	A
31	A	930	G
31	A	938	A
31	A	939	A
31	A	942	A
31	A	946	U
31	A	950	A

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Mol	Chain	Res	Type
31	A	954	C
31	A	955	A
31	A	956	C
31	A	957	C
31	A	958	C
31	A	960	C
31	A	962	C
31	A	963	C
31	A	964	C
31	A	967	A
31	A	975	A
31	A	982	A
31	A	984	C
31	A	986	G
31	A	988	G
31	A	992	U
31	A	993	A
31	A	1001	C
31	A	1002	C
31	A	1004	G
31	A	1007	G
31	A	1009	C
31	A	1011	C
31	A	1019	A
31	A	1028	G
31	A	1042	U
31	A	1043	C
31	A	1045	G
31	A	1046	A
31	A	1048	C
31	A	1049	A
31	A	1052	C
31	A	1058	C
31	A	1065	C
31	A	1069	A
31	A	1077	U
31	A	1078	A
31	A	1079	G
31	A	1082	A
31	A	1084	C
31	A	1103	A
31	A	1105	C

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Mol	Chain	Res	Type
31	A	1107	U
31	A	1109	A
31	A	1110	A
31	A	1117	A
31	A	1118	A
31	A	1119	U
31	A	1120	C
31	A	1121	A
31	A	1126	A
31	A	1137	A
31	A	1153	C
31	A	1155	G
31	A	1166	A
31	A	1167	A
31	A	1176	G
31	A	1179	G
31	A	1181	G
31	A	1185	C
31	A	1186	A
31	A	1187	U
31	A	1188	A
31	A	1189	U
31	A	1190	C
31	A	1193	U
31	A	1194	C
31	A	1197	G
31	A	1199	G
31	A	1200	G
31	A	1203	C
31	A	1209	C
31	A	1212	U
31	A	1215	U
31	A	1223	C
31	A	1229	U
31	A	1235	U
31	A	1236	C
31	A	1239	C
31	A	1240	A
31	A	1245	U
31	A	1246	U
31	A	1248	C
31	A	1249	U

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Mol	Chain	Res	Type
31	A	1250	C
31	A	1251	A
31	A	1254	C
31	A	1259	U
31	A	1269	U
31	A	1271	C
31	A	1272	A
31	A	1275	A
31	A	1276	A
31	A	1277	A
31	A	1278	C
31	A	1280	C
31	A	1281	U
31	A	1285	G
31	A	1286	A
31	A	1287	A
31	A	1291	U
31	A	1292	A
31	A	1293	C
31	A	1295	A
31	A	1296	A
31	A	1297	G
31	A	1298	U
31	A	1312	C
31	A	1314	C
31	A	1325	U
31	A	1326	A
31	A	1327	G
31	A	1328	G
31	A	1342	C
31	A	1343	A
31	A	1350	G
31	A	1351	G
31	A	1352	C
31	A	1353	A
31	A	1354	A
31	A	1355	G
31	A	1356	A
31	A	1358	A
31	A	1365	A
31	A	1367	A
31	A	1371	U

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Mol	Chain	Res	Type
31	A	1373	U
31	A	1377	C
31	A	1378	C
31	A	1379	A
31	A	1386	U
31	A	1387	A
31	A	1390	A
31	A	1392	A
31	A	1399	A
31	A	1402	A
31	A	1403	A
31	A	1405	C
31	A	1406	U
31	A	1415	G
31	A	1419	G
31	A	1420	U
31	A	1421	G
31	A	1422	G
31	A	1426	U
31	A	1429	C
31	A	1430	A
31	A	1431	G
31	A	1432	U
31	A	1433	A
31	A	1451	U
31	A	1456	U
31	A	1458	A
31	A	1460	C
31	A	1461	A
31	A	1462	G
31	A	1463	G
31	A	1464	G
31	A	1466	C
31	A	1468	U
31	A	1471	A
31	A	1472	G
31	A	1473	C
31	A	1478	A
31	A	1480	A
31	A	1481	C
31	A	1482	A
31	A	1483	C

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Mol	Chain	Res	Type
31	A	1484	C
31	A	1485	G
31	A	1486	C
31	A	1491	C
31	A	1501	A
31	A	1518	C
31	A	1521	U
31	A	1522	U
31	A	1523	A
31	A	1524	A
31	A	1525	C
31	A	1526	U
31	A	1527	A
31	A	1533	C
31	A	1537	C
31	A	1539	C
31	A	1546	A
31	A	1547	U
31	A	1556	C
31	A	1558	A
31	A	1559	G
31	A	1563	U
31	A	1564	A
31	A	1565	A
31	A	1566	C
31	A	1567	A
31	A	1568	U
31	A	1570	G
31	A	1571	U
31	A	1572	A
31	A	1580	U
31	A	1583	MA6
31	A	1590	A
31	A	1591	C
31	A	1594	G
31	A	1595	G
31	A	1601	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	A	1341	C

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Mol	Chain	Res	Type
31	A	1386	U
31	A	1432	U
31	A	1461	A
31	A	1483	C

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

3 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
9	5F0	I	184	9	8,8,9	0.56	0	7,9,11	1.21	1 (14%)
31	MA6	A	1584	31	23,26,27	1.28	3 (13%)	34,38,41	3.19	12 (35%)
31	MA6	A	1583	31	23,26,27	1.27	3 (13%)	34,38,41	3.14	11 (32%)

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
9	5F0	I	184	9	-	2/9/9/10	-
31	MA6	A	1584	31	-	0/11/29/30	0/3/3/3
31	MA6	A	1583	31	-	1/11/29/30	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	1583	MA6	C6-N6	3.39	1.46	1.36
31	A	1584	MA6	C6-N6	3.36	1.46	1.36
31	A	1584	MA6	C5-C4	-2.59	1.34	1.39
31	A	1583	MA6	C5-C4	-2.53	1.34	1.39
31	A	1583	MA6	C5-N7	-2.30	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	1584	MA6	C5-N7	-2.27	1.34	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1584	MA6	N1-C6-N6	-12.52	103.39	117.08
31	A	1583	MA6	N1-C6-N6	-12.20	103.75	117.08
31	A	1584	MA6	C5-C6-N6	6.39	136.43	125.30
31	A	1583	MA6	C5-C6-N6	6.19	136.09	125.30
31	A	1583	MA6	N1-C2-N3	-5.48	120.03	128.60
31	A	1584	MA6	N1-C2-N3	-5.42	120.12	128.60
31	A	1583	MA6	C5-C4-N3	-5.16	120.02	126.75
31	A	1584	MA6	C5-C4-N3	-5.16	120.02	126.75
31	A	1584	MA6	N9-C8-N7	-4.37	107.94	113.91
31	A	1583	MA6	N9-C8-N7	-4.15	108.23	113.91
31	A	1583	MA6	C4-C5-C6	3.50	119.80	115.88
31	A	1584	MA6	C4-C5-C6	3.50	119.80	115.88
31	A	1583	MA6	C2-N3-C4	3.49	120.00	111.75
31	A	1584	MA6	C2-N3-C4	3.49	119.99	111.75
31	A	1583	MA6	C2-N1-C6	3.49	119.99	111.75
31	A	1584	MA6	C2-N1-C6	3.44	119.89	111.75
31	A	1584	MA6	C5-N7-C8	3.18	108.03	103.51
31	A	1583	MA6	N3-C4-N9	3.10	132.19	127.08
31	A	1584	MA6	N3-C4-N9	3.02	132.06	127.08
31	A	1583	MA6	C5-N7-C8	3.01	107.79	103.51
9	I	184	5F0	O-C-CB	-2.80	117.26	125.43
31	A	1584	MA6	C4-N9-C8	2.19	108.10	105.73
31	A	1584	MA6	C4-C5-N7	-2.14	108.01	110.62
31	A	1583	MA6	C4-N9-C8	2.07	107.97	105.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	184	5F0	OD1-C1-CA-CB
31	A	1583	MA6	C4'-C5'-O5'-P
9	I	184	5F0	O-C-CB-CA

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	184	5F0	2	0
31	A	1584	MA6	1	0
31	A	1583	MA6	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 21 are monoatomic - leaving 7 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
38	NAD	A	1701	40	45,48,48	0.74	1 (2%)	63,73,73	0.72	1 (1%)
35	FES	P	201	6,15	0,4,4	-	-	-	-	-
36	ATP	X	501	-	29,33,33	0.28	0	44,52,52	0.69	1 (2%)
37	GDP	7	801	-	28,30,30	1.13	3 (10%)	44,47,47	1.84	7 (15%)
35	FES	T	201	12,19	0,4,4	-	-	-	-	-
37	GDP	X	502	-	28,30,30	1.13	3 (10%)	44,47,47	1.87	7 (15%)
39	SPM	A	1702	-	13,13,13	0.35	0	12,12,12	0.97	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
38	NAD	A	1701	40	-	0/30/62/62	0/5/5/5
35	FES	P	201	6,15	-	-	0/1/1/1
36	ATP	X	501	-	-	10/22/38/38	0/3/3/3
37	GDP	7	801	-	-	5/16/32/32	0/3/3/3
35	FES	T	201	12,19	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	GDP	X	502	-	-	4/16/32/32	0/3/3/3
39	SPM	A	1702	-	-	1/11/11/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	7	801	GDP	C5-C4	3.07	1.47	1.38
37	X	502	GDP	C5-C4	3.06	1.47	1.38
38	A	1701	NAD	O4D-C1D	-2.45	1.37	1.41
37	X	502	GDP	C6-N1	-2.40	1.34	1.38
37	7	801	GDP	C6-N1	-2.38	1.34	1.38
37	X	502	GDP	C5-N7	-2.14	1.34	1.39
37	7	801	GDP	C5-N7	-2.13	1.35	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	801	GDP	C5-C4-N3	-6.19	118.42	128.46
37	X	502	GDP	C5-C4-N3	-6.09	118.58	128.46
37	7	801	GDP	C2-N3-C4	4.89	121.01	112.30
37	X	502	GDP	C2-N3-C4	4.88	120.99	112.30
37	7	801	GDP	N9-C4-N3	4.63	135.24	125.94
37	X	502	GDP	N9-C4-N3	4.58	135.13	125.94
37	X	502	GDP	PA-O3A-PB	-3.85	119.63	132.83
37	7	801	GDP	PA-O3A-PB	-3.55	120.65	132.83
37	X	502	GDP	C6-C5-N7	3.27	136.34	130.25
37	7	801	GDP	C6-C5-N7	3.15	136.10	130.25
37	X	502	GDP	C4-C5-N7	-2.70	106.44	110.72
37	7	801	GDP	C4-C5-N7	-2.69	106.46	110.72
37	7	801	GDP	O6-C6-C5	-2.16	120.88	126.60
37	X	502	GDP	O6-C6-C5	-2.15	120.89	126.60
36	X	501	ATP	PB-O3B-PG	2.06	139.88	132.83
38	A	1701	NAD	O2A-PA-O1A	2.04	122.33	112.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	X	501	ATP	C5'-O5'-PA-O1A
36	X	501	ATP	C5'-O5'-PA-O2A
37	7	801	GDP	C5'-O5'-PA-O2A

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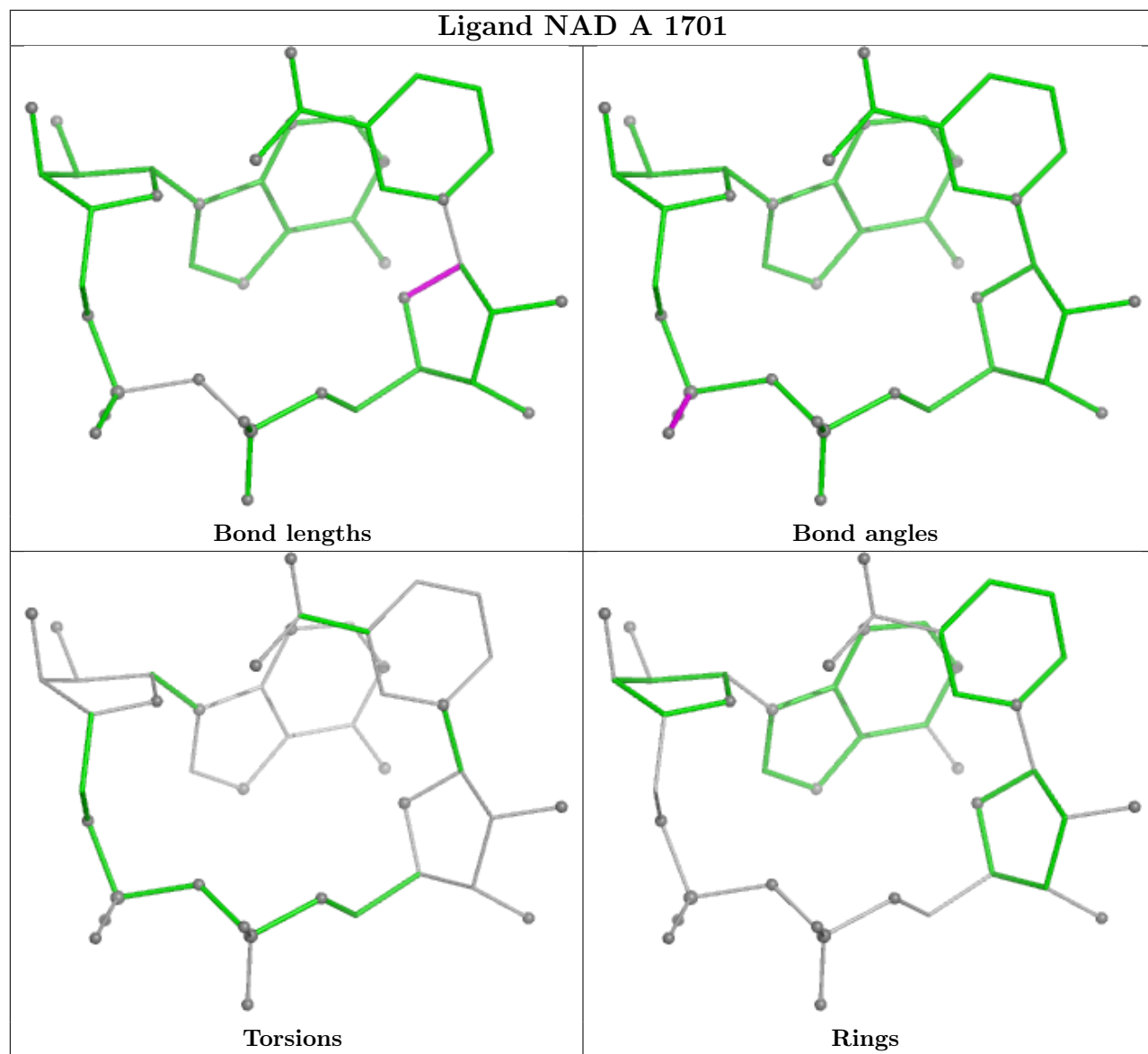
Mol	Chain	Res	Type	Atoms
36	X	501	ATP	C3'-C4'-C5'-O5'
37	7	801	GDP	O4'-C4'-C5'-O5'
36	X	501	ATP	O4'-C4'-C5'-O5'
36	X	501	ATP	C4'-C5'-O5'-PA
39	A	1702	SPM	C7-C8-C9-N10
37	7	801	GDP	C3'-C4'-C5'-O5'
37	7	801	GDP	C5'-O5'-PA-O3A
36	X	501	ATP	PG-O3B-PB-O1B
37	7	801	GDP	C5'-O5'-PA-O1A
36	X	501	ATP	PG-O3B-PB-O2B
37	X	502	GDP	O4'-C4'-C5'-O5'
37	X	502	GDP	PA-O3A-PB-O3B
36	X	501	ATP	C5'-O5'-PA-O3A
36	X	501	ATP	PB-O3A-PA-O1A
36	X	501	ATP	PB-O3A-PA-O2A
37	X	502	GDP	C5'-O5'-PA-O1A
37	X	502	GDP	PA-O3A-PB-O1B

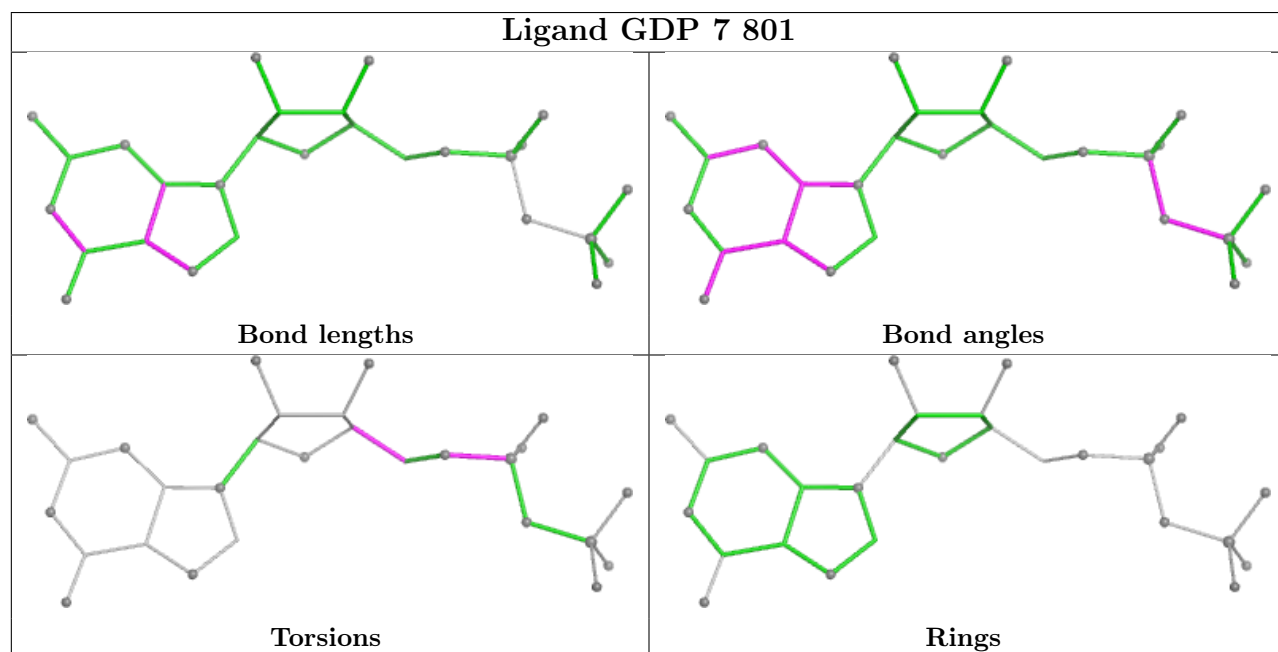
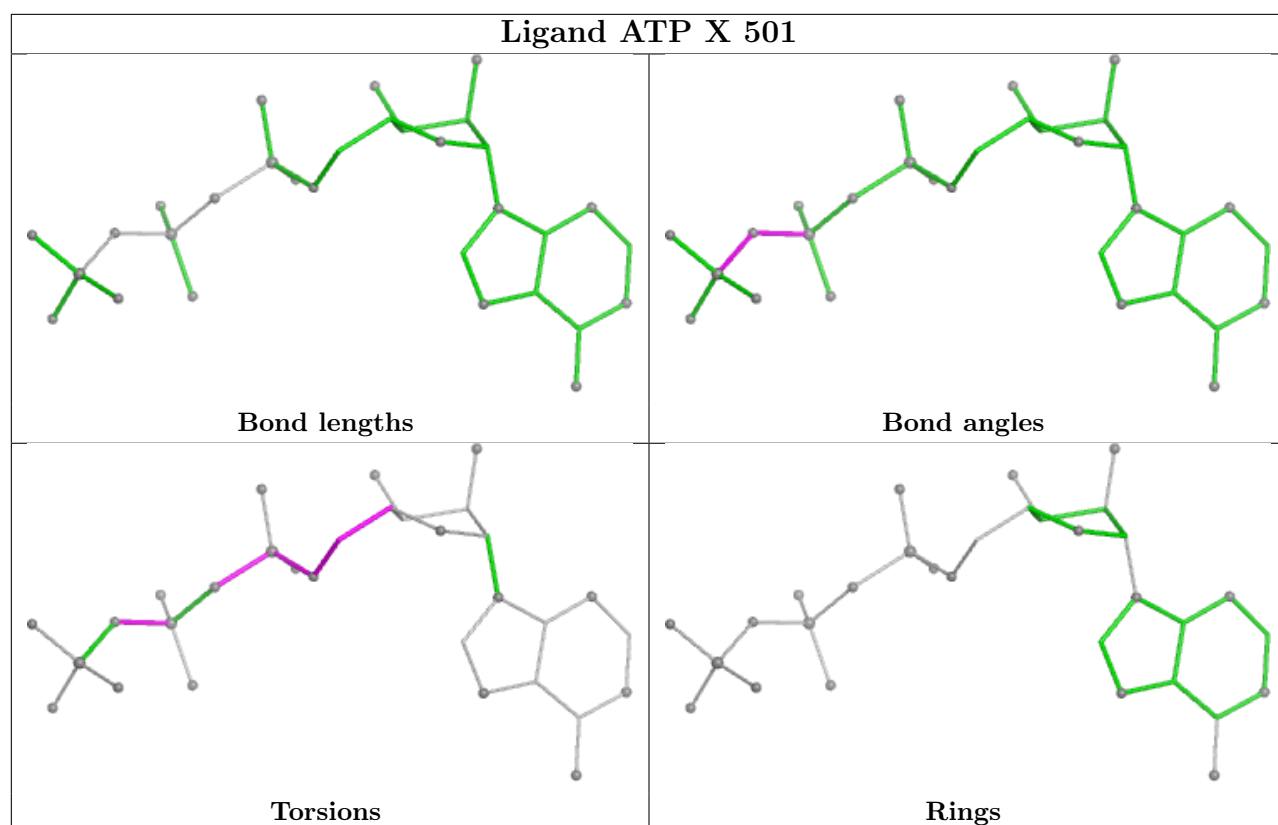
There are no ring outliers.

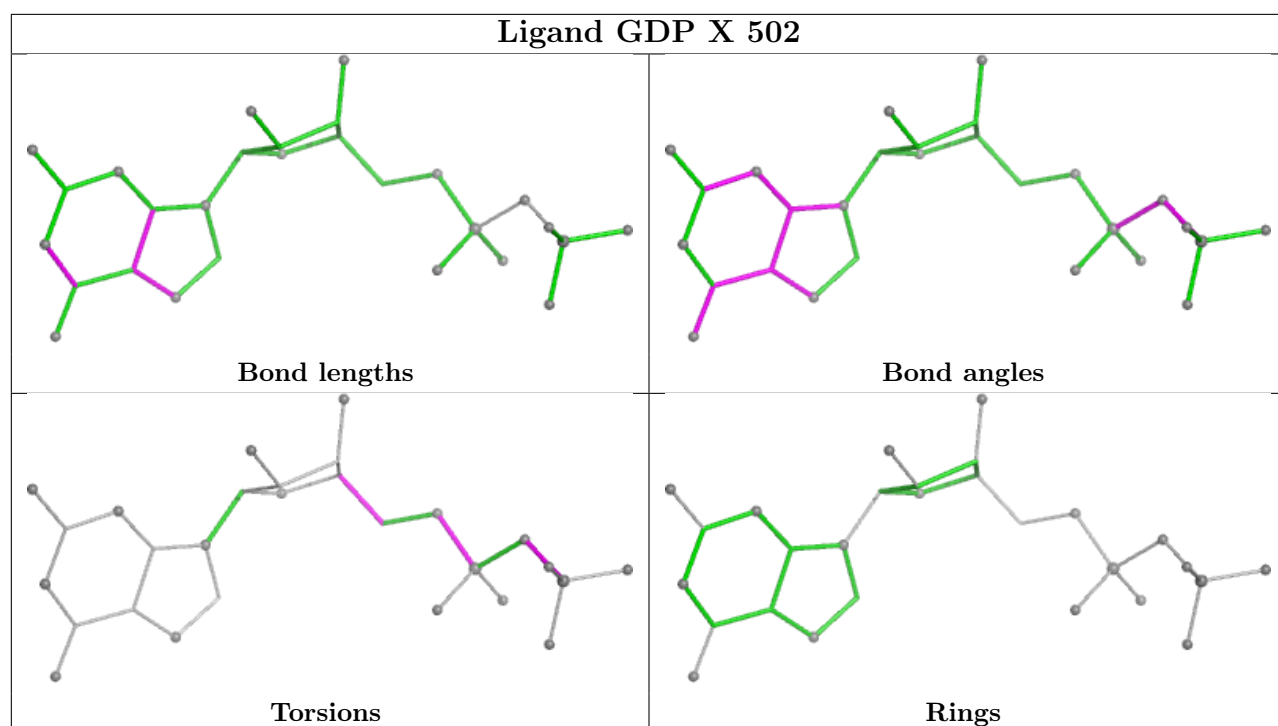
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	P	201	FES	1	0
36	X	501	ATP	1	0
37	7	801	GDP	1	0
35	T	201	FES	4	0
39	A	1702	SPM	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](#)

There are no chain breaks in this entry.

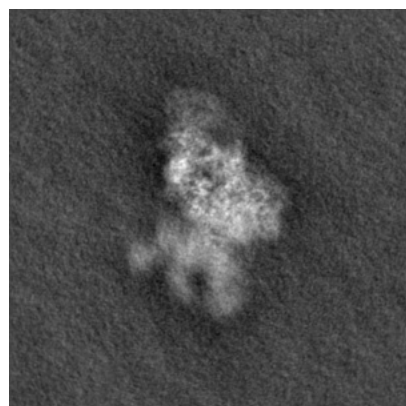
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54130. These allow visual inspection of the internal detail of the map and identification of artifacts.

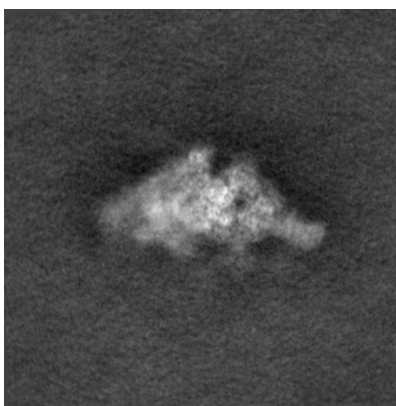
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

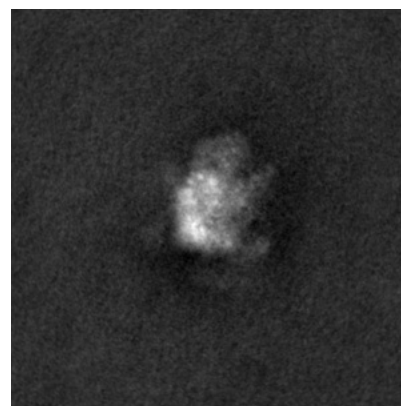
#### 6.1.1 Primary map



X

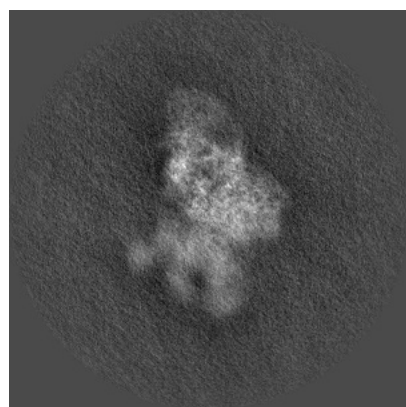


Y

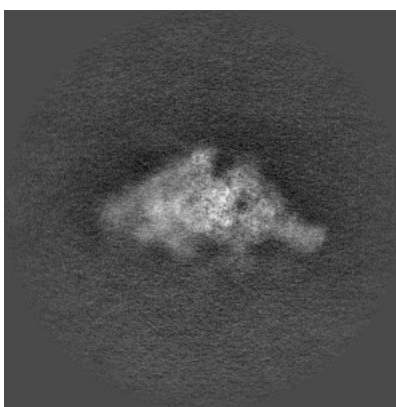


Z

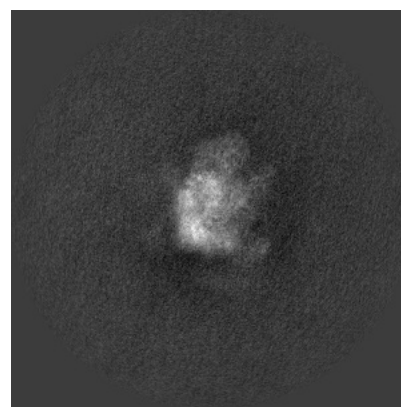
#### 6.1.2 Raw map



X



Y



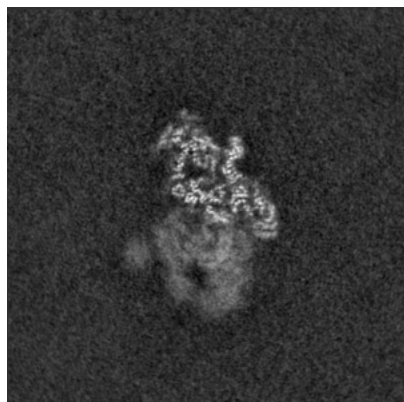
Z

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

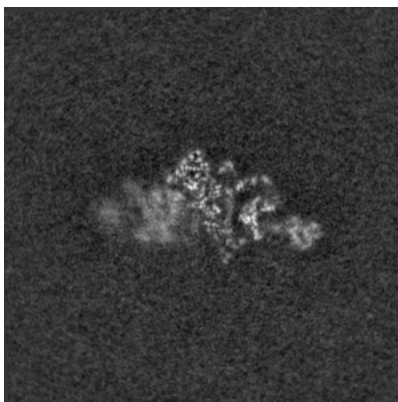


## 6.2 Central slices [i](#)

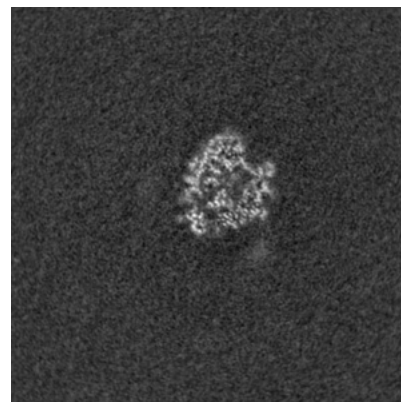
### 6.2.1 Primary map



X Index: 300

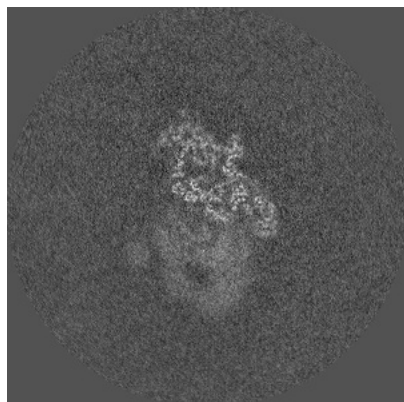


Y Index: 300

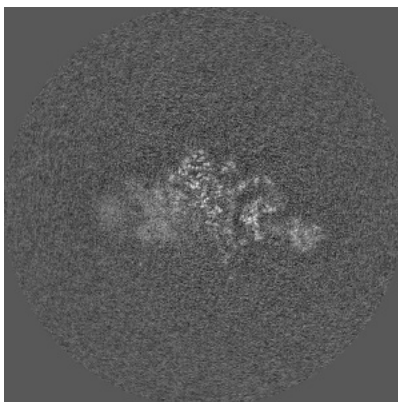


Z Index: 300

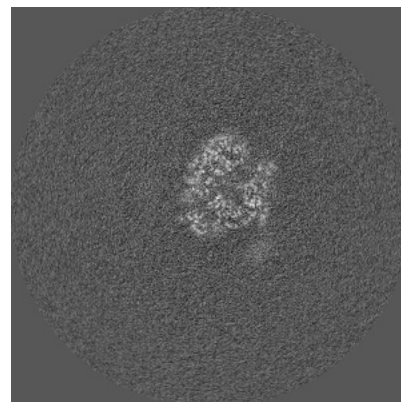
### 6.2.2 Raw map



X Index: 300



Y Index: 300

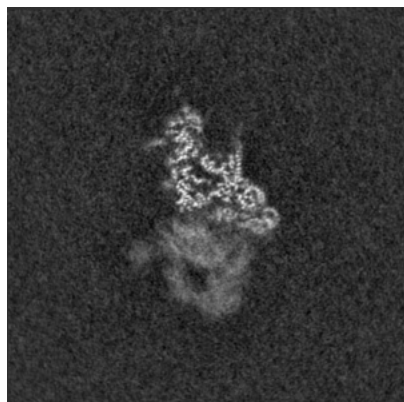


Z Index: 300

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

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

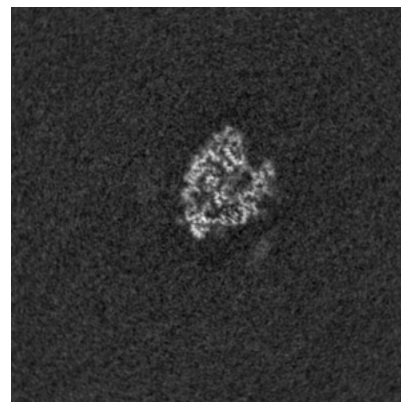
### 6.3.1 Primary map



X Index: 287

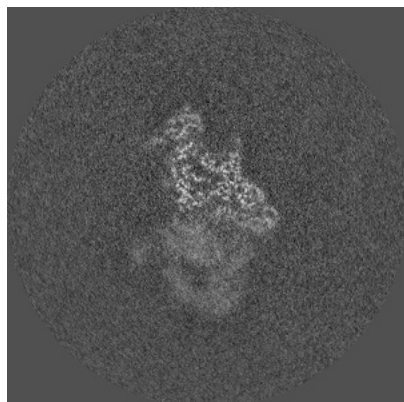


Y Index: 308

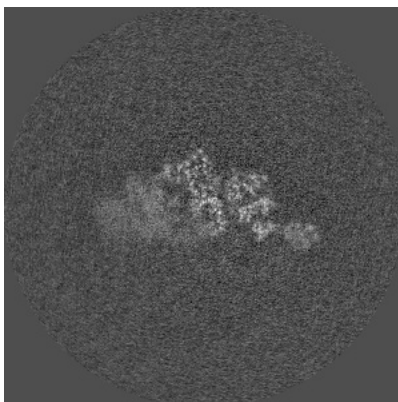


Z Index: 304

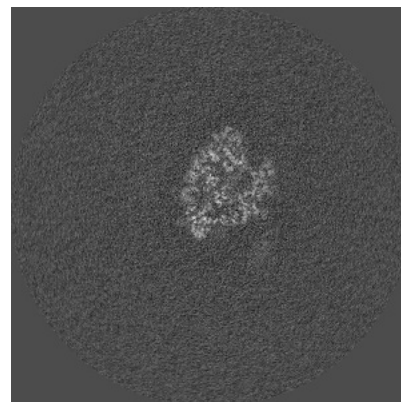
### 6.3.2 Raw map



X Index: 287



Y Index: 308

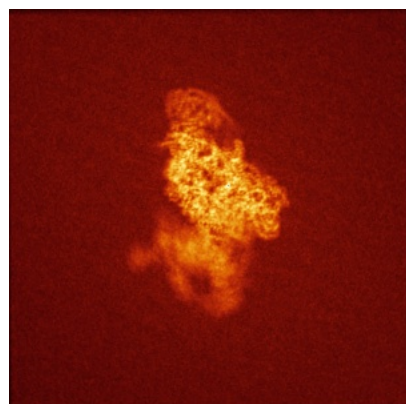


Z Index: 307

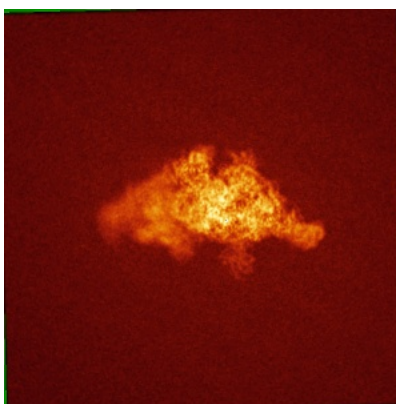
The images above show the largest variance slices of the map in three orthogonal directions.

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

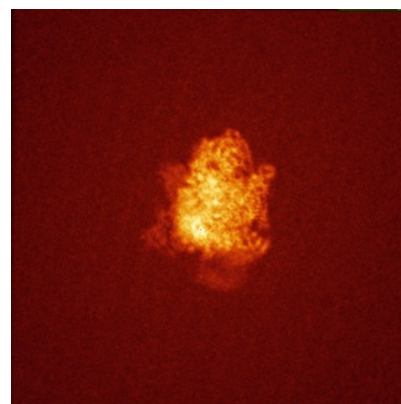
### 6.4.1 Primary map



X

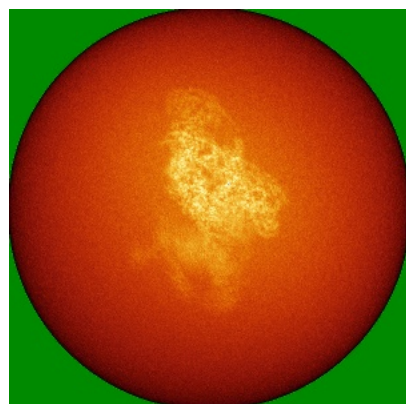


Y

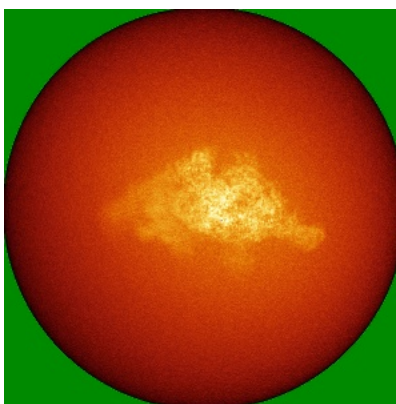


Z

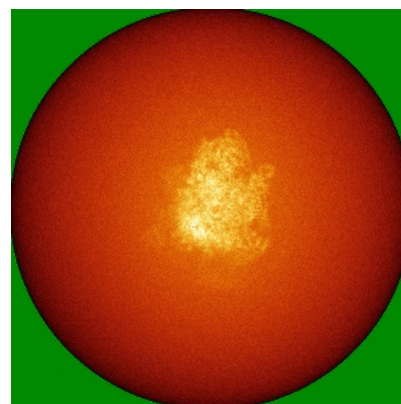
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

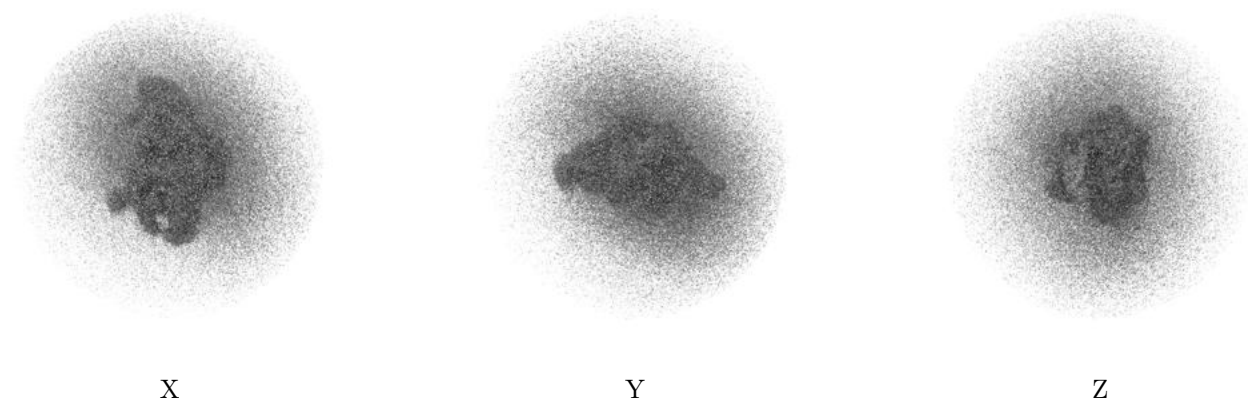
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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](#)

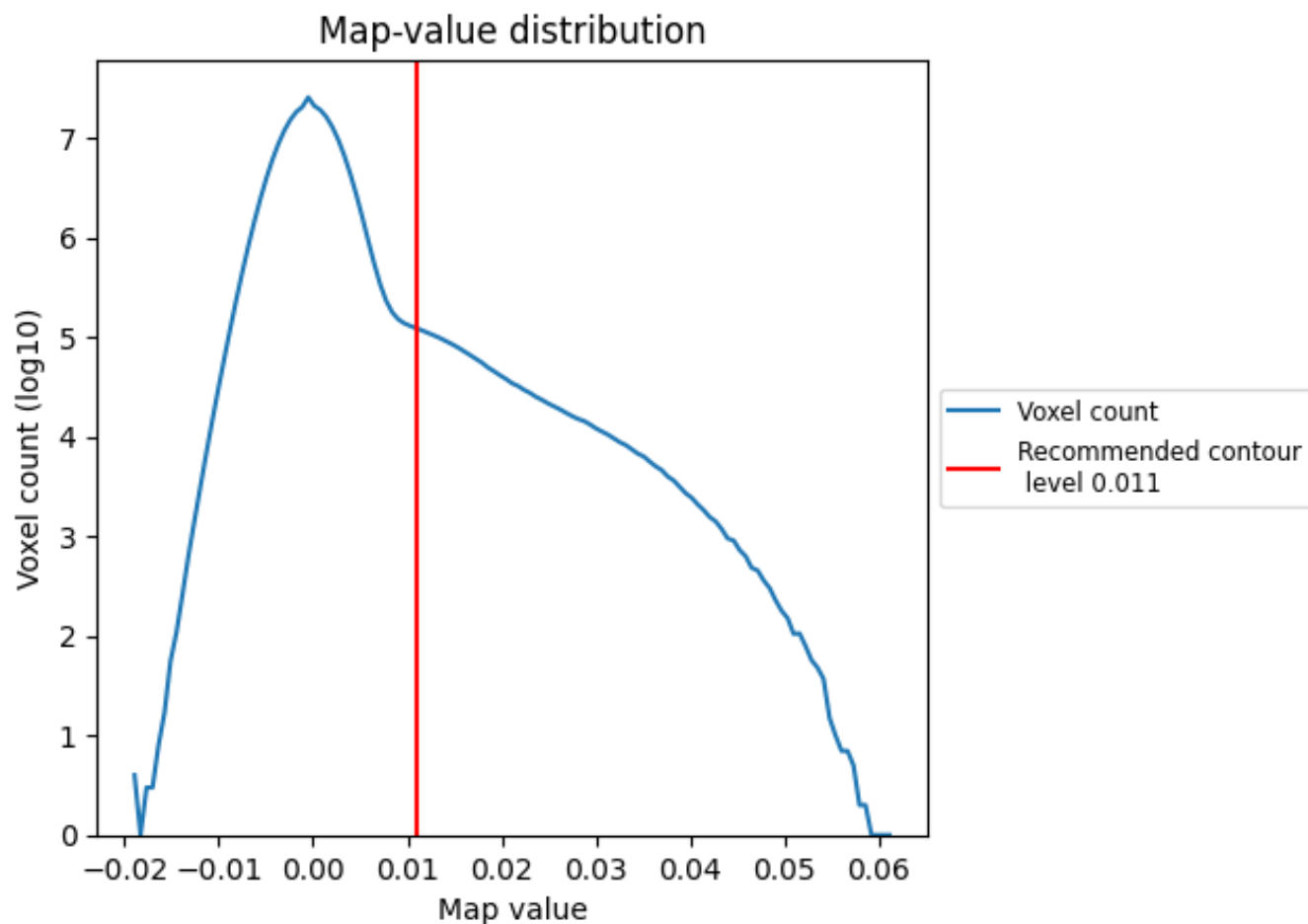
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

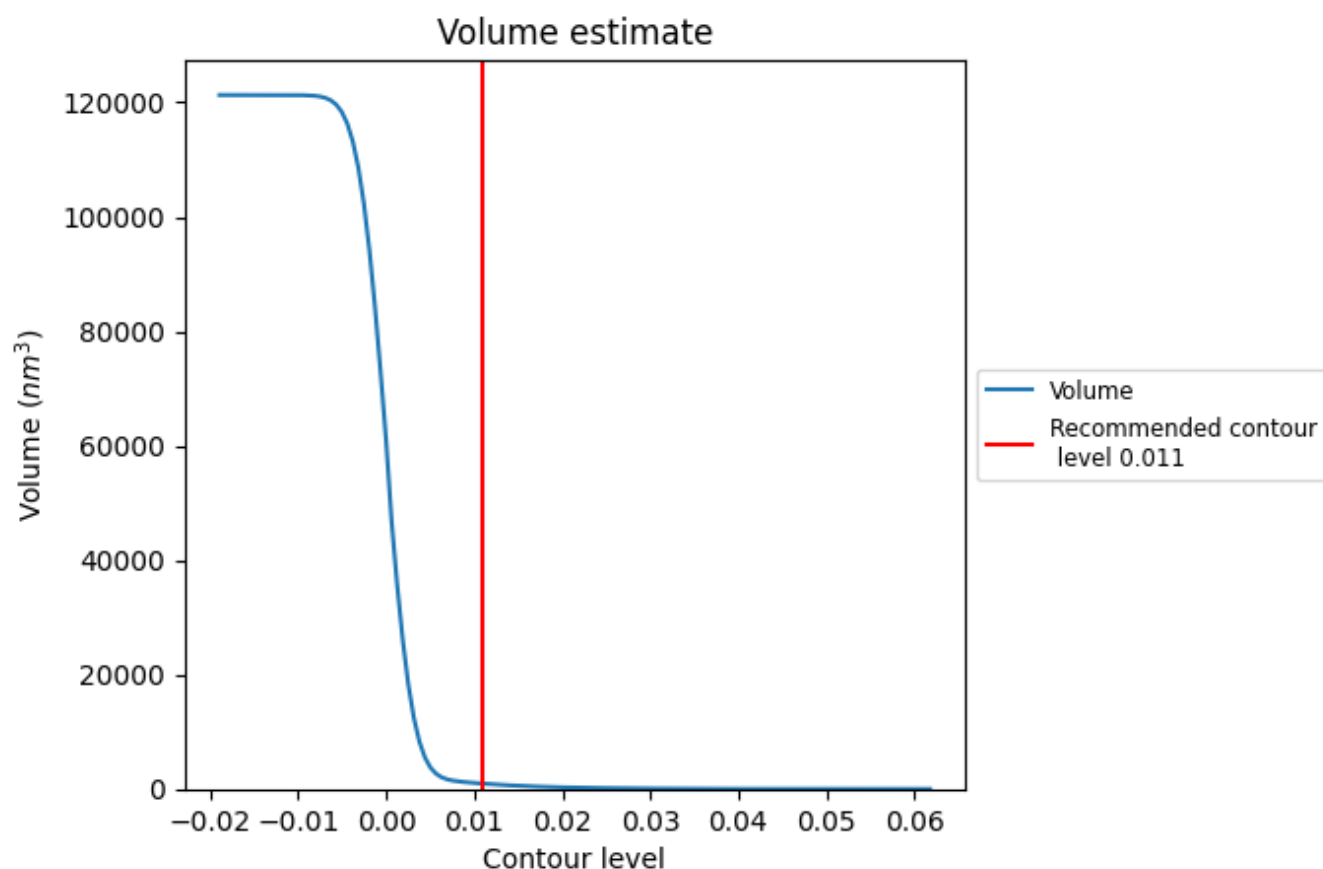
This section contains the results of statistical analysis of the map.

### 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.

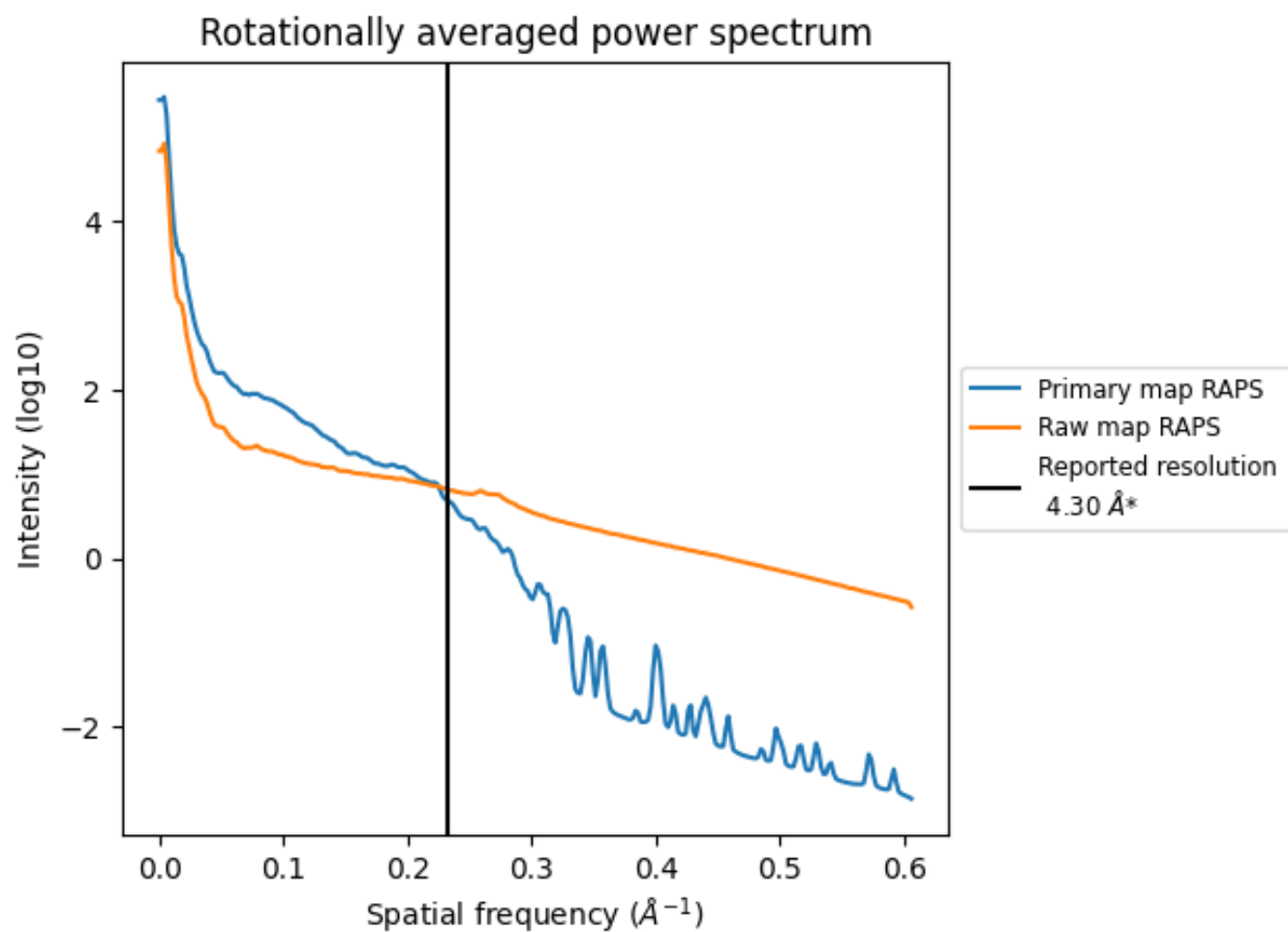
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 936 nm<sup>3</sup>; this corresponds to an approximate mass of 845 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 ⓘ

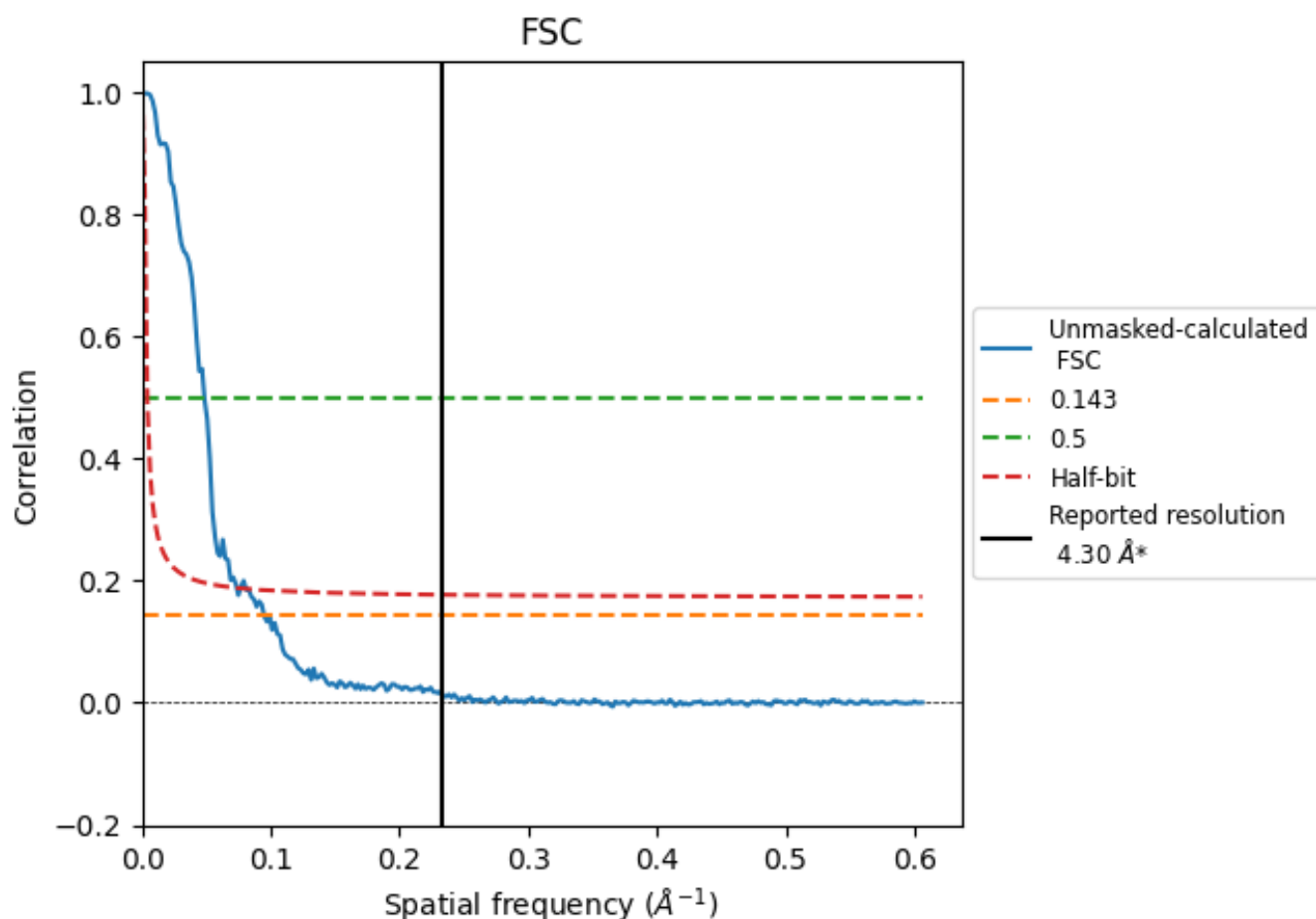


\*Reported resolution corresponds to spatial frequency of 0.233  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

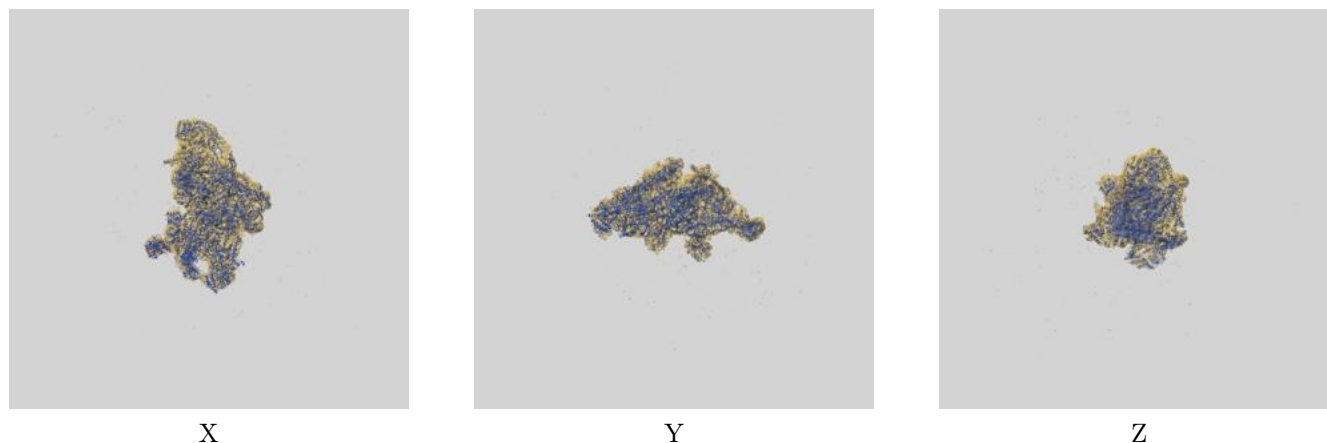
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.56	20.70	13.61

\*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 10.56 differs from the reported value 4.3 by more than 10 %

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

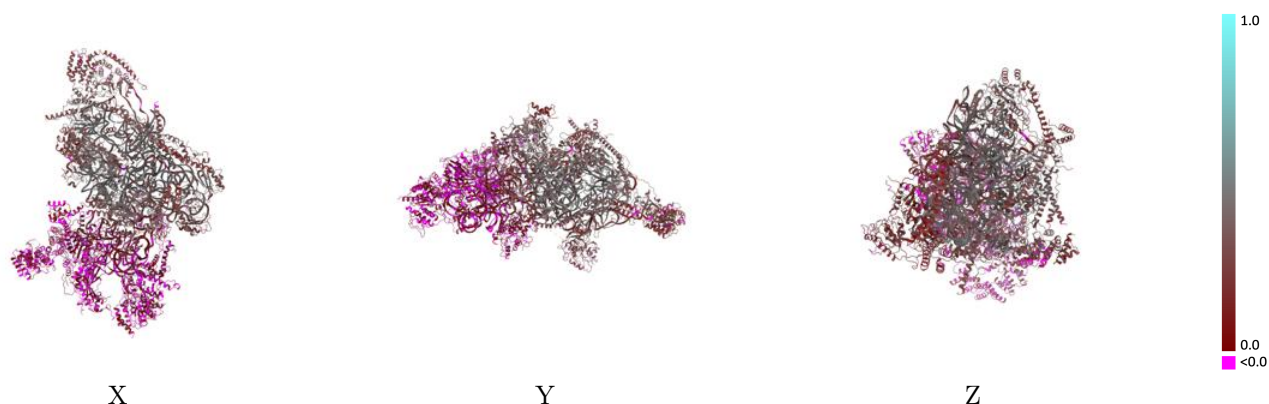
This section contains information regarding the fit between EMDB map EMD-54130 and PDB model 9ROT. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

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



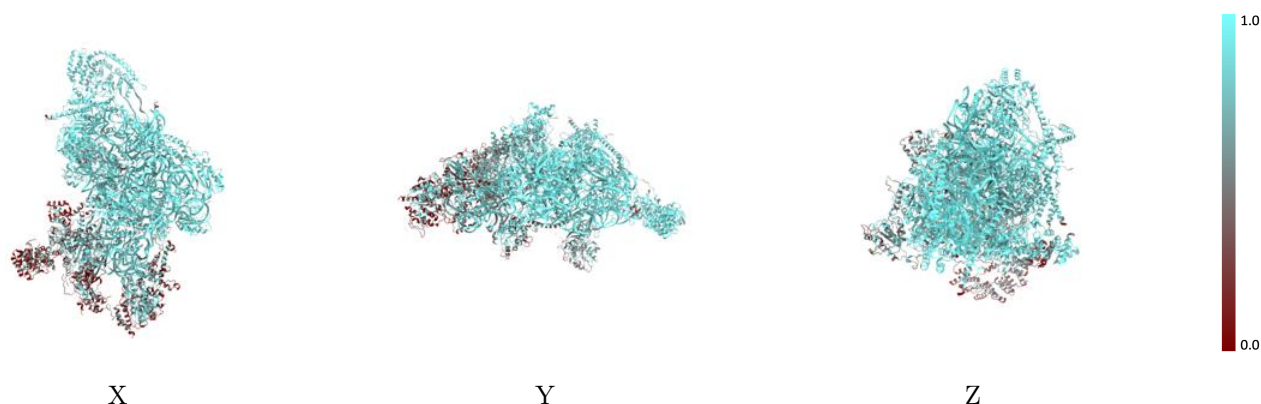
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



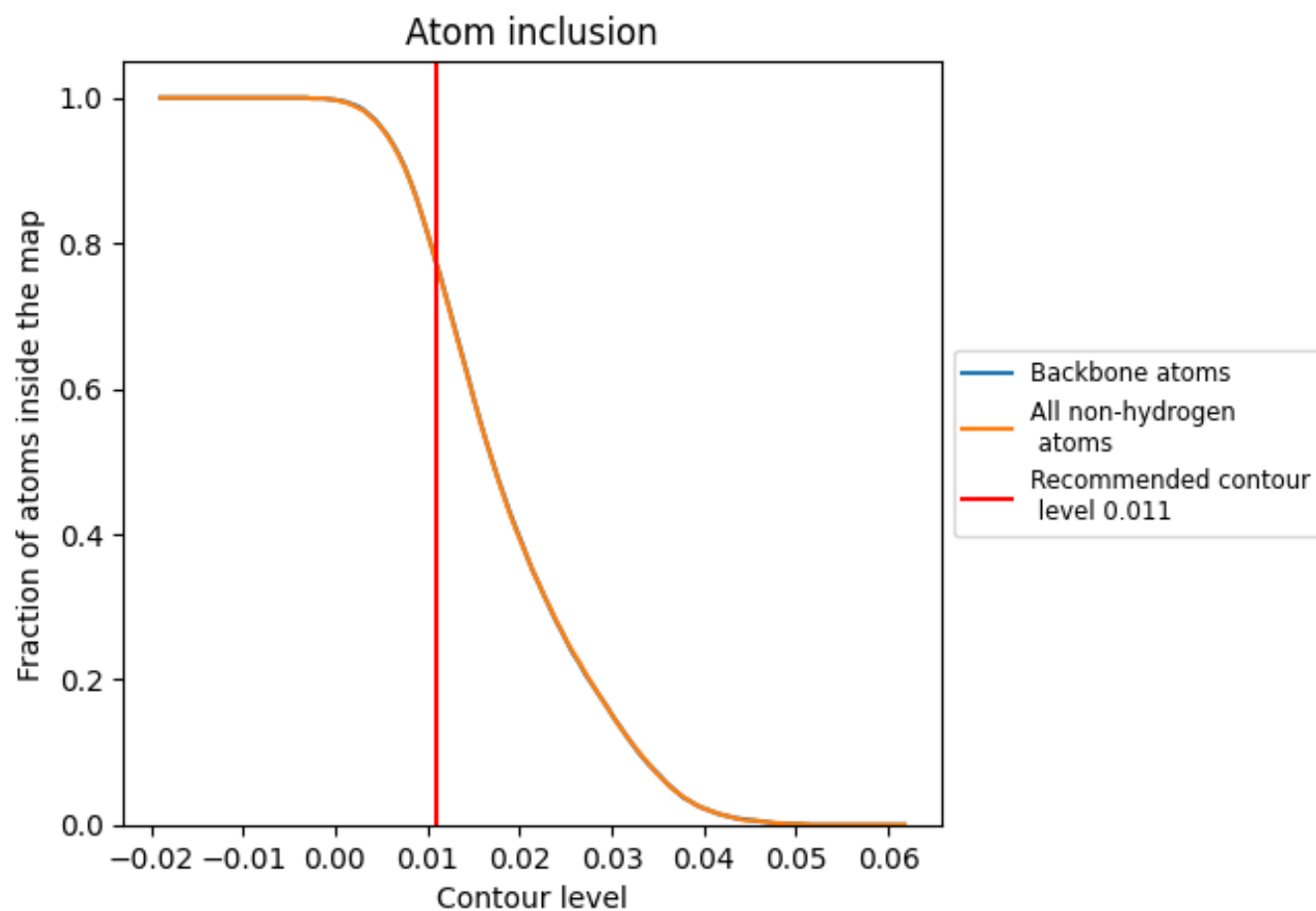
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).





































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 77% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7720	 0.2410
0	 0.8750	 0.3240
1	 0.4380	 0.0390
3	 0.8550	 0.3510
4	 0.3800	 0.0330
7	 0.5840	 0.2490
A	 0.9530	 0.3060
B	 0.8960	 0.3950
C	 0.7210	 0.0770
D	 0.7770	 0.3160
E	 0.8770	 0.3650
F	 0.5480	 0.0410
G	 0.7290	 0.1100
H	 0.4810	 0.0090
I	 0.8990	 0.3050
J	 0.8620	 0.3980
K	 0.6400	 0.0010
L	 0.8710	 0.3520
M	 0.8970	 0.4070
N	 0.9180	 0.4210
O	 0.8970	 0.4000
P	 0.8920	 0.3750
Q	 0.8500	 0.3300
R	 0.8840	 0.3620
S	 0.8830	 0.3440
T	 0.8780	 0.3920
U	 0.8720	 0.3280
V	 0.8730	 0.2140
W	 0.8960	 0.3690
X	 0.5040	 0.0200
Y	 0.3590	 0.0150
Z	 0.5440	 0.0700
a	 0.5780	 0.1280
b	 0.6110	 0.0870

