



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:04 AM UTC

PDB ID : 9IGT / pdb_00009igt
EMDB ID : EMD-52857
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 : 2025-02-20
Resolution : 5.96 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 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

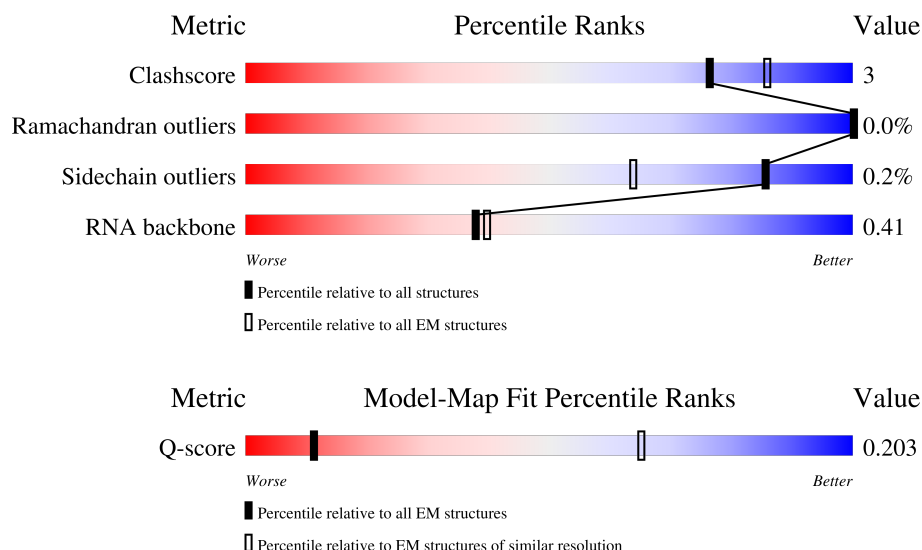
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.96 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	474 (5.47 - 6.46)

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

Mol	Chain	Length	Quality of chain
1	B	296	
2	C	167	
3	D	430	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	125	
5	F	242	
6	G	396	
7	H	201	
8	I	194	
9	J	138	
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	V	414	
22	W	187	
23	X	398	
24	Y	395	
25	Z	106	
26	0	218	
27	1	323	
28	3	199	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	4	689	
30	b	407	
31	A	954	
32	7	691	
33	t	71	
34	a	302	

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
37	FES	P	201	-	-	X	-
8	5F0	I	184	-	-	X	-

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 134086 atoms, of which 62360 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
			3643	1164	1815	331	323	10		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	327	Total	C	H	N	O	S	0	0
			5270	1641	2657	489	470	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	199	Total	C	H	N	O	S	0	0
			3320	1043	1686	293	287	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	304	Total	C	H	N	O	S	0	0
			4997	1592	2489	445	457	14		

- Molecule 7 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	140	Total	C	H	N	O	S	0	0
			2335	745	1183	194	210	3		

- Molecule 8 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	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 9 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	103	Total	C	H	N	O	S	0	0
			1629	493	835	157	138	6		

- 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
			1908	594	966	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
			3166	1019	1567	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 MRPS21 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	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 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
			2765	877	1394	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 S27, mitochondrial.

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

- Molecule 22 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	W	100	Total	C	H	N	O	S	0	0
			1590	498	801	141	146	4		

- Molecule 23 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 24 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 25 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 26 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	0	214	Total	C	H	N	O	S	0	0
			3562	1124	1784	337	312	5		

- Molecule 27 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	1	275	Total	C	H	N	O	S	0	0
			4492	1415	2262	380	424	11		

- Molecule 28 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	3	69	Total	C	H	N	O	S	0	0
			1302	395	686	132	88	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	559	Total	C	H	N	O	S	0	0
			9086	2915	4542	770	833	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
			30394	9040	10238	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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	37	MET	PHE	conflict	UNP P46199

- Molecule 33 is a protein called Large ribosomal subunit protein bL12m, short mature form.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	t	71	Total	C	H	N	O	0	0
			1146	352	599	93	102		

- Molecule 34 is a protein called Putative ribosome-binding factor A, mitochondrial.

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

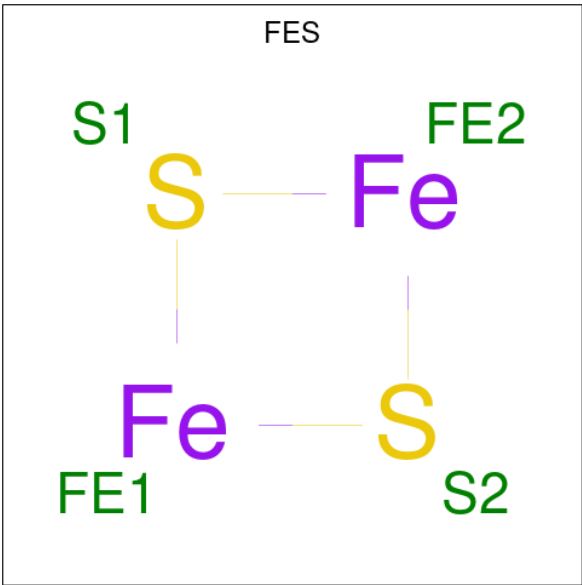
- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	B	1	Total	Mg	0
			1	1	
35	A	11	Total	Mg	0
			11	11	

- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

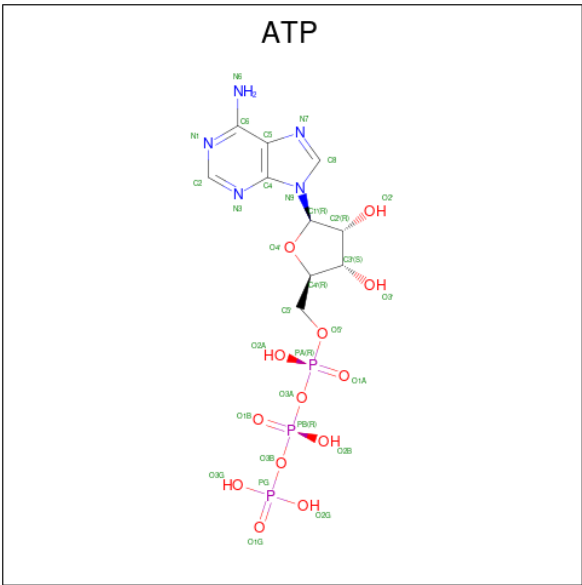
Mol	Chain	Residues	Atoms		AltConf
36	O	1	Total	Zn	0
			1	1	

- Molecule 37 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



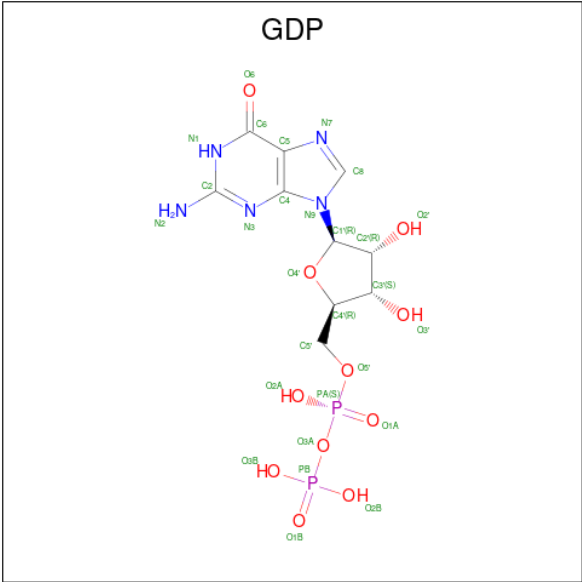
Mol	Chain	Residues	Atoms			AltConf
37	P	1	Total	Fe	S	0
			4	2	2	
37	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 38 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



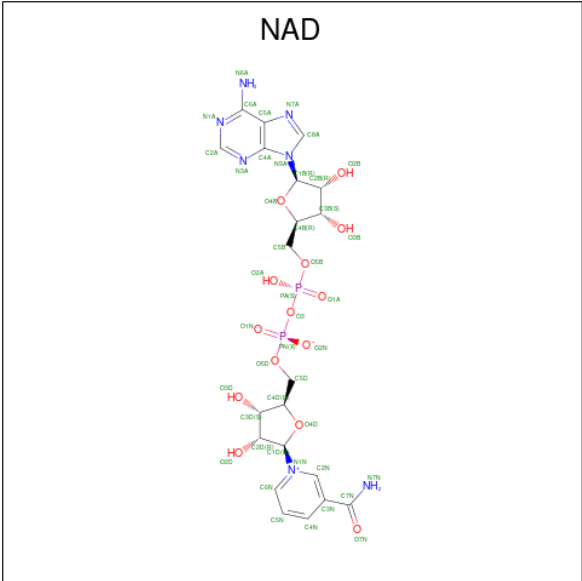
Mol	Chain	Residues	Atoms						AltConf
38	X	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 39 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



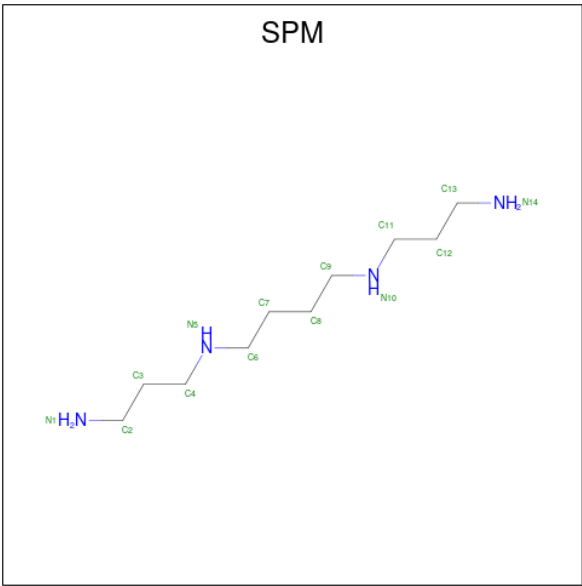
Mol	Chain	Residues	Atoms						AltConf
39	X	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	
39	7	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

- Molecule 40 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 41 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



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

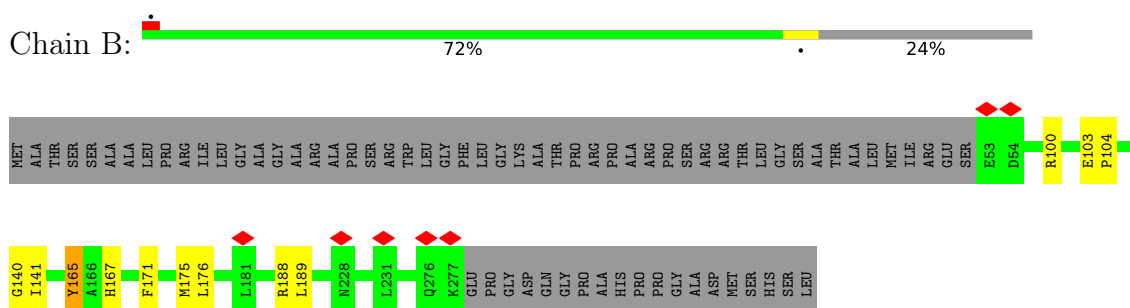
- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	C	1	Total	O	0
			1	1	
42	G	1	Total	O	0
			1	1	
42	I	1	Total	O	0
			1	1	
42	K	1	Total	O	0
			1	1	
42	T	1	Total	O	0
			1	1	
42	0	1	Total	O	0
			1	1	
42	1	1	Total	O	0
			1	1	
42	b	1	Total	O	0
			1	1	

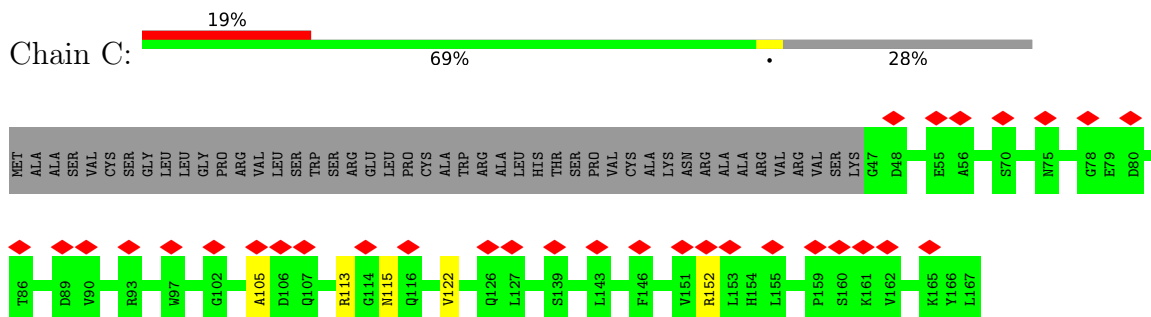
3 Residue-property plots [i](#)

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

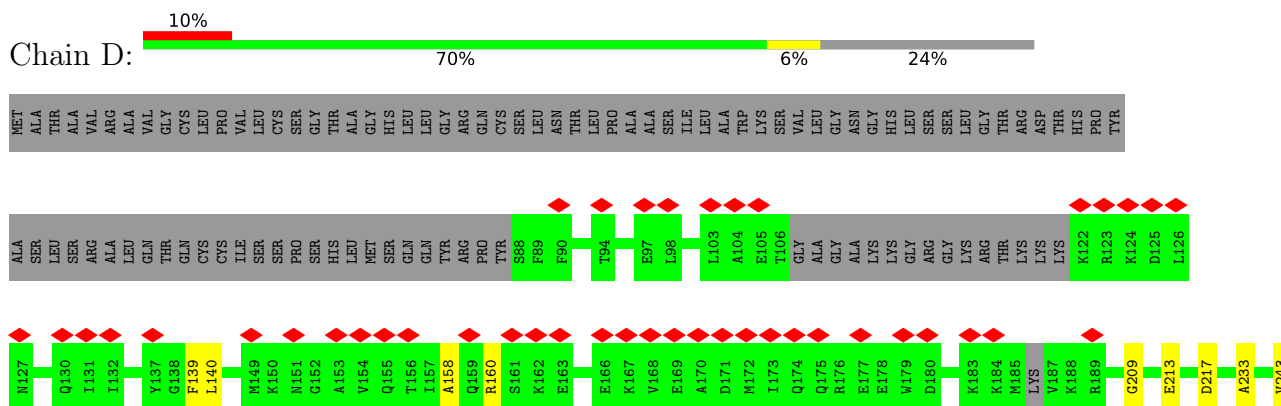
- Molecule 1: 28S ribosomal protein S2, mitochondrial

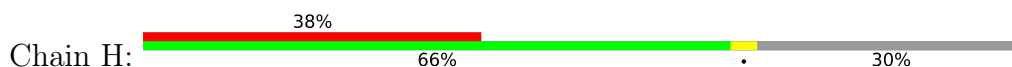


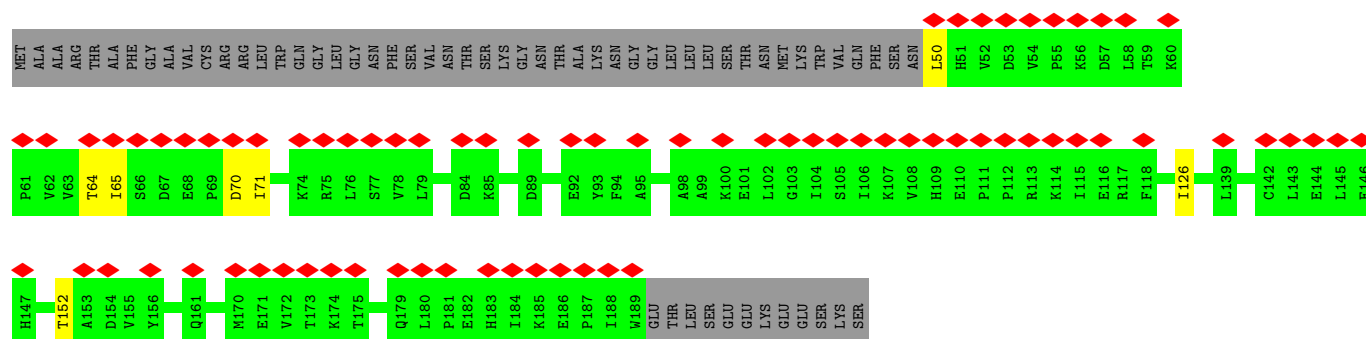
- Molecule 2: 28S ribosomal protein S24, mitochondrial



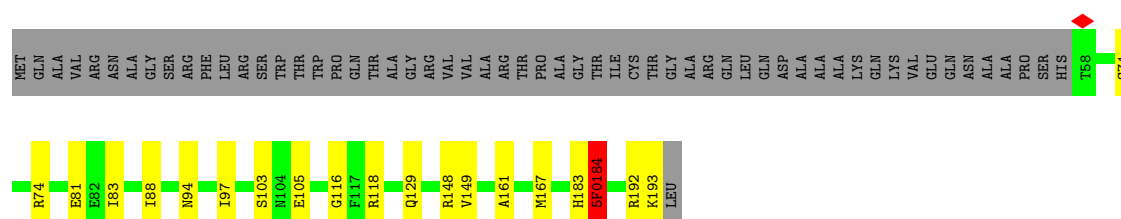
- Molecule 3: 28S ribosomal protein S5, mitochondrial



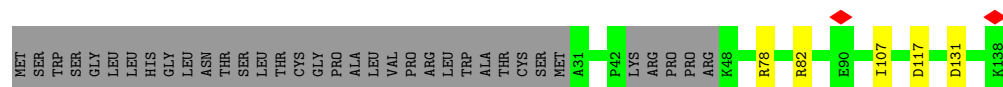




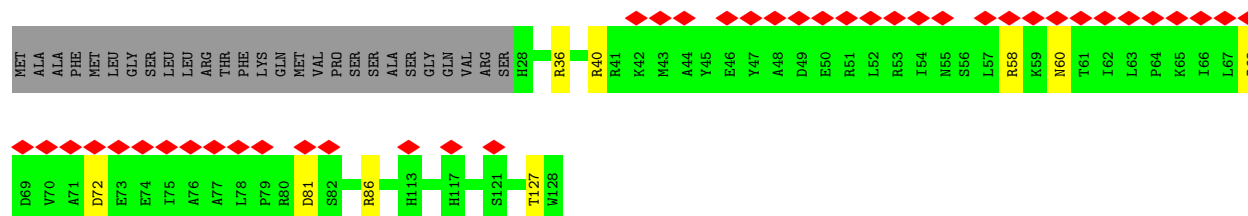
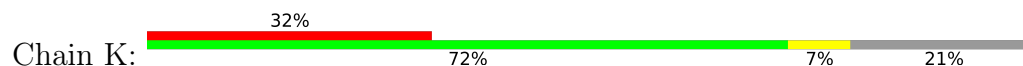
- Molecule 8: 28S ribosomal protein S11, mitochondrial



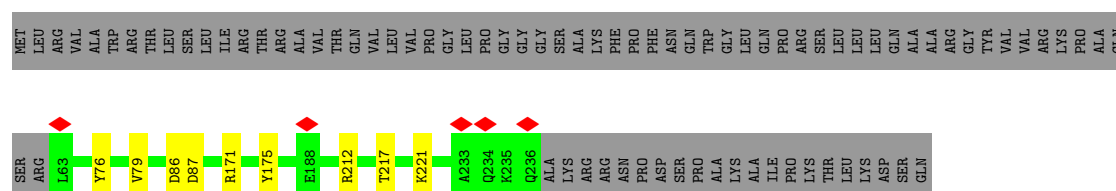
- Molecule 9: 28S ribosomal protein S12, mitochondrial




- Molecule 10: 28S ribosomal protein S14, mitochondrial

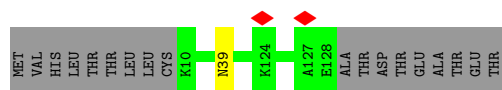


- Molecule 11: 28S ribosomal protein S15, mitochondrial




- Molecule 12: 28S ribosomal protein S16, mitochondrial

Chain M:  86% 13%



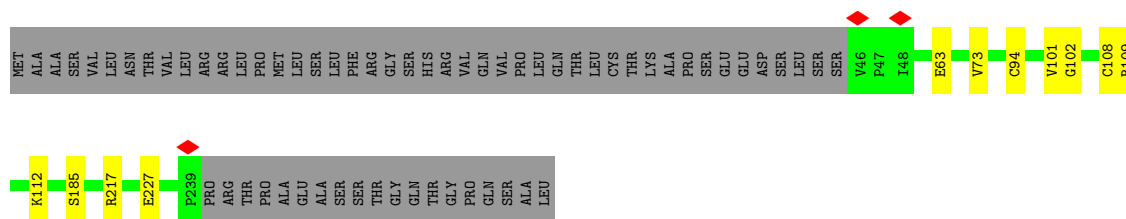
- Molecule 13: 28S ribosomal protein S17, mitochondrial

Chain N:  79% 5% 15%



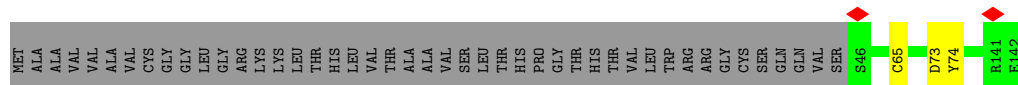
- Molecule 14: 28S ribosomal protein S18b, mitochondrial

Chain O:  71% 25%




- Molecule 15: 28S ribosomal protein S18c, mitochondrial

Chain P:  66% 32%




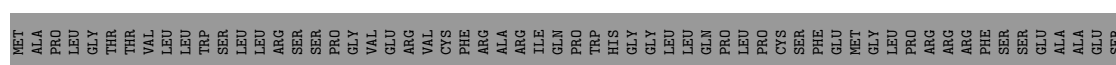
- Molecule 16: MRPS21 isoform 1

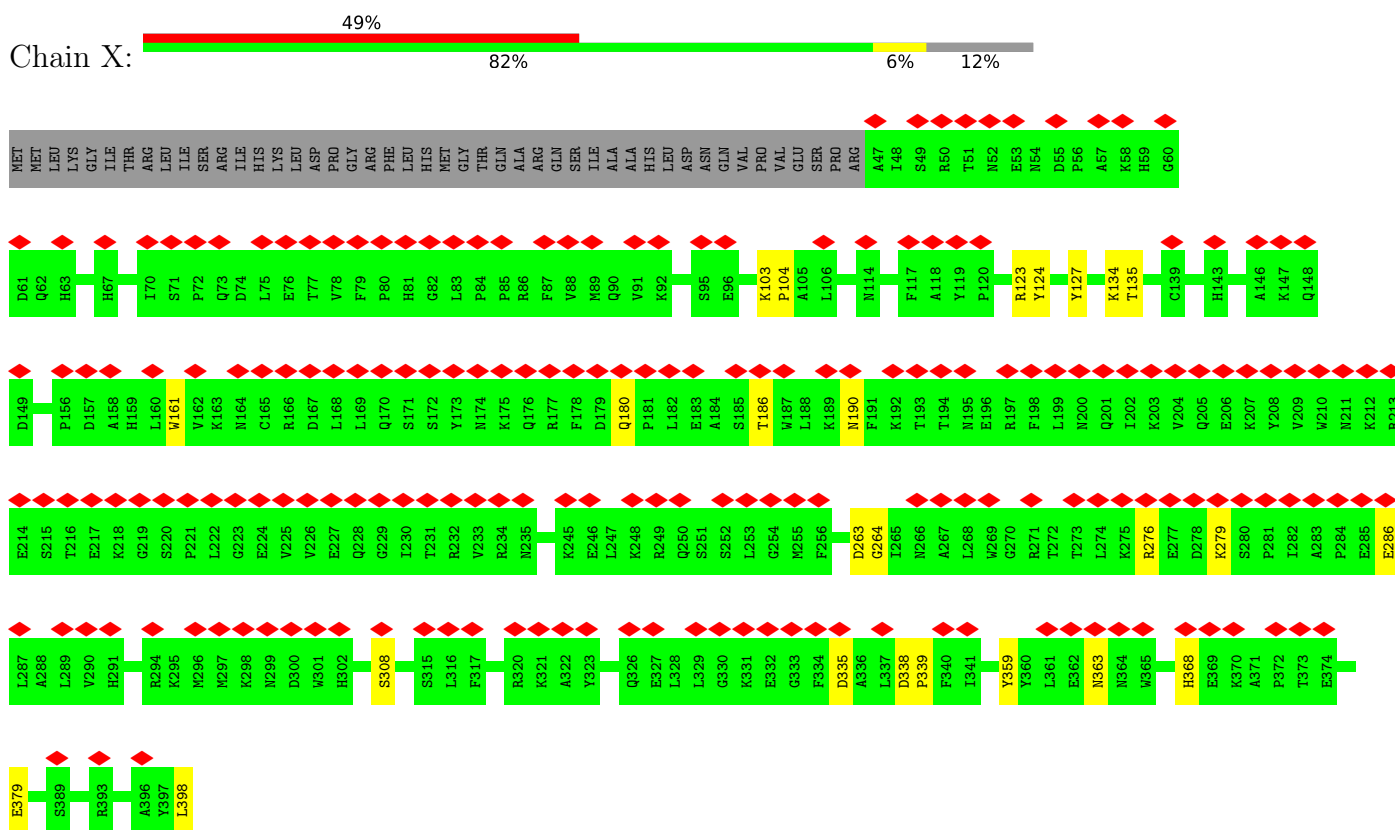
Chain Q:  91% 9%



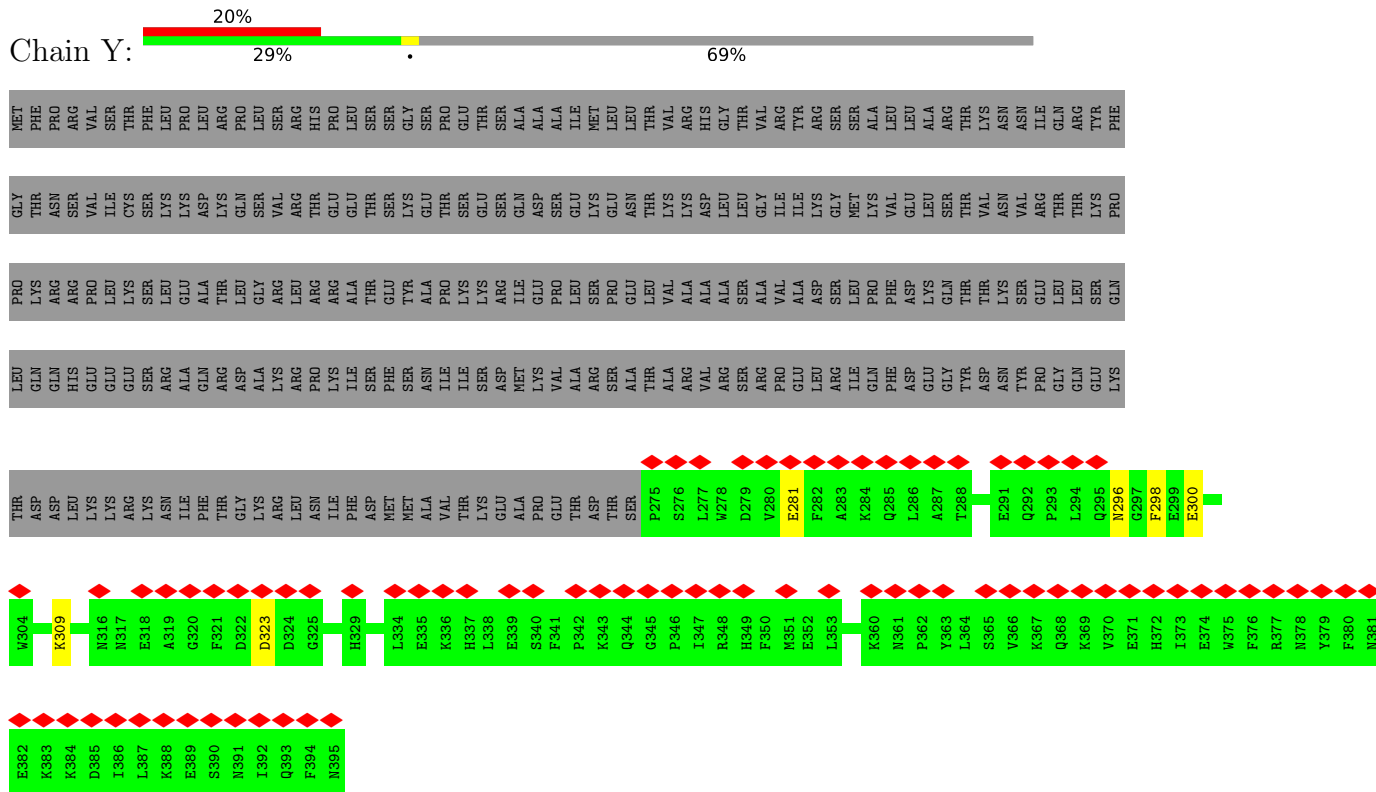
- Molecule 17: 28S ribosomal protein S22, mitochondrial

Chain R:  77% 5% 18%

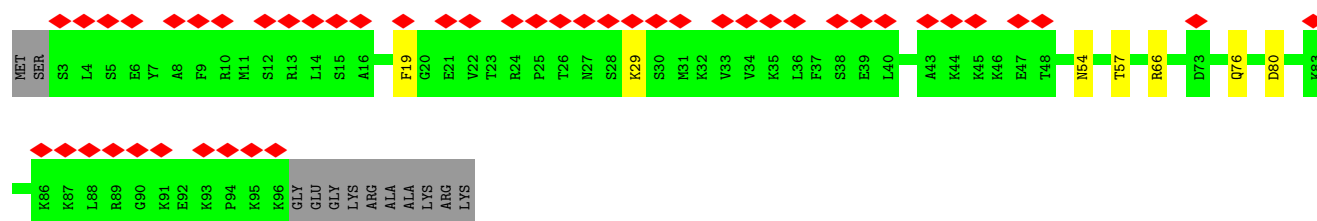
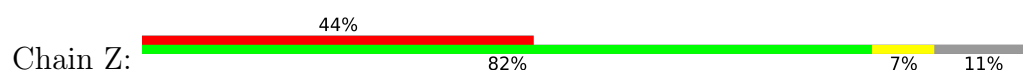




- Molecule 24: 28S ribosomal protein S31, mitochondrial



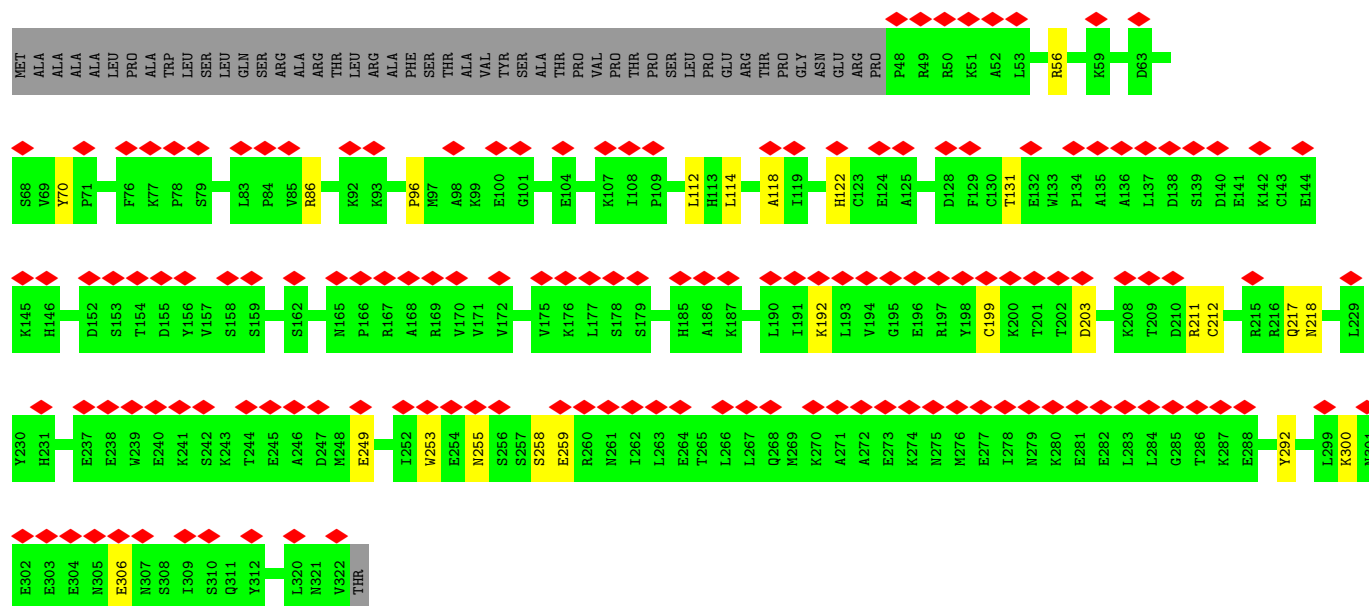
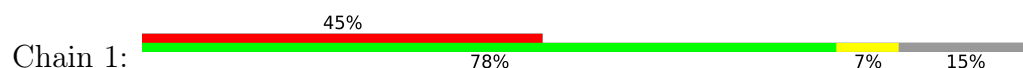
- Molecule 25: 28S ribosomal protein S33, mitochondrial



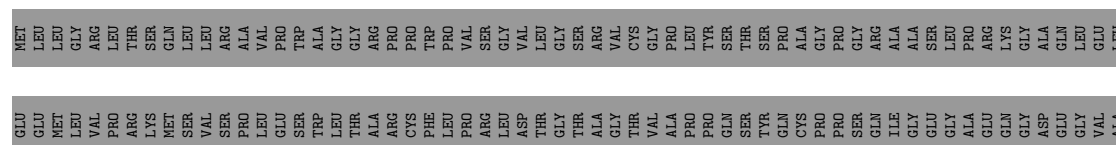
- Molecule 26: 28S ribosomal protein S34, mitochondrial



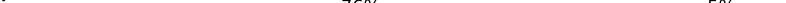
- Molecule 27: 28S ribosomal protein S35, mitochondrial

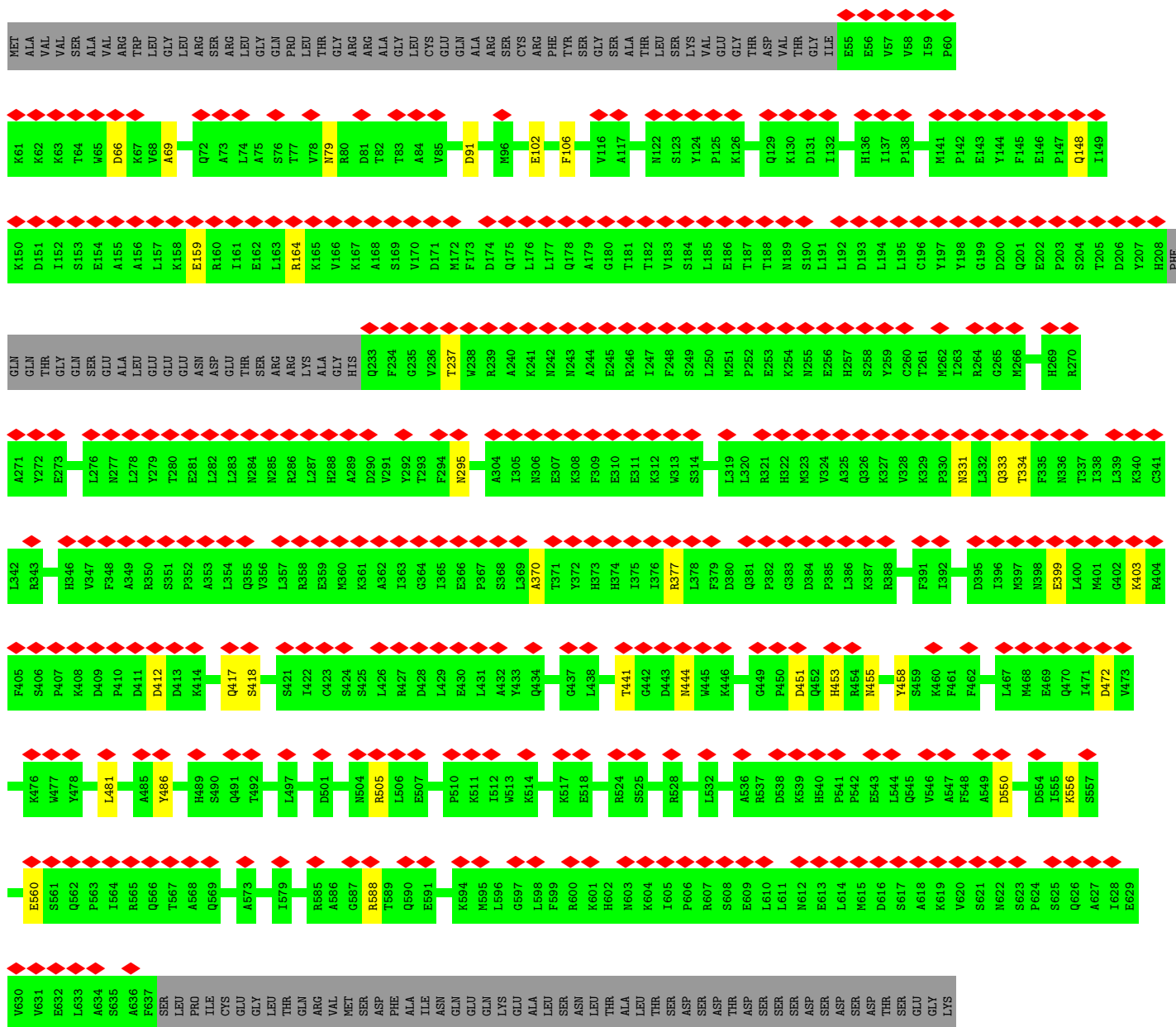


- Molecule 28: Aurora kinase A-interacting protein



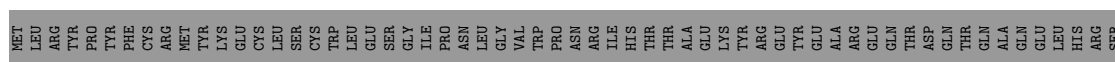
- Molecule 29: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

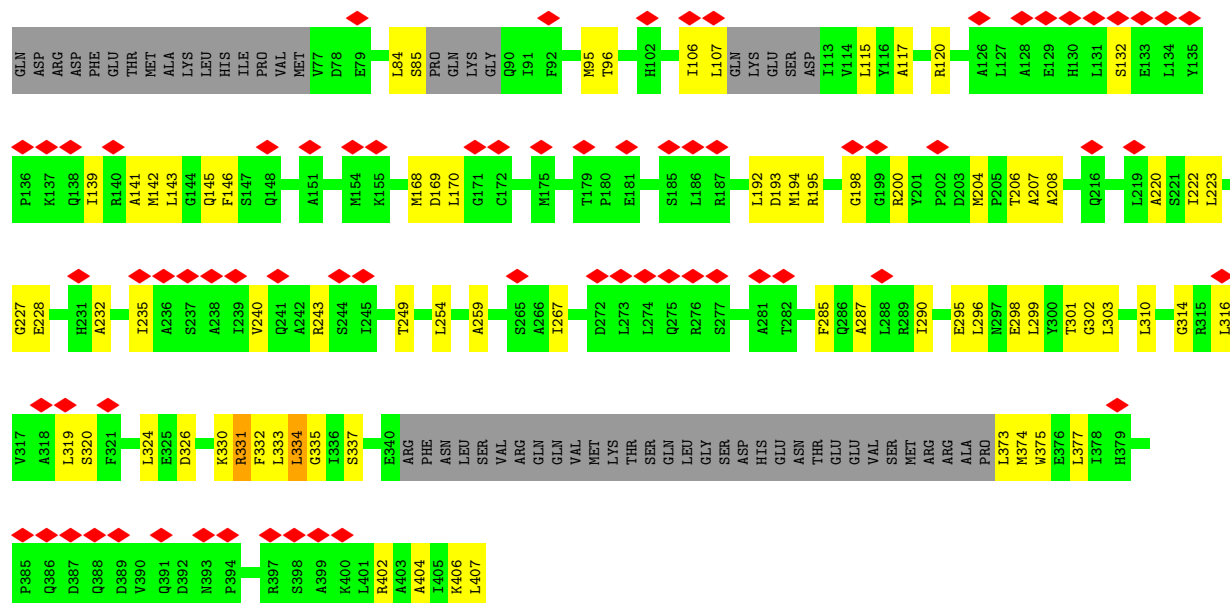
Chain 4: 



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

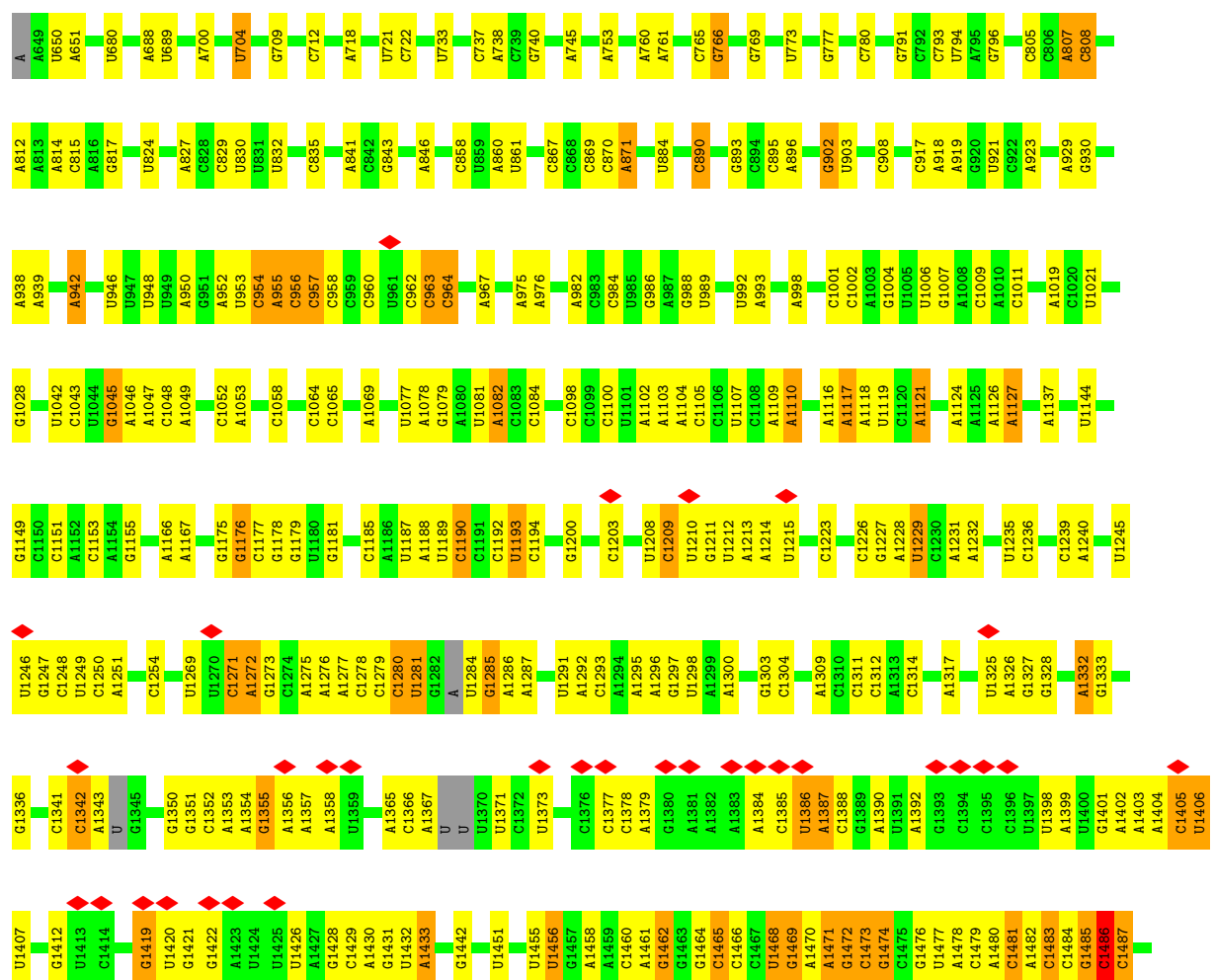
Chain b: 

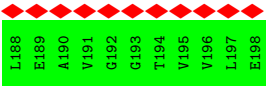




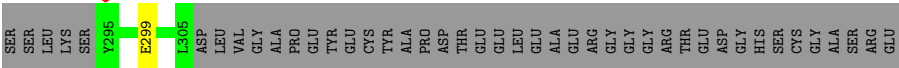
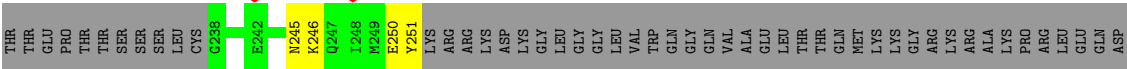
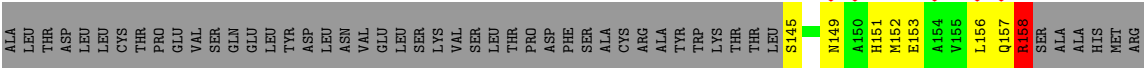
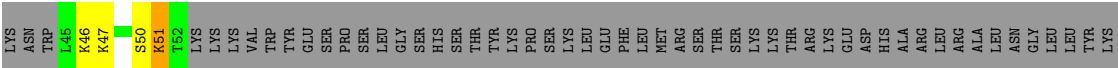
• Molecule 31: 12S mitochondrial rRNA

Chain A: 61% 31% 7% •





● Molecule 34: 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	2833	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	0.049	Depositor
Minimum map value	-0.016	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: SPM, MA6, B8T, GDP, ACE, ATP, 5MC, 5F0, FES, NAD, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.23	0/1871	0.38	1/2531 (0.0%)
2	C	0.10	0/1024	0.21	0/1388
3	D	0.09	0/2663	0.21	0/3569
4	E	0.10	0/926	0.21	0/1252
5	F	0.08	0/1670	0.20	0/2241
6	G	0.17	0/2562	0.30	1/3432 (0.0%)
7	H	0.10	0/1178	0.22	0/1598
8	I	0.09	0/1021	0.22	0/1375
9	J	0.10	0/807	0.21	0/1082
10	K	0.10	0/880	0.22	0/1182
11	L	0.15	0/1477	0.27	0/1974
12	M	0.11	0/963	0.22	0/1295
13	N	0.41	0/886	0.55	0/1199
14	O	0.11	0/1655	0.24	0/2254
15	P	0.11	0/798	0.24	0/1070
16	Q	0.46	0/754	0.70	0/1003
17	R	0.10	0/2456	0.20	0/3317
18	S	0.09	0/1138	0.19	0/1533
19	T	0.16	0/1402	0.26	0/1883
20	U	0.10	0/1510	0.20	0/2025
21	V	0.10	0/2967	0.22	0/4009
22	W	0.10	0/800	0.25	0/1076
23	X	0.09	0/2921	0.21	0/3954
24	Y	0.10	0/1054	0.21	0/1421
25	Z	0.09	0/815	0.19	0/1087
26	0	0.09	0/1825	0.22	0/2473
27	1	0.09	0/2277	0.21	0/3080
28	3	0.10	0/627	0.25	0/828
29	4	0.09	0/4651	0.22	0/6293
30	b	0.30	0/2298	0.45	2/3097 (0.1%)
31	A	0.14	0/22441	0.24	0/34928
32	7	0.08	0/3554	0.23	0/4805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	t	0.06	0/551	0.19	0/740
34	a	0.57	0/482	0.82	0/640
All	All	0.15	0/74904	0.27	4/105634 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
8	I	0	3
11	L	0	1
16	Q	0	3
30	b	0	1
34	a	0	1
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	335	GLY	CA-C-O	-6.35	117.15	122.29
1	B	165	TYR	CA-C-O	-5.96	114.39	121.66
6	G	151	PHE	N-CA-CB	-5.46	100.87	109.78
30	b	374	MET	N-CA-C	-5.06	106.42	112.59

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	ARG	Sidechain
8	I	183	HIS	Mainchain
8	I	184	5F0	Peptide,Mainchain
11	L	171	ARG	Sidechain
16	Q	42	ARG	Sidechain
16	Q	43	ARG	Sidechain
16	Q	62	ARG	Sidechain
34	a	158	ARG	Sidechain
30	b	331	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1828	1815	1815	13	0
2	C	994	985	984	4	0
3	D	2613	2657	2656	15	0
4	E	910	929	929	2	0
5	F	1634	1686	1686	5	0
6	G	2508	2489	2488	29	0
7	H	1152	1183	1183	6	0
8	I	1011	1049	1042	15	0
9	J	794	835	833	4	0
10	K	862	885	885	5	0
11	L	1453	1540	1540	4	0
12	M	942	966	966	1	0
13	N	868	928	928	4	0
14	O	1599	1567	1567	6	0
15	P	781	807	807	2	0
16	Q	744	758	758	3	0
17	R	2409	2428	2428	10	0
18	S	1111	1115	1115	6	0
19	T	1371	1394	1394	4	0
20	U	1488	1499	1499	2	0
21	V	2907	2907	2906	11	0
22	W	789	801	801	2	0
23	X	2849	2844	2844	17	0
24	Y	1023	970	970	5	0
25	Z	797	815	815	5	0
26	0	1778	1784	1783	9	0
27	1	2230	2262	2262	17	0
28	3	616	686	686	6	0
29	4	4544	4542	4542	20	0
30	b	2261	2318	2315	51	0
31	A	20156	10238	10239	117	0
32	7	3501	3548	3548	22	0
33	t	547	599	599	2	0
34	a	482	473	470	10	0
35	A	11	0	0	0	0
35	B	1	0	0	0	0
36	O	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	P	4	0	0	2	0
37	T	4	0	0	0	0
38	X	31	12	12	2	0
39	7	28	10	12	1	0
39	X	28	10	12	0	0
40	A	44	26	26	0	0
41	A	14	0	26	1	0
42	0	1	0	0	0	0
42	1	1	0	0	0	0
42	C	1	0	0	1	0
42	G	1	0	0	1	0
42	I	1	0	0	0	0
42	K	1	0	0	0	0
42	T	1	0	0	0	0
42	b	1	0	0	1	0
All	All	71726	62360	62371	379	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 (379) 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)
8:I:184:5F0:O	31:A:976:A:C2	1.73	1.40
8:I:184:5F0:O	31:A:976:A:H2	0.80	1.13
8:I:184:5F0:C	31:A:976:A:H2	1.89	0.85
32:7:198:ASP:OD1	32:7:203:THR:OG1	1.95	0.84
34:a:299:GLU:N	34:a:299:GLU:OE1	2.12	0.82
31:A:1485:G:N2	31:A:1487:C:OP1	2.15	0.80
17:R:208:ILE:O	17:R:214:ASN:ND2	2.17	0.78
6:G:379:ARG:NH1	6:G:380:LYS:O	2.19	0.75
31:A:1567:A:H3'	31:A:1568:U:H5''	1.70	0.74
5:F:155:MET:SD	5:F:179:ARG:NH1	2.62	0.73
34:a:245:ASN:OD1	34:a:246:LYS:N	2.21	0.73
28:3:148:LYS:O	28:3:151:ARG:NH1	2.22	0.73
29:4:441:THR:OG1	29:4:444:ASN:OD1	2.07	0.72
4:E:105:CYS:HB2	37:P:201:FES:S1	2.26	0.70
29:4:417:GLN:OE1	29:4:453:HIS:ND1	2.24	0.70
3:D:297:ARG:NH1	31:A:1121:A:OP2	2.24	0.70
30:b:170:LEU:HD21	30:b:299:LEU:HD13	1.73	0.70
19:T:132:ARG:NH1	19:T:136:LEU:O	2.24	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:952:A:N3	31:A:954:C:N4	2.41	0.69
23:X:134:LYS:NZ	38:X:501:ATP:O1G	2.20	0.69
31:A:1483:C:N4	31:A:1567:A:O2'	2.26	0.69
17:R:317:ALA:O	17:R:321:ALA:N	2.26	0.69
31:A:1600:A:N1	31:A:1601:C:N4	2.41	0.68
18:S:98:ARG:NH2	18:S:128:GLU:OE1	2.27	0.68
31:A:1600:A:C6	31:A:1601:C:N4	2.62	0.68
10:K:60:ASN:OD1	10:K:68:GLN:NE2	2.27	0.67
31:A:1401:G:N1	31:A:1404:A:OP2	2.28	0.67
31:A:1272:A:H61	31:A:1303:G:C2'	2.08	0.67
31:A:1366:C:O2'	31:A:1419:G:O4'	2.12	0.67
8:I:71:SER:O	8:I:74:ARG:NH1	2.28	0.66
31:A:1247:G:N2	31:A:1342:C:OP1	2.28	0.66
1:B:141:ILE:HG23	1:B:165:TYR:CE2	2.30	0.66
20:U:80:ARG:O	20:U:84:GLU:N	2.29	0.66
28:3:137:LYS:NZ	31:A:1575:U:OP2	2.22	0.65
21:V:29:LEU:N	21:V:149:ASP:OD1	2.29	0.65
31:A:1566:C:H3'	31:A:1567:A:H5''	1.79	0.65
8:I:94:ASN:ND2	31:A:989:U:OP1	2.30	0.65
31:A:1117:A:N6	31:A:1119:U:O2'	2.29	0.65
30:b:200:ARG:NE	42:b:501:HOH:O	2.30	0.65
6:G:200:LEU:O	6:G:218:TYR:OH	2.14	0.64
30:b:406:LYS:O	30:b:407:LEU:C	2.41	0.64
2:C:115:ASN:ND2	24:Y:309:LYS:O	2.31	0.64
18:S:83:ARG:NH1	18:S:93:LYS:O	2.30	0.64
6:G:276:ARG:N	42:G:2001:HOH:O	2.30	0.64
18:S:7:GLU:N	18:S:7:GLU:OE1	2.31	0.64
31:A:1177:C:O2'	31:A:1568:U:O4	2.14	0.63
6:G:69:TYR:OH	6:G:133:PRO:O	2.16	0.63
8:I:83:ILE:O	8:I:148:ARG:NH2	2.31	0.63
31:A:1486:B8T:O2'	31:A:1487:C:O4'	2.15	0.63
2:C:113:ARG:NH2	42:C:201:HOH:O	2.31	0.63
30:b:106:ILE:HB	30:b:115:LEU:HD11	1.80	0.62
25:Z:19:PHE:O	27:1:211:ARG:NH2	2.32	0.62
27:1:56:ARG:NH2	29:4:91:ASP:OD2	2.32	0.62
30:b:316:LEU:HD22	30:b:333:LEU:HD21	1.81	0.62
27:1:255:ASN:N	27:1:259:GLU:OE1	2.28	0.62
2:C:152:ARG:NH1	24:Y:300:GLU:OE1	2.33	0.61
30:b:96:THR:HG23	30:b:146:PHE:CE1	2.34	0.61
6:G:243:ARG:O	6:G:246:ARG:NH1	2.33	0.61
27:1:192:LYS:NZ	27:1:249:GLU:OE2	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:63:GLU:OE1	14:O:112:LYS:NZ	2.32	0.61
31:A:890:C:O2'	31:A:902:G:N2	2.33	0.61
30:b:298:GLU:O	30:b:301:THR:OG1	2.13	0.61
31:A:1502:A:N6	31:A:1548:A:N3	2.49	0.61
31:A:843:G:N2	31:A:846:A:OP2	2.35	0.60
31:A:942:A:N6	31:A:1047:A:OP2	2.35	0.60
29:4:550:ASP:OD1	29:4:588:ARG:NH2	2.35	0.60
23:X:263:ASP:OD1	23:X:264:GLY:N	2.36	0.59
31:A:1366:C:OP1	31:A:1388:C:O2'	2.20	0.59
29:4:458:TYR:HB3	29:4:486:TYR:CE1	2.38	0.59
1:B:176:LEU:HD23	1:B:189:LEU:HD22	1.84	0.59
3:D:217:ASP:OD2	3:D:251:LYS:NZ	2.32	0.59
10:K:81:ASP:OD1	10:K:86:ARG:NH1	2.35	0.58
17:R:195:VAL:O	19:T:137:ARG:NH1	2.34	0.58
29:4:399:GLU:OE2	29:4:403:LYS:NZ	2.21	0.58
24:Y:296:ASN:OD1	24:Y:298:PHE:N	2.37	0.58
9:J:78:ARG:NH2	9:J:117:ASP:OD2	2.36	0.58
31:A:1229:U:O2'	31:A:1442:G:O4'	2.21	0.58
6:G:158:TYR:HA	6:G:209:LEU:HD13	1.85	0.58
31:A:1569:G:O2'	31:A:1570:G:OP2	2.20	0.57
9:J:117:ASP:OD1	31:A:895:C:N4	2.37	0.57
8:I:184:5F0:C	31:A:976:A:C2	2.76	0.56
31:A:1175:G:N2	31:A:1481:C:O2'	2.37	0.56
26:0:9:ARG:NH2	31:A:805:C:O2	2.38	0.56
21:V:43:ARG:NE	21:V:77:ASP:OD1	2.36	0.56
23:X:338:ASP:OD1	27:1:292:TYR:OH	2.22	0.56
32:7:274:GLN:NE2	32:7:278:ASP:OD2	2.38	0.56
21:V:375:TYR:CZ	21:V:379:LEU:HD11	2.41	0.56
30:b:222:ILE:O	30:b:287:ALA:HB1	2.06	0.56
33:t:134:LEU:HD12	33:t:134:LEU:O	2.07	0.55
24:Y:281:GLU:OE2	29:4:164:ARG:NH2	2.37	0.55
17:R:352:ALA:O	17:R:356:HIS:ND1	2.40	0.55
31:A:1600:A:C2	31:A:1601:C:N3	2.75	0.55
26:0:53:ARG:NH1	31:A:704:U:OP1	2.39	0.55
11:L:86:ASP:OD1	11:L:87:ASP:N	2.40	0.55
31:A:1600:A:C2	31:A:1601:C:C4	2.94	0.55
34:a:187:ASN:HB3	34:a:190:LEU:HD23	1.87	0.55
3:D:139:PHE:O	3:D:160:ARG:NH2	2.40	0.54
8:I:129:GLN:NE2	8:I:167:MET:SD	2.78	0.54
9:J:107:ILE:N	9:J:131:ASP:OD2	2.33	0.54
6:G:217:ASP:OD1	6:G:218:TYR:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:295:ASN:ND2	29:4:334:THR:OG1	2.40	0.54
30:b:310:LEU:HD23	30:b:375:TRP:CH2	2.43	0.54
30:b:310:LEU:HD11	30:b:314:GLY:HA3	1.88	0.54
1:B:141:ILE:HG23	1:B:165:TYR:CD2	2.43	0.54
30:b:223:LEU:HD13	30:b:235:ILE:CG2	2.38	0.54
12:M:39:ASN:ND2	31:A:841:A:OP1	2.41	0.54
30:b:107:LEU:HG	30:b:115:LEU:HD12	1.90	0.54
30:b:227:GLY:HA3	30:b:287:ALA:HB2	1.89	0.54
31:A:1081:U:O4	31:A:1082:A:N6	2.41	0.53
31:A:1227:G:OP2	31:A:1228:A:O2'	2.16	0.53
15:P:73:ASP:OD1	15:P:74:TYR:N	2.41	0.53
32:7:261:ALA:HB2	32:7:287:VAL:CG1	2.38	0.53
17:R:263:ARG:NH2	17:R:287:ASP:OD1	2.42	0.53
23:X:127:TYR:OH	27:1:306:GLU:OE2	2.26	0.53
3:D:209:GLY:N	3:D:213:GLU:O	2.41	0.53
27:1:212:CYS:O	27:1:218:ASN:ND2	2.42	0.53
30:b:142:MET:HE3	30:b:143:LEU:O	2.09	0.53
7:H:126:ILE:HG12	31:A:1226:C:H1'	1.90	0.52
21:V:375:TYR:CE2	21:V:379:LEU:HD11	2.43	0.52
25:Z:66:ARG:NH2	25:Z:80:ASP:OD2	2.35	0.52
30:b:195:ARG:NH1	30:b:204:MET:O	2.42	0.52
31:A:1272:A:N6	31:A:1304:C:O4'	2.43	0.52
6:G:157:SER:O	6:G:209:LEU:HD22	2.09	0.52
31:A:1600:A:N1	31:A:1601:C:C4	2.77	0.52
3:D:312:TYR:OH	3:D:315:ARG:NH1	2.41	0.52
30:b:310:LEU:HD23	30:b:375:TRP:HH2	1.75	0.52
26:0:101:ARG:NH1	31:A:1528:A:OP1	2.43	0.52
1:B:103:GLU:OE2	18:S:52:ARG:NH2	2.44	0.51
26:0:84:SER:OG	26:0:138:ASP:OD2	2.25	0.51
5:F:198:ARG:NH1	31:A:1384:A:OP2	2.44	0.51
27:1:118:ALA:O	27:1:122:HIS:N	2.40	0.51
18:S:5:ARG:NH1	31:A:1279:C:O3'	2.44	0.51
31:A:917:C:O2'	31:A:921:U:OP1	2.28	0.51
31:A:1053:A:N1	31:A:1100:C:O2'	2.41	0.51
11:L:217:THR:O	11:L:221:LYS:N	2.43	0.51
26:0:43:ARG:O	26:0:47:GLY:N	2.39	0.50
31:A:1565:A:H5'	31:A:1566:C:OP2	2.11	0.50
3:D:245:VAL:HG22	3:D:271:ALA:HB1	1.91	0.50
1:B:141:ILE:HG21	6:G:152:TYR:OH	2.12	0.50
6:G:66:ARG:NH1	31:A:1300:A:O2'	2.44	0.50
31:A:1501:A:N6	31:A:1549:G:N3	2.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:7:188:HIS:ND1	32:7:268:GLN:OE1	2.42	0.50
6:G:157:SER:C	6:G:209:LEU:HD22	2.37	0.50
30:b:303:LEU:HD22	30:b:332:PHE:CD2	2.46	0.50
31:A:1570:G:H4'	31:A:1571:U:O5'	2.11	0.50
28:3:150:THR:HG22	28:3:150:THR:O	2.11	0.50
6:G:301:GLN:N	6:G:301:GLN:OE1	2.44	0.50
19:T:37:HIS:NE2	31:A:955:A:N7	2.59	0.50
32:7:321:VAL:HG13	32:7:321:VAL:O	2.11	0.50
25:Z:29:LYS:NZ	31:A:1398:U:OP1	2.45	0.49
34:a:198:ALA:O	34:a:199:VAL:C	2.55	0.49
26:0:93:CYS:SG	26:0:121:LYS:N	2.81	0.49
30:b:295:GLU:O	30:b:299:LEU:N	2.44	0.49
30:b:314:GLY:O	30:b:406:LYS:N	2.45	0.49
31:A:1175:G:H21	31:A:1481:C:HO2'	1.61	0.49
31:A:1272:A:H61	31:A:1303:G:H2'	1.76	0.49
6:G:139:GLN:O	6:G:146:PRO:HA	2.12	0.49
8:I:88:ILE:HD12	8:I:149:VAL:HG13	1.95	0.49
21:V:374:THR:O	21:V:378:ASN:N	2.38	0.49
30:b:170:LEU:CD2	30:b:299:LEU:HD13	2.43	0.49
30:b:334:LEU:HB3	30:b:377:LEU:HG	1.93	0.49
11:L:76:TYR:O	11:L:79:VAL:HG22	2.11	0.49
23:X:123:ARG:NH2	23:X:339:PRO:O	2.46	0.49
23:X:368:HIS:N	23:X:398:LEU:O	2.42	0.48
5:F:211:GLU:O	5:F:216:GLN:N	2.46	0.48
8:I:192:ARG:O	8:I:193:LYS:C	2.56	0.48
1:B:171:PHE:CE2	1:B:175:MET:HE3	2.48	0.48
3:D:284:ARG:NH1	3:D:287:ASP:O	2.46	0.48
30:b:333:LEU:HD22	30:b:404:ALA:HB3	1.94	0.48
31:A:1567:A:H5'	31:A:1568:U:O5'	2.14	0.48
31:A:1583:MA6:H93	31:A:1584:MA6:C2	2.43	0.48
8:I:116:GLY:O	8:I:118:ARG:NH1	2.45	0.48
23:X:161:TRP:O	23:X:180:GLN:NE2	2.41	0.48
6:G:139:GLN:O	6:G:147:PHE:N	2.39	0.48
14:O:94:CYS:SG	14:O:108:CYS:SG	3.12	0.48
23:X:276:ARG:NH2	23:X:286:GLU:OE1	2.46	0.48
32:7:266:MET:N	32:7:269:THR:OG1	2.41	0.48
32:7:434:VAL:HG22	32:7:435:GLU:H	1.79	0.48
1:B:167:HIS:HA	6:G:153:THR:HG22	1.96	0.48
17:R:253:ILE:O	17:R:257:GLY:N	2.47	0.48
31:A:1110:A:H4'	41:A:1702:SPM:H112	1.95	0.48
21:V:141:ASN:ND2	21:V:172:ALA:O	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:451:ASP:OD1	29:4:455:ASN:ND2	2.47	0.48
30:b:240:VAL:HG23	30:b:243:ARG:HH21	1.79	0.48
31:A:1483:C:N4	31:A:1567:A:H1'	2.29	0.48
23:X:124:TYR:O	23:X:308:SER:N	2.43	0.47
31:A:1479:C:H5''	31:A:1485:G:C2	2.49	0.47
34:a:250:GLU:O	34:a:251:TYR:C	2.55	0.47
13:N:75:LYS:NZ	31:A:766:G:OP2	2.46	0.47
25:Z:76:GLN:O	25:Z:80:ASP:N	2.46	0.47
30:b:145:GLN:OE1	30:b:145:GLN:N	2.41	0.47
30:b:228:GLU:HG3	30:b:324:LEU:HD11	1.96	0.47
23:X:135:THR:OG1	38:X:501:ATP:O1B	2.26	0.47
28:3:147:VAL:O	28:3:151:ARG:N	2.47	0.47
30:b:208:ALA:CB	30:b:249:THR:HG23	2.44	0.47
31:A:948:U:OP2	31:A:1045:G:N2	2.47	0.47
15:P:65:CYS:N	37:P:201:FES:S2	2.79	0.47
30:b:223:LEU:HD13	30:b:235:ILE:HG23	1.97	0.47
22:W:174:GLU:O	22:W:175:SER:C	2.58	0.47
30:b:228:GLU:CG	30:b:324:LEU:HD11	2.45	0.47
31:A:1461:A:H3'	31:A:1462:G:H5'	1.97	0.47
21:V:318:ASP:OD1	21:V:319:ILE:N	2.47	0.47
32:7:179:ARG:NH2	32:7:253:ASP:OD2	2.43	0.47
31:A:1464:G:H21	31:A:1465:C:H5	1.63	0.47
30:b:320:SER:CB	30:b:326:ASP:HA	2.45	0.46
31:A:1571:U:H3'	31:A:1572:A:H5'	1.97	0.46
30:b:220:ALA:HA	30:b:223:LEU:HD12	1.97	0.46
5:F:36:ARG:NH2	31:A:1311:C:O2	2.43	0.46
31:A:765:C:H5'	31:A:766:G:OP2	2.16	0.46
6:G:320:VAL:HG12	6:G:321:ASP:N	2.31	0.46
31:A:1428:G:O2'	31:A:1433:A:OP1	2.19	0.46
31:A:1455:U:O2'	31:A:1456:U:C6	2.69	0.46
6:G:116:LEU:O	6:G:122:ARG:NH2	2.46	0.46
14:O:101:VAL:HG12	14:O:102:GLY:N	2.30	0.46
23:X:359:TYR:O	23:X:363:ASN:ND2	2.47	0.46
13:N:93:ASP:O	13:N:97:GLY:N	2.44	0.46
31:A:871:A:N1	31:A:918:A:O2'	2.47	0.46
31:A:1469:G:H2'	31:A:1470:A:O4'	2.16	0.46
6:G:318:HIS:HA	6:G:323:LEU:HD12	1.98	0.46
30:b:249:THR:HG22	30:b:249:THR:O	2.16	0.46
9:J:82:ARG:NH1	31:A:1496:U:OP1	2.48	0.45
26:O:178:ARG:O	26:O:183:ASP:N	2.49	0.45
29:4:481:LEU:HB3	29:4:486:TYR:CE1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1566:C:N3	31:A:1567:A:N6	2.64	0.45
29:4:148:GLN:N	29:4:159:GLU:OE2	2.49	0.45
30:b:194:MET:HB2	30:b:207:ALA:HB2	1.98	0.45
31:A:824:U:OP1	32:7:557:SER:OG	2.29	0.45
31:A:1190:C:O2	31:A:1465:C:N4	2.49	0.45
1:B:100:ARG:NH2	31:A:1116:A:OP2	2.49	0.45
32:7:492:LEU:O	32:7:493:ARG:C	2.59	0.45
16:Q:72:ILE:HD11	31:A:1600:A:H4'	1.98	0.45
33:t:134:LEU:HD22	33:t:145:LEU:HD21	1.98	0.45
3:D:243:VAL:HG12	3:D:245:VAL:HG13	1.99	0.45
30:b:195:ARG:NH2	30:b:198:GLY:O	2.41	0.45
8:I:81:GLU:OE1	8:I:81:GLU:N	2.43	0.45
13:N:73:ARG:NH2	31:A:769:G:OP2	2.50	0.45
21:V:123:ASP:OD1	21:V:123:ASP:N	2.50	0.45
31:A:1600:A:C6	31:A:1601:C:C4	3.04	0.45
34:a:152:MET:HG2	34:a:156:LEU:HD23	1.98	0.45
23:X:279:LYS:NZ	31:A:1412:G:OP1	2.50	0.45
23:X:186:THR:O	23:X:190:ASN:ND2	2.50	0.45
30:b:84:LEU:O	30:b:85:SER:C	2.59	0.45
32:7:261:ALA:HB3	32:7:289:LYS:HB2	1.98	0.45
30:b:259:ALA:HB1	30:b:267:ILE:HD11	1.98	0.45
3:D:407:ASP:OD2	3:D:410:ASP:N	2.46	0.44
19:T:42:GLU:OE1	19:T:45:ARG:NH2	2.44	0.44
30:b:168:MET:SD	30:b:303:LEU:HD23	2.57	0.44
31:A:1473:C:H2'	31:A:1474:G:H1'	1.98	0.44
21:V:250:ILE:O	21:V:255:TYR:OH	2.32	0.44
34:a:156:LEU:HD13	34:a:158:ARG:NH1	2.32	0.44
3:D:233:ALA:HB2	31:A:1176:G:OP2	2.16	0.44
14:O:217:ARG:NH1	14:O:227:GLU:OE2	2.50	0.44
31:A:1405:C:O2'	31:A:1406:U:O4'	2.34	0.44
27:1:70:TYR:HE2	27:1:112:LEU:HD13	1.82	0.44
7:H:70:ASP:OD1	7:H:71:ILE:N	2.48	0.44
31:A:1208:U:H2'	31:A:1209:C:O4'	2.18	0.44
31:A:1499:U:OP2	31:A:1500:C:N4	2.43	0.44
32:7:309:VAL:O	32:7:309:VAL:HG23	2.17	0.44
34:a:245:ASN:OD1	34:a:245:ASN:C	2.60	0.44
1:B:140:GLY:O	6:G:145:ARG:NH1	2.49	0.44
27:1:86:ARG:NH1	27:1:96:PRO:O	2.46	0.44
30:b:192:LEU:HD21	30:b:254:LEU:HD22	2.00	0.44
31:A:1355:G:N7	31:A:1357:A:N6	2.63	0.44
31:A:1465:C:N3	31:A:1466:C:N4	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:59:ARG:NH1	31:A:1021:U:O4	2.51	0.43
30:b:169:ASP:HB3	30:b:319:LEU:HD13	2.00	0.43
30:b:120:ARG:HG3	30:b:145:GLN:HB3	2.00	0.43
30:b:331:ARG:HD2	30:b:337:SER:HB3	2.00	0.43
32:7:359:VAL:HG13	32:7:372:THR:CG2	2.48	0.43
31:A:807:A:N3	31:A:808:C:N4	2.60	0.43
25:Z:54:ASN:ND2	25:Z:57:THR:OG1	2.51	0.43
31:A:1280:C:H2'	31:A:1281:U:H5'	2.01	0.43
31:A:1468:U:O2'	31:A:1469:G:P	2.76	0.43
31:A:1481:C:O2	31:A:1481:C:H2'	2.19	0.43
14:O:73:VAL:O	14:O:109:ARG:NH2	2.49	0.43
29:4:66:ASP:OD1	29:4:69:ALA:N	2.51	0.43
1:B:165:TYR:HA	6:G:149:TYR:O	2.19	0.43
31:A:1192:C:H3'	31:A:1193:U:H5''	2.01	0.43
31:A:1210:U:H2'	31:A:1211:G:O4'	2.19	0.43
14:O:185:SER:O	17:R:183:LYS:NZ	2.49	0.43
17:R:162:SER:HB2	17:R:165:ILE:HD12	2.00	0.43
29:4:102:GLU:O	29:4:106:PHE:N	2.49	0.43
30:b:223:LEU:HB2	30:b:232:ALA:HB1	2.01	0.43
31:A:700:A:N1	31:A:709:G:O2'	2.48	0.43
32:7:188:HIS:HB3	32:7:191:HIS:CE1	2.53	0.43
3:D:345:LEU:HD23	3:D:345:LEU:C	2.44	0.43
3:D:372:GLU:N	3:D:382:ILE:O	2.49	0.43
6:G:315:PHE:CD2	6:G:369:LEU:HD21	2.54	0.43
7:H:50:LEU:HD12	29:4:79:ASN:HB3	2.01	0.43
23:X:335:ASP:OD1	27:1:300:LYS:NZ	2.47	0.43
30:b:95:MET:HE2	30:b:302:GLY:HA2	2.00	0.43
30:b:193:ASP:OD1	30:b:206:THR:HG22	2.18	0.43
1:B:141:ILE:HG23	1:B:165:TYR:HE2	1.81	0.42
6:G:243:ARG:O	6:G:246:ARG:NH2	2.51	0.42
31:A:1332:A:H2'	31:A:1333:G:O4'	2.18	0.42
32:7:538:TYR:OH	32:7:544:CYS:O	2.26	0.42
4:E:5:GLU:N	4:E:94:VAL:O	2.47	0.42
24:Y:323:ASP:OD2	27:1:217:GLN:NE2	2.47	0.42
31:A:689:U:OP1	31:A:827:A:O2'	2.36	0.42
32:7:591:VAL:HG12	32:7:592:LYS:N	2.33	0.42
7:H:64:THR:HG22	7:H:65:ILE:H	1.85	0.42
10:K:58:ARG:NE	10:K:72:ASP:OD1	2.45	0.42
10:K:127:THR:HG23	31:A:1309:A:H1'	2.01	0.42
22:W:84:LEU:O	22:W:90:THR:OG1	2.32	0.42
23:X:103:LYS:N	23:X:104:PRO:CD	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:69:THR:OG1	17:R:72:ASP:OD1	2.34	0.42
21:V:132:LYS:O	21:V:136:GLY:N	2.42	0.42
30:b:330:LYS:HA	30:b:402:ARG:HD3	2.02	0.42
32:7:376:ILE:HG22	32:7:377:GLN:N	2.34	0.42
23:X:127:TYR:HH	27:1:306:GLU:CD	2.26	0.42
29:4:472:ASP:OD1	29:4:505:ARG:NH1	2.53	0.42
30:b:254:LEU:HD23	30:b:285:PHE:CE1	2.55	0.42
21:V:167:VAL:HG13	21:V:172:ALA:HB3	2.00	0.42
29:4:331:ASN:ND2	29:4:333:GLN:OE1	2.53	0.42
31:A:1471:A:C5	31:A:1472:G:C2	3.08	0.42
31:A:1567:A:C3'	31:A:1568:U:H5''	2.45	0.42
26:0:63:ARG:NH2	26:0:110:ASP:OD2	2.53	0.42
31:A:1271:C:H5'	31:A:1272:A:OP2	2.20	0.42
31:A:1284:U:H2'	31:A:1285:G:OP2	2.20	0.42
6:G:217:ASP:OD1	6:G:217:ASP:C	2.61	0.42
31:A:963:C:H2'	31:A:964:C:H5'	2.02	0.42
31:A:1571:U:H4'	31:A:1572:A:OP2	2.19	0.42
31:A:1590:A:O2'	31:A:1591:C:H5''	2.20	0.42
34:a:152:MET:O	34:a:153:GLU:C	2.63	0.42
2:C:105:ALA:N	2:C:122:VAL:O	2.47	0.41
31:A:1503:G:C2	31:A:1546:A:C4	3.07	0.41
29:4:556:LYS:NZ	29:4:560:GLU:OE2	2.50	0.41
8:I:192:ARG:O	8:I:192:ARG:CG	2.69	0.41
31:A:1102:A:OP2	31:A:1104:A:N6	2.46	0.41
1:B:103:GLU:N	1:B:104:PRO:CD	2.83	0.41
17:R:275:PHE:O	17:R:279:LYS:N	2.53	0.41
30:b:375:TRP:CE3	30:b:406:LYS:HA	2.56	0.41
31:A:952:A:C5	31:A:953:U:C4	3.09	0.41
3:D:140:LEU:HD12	3:D:158:ALA:HB3	2.02	0.41
10:K:36:ARG:O	10:K:40:ARG:HB2	2.20	0.41
11:L:212:ARG:NH2	28:3:187:GLU:O	2.54	0.41
27:1:199:CYS:O	27:1:203:ASP:N	2.54	0.41
27:1:253:TRP:NE1	27:1:258:SER:OG	2.51	0.41
31:A:1385:C:C5'	31:A:1386:U:H2'	2.50	0.41
31:A:1386:U:H1'	31:A:1387:A:OP1	2.21	0.41
6:G:318:HIS:NE2	23:X:379:GLU:OE2	2.54	0.41
13:N:86:PHE:O	13:N:87:LYS:C	2.63	0.41
16:Q:37:GLU:HA	16:Q:40:LYS:HD2	2.02	0.41
29:4:377:ARG:NE	29:4:418:SER:OG	2.53	0.41
30:b:290:ILE:HG21	30:b:296:LEU:HD12	2.03	0.41
31:A:760:A:N1	31:A:780:C:O2'	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1213:A:N7	31:A:1214:A:C4	2.89	0.41
31:A:1499:U:C4	31:A:1500:C:C2	3.08	0.41
32:7:321:VAL:HG22	32:7:323:VAL:HG13	2.03	0.41
3:D:243:VAL:HG11	3:D:268:PHE:CD1	2.55	0.41
6:G:110:TYR:OH	27:1:114:LEU:O	2.37	0.41
8:I:103:SER:OG	8:I:105:GLU:OE2	2.39	0.41
30:b:117:ALA:HB3	30:b:141:ALA:HA	2.02	0.41
6:G:225:LEU:HD23	6:G:225:LEU:O	2.20	0.41
1:B:165:TYR:HD1	6:G:149:TYR:HA	1.85	0.41
5:F:156:ILE:HG22	5:F:157:GLY:N	2.36	0.41
8:I:97:ILE:HD11	8:I:161:ALA:HB1	2.03	0.41
20:U:169:THR:HG22	20:U:170:ARG:N	2.36	0.41
26:0:77:GLY:N	26:0:97:LEU:O	2.48	0.41
29:4:370:ALA:N	29:4:412:ASP:OD1	2.52	0.41
31:A:1545:U:H3'	31:A:1546:A:H4'	2.03	0.41
32:7:192:GLY:N	39:7:801:GDP:H5'	2.36	0.41
29:4:237:THR:HG22	29:4:237:THR:O	2.21	0.41
30:b:132:SER:HA	30:b:139:ILE:HG23	2.03	0.41
30:b:223:LEU:HA	30:b:287:ALA:CB	2.50	0.41
34:a:50:SER:O	34:a:51:LYS:HB2	2.21	0.41
32:7:312:GLU:HA	32:7:316:GLY:O	2.22	0.40
28:3:165:LYS:NZ	31:A:1149:G:OP2	2.46	0.40
3:D:281:TYR:OH	18:S:21:ARG:NH1	2.54	0.40
6:G:379:ARG:HH21	31:A:1317:A:H4'	1.87	0.40
7:H:152:THR:OG1	27:1:131:THR:O	2.39	0.40
31:A:1124:A:N6	31:A:1127:A:OP1	2.55	0.40
32:7:240:ALA:HB2	32:7:534:ILE:HD11	2.02	0.40
32:7:251:VAL:HG22	32:7:358:THR:HG21	2.04	0.40
6:G:143:ASP:OD1	6:G:144:GLY:N	2.55	0.40
30:b:96:THR:OG1	30:b:169:ASP:OD1	2.31	0.40
31:A:956:C:C3'	31:A:957:C:H5'	2.51	0.40
31:A:1476:G:H2'	31:A:1477:U:H5'	2.02	0.40
7:H:64:THR:HG22	7:H:65:ILE:N	2.35	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%)	215 (96%)	8 (4%)	0	100	100
2	C	119/167 (71%)	117 (98%)	2 (2%)	0	100	100
3	D	321/430 (75%)	307 (96%)	14 (4%)	0	100	100
4	E	113/125 (90%)	109 (96%)	4 (4%)	0	100	100
5	F	197/242 (81%)	194 (98%)	3 (2%)	0	100	100
6	G	300/396 (76%)	287 (96%)	13 (4%)	0	100	100
7	H	138/201 (69%)	132 (96%)	6 (4%)	0	100	100
8	I	133/194 (69%)	124 (93%)	9 (7%)	0	100	100
9	J	99/138 (72%)	94 (95%)	5 (5%)	0	100	100
10	K	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
11	L	172/257 (67%)	169 (98%)	3 (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%)	184 (96%)	8 (4%)	0	100	100
15	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
16	Q	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
17	R	293/360 (81%)	284 (97%)	9 (3%)	0	100	100
18	S	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
19	T	166/173 (96%)	162 (98%)	4 (2%)	0	100	100
20	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
21	V	351/414 (85%)	345 (98%)	6 (2%)	0	100	100
22	W	97/187 (52%)	94 (97%)	3 (3%)	0	100	100
23	X	350/398 (88%)	340 (97%)	10 (3%)	0	100	100
24	Y	119/395 (30%)	119 (100%)	0	0	100	100
25	Z	92/106 (87%)	91 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	0	212/218 (97%)	207 (98%)	5 (2%)	0	100	100
27	1	273/323 (84%)	262 (96%)	11 (4%)	0	100	100
28	3	67/199 (34%)	67 (100%)	0	0	100	100
29	4	555/689 (81%)	535 (96%)	20 (4%)	0	100	100
30	b	282/407 (69%)	260 (92%)	22 (8%)	0	100	100
32	7	449/691 (65%)	417 (93%)	32 (7%)	0	100	100
33	t	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
34	a	52/302 (17%)	47 (90%)	4 (8%)	1 (2%)	6	31
All	All	6245/8656 (72%)	6022 (96%)	222 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	a	51	LYS

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	106/143 (74%)	106 (100%)	0	100	100
3	D	276/357 (77%)	276 (100%)	0	100	100
4	E	97/107 (91%)	97 (100%)	0	100	100
5	F	178/209 (85%)	178 (100%)	0	100	100
6	G	264/342 (77%)	264 (100%)	0	100	100
7	H	130/180 (72%)	130 (100%)	0	100	100
8	I	103/146 (70%)	103 (100%)	0	100	100
9	J	88/118 (75%)	88 (100%)	0	100	100
10	K	91/113 (80%)	91 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	158/226 (70%)	157 (99%)	1 (1%)	78	82
12	M	97/113 (86%)	97 (100%)	0	100	100
13	N	96/115 (84%)	95 (99%)	1 (1%)	68	77
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%)	77 (99%)	1 (1%)	61	73
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	V	319/364 (88%)	319 (100%)	0	100	100
22	W	87/158 (55%)	87 (100%)	0	100	100
23	X	311/351 (89%)	311 (100%)	0	100	100
24	Y	112/357 (31%)	112 (100%)	0	100	100
25	Z	87/95 (92%)	87 (100%)	0	100	100
26	0	187/190 (98%)	187 (100%)	0	100	100
27	1	253/291 (87%)	253 (100%)	0	100	100
28	3	64/166 (39%)	64 (100%)	0	100	100
29	4	500/609 (82%)	500 (100%)	0	100	100
30	b	242/350 (69%)	240 (99%)	2 (1%)	73	79
32	7	377/587 (64%)	377 (100%)	0	100	100
33	t	59/59 (100%)	59 (100%)	0	100	100
34	a	50/260 (19%)	43 (86%)	7 (14%)	3	14
All	All	5556/7499 (74%)	5544 (100%)	12 (0%)	85	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	L	175	TYR
13	N	90	LYS
16	Q	66	MET
30	b	334	LEU
30	b	373	LEU
34	a	46	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	47	LYS
34	a	145	SER
34	a	149	ASN
34	a	151	HIS
34	a	157	GLN
34	a	158	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	356	GLN
4	E	54	HIS
4	E	58	HIS
4	E	92	ASN
5	F	214	HIS
6	G	90	ASN
6	G	139	GLN
8	I	87	HIS
12	M	75	HIS
14	O	80	ASN
14	O	98	ASN
14	O	147	HIS
15	P	137	ASN
21	V	87	HIS
21	V	245	HIS
21	V	329	GLN
21	V	402	GLN
23	X	63	HIS
23	X	110	HIS
25	Z	54	ASN
27	1	268	GLN
28	3	140	HIS
28	3	166	GLN
29	4	295	ASN
29	4	373	HIS
29	4	540	HIS
30	b	253	GLN
32	7	352	ASN
34	a	157	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	A	945/954 (99%)	278 (29%)	10 (1%)

All (278) 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
31	A	738	A
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	777	G
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	858	C
31	A	860	A
31	A	861	U
31	A	867	C
31	A	869	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	998	A
31	A	1001	C
31	A	1002	C
31	A	1004	G
31	A	1006	U
31	A	1007	G
31	A	1009	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1064	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	1098	C
31	A	1103	A
31	A	1105	C
31	A	1107	U
31	A	1109	A
31	A	1110	A
31	A	1117	A
31	A	1118	A
31	A	1121	A
31	A	1126	A
31	A	1127	A
31	A	1137	A
31	A	1144	U
31	A	1151	C
31	A	1153	C
31	A	1155	G
31	A	1166	A
31	A	1167	A
31	A	1176	G
31	A	1178	G
31	A	1179	G
31	A	1181	G
31	A	1185	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	1231	A
31	A	1232	A
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
31	A	1250	C
31	A	1251	A
31	A	1254	C
31	A	1269	U
31	A	1271	C
31	A	1272	A
31	A	1273	G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1332	A
31	A	1336	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
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	1407	U
31	A	1419	G
31	A	1420	U
31	A	1421	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1462	G
31	A	1465	C
31	A	1468	U
31	A	1469	G
31	A	1471	A
31	A	1472	G
31	A	1473	C
31	A	1474	G
31	A	1478	A
31	A	1480	A
31	A	1481	C
31	A	1482	A
31	A	1483	C
31	A	1484	C
31	A	1485	G
31	A	1486	B8T
31	A	1487	C
31	A	1491	C
31	A	1492	A
31	A	1500	C
31	A	1503	G
31	A	1513	A
31	A	1519	A
31	A	1520	U
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	A	1530	A
31	A	1532	C
31	A	1533	C
31	A	1537	C
31	A	1539	C
31	A	1546	A
31	A	1556	C
31	A	1557	A
31	A	1558	A
31	A	1559	G
31	A	1560	U
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	1569	G
31	A	1570	G
31	A	1571	U
31	A	1572	A
31	A	1573	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	1599	A
31	A	1601	C

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	A	1341	C
31	A	1386	U
31	A	1432	U
31	A	1472	G
31	A	1473	C
31	A	1483	C
31	A	1520	U
31	A	1531	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	A	1567	A
31	A	1570	G

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

5 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	$\# Z > 2$
31	MA6	A	1584	31	23,26,27	1.34	3 (13%)	33,38,41	3.05	12 (36%)
31	MA6	A	1583	31	23,26,27	1.34	3 (13%)	33,38,41	3.00	11 (33%)
31	B8T	A	1486	31	19,22,23	3.30	8 (42%)	25,31,34	0.80	1 (4%)
31	5MC	A	1488	31	19,22,23	0.49	0	26,32,35	0.51	0
8	5F0	I	184	8	8,8,9	0.53	0	8,9,11	1.17	1 (12%)

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
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
31	B8T	A	1486	31	-	0/7/27/28	0/2/2/2
31	5MC	A	1488	31	-	0/7/25/26	0/2/2/2
8	5F0	I	184	8	-	2/9/9/10	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	1486	B8T	C4-N3	7.87	1.46	1.32
31	A	1486	B8T	C2-N3	6.00	1.48	1.36
31	A	1486	B8T	C6-C5	5.91	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	1486	B8T	C4-N4	4.64	1.45	1.36
31	A	1486	B8T	C2-N1	4.50	1.49	1.40
31	A	1583	MA6	C6-N6	3.62	1.46	1.36
31	A	1584	MA6	C6-N6	3.56	1.46	1.36
31	A	1486	B8T	C6-N1	3.37	1.46	1.38
31	A	1486	B8T	C5-C4	3.28	1.48	1.41
31	A	1486	B8T	O2-C2	-2.98	1.18	1.23
31	A	1584	MA6	C5-C4	-2.78	1.34	1.39
31	A	1583	MA6	C5-C4	-2.76	1.34	1.39
31	A	1583	MA6	C5-N7	-2.44	1.34	1.39
31	A	1584	MA6	C5-N7	-2.40	1.34	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1584	MA6	N1-C6-N6	-10.89	103.59	116.86
31	A	1583	MA6	N1-C6-N6	-10.47	104.11	116.86
31	A	1584	MA6	C5-C6-N6	6.83	136.14	125.33
31	A	1583	MA6	C5-C6-N6	6.51	135.64	125.33
31	A	1583	MA6	N1-C2-N3	-5.66	120.02	128.58
31	A	1584	MA6	N1-C2-N3	-5.62	120.07	128.58
31	A	1583	MA6	C5-C4-N3	-4.97	119.87	126.72
31	A	1584	MA6	C5-C4-N3	-4.83	120.07	126.72
31	A	1584	MA6	N9-C8-N7	-4.18	108.01	113.94
31	A	1583	MA6	N9-C8-N7	-3.89	108.42	113.94
31	A	1583	MA6	C4-C5-C6	3.87	119.91	115.91
31	A	1584	MA6	C4-C5-C6	3.65	119.69	115.91
31	A	1583	MA6	C2-N3-C4	3.39	120.11	111.83
31	A	1584	MA6	C2-N3-C4	3.36	120.03	111.83
31	A	1584	MA6	C2-N1-C6	3.30	119.88	111.83
31	A	1583	MA6	C2-N1-C6	3.28	119.83	111.83
31	A	1583	MA6	N3-C4-N9	3.10	132.43	127.17
31	A	1584	MA6	N3-C4-N9	2.87	132.05	127.17
31	A	1584	MA6	C5-N7-C8	2.82	107.89	103.45
8	I	184	5F0	O-C-CB	-2.77	117.32	125.38
31	A	1583	MA6	C5-N7-C8	2.61	107.56	103.45
31	A	1584	MA6	C4-N9-C8	2.26	108.11	105.74
31	A	1486	B8T	C6-C5-C4	2.24	119.70	117.00
31	A	1584	MA6	C4-C5-N7	-2.16	108.11	110.58
31	A	1583	MA6	C4-N9-C8	2.02	107.86	105.74

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	1584	MA6	1	0
31	A	1583	MA6	1	0
31	A	1486	B8T	1	0
8	I	184	5F0	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 13 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	ATP	X	501	-	32,33,33	0.33	0	48,52,52	0.62	0
39	GDP	X	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.79	7 (15%)
39	GDP	7	801	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
37	FES	P	201	4,15	0,4,4	-	-	-	-	-
37	FES	T	201	19	0,4,4	-	-	-	-	-
41	SPM	A	1702	-	13,13,13	0.35	0	12,12,12	0.99	0
40	NAD	A	1701	35	46,48,48	1.20	3 (6%)	64,73,73	0.85	2 (3%)

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	ATP	X	501	-	-	1/22/38/38	0/3/3/3
39	GDP	X	502	-	-	2/16/32/32	0/3/3/3
39	GDP	7	801	-	-	2/16/32/32	0/3/3/3
37	FES	P	201	4,15	-	-	0/1/1/1
37	FES	T	201	19	-	-	0/1/1/1
41	SPM	A	1702	-	-	1/11/11/11	-
40	NAD	A	1701	35	-	0/30/62/62	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	A	1701	NAD	PA-O3	5.44	1.65	1.59
40	A	1701	NAD	PN-O3	3.55	1.63	1.59
39	7	801	GDP	C5-C4	3.08	1.47	1.38
39	X	502	GDP	C5-C4	3.02	1.47	1.38
40	A	1701	NAD	O4D-C1D	-2.42	1.37	1.40
39	X	502	GDP	C6-N1	-2.39	1.34	1.38
39	7	801	GDP	C6-N1	-2.35	1.34	1.38
39	7	801	GDP	C5-N7	-2.08	1.34	1.39
39	X	502	GDP	C5-N7	-2.00	1.35	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	7	801	GDP	C5-C4-N3	-6.20	118.52	128.39
39	X	502	GDP	C5-C4-N3	-6.16	118.59	128.39
39	7	801	GDP	C2-N3-C4	5.04	120.99	112.30
39	X	502	GDP	C2-N3-C4	5.04	120.98	112.30
39	7	801	GDP	N9-C4-N3	4.60	135.16	125.95
39	X	502	GDP	N9-C4-N3	4.56	135.08	125.95
39	X	502	GDP	C6-C5-N7	3.31	136.32	130.29
39	7	801	GDP	C6-C5-N7	3.21	136.13	130.29
39	X	502	GDP	C4-C5-N7	-2.68	106.43	110.67
39	7	801	GDP	C4-C5-N7	-2.62	106.52	110.67
40	A	1701	NAD	O2A-PA-O1A	2.18	122.58	112.44
39	X	502	GDP	O6-C6-C5	-2.13	120.91	126.53
39	7	801	GDP	O6-C6-C5	-2.13	120.92	126.53
40	A	1701	NAD	O3-PA-O1A	-2.12	104.32	110.70
39	X	502	GDP	C8-N7-C5	2.03	107.87	104.26

There are no chirality outliers.

All (6) torsion outliers are listed below:

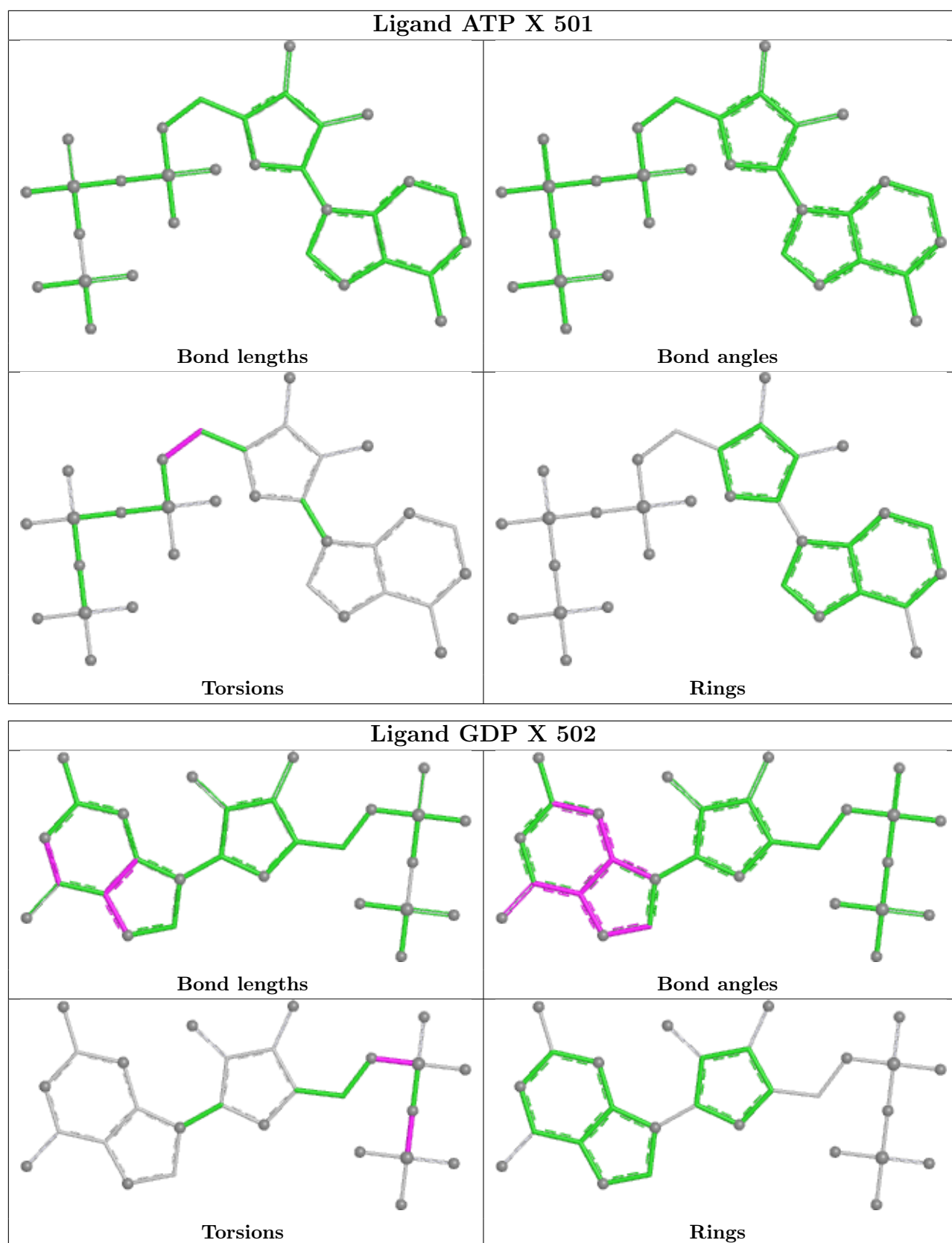
Mol	Chain	Res	Type	Atoms
39	7	801	GDP	O4'-C4'-C5'-O5'
39	7	801	GDP	C3'-C4'-C5'-O5'
41	A	1702	SPM	C7-C8-C9-N10
39	X	502	GDP	C5'-O5'-PA-O1A
38	X	501	ATP	C4'-C5'-O5'-PA
39	X	502	GDP	PA-O3A-PB-O3B

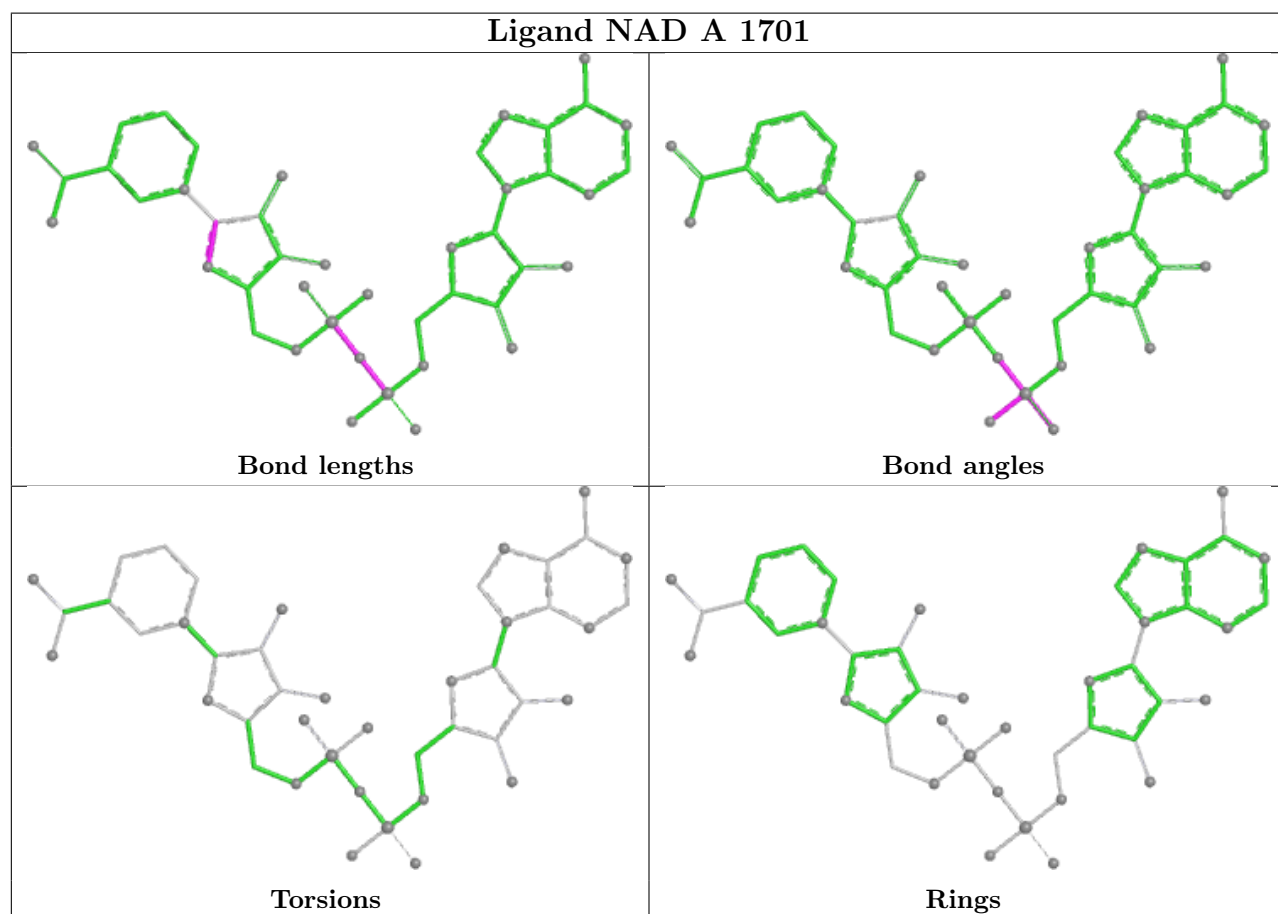
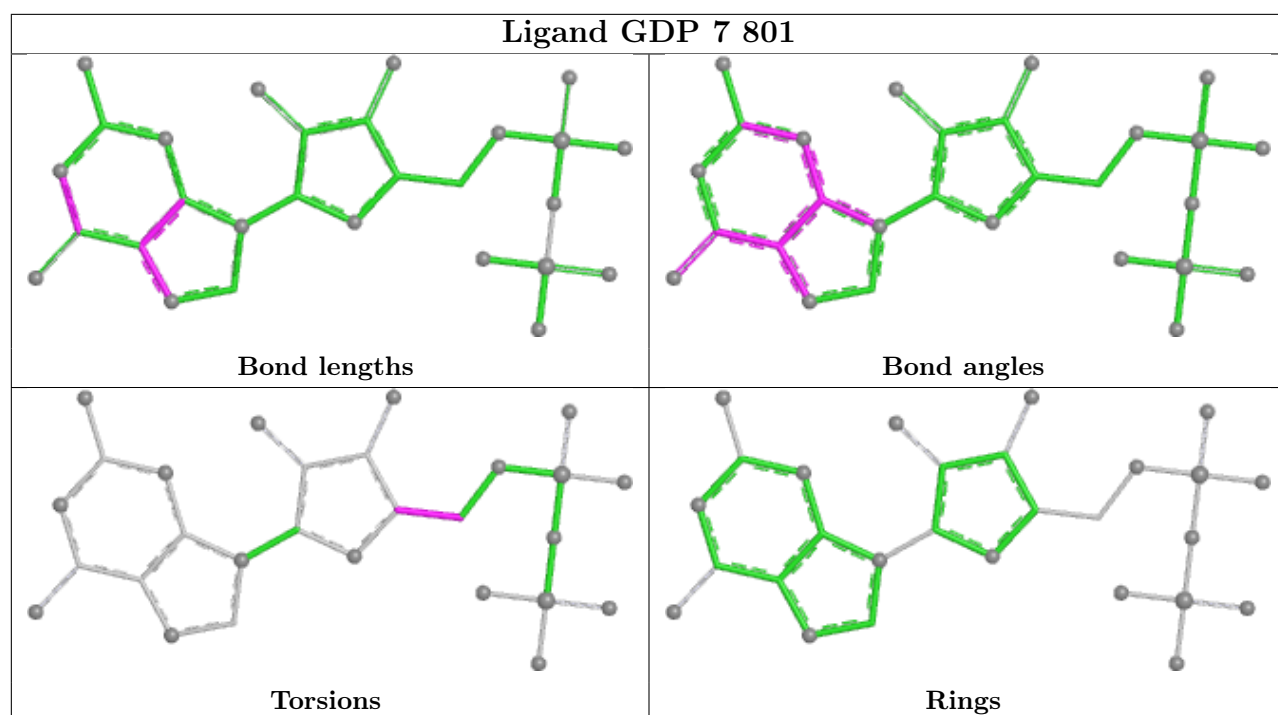
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	X	501	ATP	2	0
39	7	801	GDP	1	0
37	P	201	FES	2	0
41	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	76:ASN	C	77:VAL	N	3.05

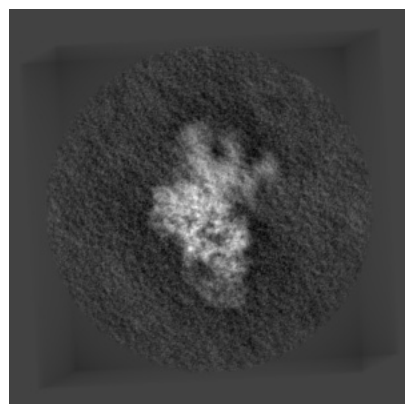
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52857. These allow visual inspection of the internal detail of the map and identification of artifacts.

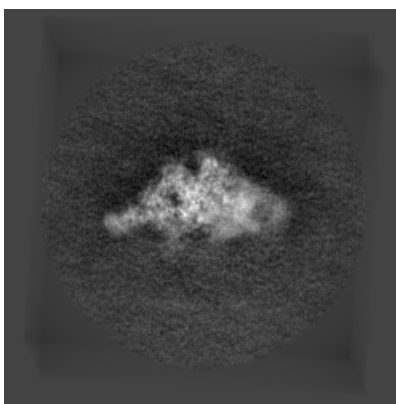
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

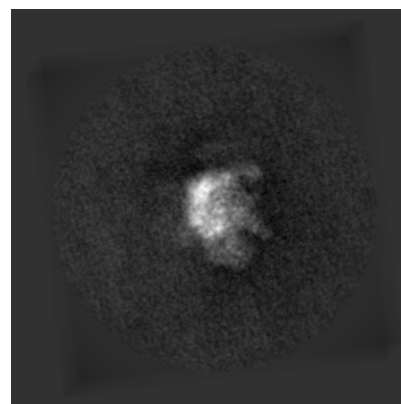
6.1.1 Primary map



X

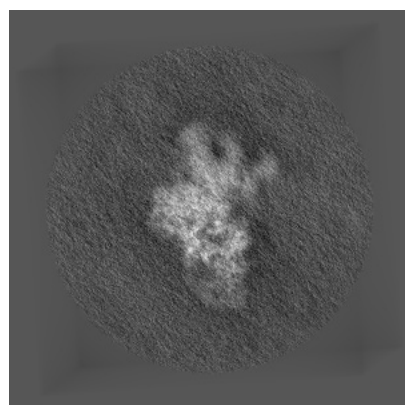


Y

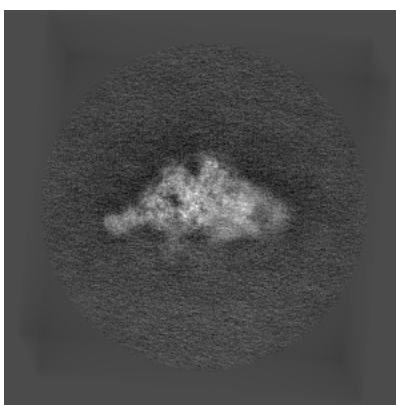


Z

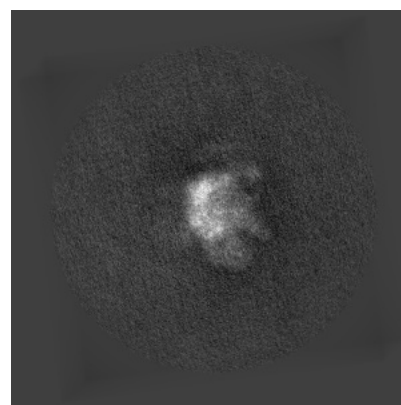
6.1.2 Raw map



X



Y

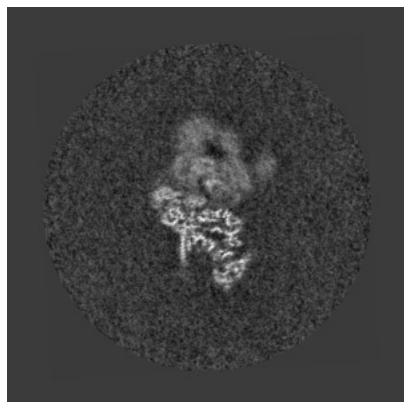


Z

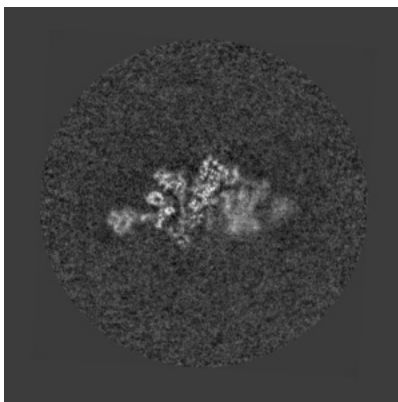
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

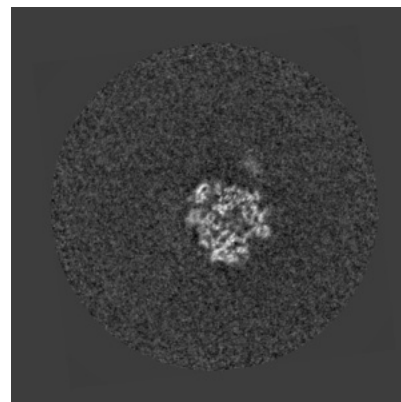
6.2.1 Primary map



X Index: 300

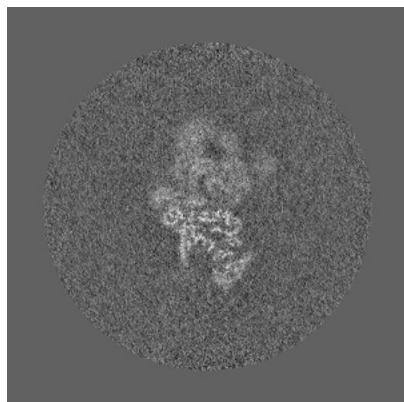


Y Index: 300

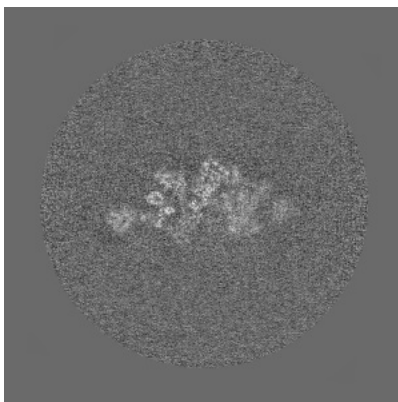


Z Index: 300

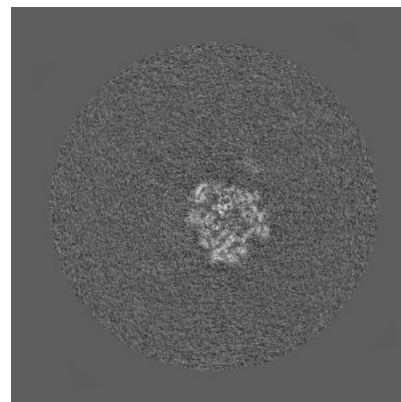
6.2.2 Raw map



X Index: 300



Y Index: 300

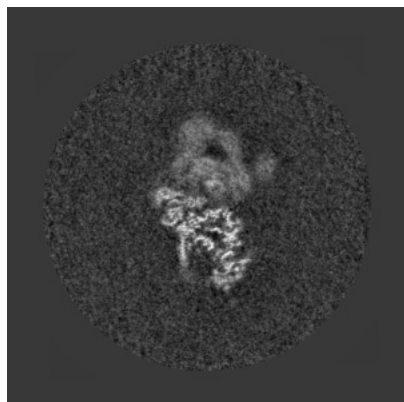


Z Index: 300

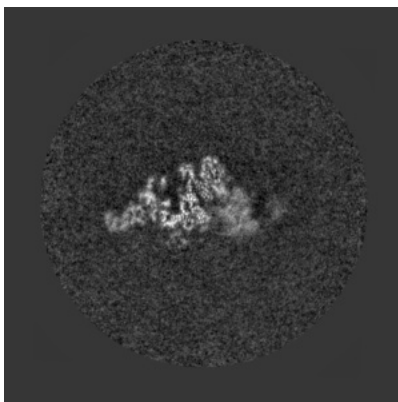
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

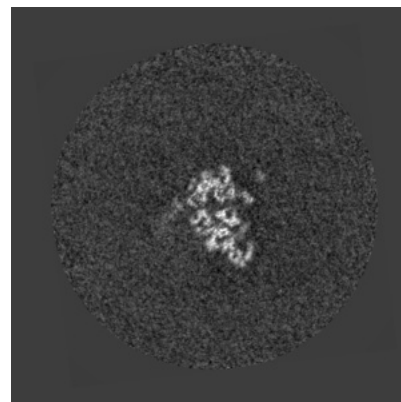
6.3.1 Primary map



X Index: 298

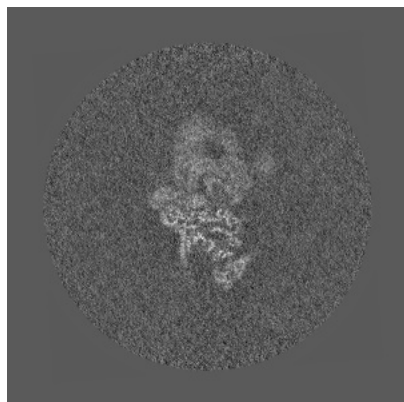


Y Index: 312

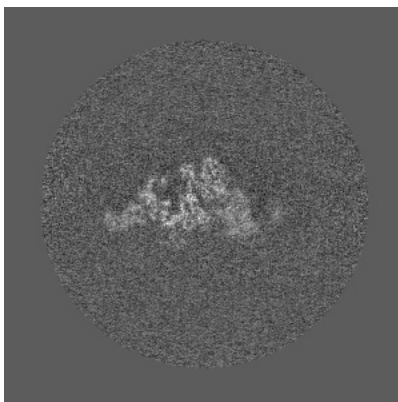


Z Index: 274

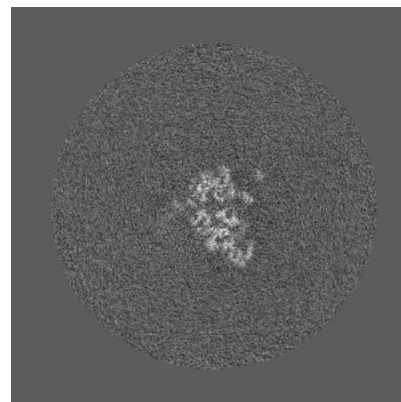
6.3.2 Raw map



X Index: 301



Y Index: 312

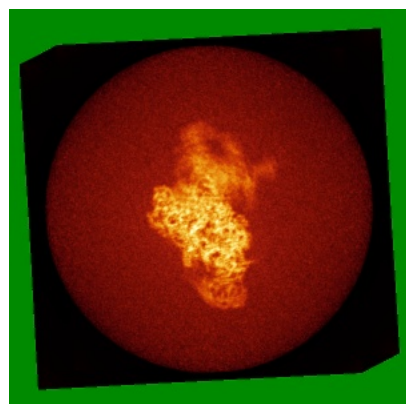


Z Index: 274

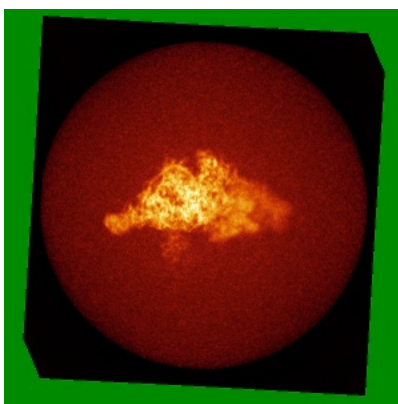
The images above show the largest variance slices of the map in three orthogonal directions.

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

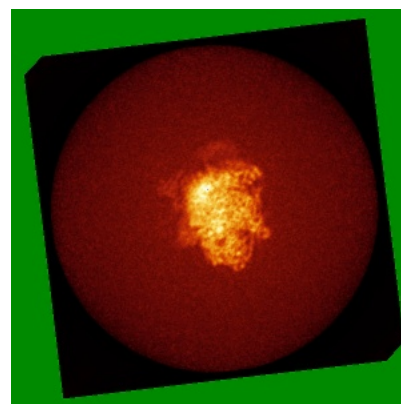
6.4.1 Primary map



X

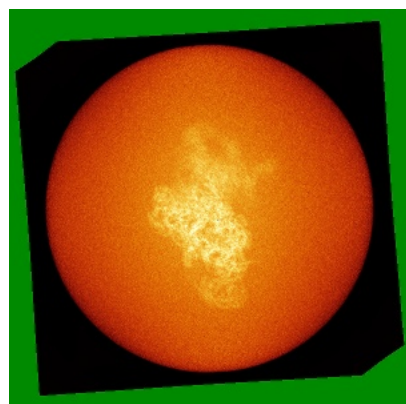


Y

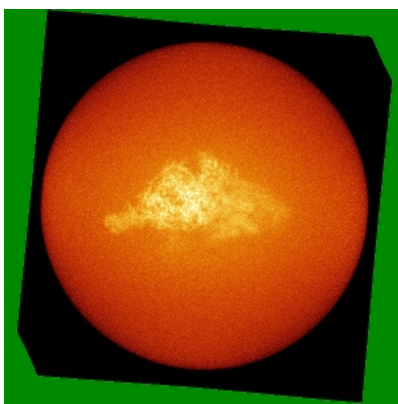


Z

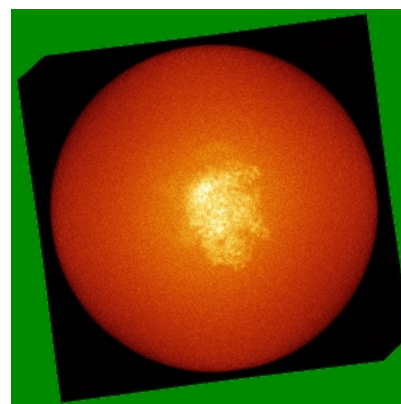
6.4.2 Raw map



X



Y

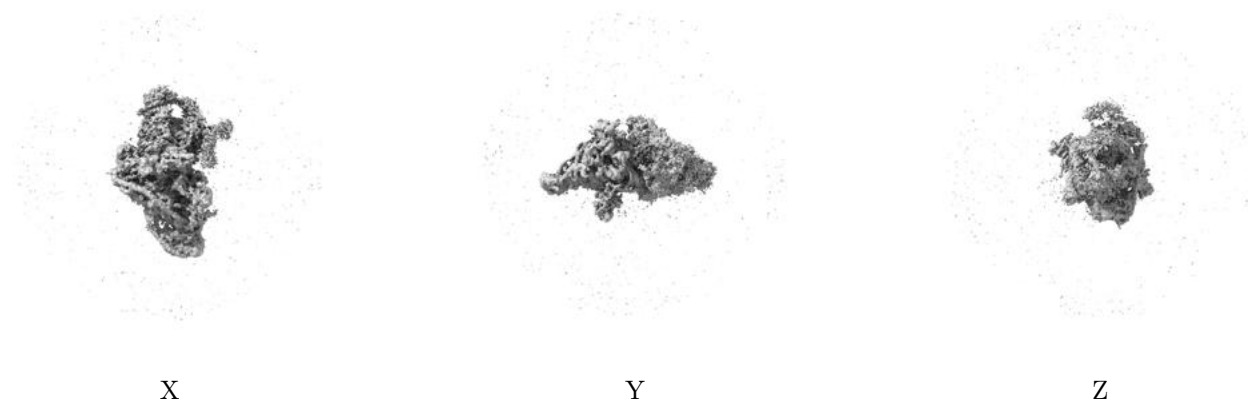


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

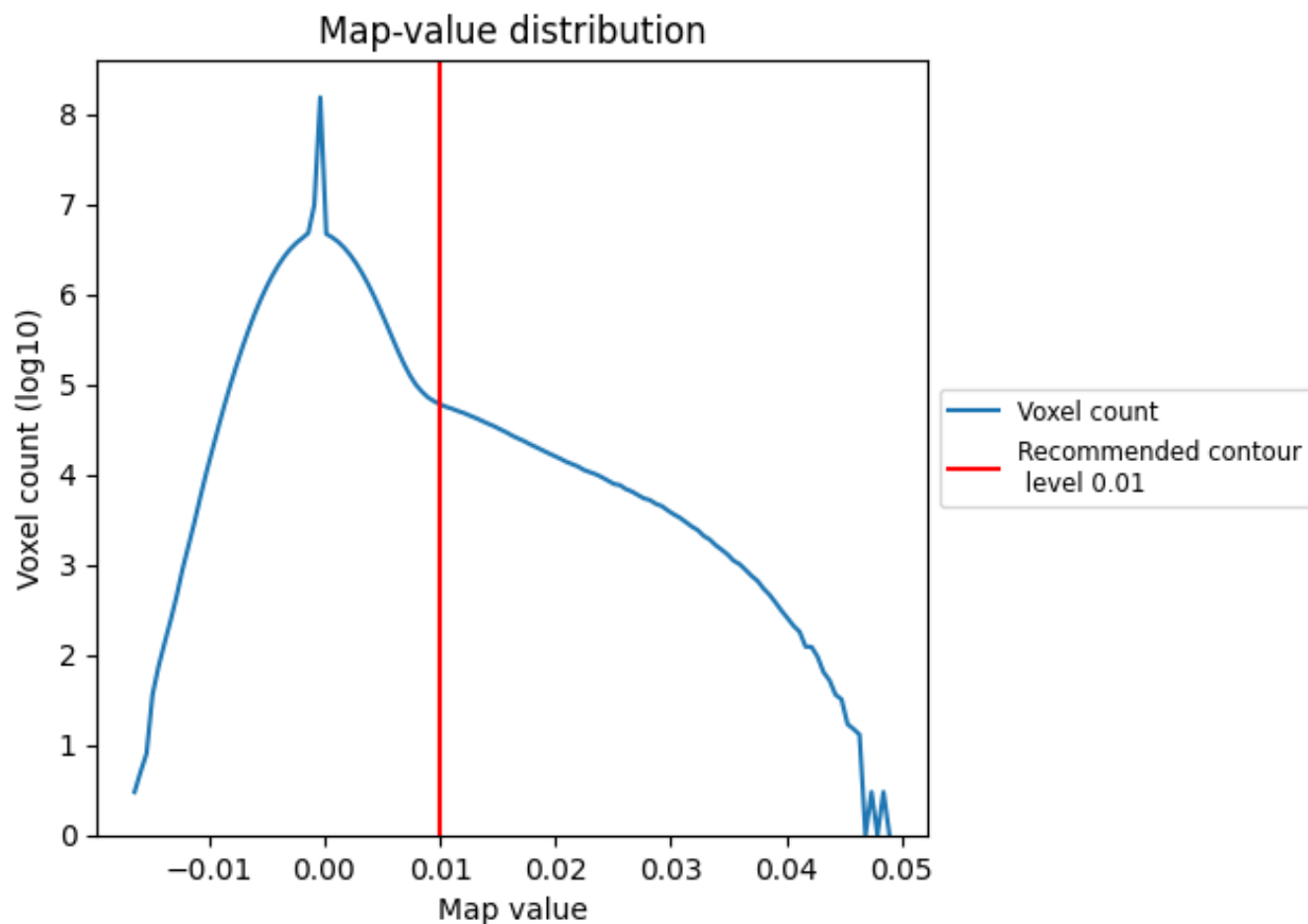
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

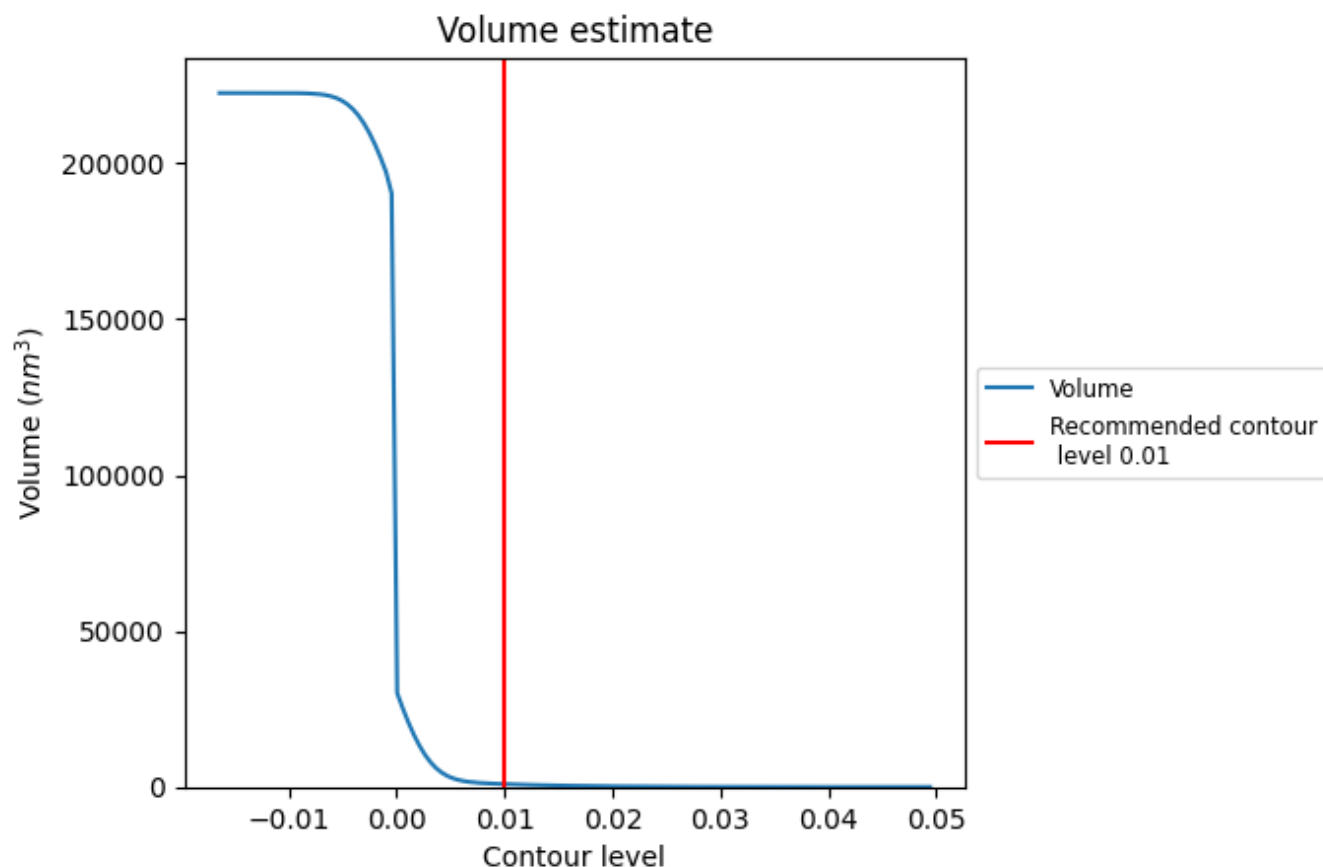
This section contains the results of statistical analysis of the map.

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.

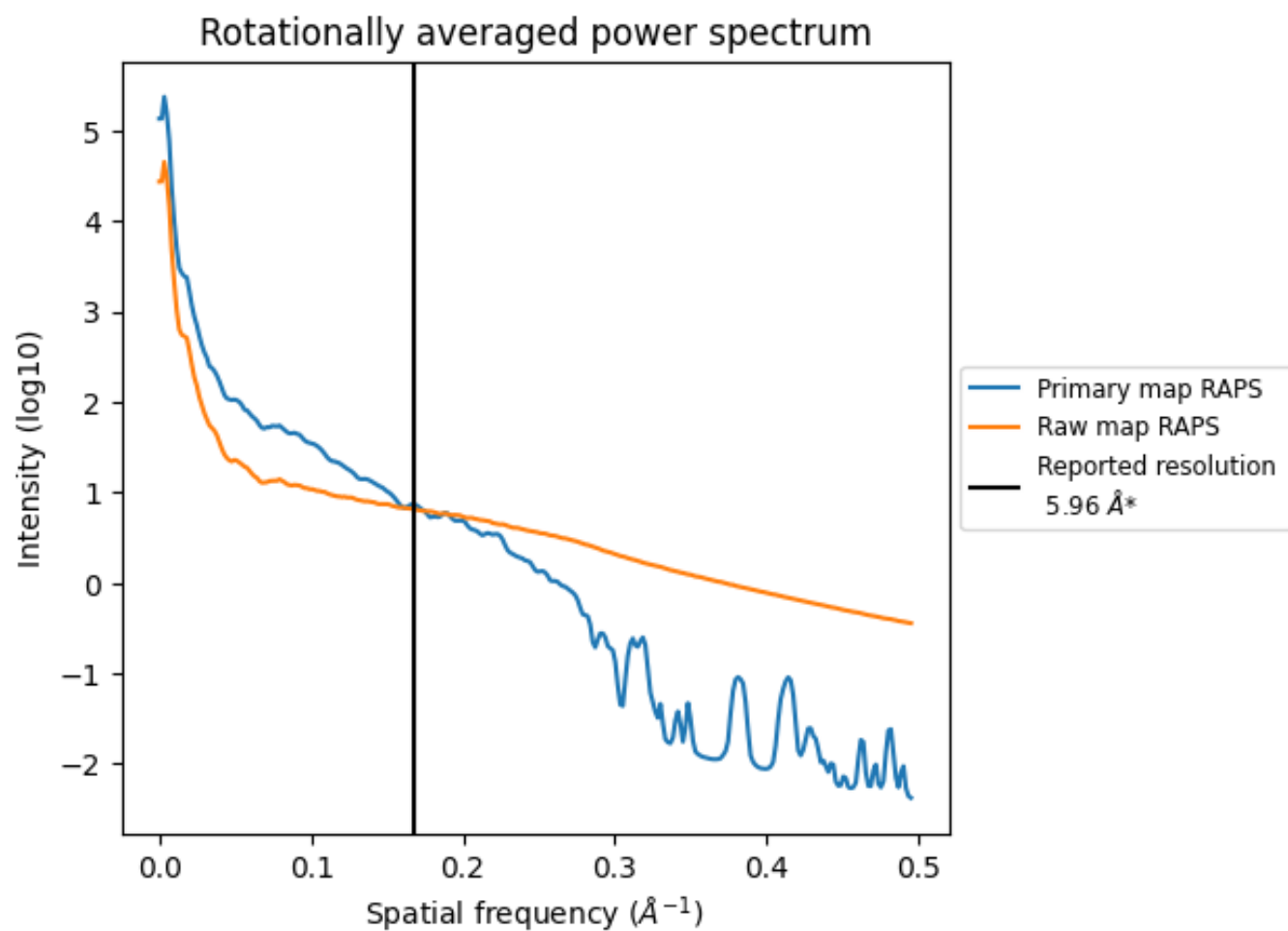
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 920 nm^3 ; this corresponds to an approximate mass of 831 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 ⓘ

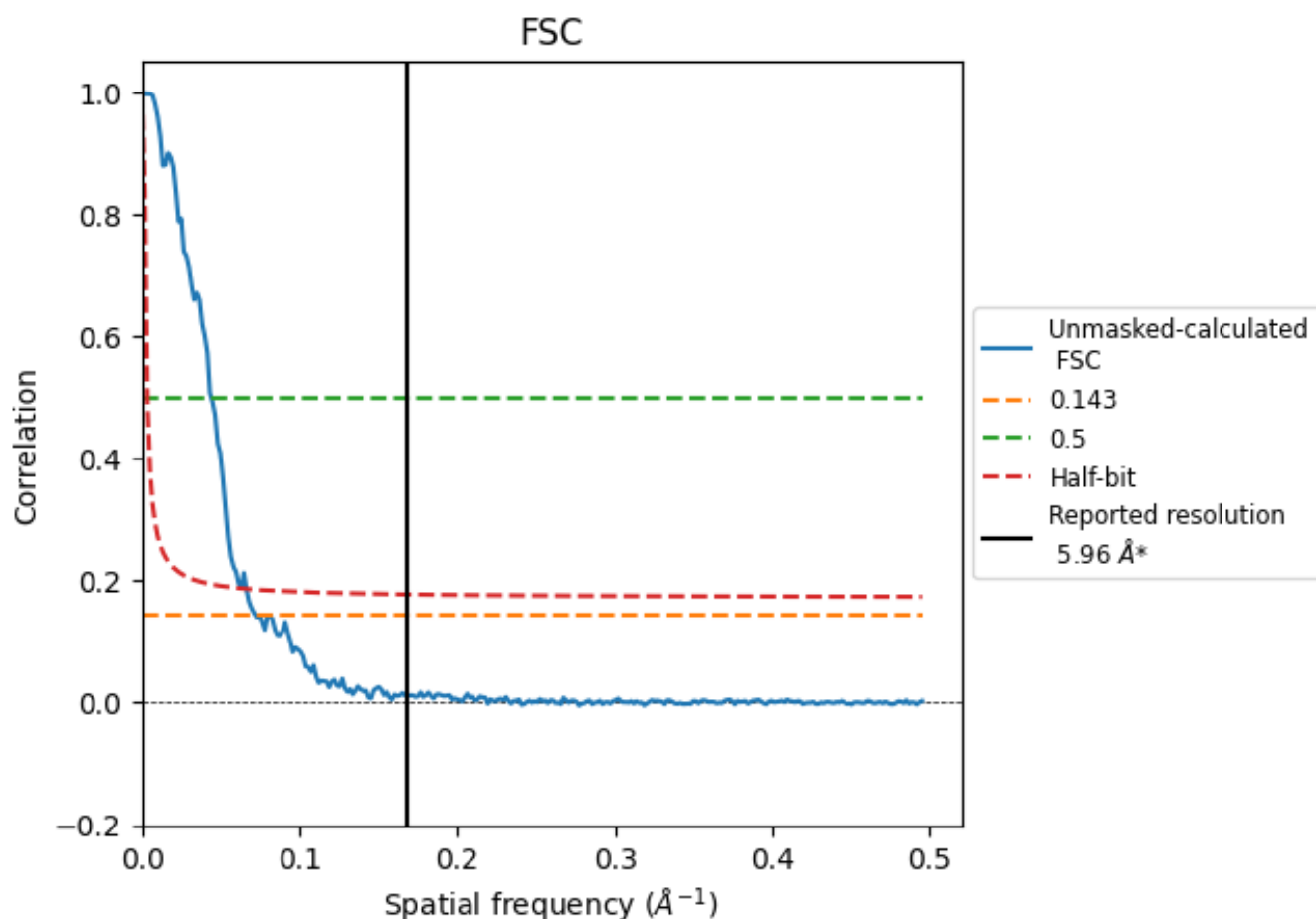


*Reported resolution corresponds to spatial frequency of 0.168 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.168 Å⁻¹

8.2 Resolution estimates [i](#)

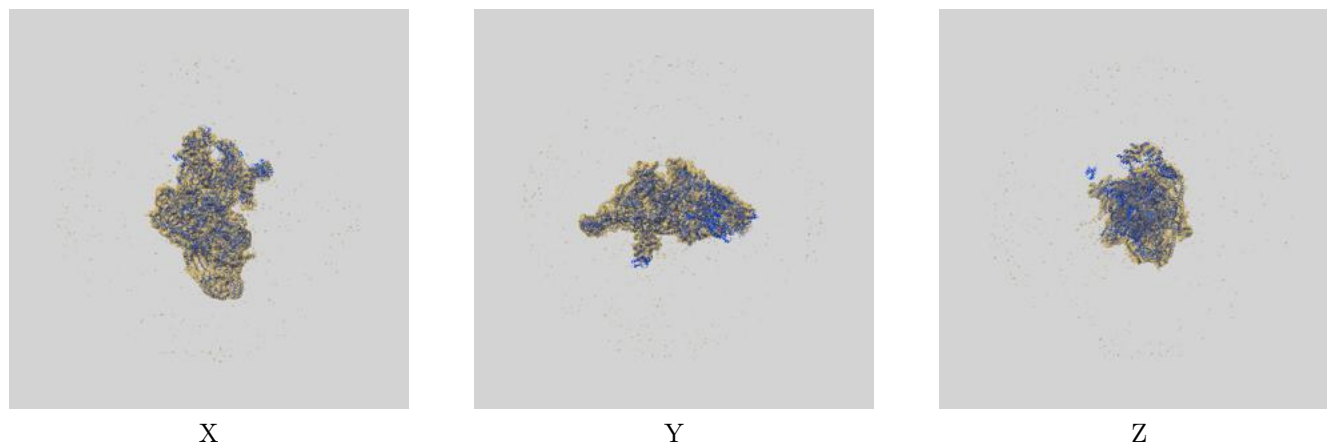
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	13.93	22.94	15.15

*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 13.93 differs from the reported value 5.96 by more than 10 %

9 Map-model fit [i](#)

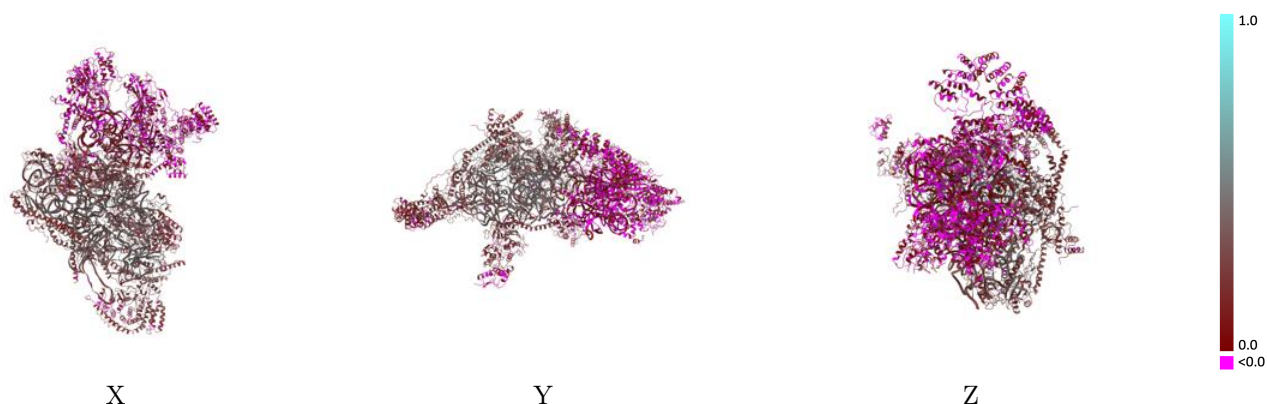
This section contains information regarding the fit between EMDB map EMD-52857 and PDB model 9IGT. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



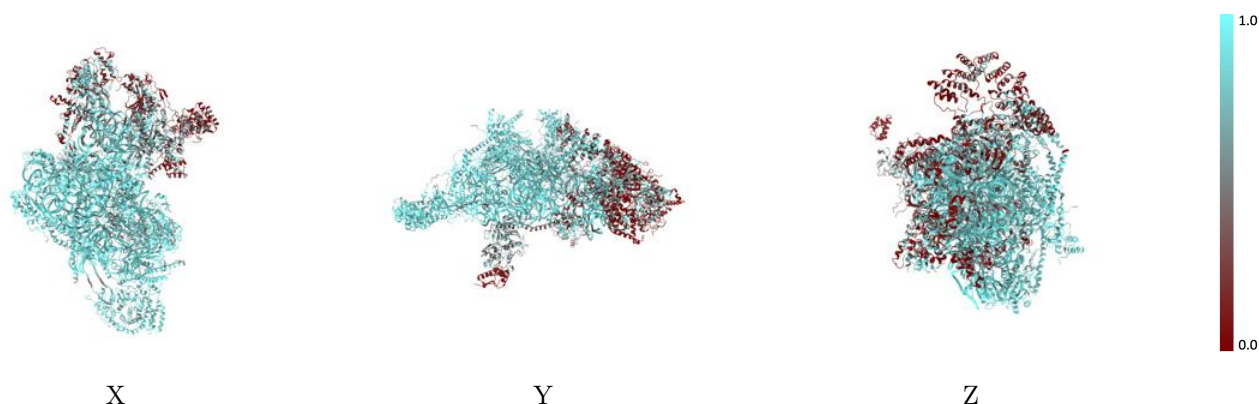
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



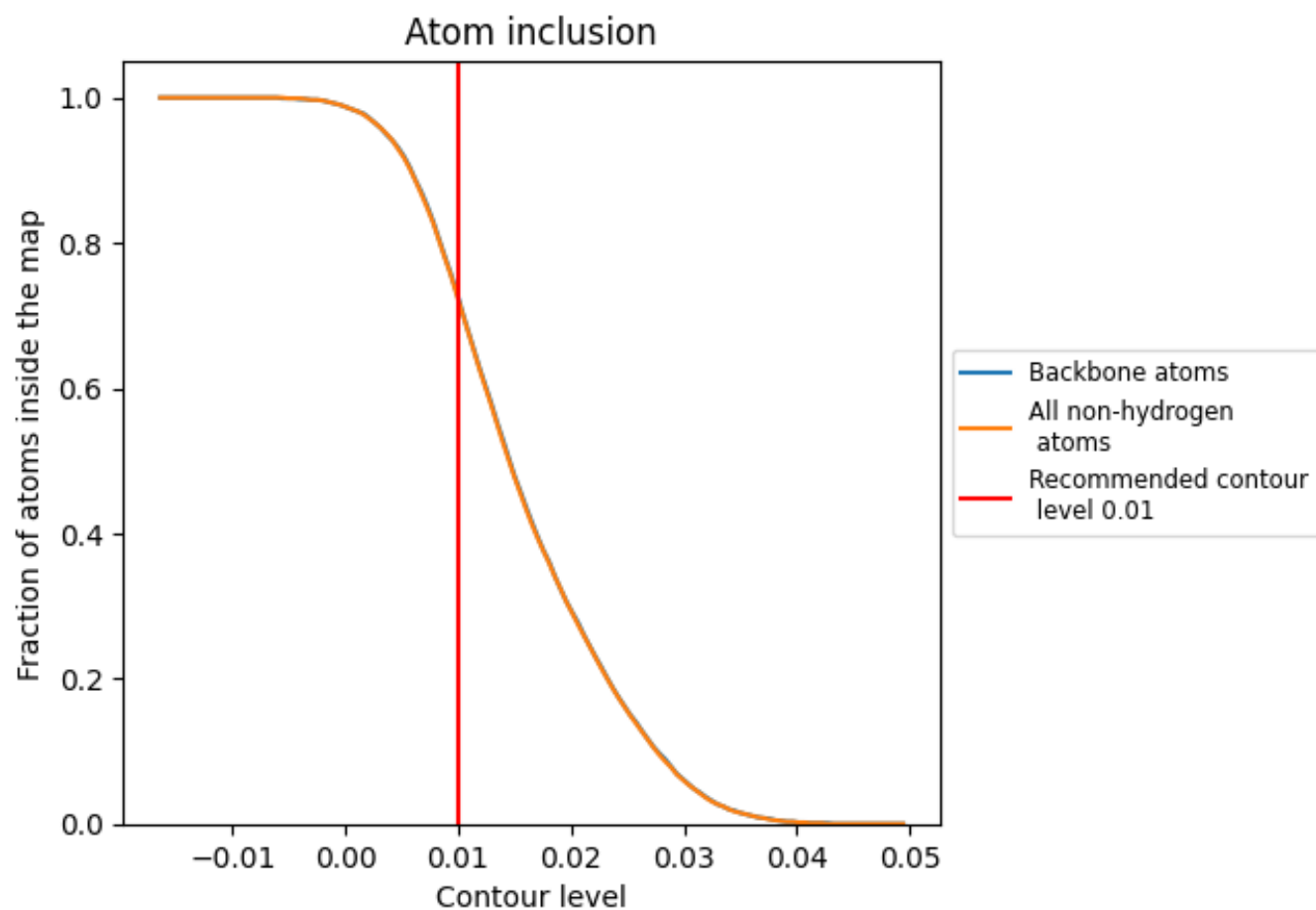
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 72% of all backbone atoms, 72% 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	 0.7220	 0.2030
0	 0.8400	 0.2540
1	 0.3960	 0.0290
3	 0.8190	 0.2980
4	 0.2950	 0.0150
7	 0.4950	 0.1930
A	 0.9160	 0.2740
B	 0.8620	 0.2970
C	 0.6390	 0.0590
D	 0.7250	 0.2680
E	 0.8430	 0.2950
F	 0.4350	 0.0130
G	 0.6980	 0.1010
H	 0.4070	 0.0110
I	 0.8850	 0.2750
J	 0.8450	 0.3510
K	 0.5470	 0.0110
L	 0.8360	 0.3100
M	 0.8850	 0.3630
N	 0.8990	 0.3740
O	 0.8990	 0.3440
P	 0.8550	 0.3020
Q	 0.8020	 0.2720
R	 0.8790	 0.3080
S	 0.8650	 0.2670
T	 0.8660	 0.3590
U	 0.8590	 0.2790
V	 0.8460	 0.1630
W	 0.8530	 0.2710
X	 0.3900	 0.0200
Y	 0.2640	 0.0360
Z	 0.4810	 0.0590
a	 0.5960	 0.1290
b	 0.6650	 0.0870
t	 0.0040	 0.0010

