Full wwPDB EM Validation Report ⓘ

Feb 6, 2023 – 01:04 PM EST

PDB ID	:	8D8L
EMDB ID	:	EMD-27251
Title	:	Yeast mitochondrial small subunit assembly intermediate (State 3)
Authors	:	Burnside, C.; Harper, N.; Klinge, S.
Deposited on	:	2022-06-08
Resolution	:	2.60 Å(reported)
Based on initial model	:	5MRC

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

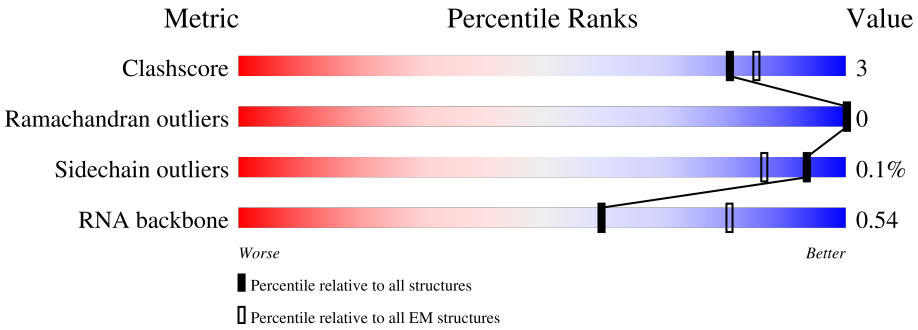
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	628	8% 61% 10% 29%
2	5	339	63% 71% 9% 20%
3	C	398	56% 5% 40%
4	M	143	12% 58% 42%
5	N	115	95%
6	O	286	67% 6% 27%
7	P	121	6% 83% 12%

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Mol	Chain	Length	Quality of chain
8	Q	237	21% 81% 5% 14%
9	R	138	59% 7% 34%
10	S	91	80% 18%
11	T	177	12% 48% 48%
12	U	264	82% 6% 12%
13	V	318	7% 63% 10% 27%
14	W	450	84% 12%
15	X	110	85% 13%
16	Y	319	79% 18%
17	Z	95	11% 87% 12%
18	A	344	5% 53% 5% 42%
19	B	394	62% 5% 32%
20	2	130	9% 70% 6% 24%
21	3	266	87% 5% 8%
22	D	486	8% 64% 33%
23	4	321	15% 77% 8% 16%
24	E	307	86% 7% 7%
25	F	131	85% 10% 5%
26	6	345	7% 85% 12%
27	G	247	55% 41%
28	H	155	92% 8%
29	8	500	14% 86% 5% 10%
30	I	278	71% 25%
31	a	1713	9% 68% 20% 12%
32	J	203	67% 29%

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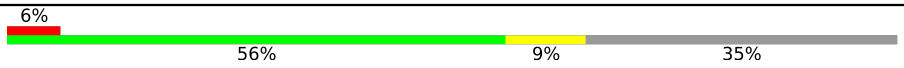
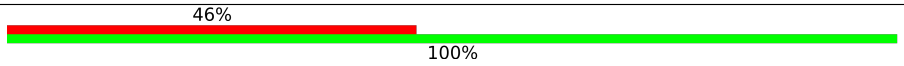
Mol	Chain	Length	Quality of chain
33	K	217	
34	c	94	
35	L	153	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 87007 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Probable S-adenosyl-L-methionine-dependent RNA methyltransferase RSM22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	447	Total	C	N	O	S	0	0
			3626	2298	657	658	13		

- Molecule 2 is a protein called 37S ribosomal protein MRP13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	270	Total	C	N	O	S	0	0
			2199	1426	375	394	4		

- Molecule 3 is a protein called Ribosomal protein VAR1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	240	Total	C	N	O	S	0	0
			2018	1277	349	365	27		

- Molecule 4 is a protein called 37S ribosomal protein SWS2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	83	Total	C	N	O	S	0	0
			645	417	111	112	5		

- Molecule 5 is a protein called 37S ribosomal protein MRP2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	112	Total	C	N	O	S	0	0
			923	590	178	151	4		

- Molecule 6 is a protein called 37S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	210	Total	C	N	O	S	0	0
			1727	1081	321	317	8		

- Molecule 7 is a protein called 37S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	116	Total	C	N	O	S	0	0
			919	586	172	159	2		

- Molecule 8 is a protein called 37S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	204	Total	C	N	O	S	0	0
			1683	1055	315	308	5		

- Molecule 9 is a protein called 37S ribosomal protein RSM18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	91	Total	C	N	O	S	0	0
			738	463	143	128	4		

- Molecule 10 is a protein called 37S ribosomal protein S19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	75	Total	C	N	O	S	0	0
			595	383	109	101	2		

- Molecule 11 is a protein called 37S ribosomal protein MRP21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	92	Total	C	N	O	S	0	0
			760	475	150	130	5		

- Molecule 12 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	233	Total	C	N	O	S	0	0
			1907	1211	331	358	7		

- Molecule 13 is a protein called 37S ribosomal protein PET123, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	233	Total	C	N	O	S	0	0
			1879	1192	338	346	3		

- Molecule 14 is a protein called 37S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	395	Total	C	N	O	S	0	0
			3174	2047	531	588	8		

- Molecule 15 is a protein called Mitochondrial 37S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	96	Total	C	N	O	S	0	0
			774	496	140	135	3		

- Molecule 16 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	263	Total	C	N	O	S	0	0
			2208	1400	393	411	4		

- Molecule 17 is a protein called 37S ribosomal protein MRP10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	84	Total	C	N	O	S	0	0
			660	418	121	115	6		

- Molecule 18 is a protein called 37S ribosomal protein MRP51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	199	Total	C	N	O	S	0	0
			1585	1023	278	279	5		

- Molecule 19 is a protein called 37S ribosomal protein MRP4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B	266	Total	C	N	O	S	0	0
			2085	1313	366	404	2		

- Molecule 20 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	99	Total	C	N	O	S	0	0
			833	530	156	146	1		

- Molecule 21 is a protein called 37S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3	244	Total	C	N	O	S	0	0
			1953	1261	328	359	5		

- Molecule 22 is a protein called 37S ribosomal protein NAM9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	326	Total	C	N	O	S	0	0
			2713	1767	477	464	5		

- Molecule 23 is a protein called 37S ribosomal protein MRP1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4	271	Total	C	N	O	S	0	0
			2182	1390	373	412	7		

- Molecule 24 is a protein called 37S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	287	Total	C	N	O	S	0	0
			2297	1467	406	416	8		

- Molecule 25 is a protein called 37S ribosomal protein MRP17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	125	Total	C	N	O	S	0	0
			1002	639	182	177	4		

- Molecule 26 is a protein called 37S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	305	Total	C	N	O	S	0	0
			2488	1587	445	450	6		

- Molecule 27 is a protein called 37S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	G	146	Total	C	N	O	S	0	0
			1168	737	217	209	5		

- Molecule 28 is a protein called 37S ribosomal protein S8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	154	Total	C	N	O	S	0	0
			1213	767	217	220	9		

- Molecule 29 is a protein called 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	8	452	Total	C	N	O	S	0	0
			3573	2272	600	681	20		

- Molecule 30 is a protein called 37S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	I	209	Total	C	N	O	S	0	0
			1676	1073	301	298	4		

- Molecule 31 is a RNA chain called 15S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1506	Total	C	N	O	P	0	0
			31987	14385	5649	10447	1506		

- Molecule 32 is a protein called 37S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	144	Total	C	N	O	S	0	0
			1186	768	204	210	4		

- Molecule 33 is a protein called 37S ribosomal protein S18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	142	Total	C	N	O	S	0	0
			1121	717	195	203	6		

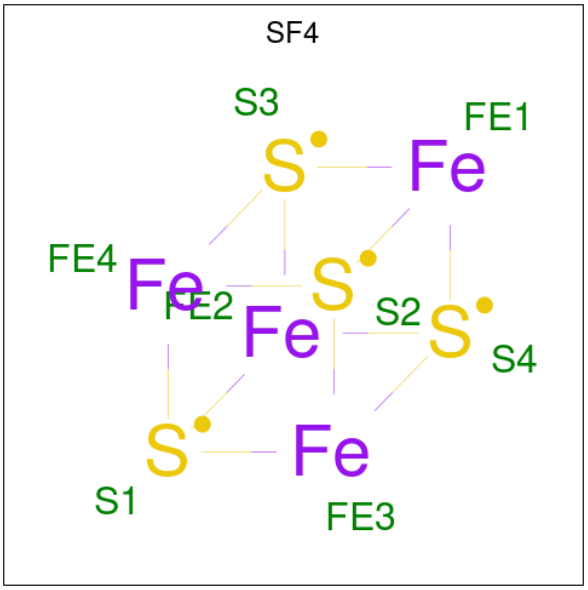
- Molecule 34 is a protein called unknown protein sequence.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	c	94	Total	C	N	O	0	0
			470	282	94	94		

- Molecule 35 is a protein called 37S ribosomal protein S12, mitochondrial.

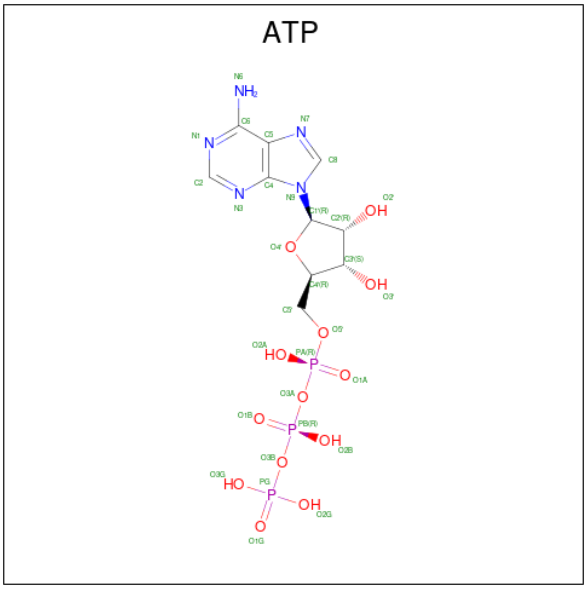
Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	121	Total	C	N	O	S	0	0
			926	571	190	161	4		

- Molecule 36 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
37	W	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	W	1	Total	Mg	0
			1	1	
38	B	1	Total	Mg	0
			1	1	
38	a	69	Total	Mg	0
			69	69	
38	L	1	Total	Mg	0
			1	1	

- Molecule 39 is water.

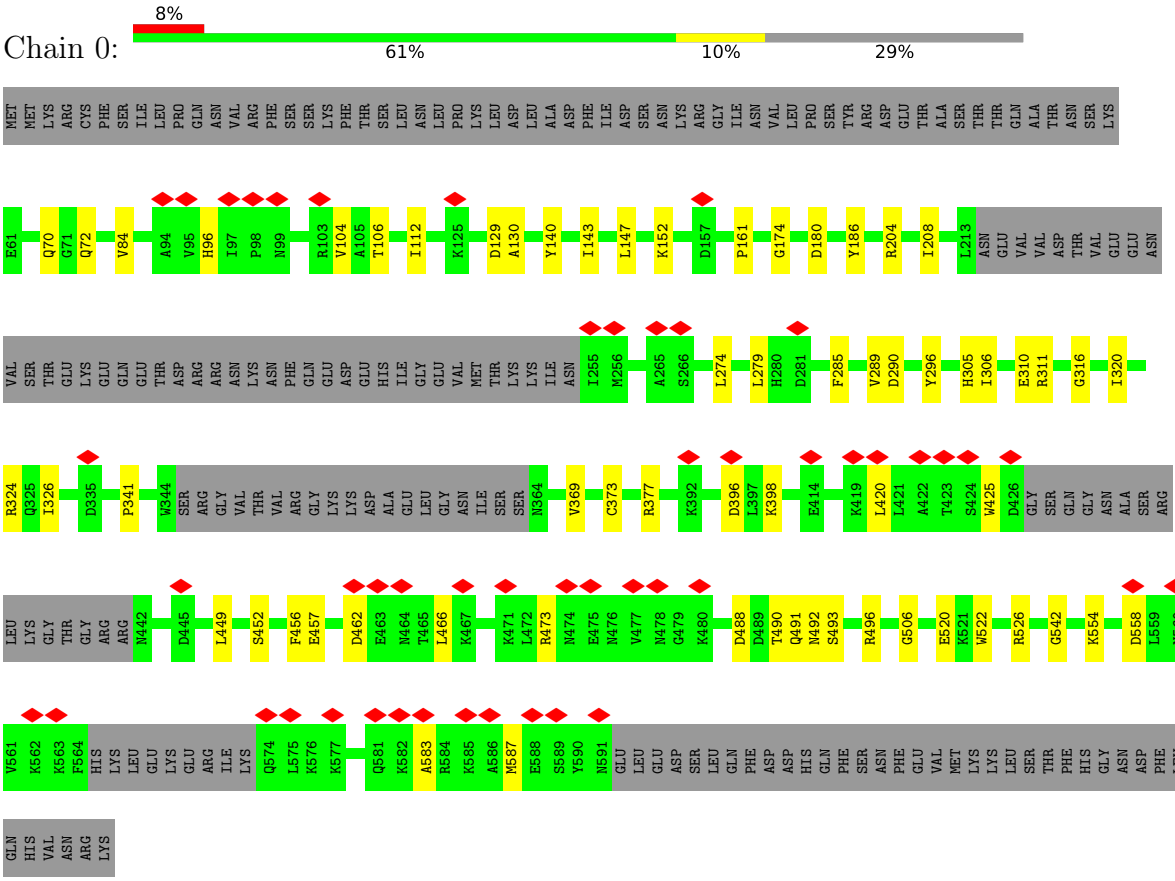
Mol	Chain	Residues	Atoms		AltConf
39	W	3	Total	O	0
			3	3	

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.

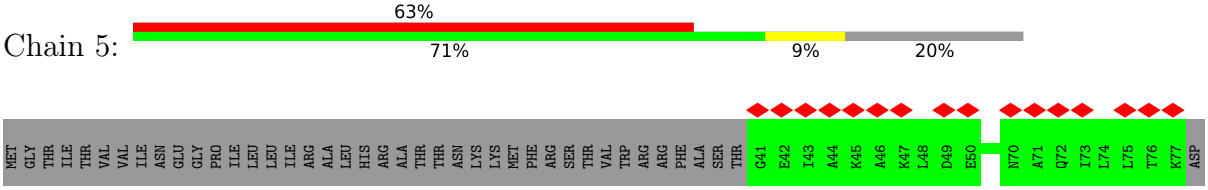
• Molecule 1: Probable S-adenosyl-L-methionine-dependent RNA methyltransferase RSM22, mitochondrial

Chain 0:



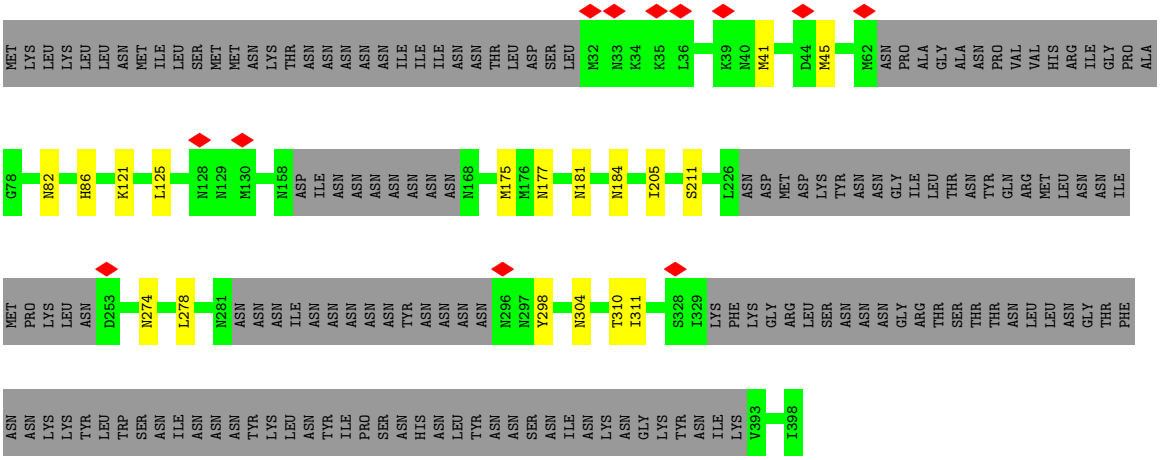
• Molecule 2: 37S ribosomal protein MRP13, mitochondrial

Chain 5:



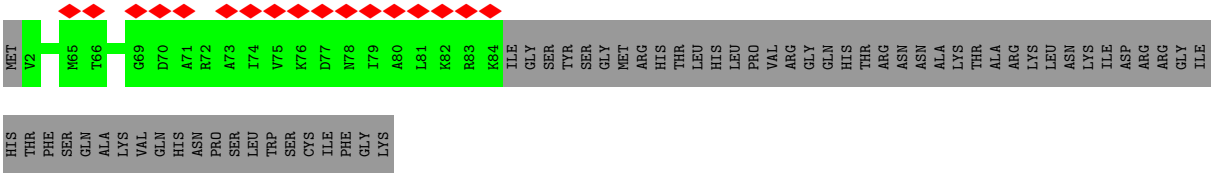
• Molecule 3: Ribosomal protein VAR1, mitochondrial

Chain C:



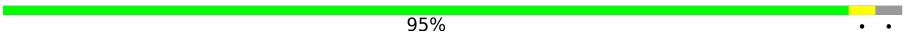
• Molecule 4: 37S ribosomal protein SWS2, mitochondrial

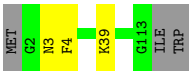
Chain M:



• Molecule 5: 37S ribosomal protein MRP2, mitochondrial

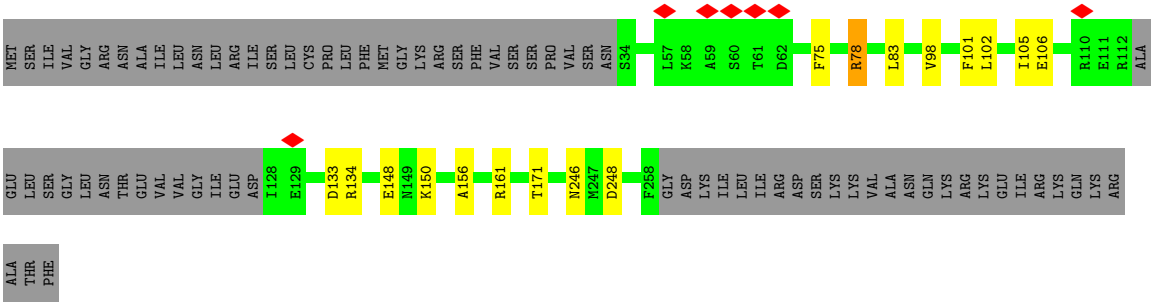
Chain N:





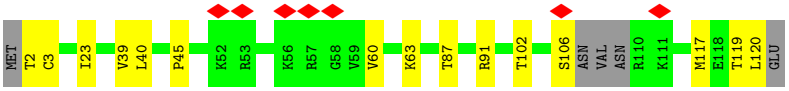
• Molecule 6: 37S ribosomal protein S28, mitochondrial

Chain O:



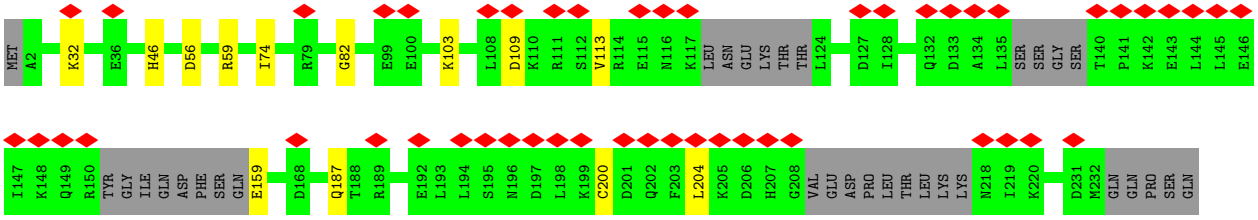
• Molecule 7: 37S ribosomal protein S16, mitochondrial

Chain P:



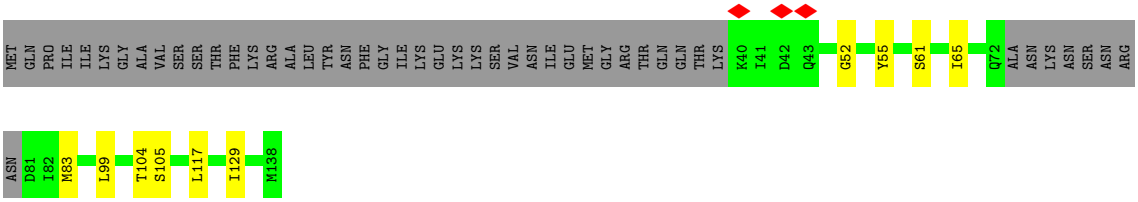
• Molecule 8: 37S ribosomal protein S17, mitochondrial

Chain Q:



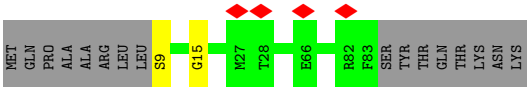
• Molecule 9: 37S ribosomal protein RSM18, mitochondrial

Chain R:

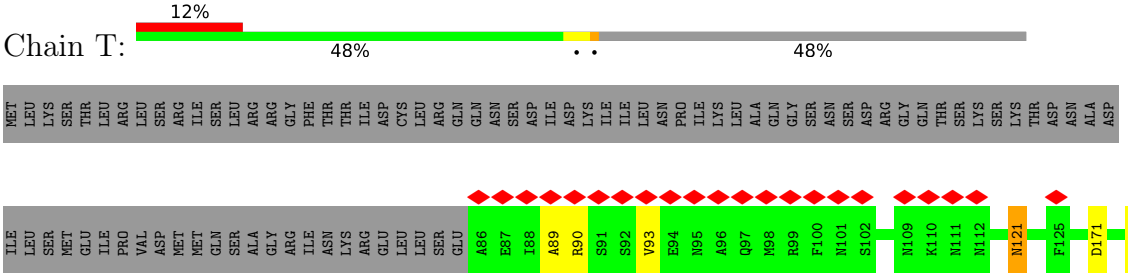


• Molecule 10: 37S ribosomal protein S19, mitochondrial

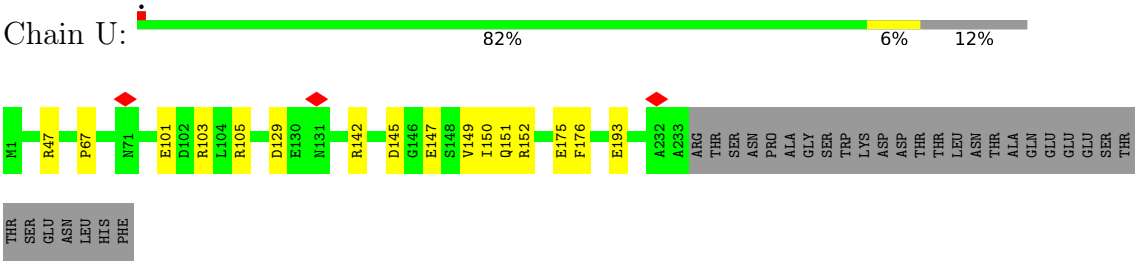
Chain S:



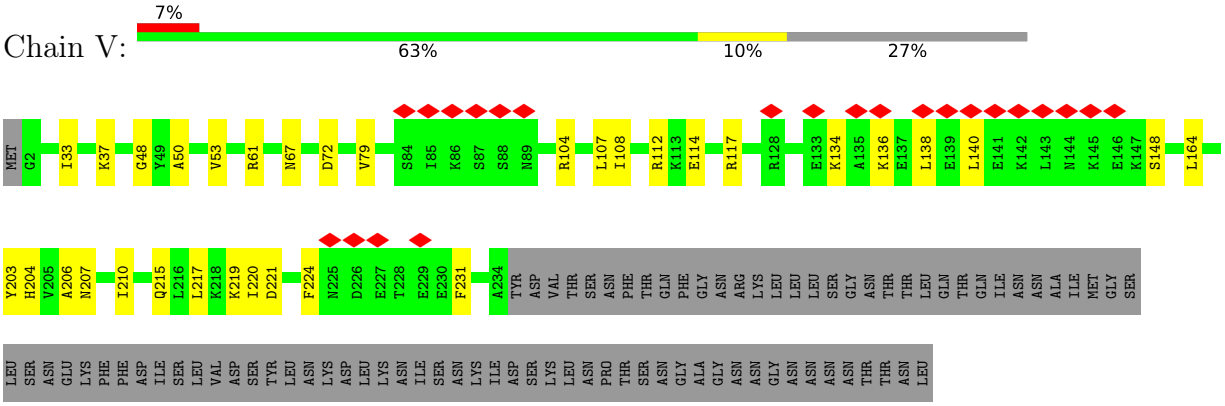
• Molecule 11: 37S ribosomal protein MRP21, mitochondrial



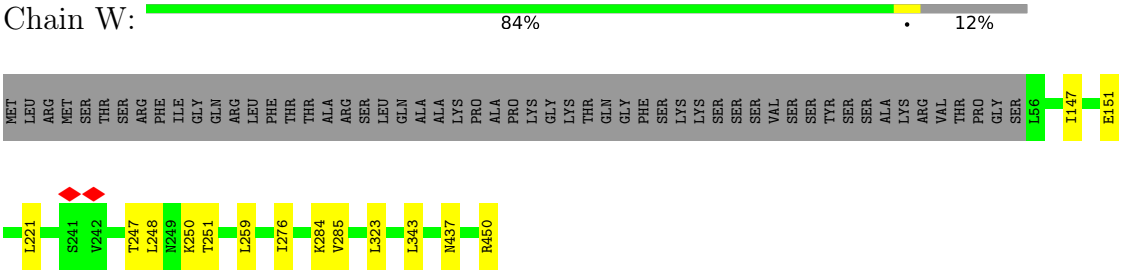
• Molecule 12: 37S ribosomal protein S25, mitochondrial



• Molecule 13: 37S ribosomal protein PET123, mitochondrial

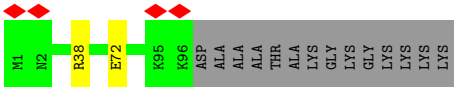


• Molecule 14: 37S ribosomal protein S23, mitochondrial



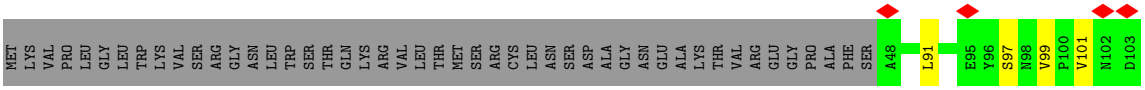
• Molecule 15: Mitochondrial 37S ribosomal protein S27

Chain X:



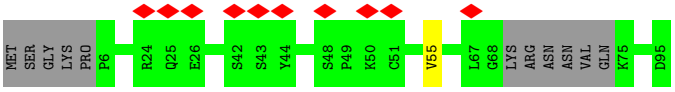
• Molecule 16: 37S ribosomal protein S24, mitochondrial

Chain Y:



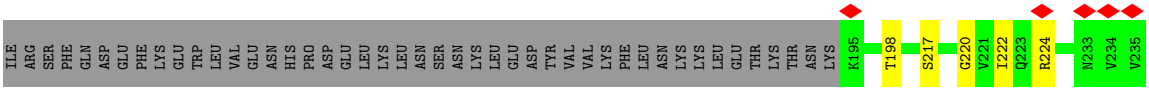
• Molecule 17: 37S ribosomal protein MRP10, mitochondrial

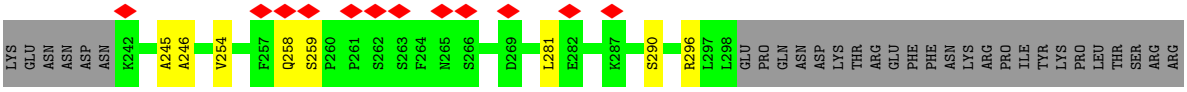
Chain Z:

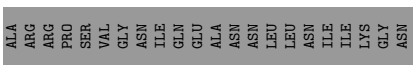


• Molecule 18: 37S ribosomal protein MRP51, mitochondrial

Chain A:

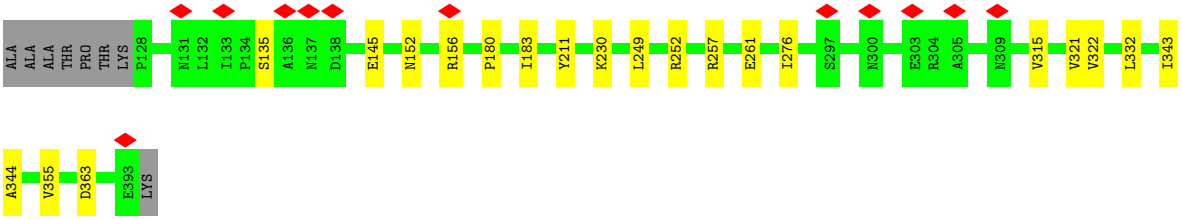






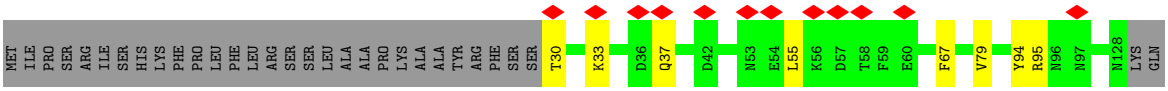
• Molecule 19: 37S ribosomal protein MRP4, mitochondrial

Chain B:



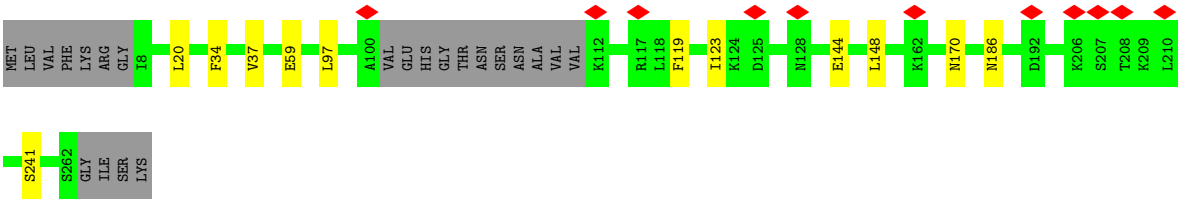
• Molecule 20: Protein FYV4, mitochondrial

Chain 2:



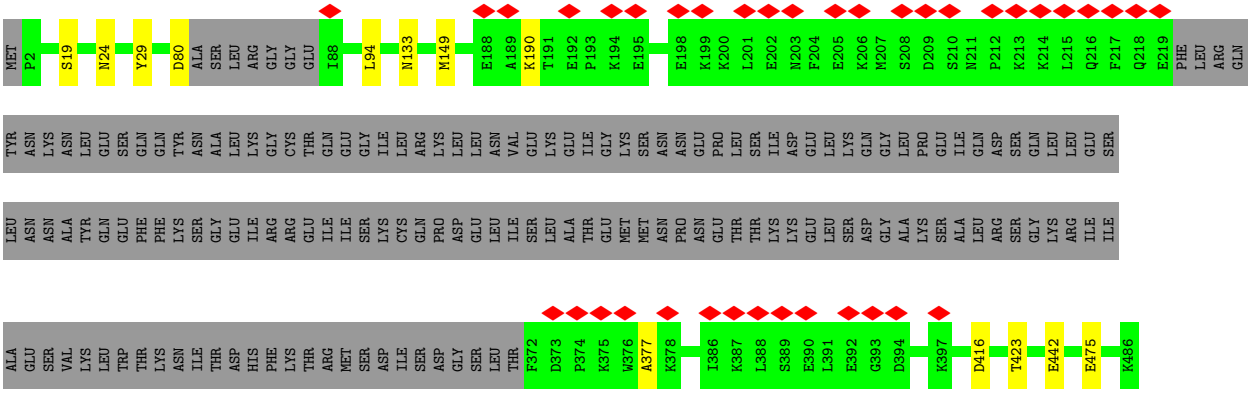
• Molecule 21: 37S ribosomal protein S26, mitochondrial

Chain 3:



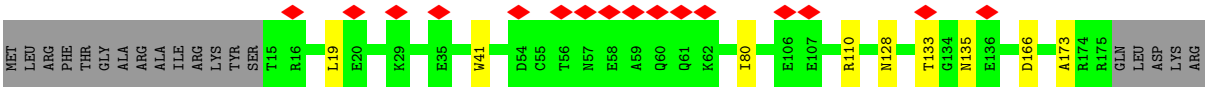
• Molecule 22: 37S ribosomal protein NAM9, mitochondrial

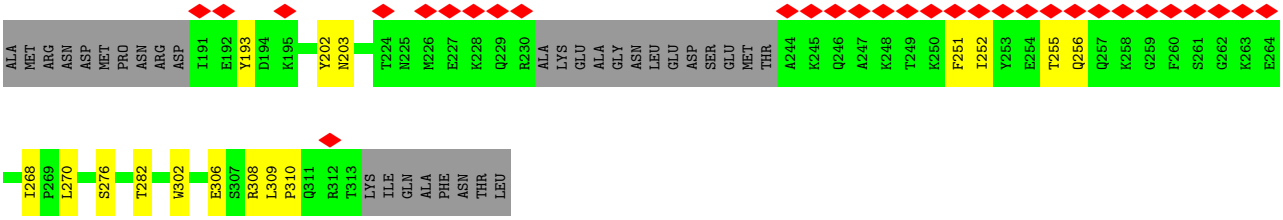
Chain D:



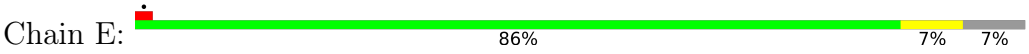
• Molecule 23: 37S ribosomal protein MRP1, mitochondrial

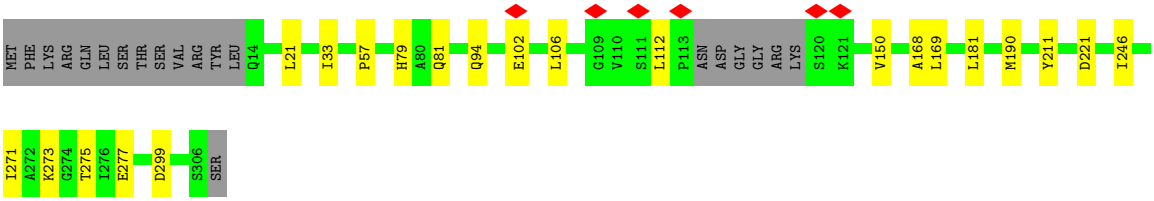
Chain 4:



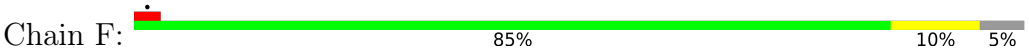


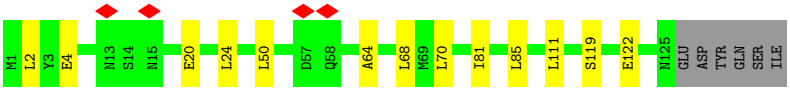
• Molecule 24: 37S ribosomal protein S5, mitochondrial



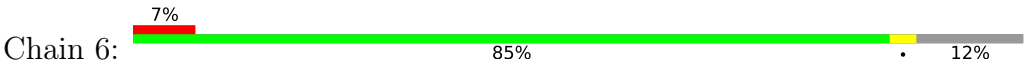


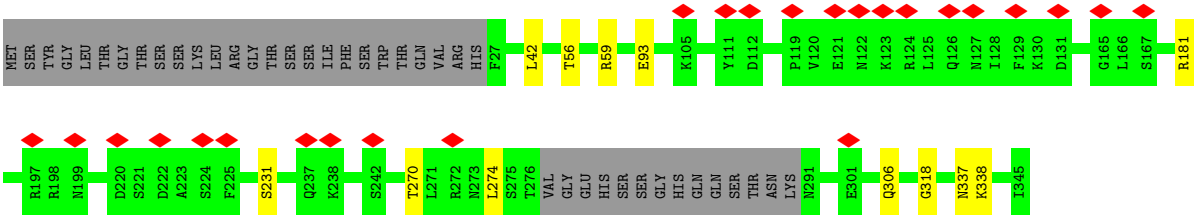
• Molecule 25: 37S ribosomal protein MRP17, mitochondrial



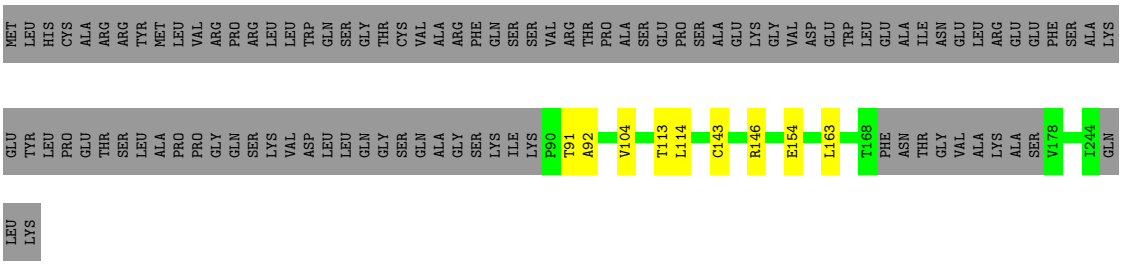


• Molecule 26: 37S ribosomal protein S35, mitochondrial



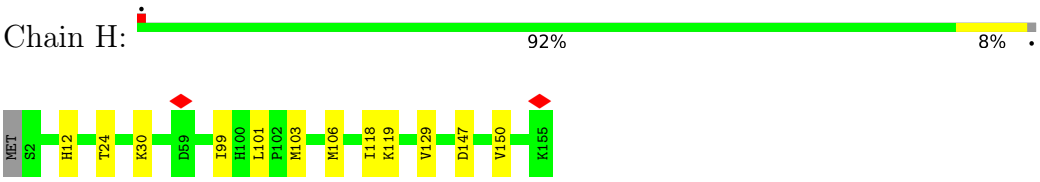


• Molecule 27: 37S ribosomal protein S7, mitochondrial



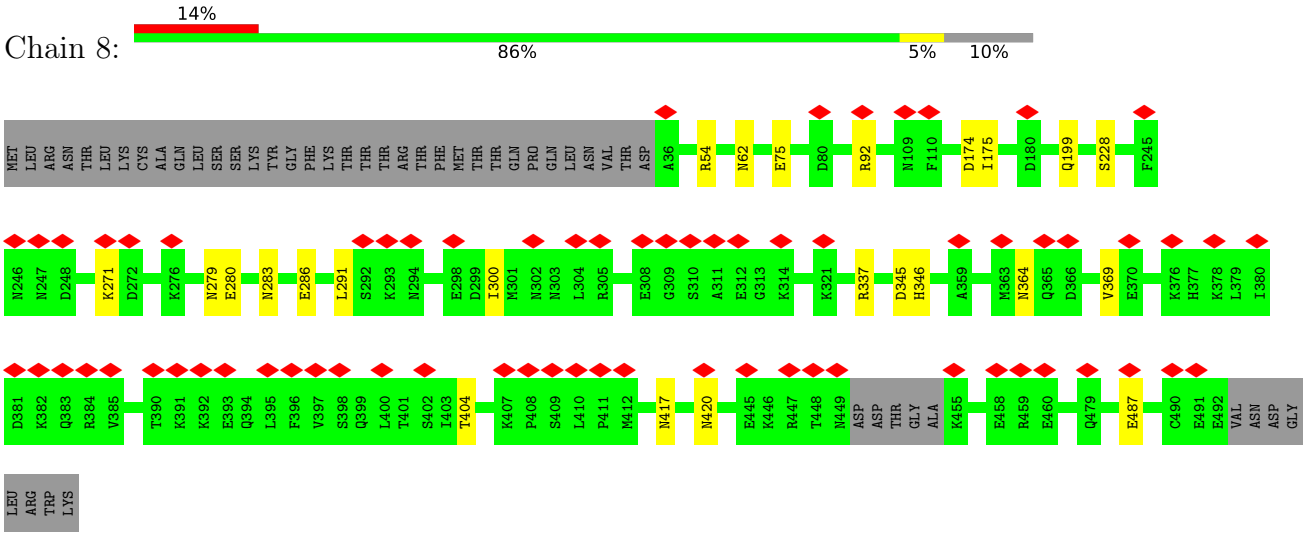
• Molecule 28: 37S ribosomal protein S8, mitochondrial

Chain H:



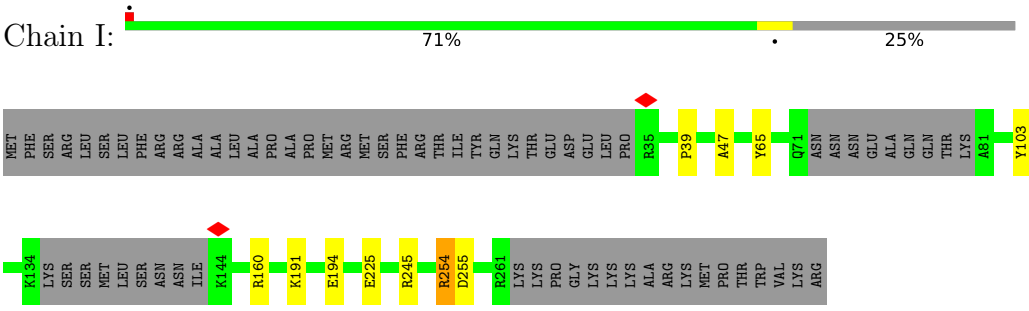
• Molecule 29: 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial

Chain 8:



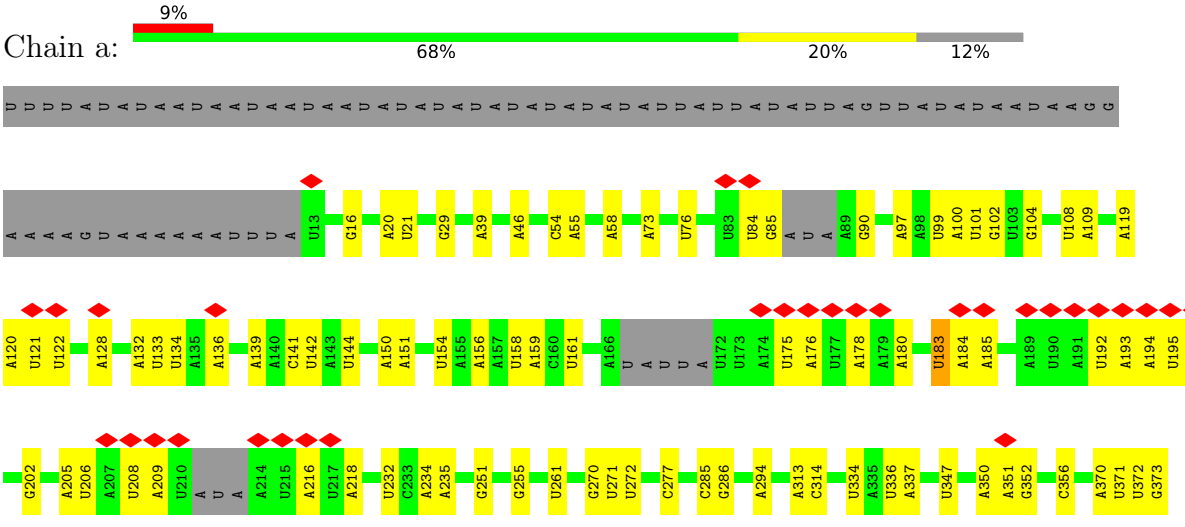
• Molecule 30: 37S ribosomal protein S9, mitochondrial

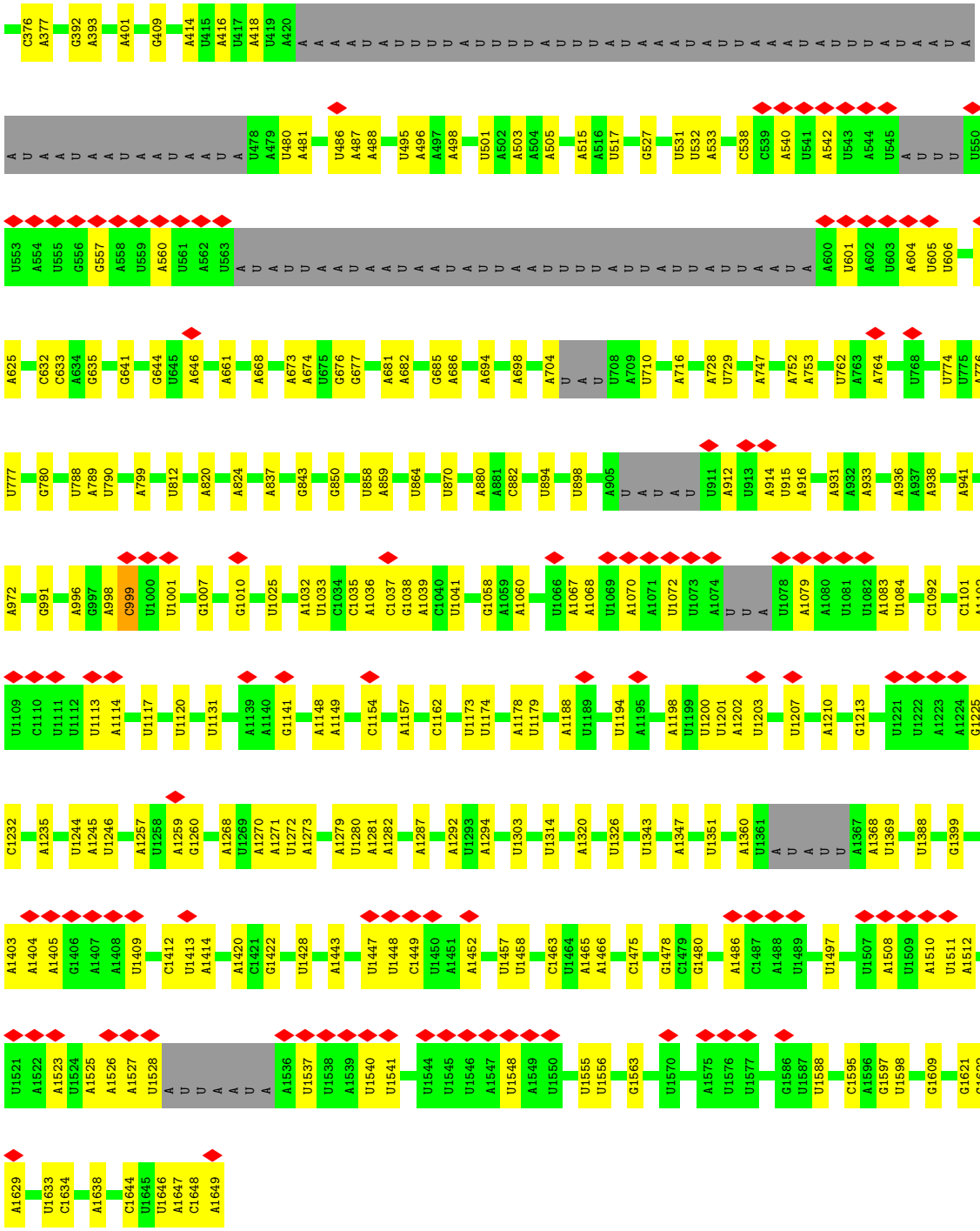
Chain I:



• Molecule 31: 15S ribosomal RNA

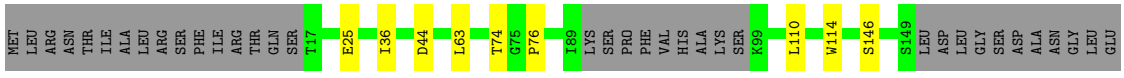
Chain a:

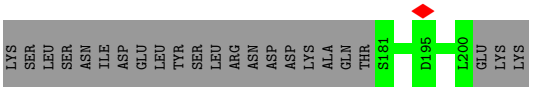




• Molecule 32: 37S ribosomal protein S10, mitochondrial

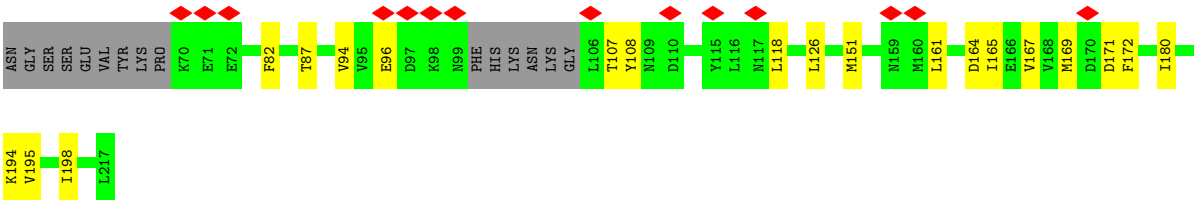
Chain J:





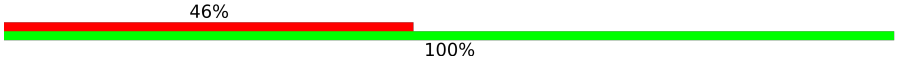
• Molecule 33: 37S ribosomal protein S18, mitochondrial

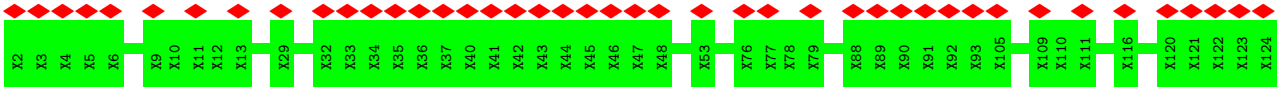
Chain K:



• Molecule 34: unknown protein sequence

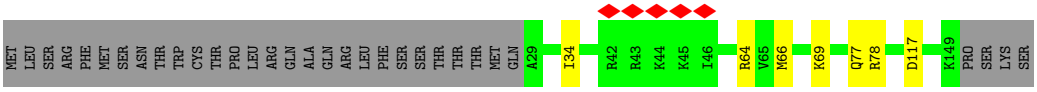
Chain c:





• Molecule 35: 37S ribosomal protein S12, mitochondrial

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	381285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61.73	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	39.186	Depositor
Minimum map value	-15.756	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.970	Depositor
Recommended contour level	3.46	Depositor
Map size (Å)	422.80002, 422.80002, 422.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, SF4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.30	0/3699	0.56	0/4979
2	5	0.27	0/2249	0.52	0/3040
3	C	0.32	0/2044	0.47	0/2740
4	M	0.28	0/655	0.48	0/874
5	N	0.30	0/940	0.58	0/1256
6	O	0.28	0/1749	0.55	0/2338
7	P	0.29	0/934	0.60	0/1260
8	Q	0.28	0/1694	0.57	0/2252
9	R	0.28	0/749	0.58	0/998
10	S	0.28	0/610	0.56	0/824
11	T	0.31	0/771	0.58	0/1019
12	U	0.30	0/1950	0.50	0/2636
13	V	0.28	0/1907	0.53	0/2549
14	W	0.32	0/3239	0.50	0/4379
15	X	0.32	0/788	0.52	0/1052
16	Y	0.31	0/2263	0.53	0/3053
17	Z	0.27	0/674	0.51	0/908
18	A	0.30	0/1621	0.53	0/2186
19	B	0.32	0/2128	0.55	0/2892
20	2	0.26	0/852	0.47	0/1142
21	3	0.30	0/2002	0.47	0/2721
22	D	0.30	0/2790	0.51	0/3758
23	4	0.27	0/2228	0.51	0/3009
24	E	0.32	0/2351	0.55	0/3169
25	F	0.29	0/1014	0.58	0/1358
26	6	0.30	0/2547	0.53	0/3438
27	G	0.29	0/1189	0.52	0/1607
28	H	0.30	0/1232	0.53	0/1660
29	8	0.28	0/3646	0.51	0/4935
30	I	0.30	0/1707	0.55	0/2298
31	a	0.47	0/35818	0.81	8/55721 (0.0%)
32	J	0.35	0/1216	0.54	0/1646

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	K	0.27	0/1136	0.53	0/1515
35	L	0.29	0/940	0.63	0/1261
All	All	0.38	0/91332	0.66	8/130473 (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
6	O	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	183	U	C2-N1-C1'	8.09	127.41	117.70
31	a	999	C	C6-N1-C2	-5.91	117.94	120.30
31	a	183	U	N1-C2-O2	5.89	126.92	122.80
31	a	183	U	N3-C2-O2	-5.80	118.14	122.20
31	a	392	G	C8-N9-C4	-5.65	104.14	106.40
31	a	1399	G	O4'-C1'-N9	5.56	112.65	108.20
31	a	183	U	C6-N1-C1'	-5.31	113.76	121.20
31	a	999	C	N3-C2-O2	-5.07	118.35	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	O	78	ARG	Sidechain

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	3626	0	3671	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5	2199	0	2246	18	0
3	C	2018	0	2041	13	0
4	M	645	0	691	0	0
5	N	923	0	974	2	0
6	O	1727	0	1770	12	0
7	P	919	0	982	10	0
8	Q	1683	0	1769	10	0
9	R	738	0	771	7	0
10	S	595	0	618	1	0
11	T	760	0	791	5	0
12	U	1907	0	1898	10	0
13	V	1879	0	1984	24	0
14	W	3174	0	3270	8	0
15	X	774	0	823	2	0
16	Y	2208	0	2177	9	0
17	Z	660	0	684	1	0
18	A	1585	0	1618	15	0
19	B	2085	0	2094	14	0
20	2	833	0	839	5	0
21	3	1953	0	1913	8	0
22	D	2713	0	2775	10	0
23	4	2182	0	2172	19	0
24	E	2297	0	2311	15	0
25	F	1002	0	1086	7	0
26	6	2488	0	2520	9	0
27	G	1168	0	1211	6	0
28	H	1213	0	1277	8	0
29	8	3573	0	3576	13	0
30	I	1676	0	1732	8	0
31	a	31987	0	16047	0	0
32	J	1186	0	1193	7	0
33	K	1121	0	1172	13	0
34	c	470	0	102	0	0
35	L	926	0	980	4	0
36	0	8	0	0	0	0
37	W	31	0	12	0	0
38	B	1	0	0	0	0
38	L	1	0	0	0	0
38	W	1	0	0	0	0
38	a	69	0	0	0	0
39	W	3	0	0	0	0
All	All	87007	0	71790	290	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 (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:324:ARG:NH2	1:0:377:ARG:O	2.09	0.84
25:F:119:SER:OG	25:F:122:GLU:OE1	1.97	0.79
1:0:70:GLN:OE1	1:0:491:GLN:NE2	2.16	0.78
30:I:254:ARG:NH1	30:I:255:ASP:O	2.18	0.77
6:O:161:ARG:HD2	6:O:171:THR:HG22	1.65	0.77
12:U:193:GLU:OE2	21:3:170:ASN:ND2	2.18	0.77
6:O:106:GLU:OE2	13:V:203:TYR:OH	2.02	0.76
16:Y:91:LEU:HD22	16:Y:101:VAL:HG13	1.69	0.75
6:O:83:LEU:HD11	6:O:156:ALA:HB2	1.67	0.74
22:D:442:GLU:OE2	26:6:181:ARG:NE	2.20	0.74
24:E:150:VAL:HG12	24:E:169:LEU:HB3	1.68	0.74
29:8:92:ARG:NH2	29:8:228:SER:O	2.21	0.73
3:C:45:MET:HG2	16:Y:316:LEU:HD11	1.70	0.73
27:G:143:CYS:O	27:G:146:ARG:NH1	2.22	0.72
1:0:96:HIS:NE2	1:0:129:ASP:OD2	2.22	0.72
1:0:72:GLN:O	1:0:152:LYS:NZ	2.21	0.72
1:0:161:PRO:O	1:0:186:TYR:OH	2.04	0.72
22:D:29:TYR:OH	26:6:93:GLU:OE2	2.06	0.72
8:Q:59:ARG:NH2	13:V:48:GLY:O	2.23	0.71
2:5:218:VAL:O	2:5:221:ARG:NH1	2.24	0.71
33:K:161:LEU:O	33:K:194:LYS:NZ	2.22	0.71
20:2:67:PHE:O	20:2:95:ARG:NH2	2.25	0.69
19:B:252:ARG:NH1	19:B:363:ASP:O	2.26	0.69
18:A:281:LEU:HD21	18:A:296:ARG:HE	1.58	0.68
24:E:246:ILE:HG12	24:E:275:THR:HG21	1.75	0.67
12:U:152:ARG:NH1	12:U:175:GLU:OE1	2.26	0.67
13:V:148:SER:OG	29:8:75:GLU:OE2	2.12	0.67
1:0:310:GLU:HB2	1:0:320:ILE:HD11	1.77	0.67
3:C:211:SER:OG	16:Y:136:GLU:OE1	2.04	0.67
6:O:101:PHE:CE2	6:O:105:ILE:HD11	2.30	0.66
7:P:45:PRO:O	7:P:63:LYS:NZ	2.29	0.66
3:C:298:TYR:OH	32:J:25:GLU:OE2	2.08	0.65
9:R:52:GLY:O	18:A:290:SER:OG	2.14	0.65
35:L:69:LYS:NZ	35:L:77:GLN:OE1	2.27	0.65
30:I:65:TYR:OH	30:I:124:GLU:OE1	2.09	0.65
1:0:106:THR:HG23	1:0:425:TRP:CZ2	2.33	0.64
24:E:271:ILE:O	24:E:275:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:K:169:MET:CE	33:K:180:ILE:HD11	2.28	0.63
1:0:420:LEU:O	1:0:425:TRP:NE1	2.30	0.63
33:K:126:LEU:HD12	33:K:151:MET:HE2	1.81	0.62
10:S:9:SER:N	10:S:15:GLY:O	2.33	0.62
13:V:104:ARG:O	13:V:108:ILE:HD12	1.99	0.62
33:K:94:VAL:HG12	33:K:118:LEU:HD23	1.82	0.61
5:N:3:ASN:OD1	5:N:4:PHE:N	2.34	0.61
2:5:324:LEU:HD12	2:5:325:LEU:HD12	1.82	0.61
1:0:496:ARG:NH2	1:0:542:GLY:O	2.33	0.61
1:0:462:ASP:O	1:0:466:LEU:HD23	2.00	0.61
23:4:270:LEU:HD21	23:4:309:LEU:HD23	1.83	0.61
1:0:140:TYR:OH	1:0:180:ASP:OD2	2.18	0.60
29:8:345:ASP:OD1	29:8:346:HIS:N	2.34	0.59
1:0:274:LEU:HD13	1:0:306:ILE:HD11	1.84	0.59
28:H:101:LEU:HD12	28:H:150:VAL:HG21	1.83	0.59
20:2:37:GLN:N	20:2:37:GLN:OE1	2.35	0.59
30:I:160:ARG:NE	30:I:225:GLU:OE1	2.35	0.59
13:V:210:ILE:HD11	13:V:219:LYS:HD2	1.84	0.59
19:B:180:PRO:O	19:B:230:LYS:NZ	2.35	0.58
2:5:89:GLN:O	2:5:91:ARG:NH1	2.35	0.58
29:8:337:ARG:NH1	29:8:404:THR:OG1	2.36	0.58
13:V:134:LYS:O	13:V:138:LEU:HD23	2.04	0.58
21:3:186:ASN:ND2	23:4:202:TYR:O	2.37	0.58
14:W:284:LYS:HG3	14:W:285:VAL:HG23	1.84	0.57
23:4:251:PHE:O	23:4:255:THR:HG22	2.05	0.57
33:K:167:VAL:HB	33:K:198:ILE:HG22	1.85	0.57
1:0:143:ILE:HG21	1:0:174:GLY:HA2	1.87	0.57
1:0:316:GLY:O	1:0:320:ILE:HD12	2.03	0.57
12:U:105:ARG:HG3	12:U:150:ILE:HD13	1.85	0.57
1:0:320:ILE:HD13	1:0:452:SER:HB3	1.86	0.57
24:E:211:TYR:OH	24:E:299:ASP:OD2	2.22	0.57
24:E:21:LEU:CD2	24:E:33:ILE:HG21	2.35	0.56
29:8:54:ARG:NH1	29:8:62:ASN:OD1	2.39	0.56
27:G:104:VAL:O	30:I:245:ARG:NH2	2.39	0.56
19:B:321:VAL:HG12	19:B:343:ILE:HB	1.88	0.56
26:6:337:ASN:OD1	26:6:338:LYS:N	2.39	0.56
1:0:320:ILE:HD13	1:0:452:SER:CB	2.36	0.55
28:H:99:ILE:HG21	28:H:118:ILE:HD11	1.87	0.55
22:D:416:ASP:H	22:D:423:THR:HG21	1.71	0.55
1:0:488:ASP:N	1:0:493:SER:OG	2.40	0.55
8:Q:200:CYS:O	8:Q:204:LEU:HD23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:106:MET:HE3	28:H:129:VAL:HG21	1.87	0.55
32:J:74:THR:HG23	32:J:114:TRP:HE1	1.72	0.55
29:8:417:ASN:O	29:8:420:ASN:ND2	2.39	0.55
23:4:268:ILE:HD13	23:4:310:PRO:HG3	1.87	0.55
1:0:369:VAL:HG11	1:0:373:CYS:HB2	1.89	0.54
23:4:135:ASN:ND2	23:4:306:GLU:OE1	2.36	0.54
18:A:281:LEU:HD11	18:A:296:ARG:HH21	1.72	0.54
23:4:110:ARG:NH2	23:4:282:THR:O	2.40	0.54
2:5:185:PHE:CE1	2:5:189:ILE:HD13	2.43	0.54
14:W:221:LEU:HD21	14:W:259:LEU:CD2	2.38	0.53
18:A:224:ARG:HH12	23:4:255:THR:HG23	1.73	0.53
12:U:147:GLU:OE2	12:U:151:GLN:NE2	2.40	0.53
1:0:490:THR:OG1	1:0:492:ASN:OD1	2.25	0.53
1:0:112:ILE:O	1:0:311:ARG:NH2	2.41	0.53
24:E:106:LEU:HD11	24:E:112:LEU:HD11	1.90	0.53
2:5:224:ASN:OD1	2:5:225:THR:N	2.41	0.53
2:5:266:GLU:O	2:5:270:LEU:HD13	2.08	0.53
12:U:47:ARG:NH1	19:B:211:TYR:O	2.41	0.53
2:5:324:LEU:CD1	2:5:325:LEU:HD12	2.39	0.52
32:J:74:THR:HG23	32:J:114:TRP:NE1	2.24	0.52
3:C:177:ASN:O	3:C:181:ASN:ND2	2.42	0.52
22:D:190:LYS:NZ	22:D:377:ALA:O	2.41	0.52
14:W:250:LYS:HG2	14:W:251:THR:HG23	1.90	0.52
23:4:128:ASN:OD1	23:4:302:TRP:NE1	2.41	0.52
19:B:315:VAL:HG21	30:I:39:PRO:HD3	1.91	0.52
24:E:79:HIS:O	24:E:81:GLN:NE2	2.39	0.52
21:3:148:LEU:O	23:4:203:ASN:ND2	2.43	0.52
22:D:80:ASP:OD1	26:6:231:SER:OG	2.24	0.52
27:G:113:THR:HG21	27:G:154:GLU:OE2	2.10	0.52
25:F:4:GLU:OE1	25:F:68:LEU:HD11	2.09	0.52
20:2:30:THR:O	20:2:95:ARG:NH1	2.44	0.51
33:K:165:ILE:HB	33:K:195:VAL:HG12	1.92	0.51
6:O:102:LEU:HA	6:O:105:ILE:HD12	1.92	0.51
19:B:135:SER:N	19:B:145:GLU:OE2	2.39	0.51
1:0:279:LEU:HD11	1:0:285:PHE:HA	1.92	0.51
8:Q:46:HIS:O	8:Q:74:ILE:HD12	2.10	0.51
16:Y:250:TYR:CE2	16:Y:254:ILE:HD11	2.46	0.51
21:3:34:PHE:HA	21:3:37:VAL:HG12	1.92	0.51
8:Q:56:ASP:OD1	8:Q:82:GLY:N	2.42	0.51
17:Z:55:VAL:HG13	27:G:163:LEU:HD11	1.92	0.51
23:4:19:LEU:HD23	23:4:41:TRP:CH2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:E:168:ALA:HB2	24:E:190:MET:HE3	1.93	0.51
18:A:217:SER:OG	18:A:220:GLY:O	2.21	0.50
14:W:147:ILE:HD12	14:W:343:LEU:HB2	1.92	0.50
19:B:315:VAL:HG13	19:B:315:VAL:O	2.12	0.50
28:H:106:MET:CE	28:H:129:VAL:HG21	2.41	0.50
24:E:169:LEU:HD11	24:E:181:LEU:HD22	1.93	0.50
1:0:84:VAL:HG13	1:0:208:ILE:HG23	1.94	0.50
6:O:133:ASP:OD2	13:V:215:GLN:NE2	2.44	0.50
8:Q:187:GLN:NE2	12:U:67:PRO:O	2.40	0.49
25:F:81:ILE:O	25:F:85:LEU:HD23	2.12	0.49
1:0:520:GLU:OE1	1:0:522:TRP:NE1	2.43	0.49
22:D:416:ASP:HB3	22:D:423:THR:HG21	1.93	0.49
23:4:133:THR:HG22	23:4:133:THR:O	2.12	0.49
13:V:217:LEU:HD23	13:V:221:ASP:OD1	2.12	0.49
25:F:2:LEU:HD11	25:F:70:LEU:HG	1.93	0.49
11:T:177:TYR:OH	18:A:75:THR:HG22	2.11	0.49
2:5:266:GLU:N	2:5:266:GLU:OE1	2.46	0.49
3:C:274:ASN:O	3:C:278:LEU:HD23	2.12	0.49
12:U:142:ARG:NH2	12:U:145:ASP:OD1	2.46	0.49
18:A:258:GLN:OE1	18:A:259:SER:OG	2.29	0.48
23:4:252:ILE:HG22	23:4:256:GLN:OE1	2.14	0.48
2:5:244:GLU:C	2:5:245:LEU:HD12	2.33	0.48
22:D:19:SER:O	22:D:24:ASN:ND2	2.44	0.48
24:E:94:GLN:N	24:E:94:GLN:OE1	2.46	0.48
1:0:396:ASP:O	1:0:398:LYS:NZ	2.46	0.48
13:V:136:LYS:O	13:V:140:LEU:HD23	2.14	0.48
18:A:281:LEU:HD11	18:A:296:ARG:NH2	2.29	0.48
33:K:96:GLU:HB2	33:K:118:LEU:HD21	1.96	0.48
9:R:104:THR:HG22	9:R:105:SER:N	2.29	0.47
33:K:107:THR:HG22	33:K:108:TYR:N	2.29	0.47
8:Q:159:GLU:N	8:Q:159:GLU:OE1	2.46	0.47
6:O:148:GLU:OE1	6:O:150:LYS:NZ	2.40	0.47
23:4:308:ARG:O	23:4:310:PRO:HD3	2.14	0.47
24:E:21:LEU:HD21	24:E:33:ILE:HG21	1.97	0.47
25:F:20:GLU:O	25:F:24:LEU:HD23	2.14	0.47
33:K:164:ASP:OD1	33:K:164:ASP:N	2.43	0.47
1:0:341:PRO:O	1:0:473:ARG:NH1	2.38	0.47
16:Y:91:LEU:HD23	16:Y:104:ILE:HD11	1.97	0.47
28:H:12:HIS:HE2	28:H:24:THR:HG1	1.60	0.47
29:8:279:ASN:ND2	29:8:487:GLU:OE1	2.48	0.47
1:0:506:GLY:HA2	1:0:526:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:129:ASP:OD1	29:8:271:LYS:NZ	2.48	0.47
13:V:231:PHE:CE2	25:F:111:LEU:HD22	2.50	0.47
20:2:33:LYS:O	20:2:94:TYR:OH	2.31	0.47
22:D:133:ASN:N	22:D:149:MET:O	2.40	0.47
22:D:416:ASP:N	22:D:423:THR:HG21	2.30	0.47
3:C:278:LEU:HD21	3:C:304:ASN:HB3	1.97	0.46
21:3:144:GLU:OE1	21:3:241:SER:OG	2.33	0.46
6:O:134:ARG:HG2	13:V:206:ALA:HB3	1.98	0.46
12:U:149:VAL:HG22	12:U:176:PHE:HB2	1.97	0.46
23:4:80:ILE:HD12	23:4:80:ILE:H	1.81	0.46
19:B:249:LEU:HD23	19:B:322:VAL:HG12	1.98	0.46
26:6:56:THR:HG22	26:6:59:ARG:NH2	2.31	0.46
19:B:180:PRO:HA	19:B:183:ILE:HD12	1.97	0.45
19:B:257:ARG:NH1	19:B:261:GLU:OE2	2.45	0.45
33:K:169:MET:HE1	33:K:180:ILE:HD11	1.98	0.45
33:K:169:MET:HE3	33:K:180:ILE:HD11	1.98	0.45
7:P:117:MET:SD	7:P:119:THR:OG1	2.75	0.45
13:V:79:VAL:HG13	13:V:107:LEU:HD23	1.99	0.45
13:V:164:LEU:HD21	28:H:30:LYS:HA	1.99	0.45
14:W:276:ILE:HG13	14:W:323:LEU:HD11	1.99	0.45
28:H:103:MET:N	28:H:147:ASP:OD1	2.47	0.45
9:R:83:MET:HB2	9:R:117:LEU:HD21	1.99	0.45
14:W:151:GLU:OE2	14:W:437:ASN:ND2	2.47	0.45
14:W:247:THR:C	14:W:248:LEU:HD12	2.36	0.45
24:E:273:LYS:O	24:E:277:GLU:OE1	2.35	0.45
2:5:106:ILE:HG12	2:5:116:LEU:HD11	1.99	0.44
21:3:119:PHE:CE2	21:3:123:ILE:HD11	2.52	0.44
27:G:113:THR:HG23	27:G:114:LEU:N	2.32	0.44
13:V:33:ILE:HG22	13:V:37:LYS:HE2	1.99	0.44
14:W:450:ARG:NH1	30:I:194:GLU:OE2	2.49	0.44
19:B:152:ASN:OD1	19:B:156:ARG:NH2	2.50	0.44
2:5:146:LEU:HD11	2:5:163:LEU:HD22	1.99	0.44
3:C:121:LYS:NZ	15:X:72:GLU:OE2	2.46	0.44
5:N:39:LYS:NZ	15:X:38:ARG:O	2.50	0.44
7:P:60:VAL:HG11	26:6:306:GLN:HB2	2.00	0.44
13:V:53:VAL:O	13:V:61:ARG:NH2	2.45	0.44
18:A:224:ARG:NH2	23:4:255:THR:OG1	2.50	0.44
22:D:94:LEU:HD13	22:D:475:GLU:HG2	2.00	0.44
29:8:199:GLN:HG3	29:8:286:GLU:HA	1.99	0.44
2:5:118:ASP:O	2:5:122:GLU:OE1	2.35	0.44
1:0:274:LEU:HD21	1:0:296:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:119:THR:HG22	7:P:120:LEU:N	2.33	0.44
13:V:79:VAL:HG23	13:V:79:VAL:O	2.17	0.44
18:A:75:THR:HG23	18:A:77:PHE:CD1	2.53	0.44
23:4:173:ALA:HB1	23:4:193:TYR:HB2	1.98	0.44
11:T:171:ASP:OD1	11:T:175:LYS:NZ	2.40	0.44
12:U:101:GLU:O	12:U:105:ARG:N	2.50	0.44
26:6:42:LEU:HD21	26:6:56:THR:HG21	1.99	0.44
3:C:82:ASN:OD1	24:E:57:PRO:HG3	2.18	0.43
18:A:198:THR:O	18:A:198:THR:HG22	2.18	0.43
33:K:171:ASP:OD1	33:K:172:PHE:N	2.49	0.43
11:T:89:ALA:O	11:T:93:VAL:HG13	2.17	0.43
1:0:129:ASP:OD1	1:0:204:ARG:NE	2.50	0.43
1:0:305:HIS:ND1	1:0:457:GLU:HG2	2.33	0.43
2:5:236:GLY:O	2:5:240:GLY:N	2.47	0.43
13:V:72:ASP:OD2	13:V:112:ARG:NH2	2.51	0.43
19:B:322:VAL:HG22	19:B:344:ALA:HB2	2.01	0.43
7:P:39:VAL:HG11	26:6:318:GLY:HA3	2.01	0.43
23:4:268:ILE:HG21	23:4:310:PRO:HG3	2.01	0.43
23:4:166:ASP:OD2	23:4:276:SER:OG	2.31	0.43
1:0:449:LEU:HD23	1:0:449:LEU:H	1.84	0.43
29:8:364:ASN:ND2	29:8:369:VAL:O	2.51	0.43
18:A:222:ILE:HD12	23:4:256:GLN:NE2	2.34	0.43
24:E:221:ASP:OD2	28:H:119:LYS:NZ	2.52	0.43
1:0:143:ILE:HG22	1:0:147:LEU:HD12	2.01	0.43
6:O:78:ARG:NH1	8:Q:103:LYS:HB2	2.34	0.43
19:B:276:ILE:HD11	30:I:47:ALA:HB2	2.01	0.43
13:V:50:ALA:O	13:V:61:ARG:NH2	2.52	0.42
3:C:41:MET:HE1	16:Y:312:VAL:HA	2.00	0.42
18:A:245:ALA:HB2	18:A:254:VAL:HG21	2.02	0.42
21:3:20:LEU:HD11	21:3:97:LEU:HD22	2.00	0.42
26:6:270:THR:O	26:6:274:LEU:HD13	2.19	0.42
6:O:246:ASN:O	6:O:248:ASP:N	2.52	0.42
13:V:114:GLU:OE2	13:V:117:ARG:NH2	2.52	0.42
29:8:174:ASP:OD2	29:8:175:ILE:HG23	2.19	0.42
33:K:82:PHE:HD1	33:K:87:THR:HG1	1.63	0.42
1:0:506:GLY:CA	1:0:526:ARG:HE	2.32	0.42
27:G:91:THR:HG22	27:G:92:ALA:N	2.35	0.42
9:R:55:TYR:CZ	18:A:246:ALA:HB1	2.54	0.42
32:J:63:LEU:HD11	32:J:76:PRO:HD3	2.01	0.42
11:T:121:ASN:O	11:T:121:ASN:ND2	2.51	0.42
19:B:332:LEU:HD22	19:B:355:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:279:LEU:HD13	1:0:289:VAL:HG23	2.02	0.42
2:5:315:TYR:O	2:5:319:LEU:HD23	2.19	0.42
30:I:103:TYR:CE2	30:I:107:LEU:HD11	2.54	0.42
1:0:306:ILE:HG22	1:0:456:PHE:HB2	2.02	0.42
7:P:2:THR:HG22	7:P:3:CYS:N	2.34	0.42
13:V:79:VAL:CG1	13:V:107:LEU:HD23	2.49	0.42
6:O:98:VAL:O	6:O:102:LEU:HD13	2.19	0.42
1:0:583:ALA:O	1:0:587:MET:HG2	2.19	0.41
29:8:280:GLU:HA	29:8:283:ASN:ND2	2.34	0.41
20:2:55:LEU:HD11	20:2:79:VAL:HG22	2.02	0.41
7:P:102:THR:O	7:P:106:SER:N	2.53	0.41
7:P:23:ILE:O	7:P:40:LEU:N	2.52	0.41
13:V:220:ILE:HD12	13:V:224:PHE:CD2	2.55	0.41
18:A:39:LYS:HZ1	21:3:59:GLU:HG2	1.85	0.41
32:J:44:ASP:HB2	32:J:110:LEU:HD11	2.02	0.41
35:L:64:ARG:NH1	35:L:66:MET:SD	2.93	0.41
2:5:263:SER:O	2:5:267:LEU:N	2.45	0.41
7:P:2:THR:HG22	7:P:3:CYS:H	1.85	0.41
9:R:65:ILE:HD12	9:R:65:ILE:H	1.85	0.41
13:V:67:ASN:OD1	13:V:67:ASN:O	2.38	0.41
29:8:291:LEU:HD11	29:8:300:ILE:HD11	2.03	0.41
8:Q:32:LYS:NZ	35:L:34:ILE:O	2.53	0.41
8:Q:74:ILE:HD12	8:Q:74:ILE:H	1.85	0.41
13:V:217:LEU:O	13:V:220:ILE:HG22	2.21	0.41
1:0:104:VAL:HG13	1:0:130:ALA:HB2	2.03	0.41
1:0:290:ASP:HA	1:0:326:ILE:HD12	2.03	0.41
2:5:151:PHE:CD2	2:5:322:LEU:HD21	2.55	0.41
3:C:125:LEU:HD13	3:C:175:MET:HB3	2.03	0.41
3:C:310:THR:HG22	3:C:311:ILE:N	2.36	0.41
9:R:61:SER:O	9:R:65:ILE:HD12	2.20	0.41
24:E:102:GLU:N	24:E:102:GLU:OE1	2.54	0.41
2:5:185:PHE:O	2:5:189:ILE:HD12	2.21	0.41
16:Y:250:TYR:CZ	16:Y:254:ILE:HD11	2.57	0.41
32:J:36:ILE:HD11	32:J:74:THR:HG22	2.02	0.41
35:L:78:ARG:NE	35:L:117:ASP:OD2	2.51	0.41
2:5:230:ILE:HD12	2:5:230:ILE:H	1.85	0.40
1:0:554:LYS:NZ	1:0:558:ASP:OD1	2.54	0.40
3:C:82:ASN:O	3:C:86:HIS:ND1	2.48	0.40
6:O:75:PHE:O	6:O:78:ARG:HG2	2.21	0.40
25:F:50:LEU:HD21	25:F:64:ALA:HB3	2.01	0.40
3:C:184:ASN:ND2	3:C:205:ILE:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:97:SER:O	16:Y:99:VAL:N	2.55	0.40
7:P:87:THR:HG22	7:P:91:ARG:HD3	2.03	0.40
8:Q:109:ASP:O	8:Q:113:VAL:HG23	2.22	0.40
9:R:99:LEU:HD13	9:R:129:ILE:HG12	2.04	0.40
11:T:90:ARG:O	11:T:93:VAL:HG22	2.22	0.40
16:Y:182:VAL:O	32:J:146:SER:N	2.50	0.40
13:V:204:HIS:O	13:V:207:ASN:ND2	2.55	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	437/628 (70%)	418 (96%)	19 (4%)	0	100	100
2	5	264/339 (78%)	250 (95%)	14 (5%)	0	100	100
3	C	228/398 (57%)	218 (96%)	10 (4%)	0	100	100
4	M	81/143 (57%)	79 (98%)	2 (2%)	0	100	100
5	N	110/115 (96%)	110 (100%)	0	0	100	100
6	O	206/286 (72%)	204 (99%)	2 (1%)	0	100	100
7	P	112/121 (93%)	111 (99%)	1 (1%)	0	100	100
8	Q	194/237 (82%)	189 (97%)	5 (3%)	0	100	100
9	R	87/138 (63%)	84 (97%)	3 (3%)	0	100	100
10	S	73/91 (80%)	71 (97%)	2 (3%)	0	100	100
11	T	90/177 (51%)	90 (100%)	0	0	100	100
12	U	231/264 (88%)	228 (99%)	3 (1%)	0	100	100
13	V	231/318 (73%)	223 (96%)	8 (4%)	0	100	100
14	W	393/450 (87%)	380 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	X	94/110 (86%)	93 (99%)	1 (1%)	0	100	100
16	Y	259/319 (81%)	253 (98%)	6 (2%)	0	100	100
17	Z	80/95 (84%)	80 (100%)	0	0	100	100
18	A	191/344 (56%)	186 (97%)	5 (3%)	0	100	100
19	B	264/394 (67%)	258 (98%)	6 (2%)	0	100	100
20	2	97/130 (75%)	92 (95%)	5 (5%)	0	100	100
21	3	240/266 (90%)	235 (98%)	5 (2%)	0	100	100
22	D	320/486 (66%)	312 (98%)	8 (2%)	0	100	100
23	4	265/321 (83%)	255 (96%)	10 (4%)	0	100	100
24	E	283/307 (92%)	277 (98%)	6 (2%)	0	100	100
25	F	123/131 (94%)	117 (95%)	6 (5%)	0	100	100
26	6	301/345 (87%)	297 (99%)	4 (1%)	0	100	100
27	G	142/247 (58%)	141 (99%)	1 (1%)	0	100	100
28	H	152/155 (98%)	149 (98%)	3 (2%)	0	100	100
29	8	448/500 (90%)	430 (96%)	18 (4%)	0	100	100
30	I	203/278 (73%)	201 (99%)	2 (1%)	0	100	100
32	J	138/203 (68%)	133 (96%)	5 (4%)	0	100	100
33	K	138/217 (64%)	135 (98%)	3 (2%)	0	100	100
35	L	119/153 (78%)	119 (100%)	0	0	100	100
All	All	6594/8706 (76%)	6418 (97%)	176 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	398/564 (71%)	398 (100%)	0	100	100
2	5	239/303 (79%)	239 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	237/385 (62%)	237 (100%)	0	100	100
4	M	69/121 (57%)	69 (100%)	0	100	100
5	N	100/103 (97%)	100 (100%)	0	100	100
6	O	183/250 (73%)	183 (100%)	0	100	100
7	P	101/106 (95%)	101 (100%)	0	100	100
8	Q	187/218 (86%)	187 (100%)	0	100	100
9	R	80/121 (66%)	80 (100%)	0	100	100
10	S	64/78 (82%)	64 (100%)	0	100	100
11	T	81/159 (51%)	80 (99%)	1 (1%)	71	87
12	U	208/236 (88%)	207 (100%)	1 (0%)	88	96
13	V	210/287 (73%)	210 (100%)	0	100	100
14	W	363/409 (89%)	363 (100%)	0	100	100
15	X	84/92 (91%)	84 (100%)	0	100	100
16	Y	242/289 (84%)	242 (100%)	0	100	100
17	Z	75/85 (88%)	75 (100%)	0	100	100
18	A	174/309 (56%)	174 (100%)	0	100	100
19	B	233/350 (67%)	233 (100%)	0	100	100
20	2	90/117 (77%)	90 (100%)	0	100	100
21	3	216/240 (90%)	216 (100%)	0	100	100
22	D	294/437 (67%)	294 (100%)	0	100	100
23	4	239/281 (85%)	239 (100%)	0	100	100
24	E	248/266 (93%)	248 (100%)	0	100	100
25	F	114/120 (95%)	114 (100%)	0	100	100
26	6	277/312 (89%)	277 (100%)	0	100	100
27	G	126/211 (60%)	126 (100%)	0	100	100
28	H	141/142 (99%)	141 (100%)	0	100	100
29	8	401/444 (90%)	401 (100%)	0	100	100
30	I	181/245 (74%)	179 (99%)	2 (1%)	73	88
32	J	130/183 (71%)	130 (100%)	0	100	100
33	K	122/192 (64%)	122 (100%)	0	100	100
35	L	100/131 (76%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6007/7786 (77%)	6003 (100%)	4 (0%)	93 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	T	121	ASN
12	U	103	ARG
30	I	191	LYS
30	I	254	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	70	GLN
1	0	119	HIS
1	0	139	ASN
1	0	276	HIS
1	0	391	HIS
1	0	491	GLN
1	0	507	HIS
2	5	141	HIS
12	U	4	GLN
13	V	60	HIS
13	V	204	HIS
14	W	106	HIS
14	W	449	HIS
16	Y	148	HIS
16	Y	217	HIS
16	Y	243	HIS
16	Y	246	GLN
16	Y	252	HIS
17	Z	46	HIS
20	2	92	HIS
24	E	198	HIS
25	F	61	HIS
29	8	224	HIS
29	8	259	ASN
32	J	199	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1494/1713 (87%)	343 (22%)	0

All (343) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	a	16	G
31	a	20	A
31	a	21	U
31	a	29	G
31	a	39	A
31	a	46	A
31	a	54	C
31	a	55	A
31	a	58	A
31	a	73	A
31	a	76	U
31	a	84	U
31	a	85	G
31	a	90	G
31	a	97	A
31	a	99	U
31	a	100	A
31	a	101	U
31	a	102	G
31	a	104	G
31	a	108	U
31	a	109	A
31	a	119	A
31	a	120	A
31	a	121	U
31	a	122	U
31	a	128	A
31	a	132	A
31	a	133	U
31	a	134	U
31	a	136	A
31	a	139	A
31	a	141	C
31	a	142	U
31	a	144	U
31	a	150	A
31	a	151	A
31	a	154	U

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Mol	Chain	Res	Type
31	a	156	A
31	a	158	U
31	a	159	A
31	a	161	U
31	a	175	U
31	a	176	A
31	a	178	A
31	a	180	A
31	a	183	U
31	a	184	A
31	a	185	A
31	a	192	U
31	a	193	A
31	a	194	A
31	a	195	U
31	a	196	A
31	a	197	A
31	a	202	G
31	a	205	A
31	a	206	U
31	a	208	U
31	a	209	A
31	a	216	A
31	a	218	A
31	a	232	U
31	a	234	A
31	a	235	A
31	a	251	G
31	a	255	G
31	a	261	U
31	a	270	G
31	a	271	U
31	a	272	U
31	a	277	C
31	a	285	C
31	a	286	G
31	a	294	A
31	a	313	A
31	a	314	C
31	a	334	U
31	a	336	U
31	a	337	A

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Mol	Chain	Res	Type
31	a	347	U
31	a	350	A
31	a	351	A
31	a	352	G
31	a	356	C
31	a	370	A
31	a	371	U
31	a	372	U
31	a	373	G
31	a	376	C
31	a	377	A
31	a	393	A
31	a	401	A
31	a	409	G
31	a	414	A
31	a	416	A
31	a	418	A
31	a	480	U
31	a	481	A
31	a	486	U
31	a	487	A
31	a	488	A
31	a	495	U
31	a	496	A
31	a	498	A
31	a	501	U
31	a	503	A
31	a	505	A
31	a	515	A
31	a	517	U
31	a	527	G
31	a	531	U
31	a	532	U
31	a	533	A
31	a	538	C
31	a	540	A
31	a	542	A
31	a	551	U
31	a	552	A
31	a	557	G
31	a	560	A
31	a	601	U

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Mol	Chain	Res	Type
31	a	604	A
31	a	605	U
31	a	606	U
31	a	611	U
31	a	612	A
31	a	613	G
31	a	624	U
31	a	625	A
31	a	632	C
31	a	633	C
31	a	635	G
31	a	641	G
31	a	644	G
31	a	646	A
31	a	661	A
31	a	668	A
31	a	673	A
31	a	674	A
31	a	676	G
31	a	677	G
31	a	681	A
31	a	682	A
31	a	685	G
31	a	686	A
31	a	694	A
31	a	698	A
31	a	704	A
31	a	710	U
31	a	716	A
31	a	728	A
31	a	729	U
31	a	747	A
31	a	752	A
31	a	753	A
31	a	762	U
31	a	764	A
31	a	774	U
31	a	776	A
31	a	777	U
31	a	780	G
31	a	788	U
31	a	789	A

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Mol	Chain	Res	Type
31	a	790	U
31	a	799	A
31	a	812	U
31	a	820	A
31	a	824	A
31	a	837	A
31	a	843	G
31	a	850	G
31	a	858	U
31	a	859	A
31	a	864	U
31	a	870	U
31	a	880	A
31	a	882	C
31	a	894	U
31	a	898	U
31	a	912	A
31	a	914	A
31	a	915	U
31	a	916	A
31	a	931	A
31	a	933	A
31	a	936	A
31	a	938	A
31	a	941	A
31	a	972	A
31	a	991	G
31	a	996	A
31	a	998	A
31	a	999	C
31	a	1001	U
31	a	1007	G
31	a	1010	G
31	a	1025	U
31	a	1032	A
31	a	1033	U
31	a	1035	C
31	a	1036	A
31	a	1037	C
31	a	1038	G
31	a	1039	A
31	a	1041	U

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Mol	Chain	Res	Type
31	a	1058	G
31	a	1060	A
31	a	1067	A
31	a	1068	A
31	a	1070	A
31	a	1072	U
31	a	1079	A
31	a	1083	A
31	a	1084	U
31	a	1092	C
31	a	1101	C
31	a	1102	A
31	a	1104	U
31	a	1105	G
31	a	1113	U
31	a	1114	A
31	a	1117	U
31	a	1120	U
31	a	1131	U
31	a	1141	G
31	a	1148	A
31	a	1149	A
31	a	1154	C
31	a	1157	A
31	a	1162	C
31	a	1173	U
31	a	1174	U
31	a	1178	A
31	a	1179	U
31	a	1188	A
31	a	1194	U
31	a	1198	A
31	a	1200	U
31	a	1201	U
31	a	1202	A
31	a	1203	U
31	a	1207	U
31	a	1210	A
31	a	1213	G
31	a	1225	G
31	a	1231	U
31	a	1232	C

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Mol	Chain	Res	Type
31	a	1235	A
31	a	1244	U
31	a	1245	A
31	a	1246	U
31	a	1257	A
31	a	1259	A
31	a	1260	G
31	a	1268	A
31	a	1270	A
31	a	1271	A
31	a	1272	U
31	a	1273	A
31	a	1279	A
31	a	1280	U
31	a	1281	A
31	a	1282	A
31	a	1287	A
31	a	1292	A
31	a	1294	A
31	a	1303	U
31	a	1314	U
31	a	1320	A
31	a	1326	U
31	a	1343	U
31	a	1347	A
31	a	1351	U
31	a	1360	A
31	a	1368	A
31	a	1369	U
31	a	1388	U
31	a	1403	A
31	a	1404	A
31	a	1405	A
31	a	1409	U
31	a	1412	C
31	a	1413	U
31	a	1414	A
31	a	1420	A
31	a	1422	G
31	a	1428	U
31	a	1443	A
31	a	1447	U

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Mol	Chain	Res	Type
31	a	1448	U
31	a	1449	C
31	a	1452	A
31	a	1457	U
31	a	1458	U
31	a	1463	C
31	a	1465	A
31	a	1466	A
31	a	1475	C
31	a	1478	G
31	a	1480	G
31	a	1486	A
31	a	1497	U
31	a	1508	A
31	a	1510	A
31	a	1511	U
31	a	1512	A
31	a	1516	U
31	a	1517	U
31	a	1520	U
31	a	1523	A
31	a	1525	A
31	a	1526	A
31	a	1527	A
31	a	1528	U
31	a	1537	U
31	a	1540	U
31	a	1541	U
31	a	1548	U
31	a	1555	U
31	a	1556	U
31	a	1563	G
31	a	1588	U
31	a	1595	C
31	a	1597	G
31	a	1598	U
31	a	1609	G
31	a	1621	G
31	a	1622	G
31	a	1624	U
31	a	1625	U
31	a	1626	A

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Mol	Chain	Res	Type
31	a	1627	U
31	a	1628	A
31	a	1629	A
31	a	1633	U
31	a	1634	C
31	a	1638	A
31	a	1644	C
31	a	1646	U
31	a	1647	A
31	a	1648	C
31	a	1649	A

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 74 ligands modelled in this entry, 72 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
37	ATP	W	501	38	26,33,33	0.70	0	31,52,52	1.06	1 (3%)
36	SF4	0	701	1	0,12,12	-	-	-		

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
37	ATP	W	501	38	-	4/18/38/38	0/3/3/3
36	SF4	0	701	1	-	-	0/6/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	501	ATP	C5-C6-N6	2.43	124.05	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

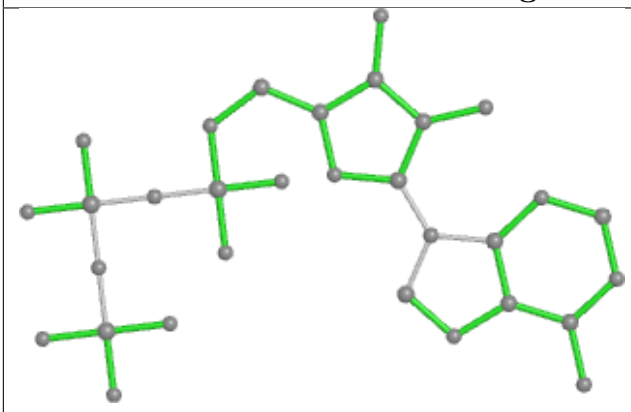
Mol	Chain	Res	Type	Atoms
37	W	501	ATP	O4'-C4'-C5'-O5'
37	W	501	ATP	C3'-C4'-C5'-O5'
37	W	501	ATP	PA-O3A-PB-O2B
37	W	501	ATP	PA-O3A-PB-O1B

There are no ring outliers.

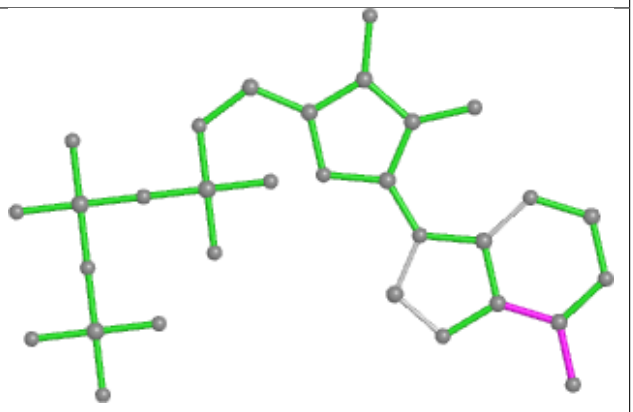
No monomer is involved in short contacts.

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

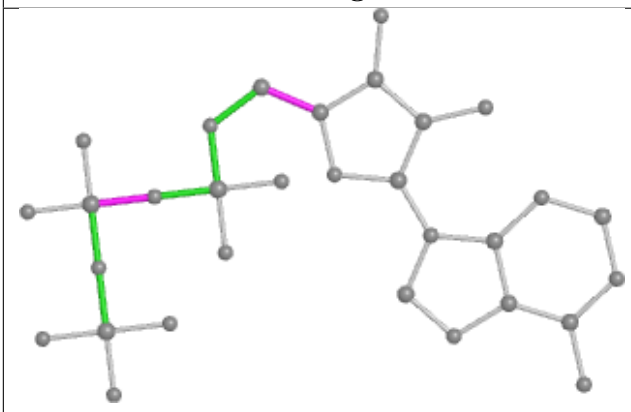
Ligand ATP W 501



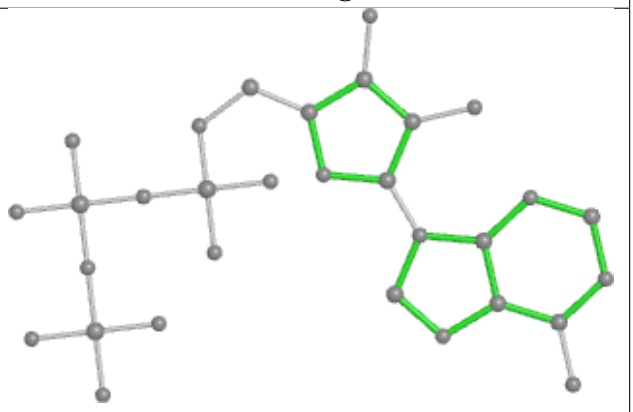
Bond lengths



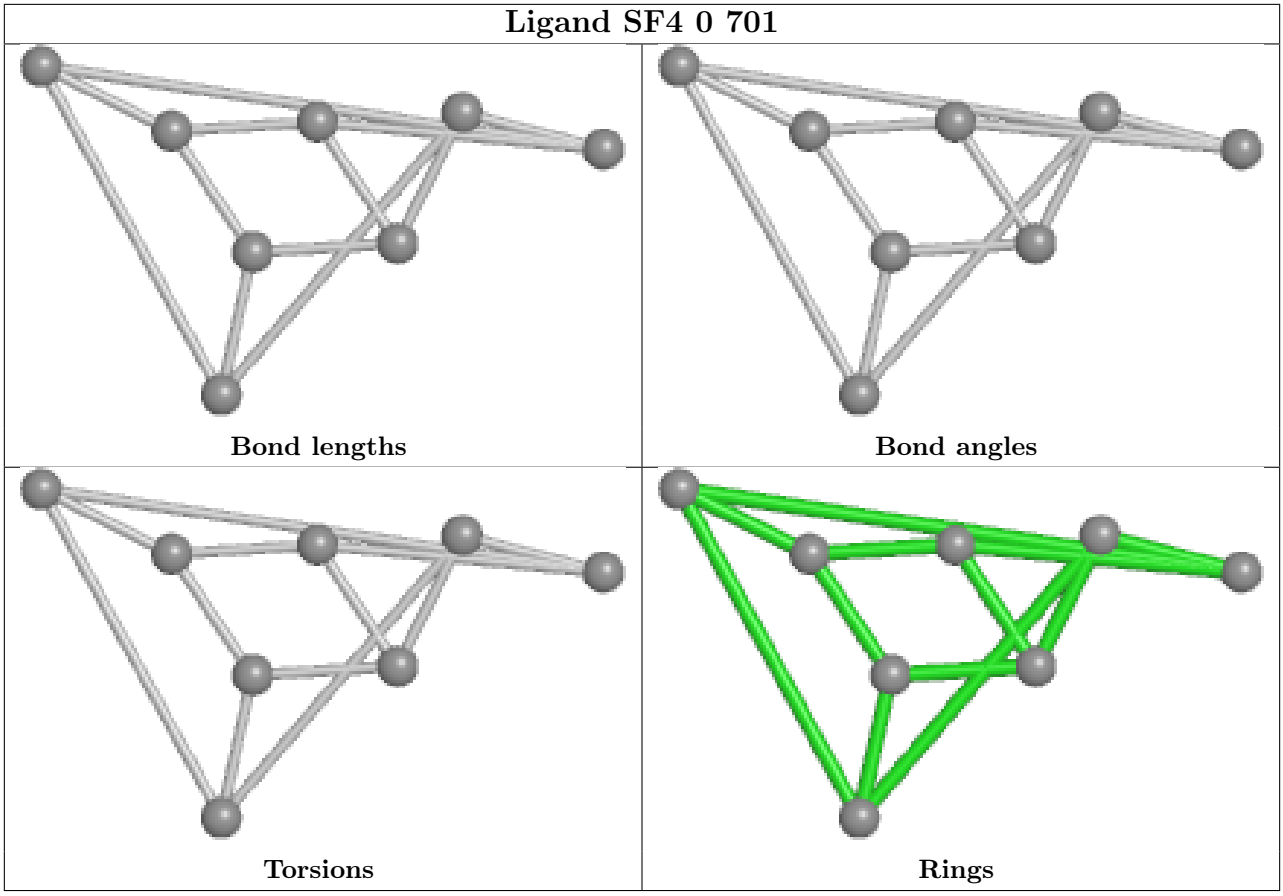
Bond angles



Torsions



Rings



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
34	c	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	59:UNK	C	76:UNK	N	23.59
1	c	93:UNK	C	105:UNK	N	20.74
1	c	37:UNK	C	40:UNK	N	10.59

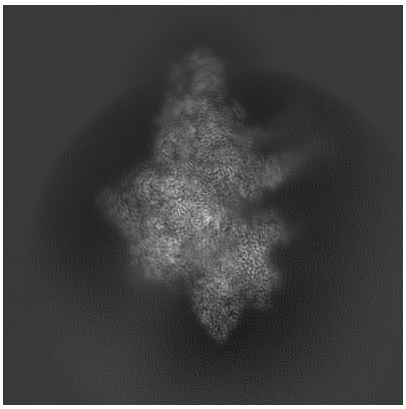
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27251. These allow visual inspection of the internal detail of the map and identification of artifacts.

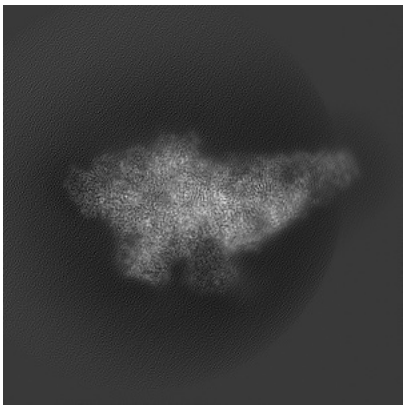
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

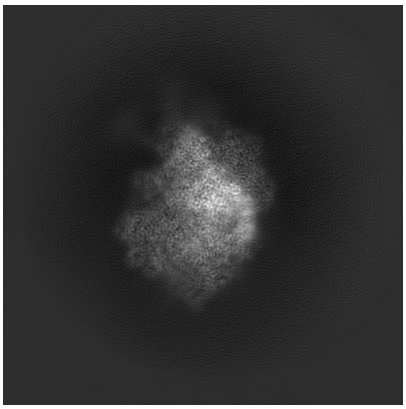
6.1.1 Primary map



X

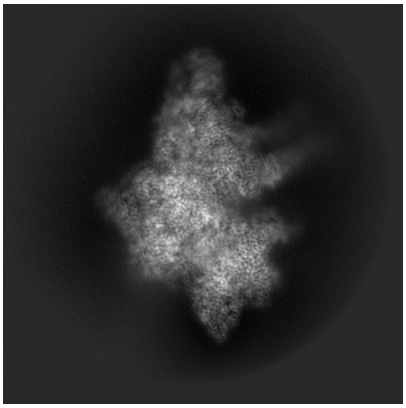


Y

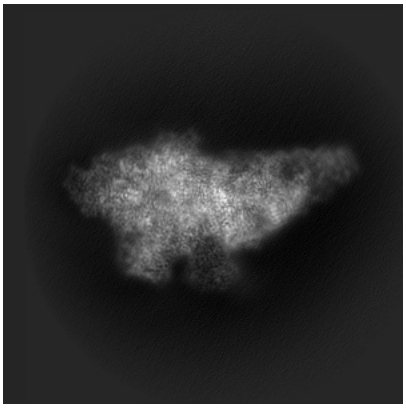


Z

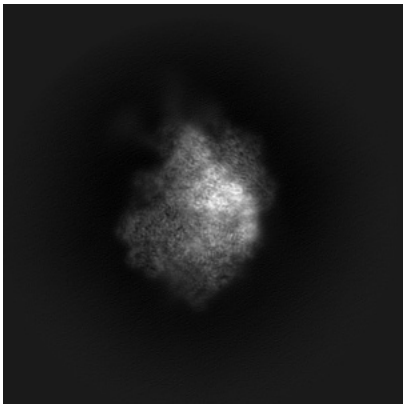
6.1.2 Raw map



X



Y

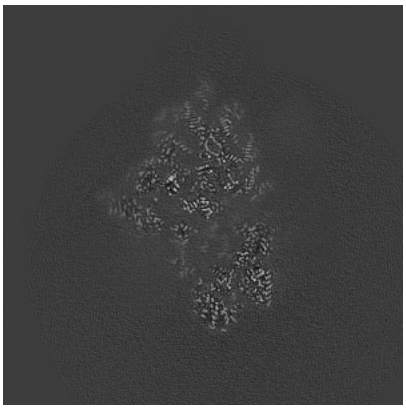


Z

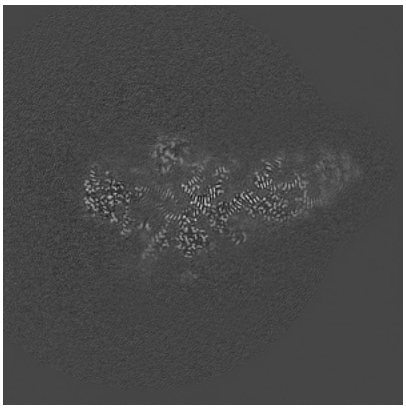
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

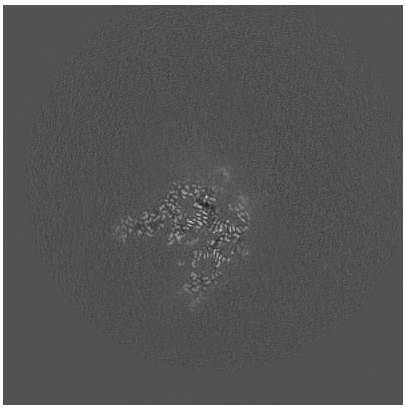
6.2.1 Primary map



X Index: 200

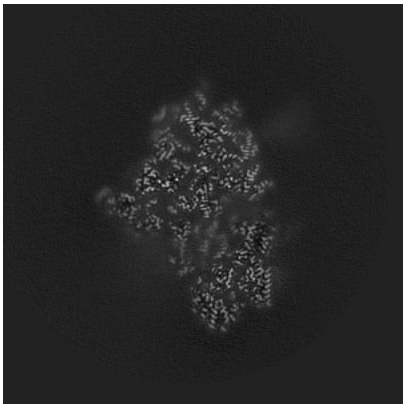


Y Index: 200

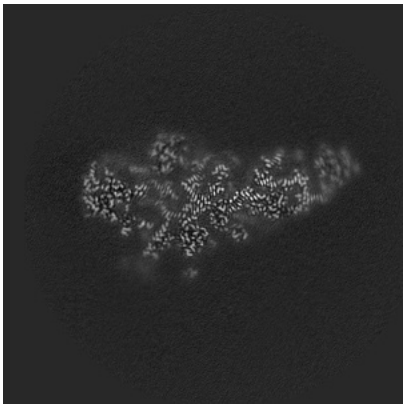


Z Index: 200

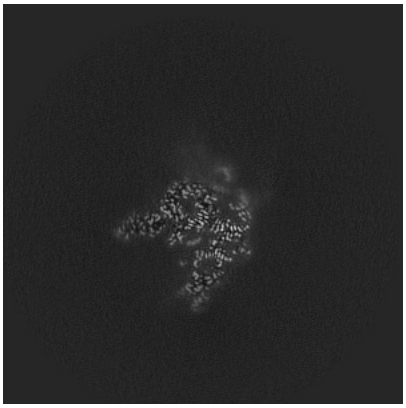
6.2.2 Raw map



X Index: 200



Y Index: 200

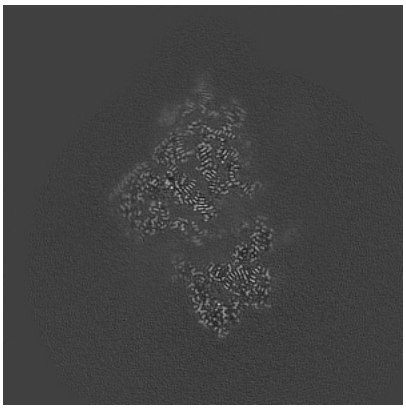


Z Index: 200

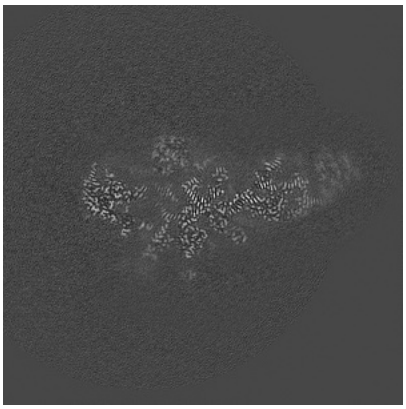
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

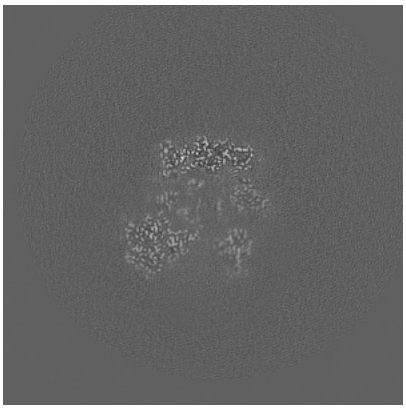
6.3.1 Primary map



X Index: 205

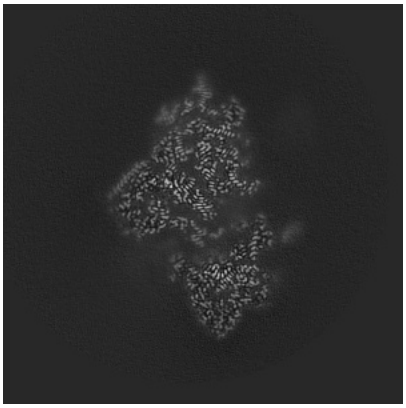


Y Index: 201

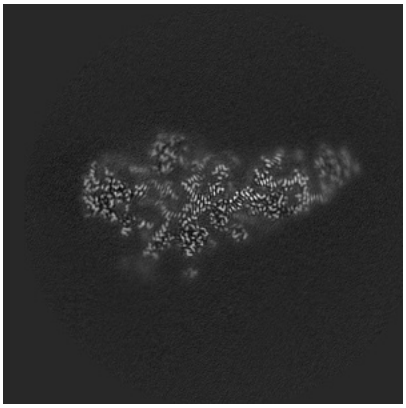


Z Index: 155

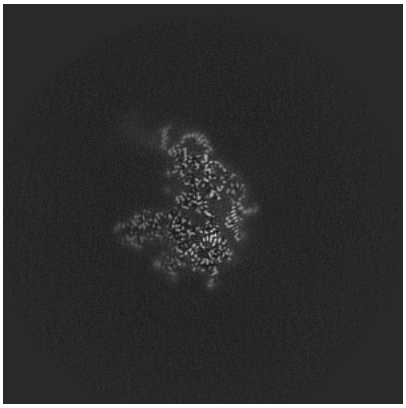
6.3.2 Raw map



X Index: 207



Y Index: 200



Z Index: 221

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

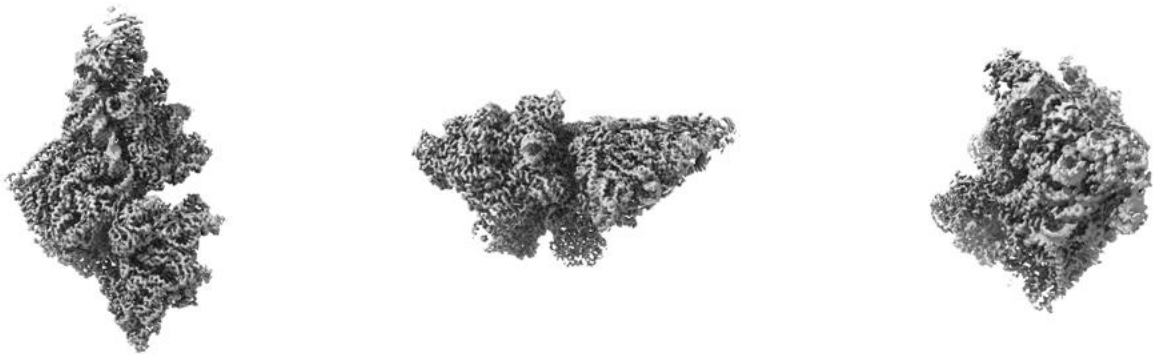
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

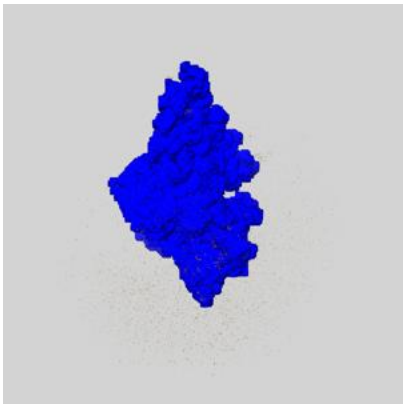
6.5 Mask visualisation

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

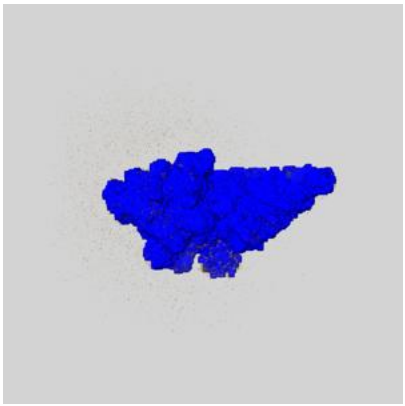
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

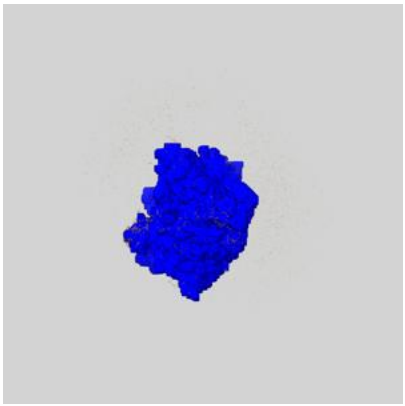
6.5.1 emd_27251_msk_1.map



X



Y

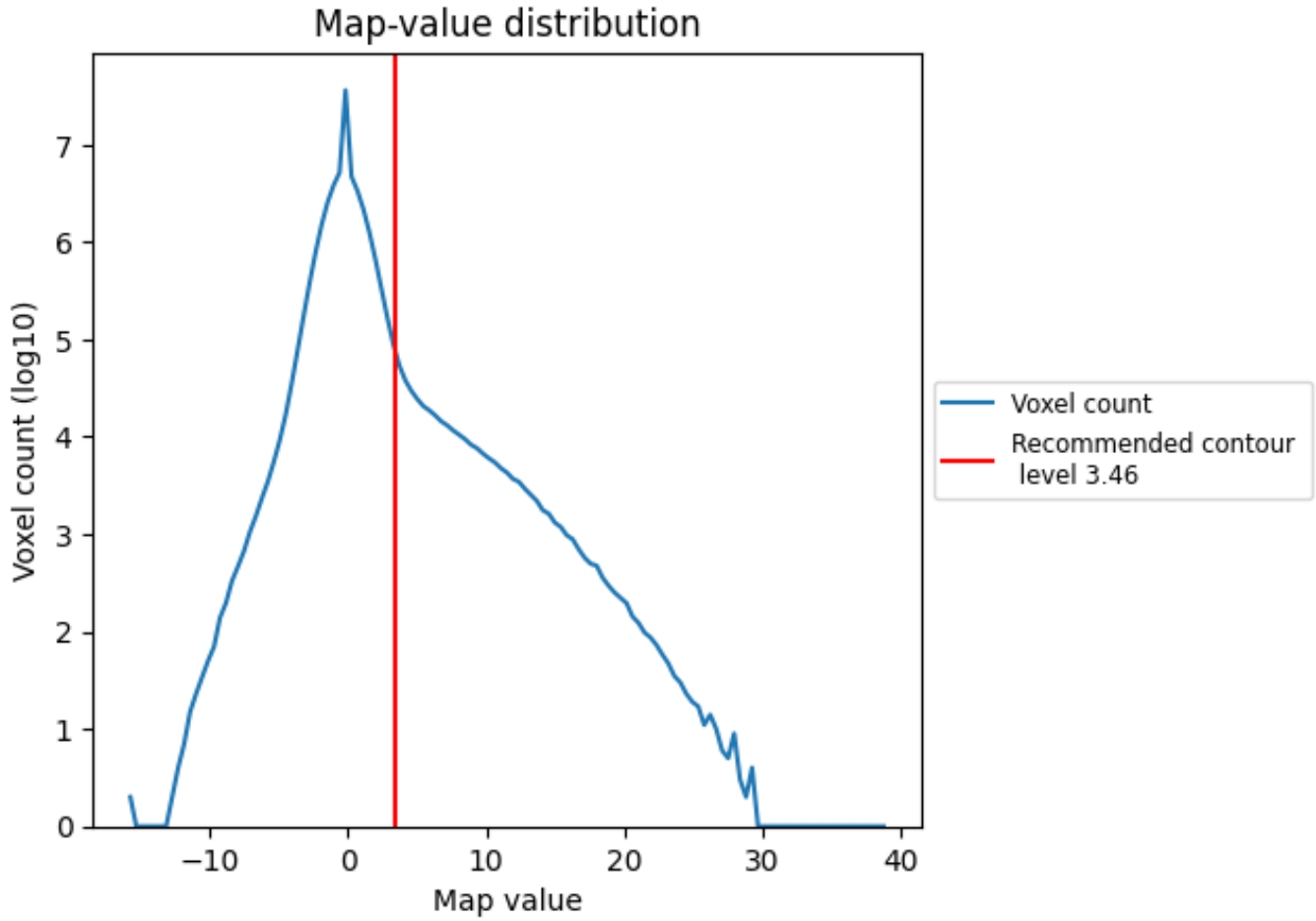


Z

7 Map analysis

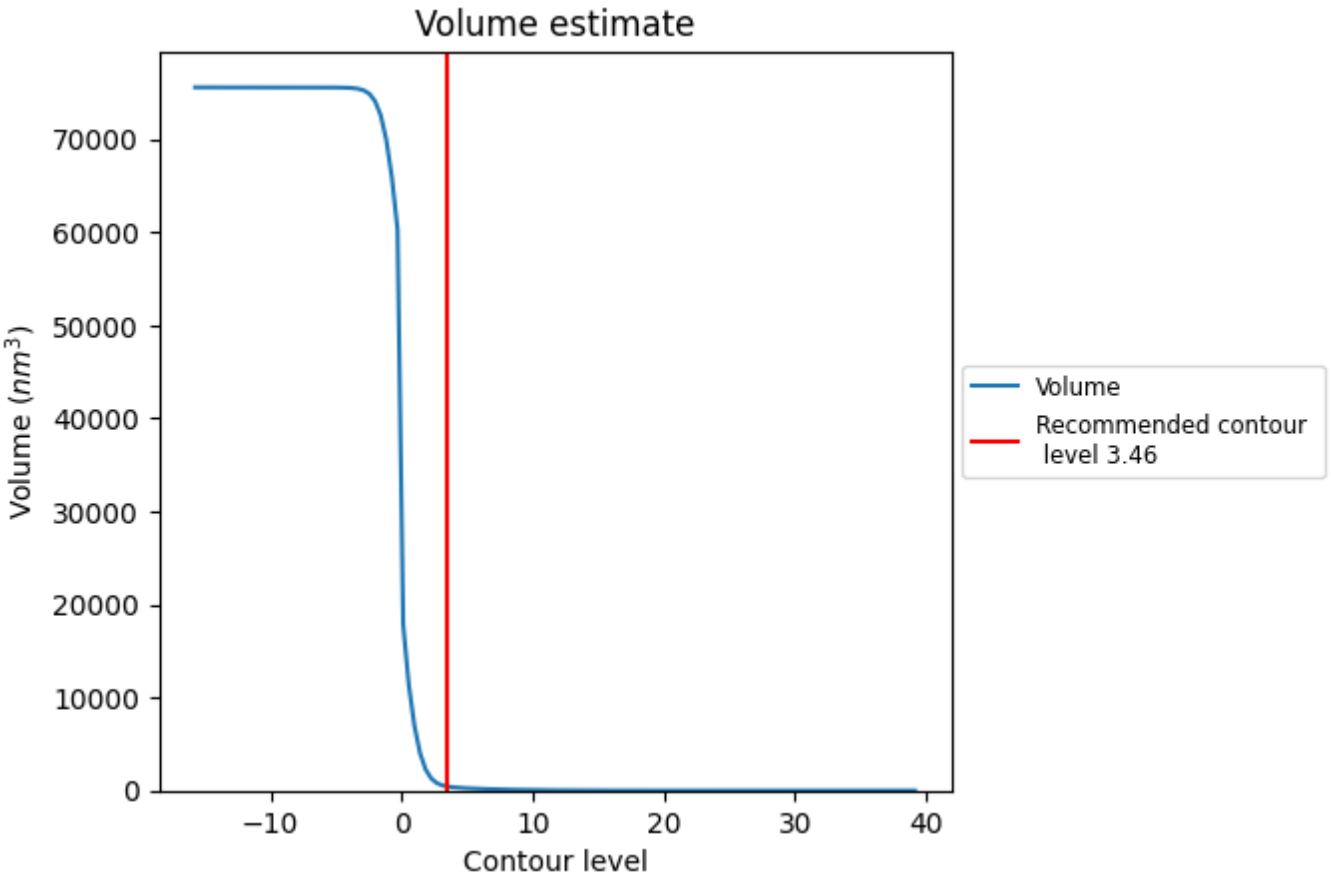
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

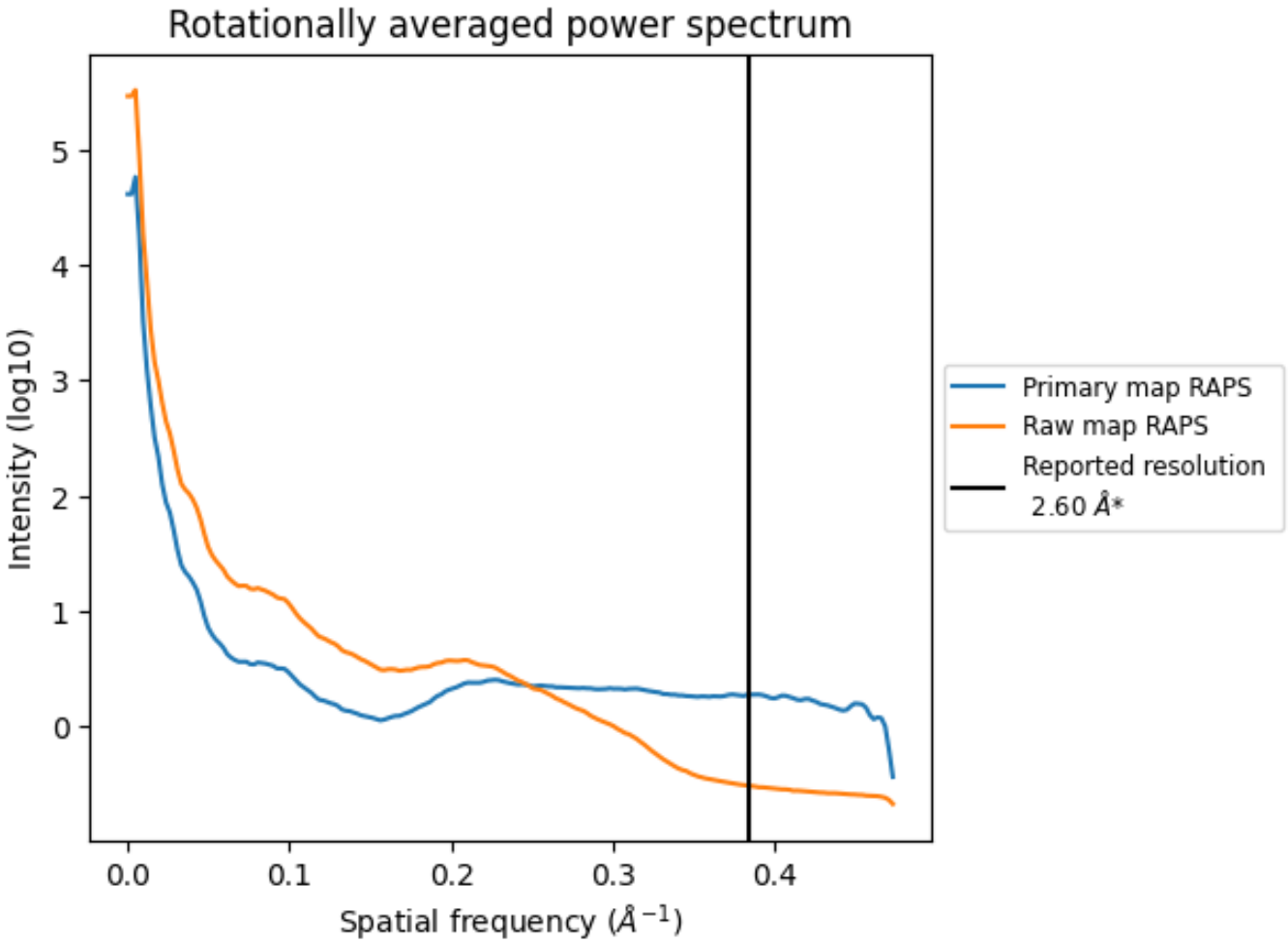
7.2 Volume estimate



The volume at the recommended contour level is 452 nm^3; this corresponds to an approximate mass of 408 kDa.

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

7.3 Rotationally averaged power spectrum (i)

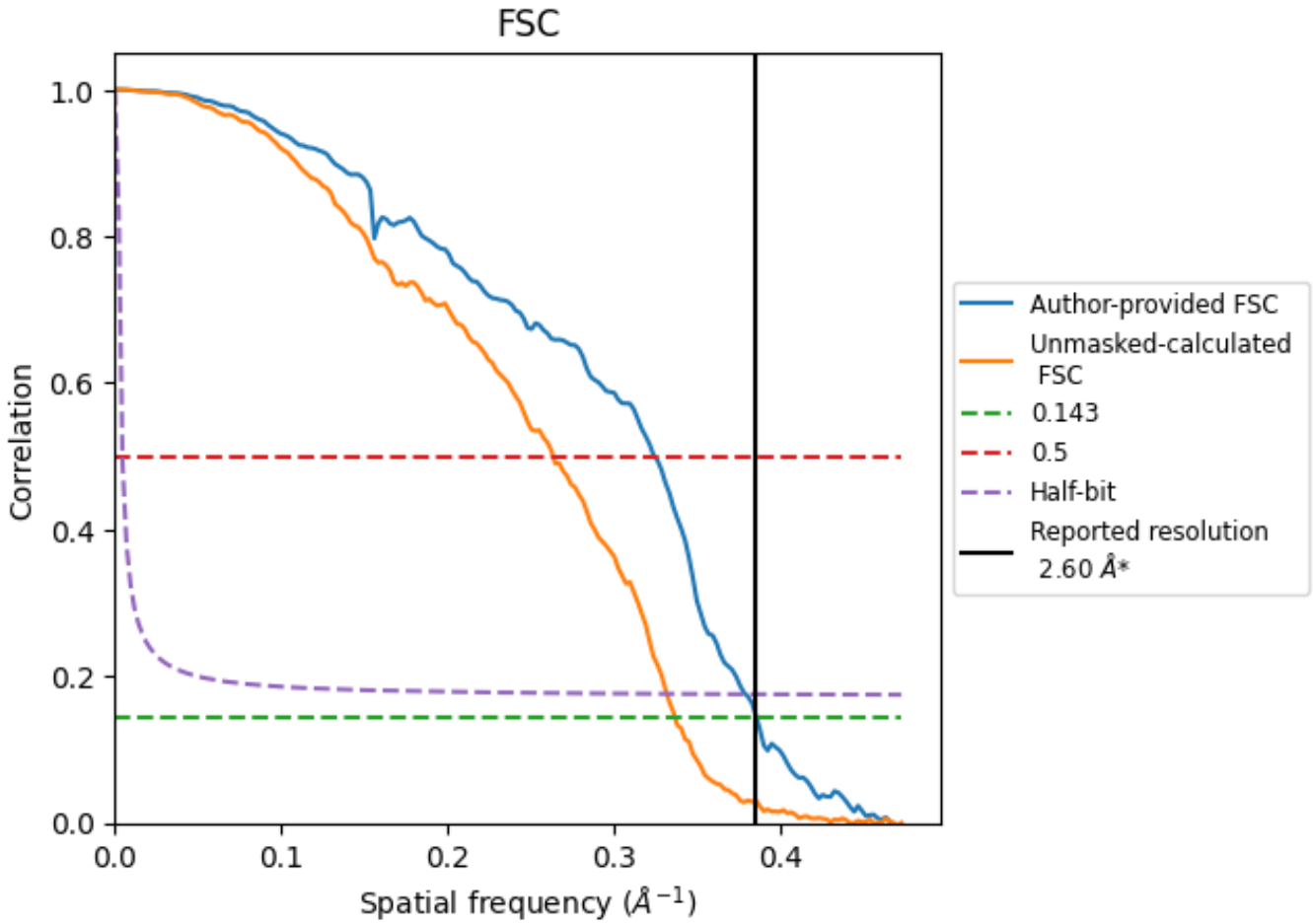


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

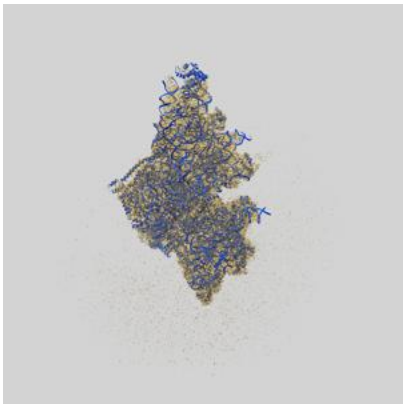
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	3.08	2.64
Unmasked-calculated*	2.97	3.79	3.01

*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 2.97 differs from the reported value 2.6 by more than 10 %

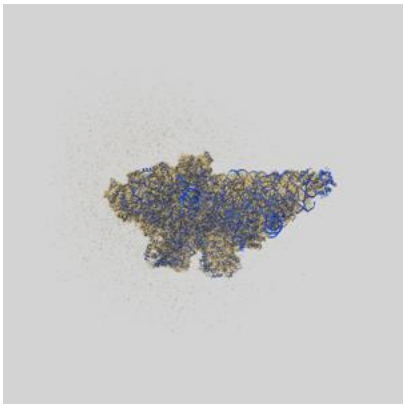
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27251 and PDB model 8D8L. Per-residue inclusion information can be found in section 3 on page 12.

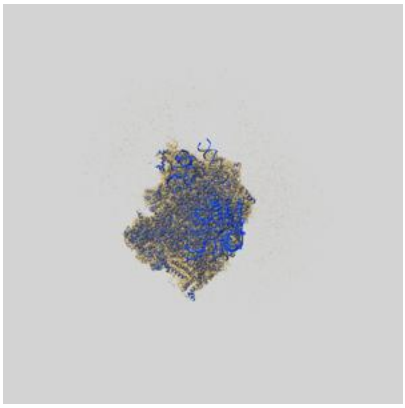
9.1 Map-model overlay



X



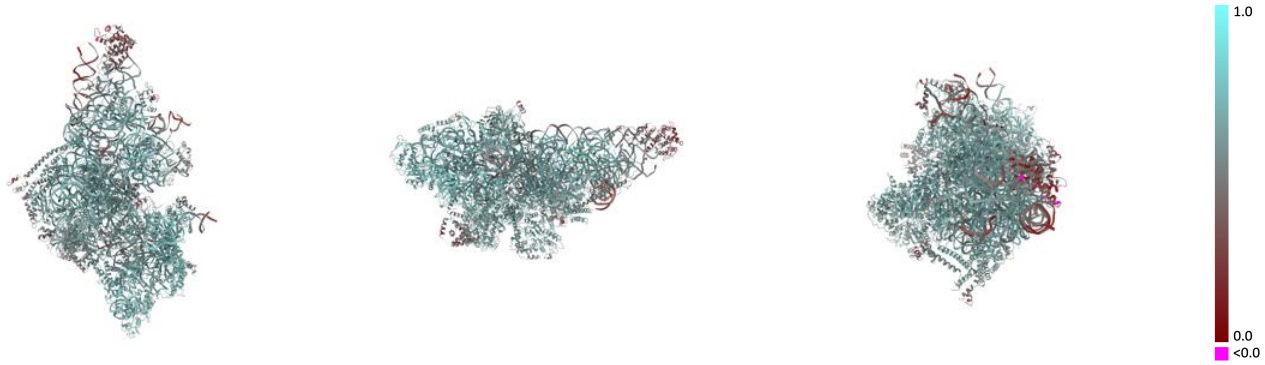
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

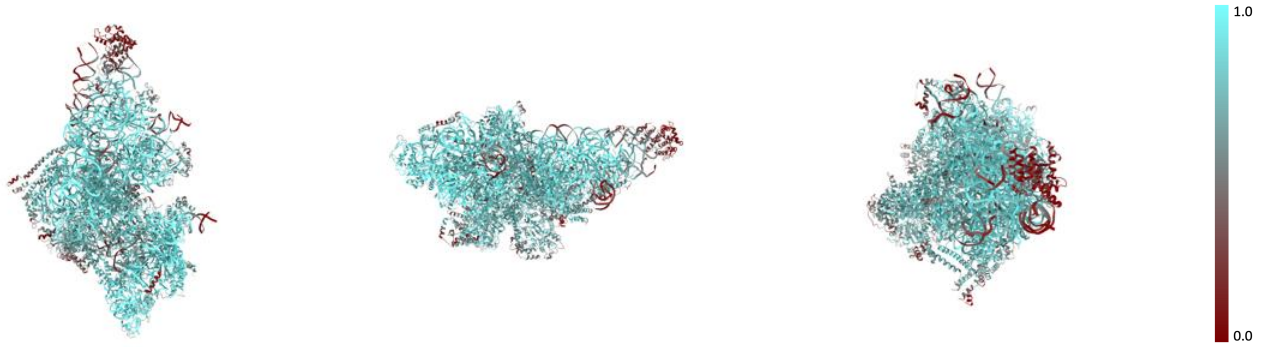
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

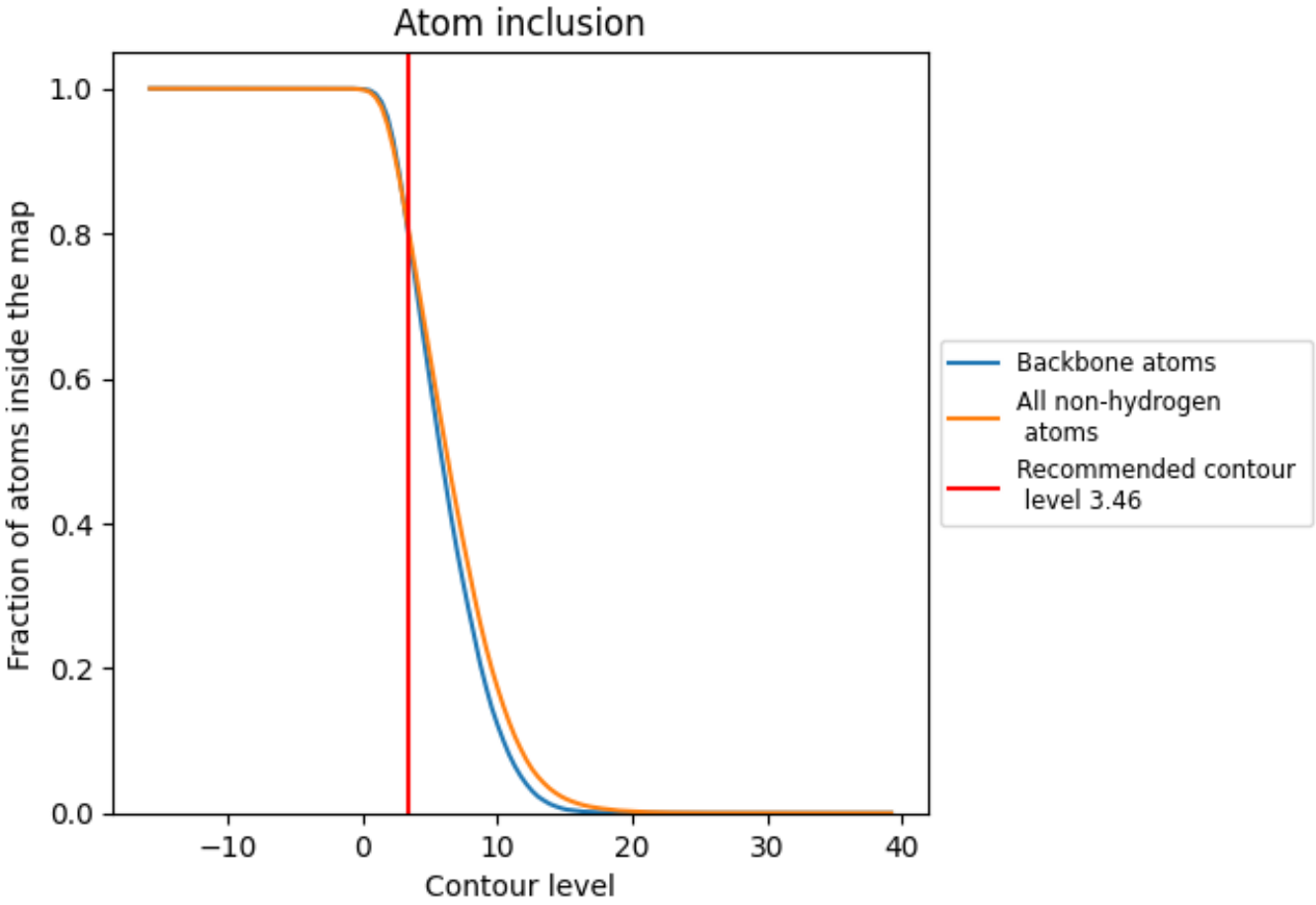
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.46).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 80% 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 (3.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.6140
0	0.7630	0.5860
2	0.6936	0.5610
3	0.8275	0.6320
4	0.6581	0.5570
5	0.2420	0.3720
6	0.7891	0.6180
8	0.6856	0.6170
A	0.7920	0.6170
B	0.8814	0.6680
C	0.8541	0.6380
D	0.8062	0.6160
E	0.8866	0.6660
F	0.7569	0.6010
G	0.8798	0.6640
H	0.9002	0.6750
I	0.8972	0.6660
J	0.9238	0.6790
K	0.6897	0.5690
L	0.8751	0.6640
M	0.7075	0.6340
N	0.9409	0.6970
O	0.8313	0.6310
P	0.8146	0.6200
Q	0.6348	0.5490
R	0.8567	0.6400
S	0.8417	0.6280
T	0.6902	0.5820
U	0.8674	0.6580
V	0.7157	0.5820
W	0.9142	0.6720
X	0.8439	0.6590
Y	0.8492	0.6380
Z	0.7442	0.6000
a	0.8371	0.6140
c	0.5277	0.4160