Full wwPDB EM Validation Report (i)

Aug 25, 2026 – 04:15 am BST

PDB ID	:	8OM2 / pdb_00008om2
EMDB ID	:	EMD-16966
Title	:	Small subunit of yeast mitochondrial ribosome in complex with METTL17/Rsm22.
Authors	:	Itoh, Y.; Chicherin, I.; Kamenski, P.; Amunts, A.
Deposited on	:	2023-03-31
Resolution	:	2.57 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 (i) 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 (i)) were used in the production of this report:

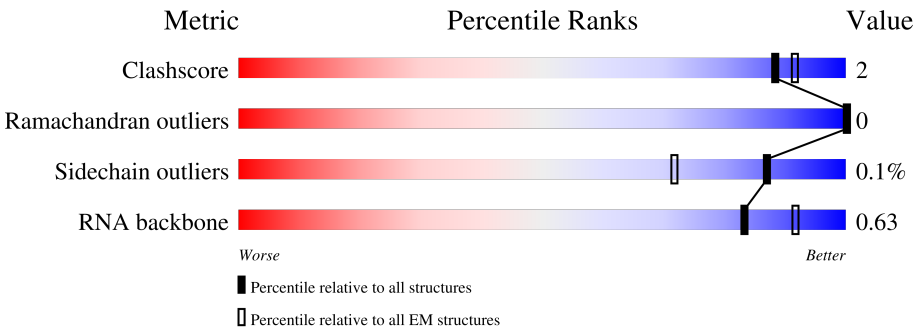
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

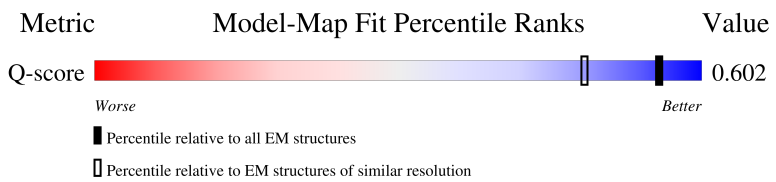
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.57 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	7615 (2.07 - 3.07)

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	A	344	29% 77% 10% 13%
2	B	394	19% 85% • 13%
3	C	398	28% 75% 5% 20%

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Mol	Chain	Length	Quality of chain
4	D	486	9% 67% 30%
5	E	307	5% 94%
6	F	131	5% 97%
7	G	247	22% 76% 6% 18%
8	H	154	96%
9	I	278	8% 79% 17%
10	J	203	7% 74% 5% 20%
11	K	217	6% 67% 30%
12	L	153	77% 20%
13	M	143	81% 17%
14	N	115	97%
15	O	286	73% 5% 22%
16	P	121	94% 5%
17	Q	237	26% 91% 8%
18	R	138	7% 68% 5% 27%
19	S	91	5% 81% 5% 13%
20	T	177	6% 47% 5% 48%
21	U	264	85% 5% 10%
22	V	318	15% 88% 10%
23	W	450	87% 11%
24	X	110	85% 11%
25	Y	319	11% 84% 15%
26	Z	95	12% 92% 5%
27	1	111	5% 26% 72%
28	2	130	75% 22%

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Mol	Chain	Length	Quality of chain
29	3	266	5% 91% 6% •
30	4	321	16% 87% 8% 6%
31	5	339	19% 78% 8% 14%
32	6	345	• 91% • 8%
33	8	500	23% 88% 5% 7%
34	r	1647	• 75% 14% • 10%
35	c	628	8% 69% 8% 23%

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 172798 atoms, of which 77593 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 37S ribosomal protein MRP51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	300	4908	1552	2481	427	441	7	1	0

- Molecule 2 is a protein called 37S ribosomal protein MRP4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	342	5436	1709	2722	467	535	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	319	5319	1661	2663	469	493	33	0	0

- Molecule 4 is a protein called 37S ribosomal protein NAM9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	341	5729	1842	2896	499	487	5	0	0

- Molecule 5 is a protein called 37S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	294	4708	1494	2360	418	428	8	0	0

- Molecule 6 is a protein called 37S ribosomal protein MRP17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	131	2184	671	1129	189	191	4	0	0

- Molecule 7 is a protein called 37S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	203	3272	1019	1660	289	299	5	0	0

- Molecule 8 is a protein called 37S ribosomal protein S8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	154	2509	774	1286	219	221	9	1	0

- Molecule 9 is a protein called 37S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	231	3783	1181	1925	334	338	5	1	0

- Molecule 10 is a protein called 37S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	162	2655	853	1334	227	237	4	0	0

- Molecule 11 is a protein called 37S ribosomal protein S18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	151	2475	775	1266	213	215	6	1	0

- Molecule 12 is a protein called 37S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	123	1932	579	993	192	164	4	0	0

- Molecule 13 is a protein called 37S ribosomal protein SWS2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	M	119	1937	591	1002	178	160	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	41	LEU	PHE	variant	UNP P53937

- Molecule 14 is a protein called 37S ribosomal protein MRP2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	N	113	1917	596	986	179	152	4	0	0

- Molecule 15 is a protein called 37S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	O	223	3668	1134	1853	334	339	8	0	0

- Molecule 16 is a protein called 37S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	P	120	1963	604	1011	178	168	2	0	0

- Molecule 17 is a protein called 37S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	Q	235	3944	1208	2014	356	361	5	1	0

- Molecule 18 is a protein called 37S ribosomal protein RSM18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	R	101	1671	507	853	162	145	4	0	0

- Molecule 19 is a protein called 37S ribosomal protein S19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	S	79	1277	404	648	114	109	2	0	0

- Molecule 20 is a protein called 37S ribosomal protein MRP21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	T	92	1569	483	800	150	131	5	1	0

- Molecule 21 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	U	237	3868	1228	1929	339	365	7	0	0

- Molecule 22 is a protein called 37S ribosomal protein PET123, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	V	286	4692	1450	2398	406	434	4	0	0

- Molecule 23 is a protein called 37S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	W	402	6555	2078	3329	542	598	8	0	0

- Molecule 24 is a protein called Mitochondrial 37S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	X	98	1619	503	832	142	139	3	0	0

- Molecule 25 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	Y	272	4514	1436	2241	408	425	4	0	0

- Molecule 26 is a protein called 37S ribosomal protein MRP10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	Z	92	1487	459	758	137	127	6	0	0

- Molecule 27 is a protein called Mitochondrial mRNA-processing protein COX24.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	1	31	613	170	334	68	39	2	0	0

- Molecule 28 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	2	102	1724	544	866	161	152	1	0	0

- Molecule 29 is a protein called 37S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	3	257	4103	1326	2040	349	383	5	0	0

- Molecule 30 is a protein called 37S ribosomal protein MRP1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	4	303	4859	1538	2423	422	466	10	0	0

- Molecule 31 is a protein called 37S ribosomal protein MRP13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	5	291	4770	1524	2409	404	429	4	0	0

- Molecule 32 is a protein called 37S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	6	319	5208	1646	2615	467	474	6	0	0

- Molecule 33 is a protein called 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	8	467	7371	2341	3681	621	708	20	0	0

- Molecule 34 is a RNA chain called 15S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
34	r	1486	47424	14203	15836	5575	10322	1488	2	0

- Molecule 35 is a protein called Probable S-adenosyl-L-methionine-dependent RNA methyltransferase RSM22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	c	483	7907	2479	3983	713	719	13	0	0

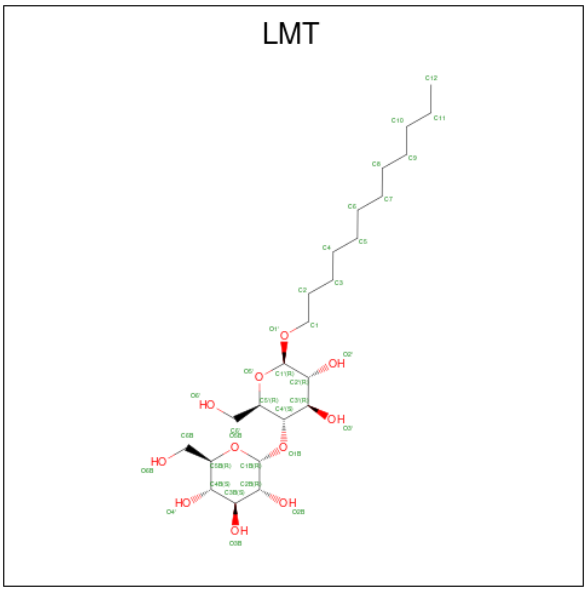
- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	B	1	1	1	0
36	K	1	1	1	0
36	W	1	1	1	0
36	r	87	87	87	0

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

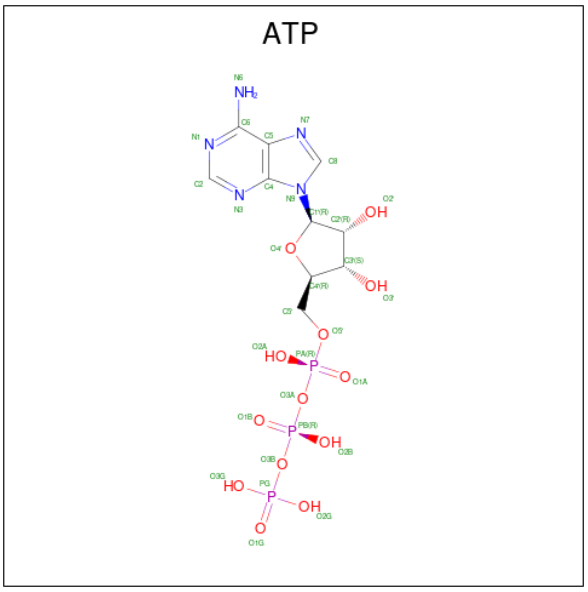
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
37	D	1	1	1	0
37	M	1	1	1	0
37	r	33	33	33	0

- Molecule 38 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



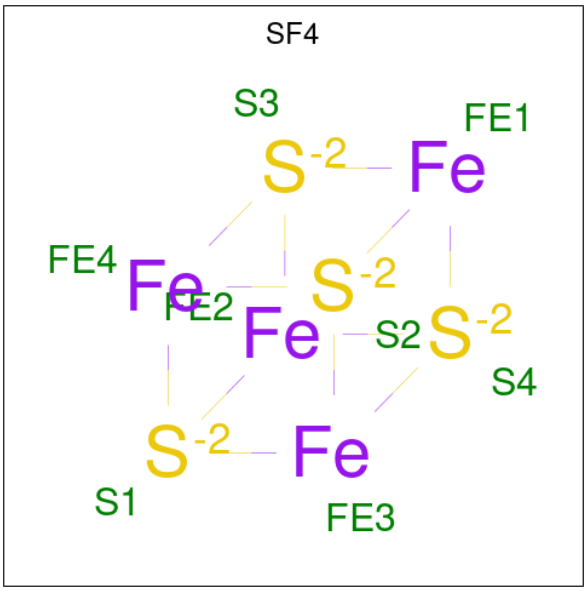
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
38	O	1	38	12	25	1	0

- Molecule 39 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 40 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
41	A	42	42	42	0
41	B	95	95	95	0
41	C	12	12	12	0
41	D	77	77	77	0
41	E	65	65	65	0
41	F	5	5	5	0
41	G	17	17	17	0
41	H	49	49	49	0
41	I	39	39	39	0
41	J	26	26	26	0
41	K	10	10	10	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
41	L	27	27	27	0
			Total	O	
41	M	10	10	10	0
			Total	O	
41	N	42	42	42	0
			Total	O	
41	O	39	39	39	0
			Total	O	
41	P	43	43	43	0
			Total	O	
41	Q	18	18	18	0
			Total	O	
41	R	7	7	7	0
			Total	O	
41	S	9	9	9	0
			Total	O	
41	T	24	24	24	0
			Total	O	
41	U	55	55	55	0
			Total	O	
41	V	18	18	18	0
			Total	O	
41	W	50	50	50	0
			Total	O	
41	X	6	6	6	0
			Total	O	
41	Y	28	28	28	0
			Total	O	
41	Z	11	11	11	0
			Total	O	
41	1	9	9	9	0
			Total	O	
41	2	12	12	12	0
			Total	O	
41	3	9	9	9	0
			Total	O	
41	4	2	2	2	0
			Total	O	
41	5	1	1	1	0
			Total	O	
41	6	53	53	53	0

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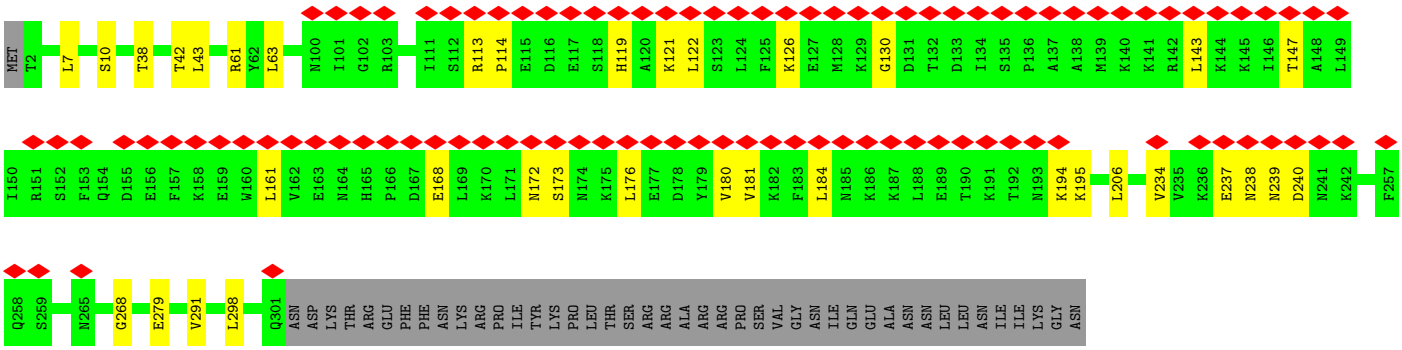
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
41	8	11	11	11	0
			Total	O	
41	r	2070	2070	2070	0
			Total	O	
41	c	23	23	23	0

3 Residue-property plots (i)

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

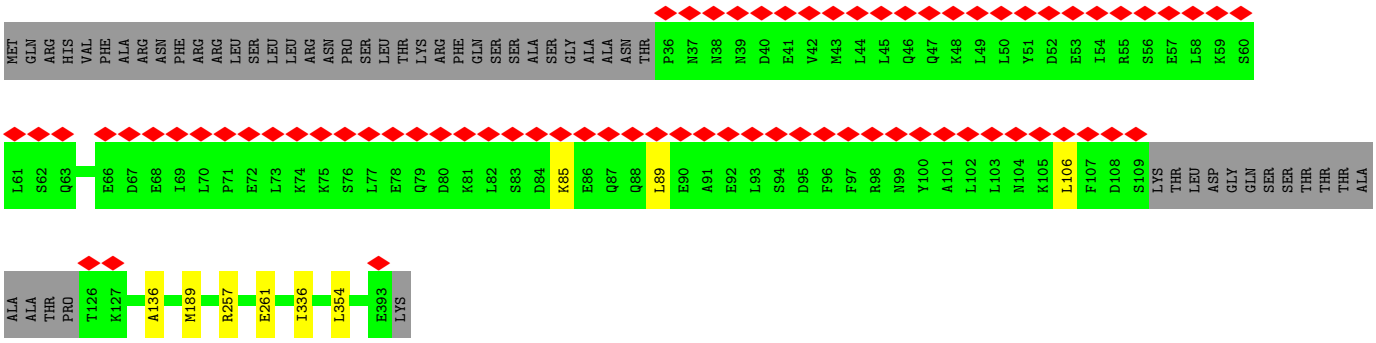
- Molecule 1: 37S ribosomal protein MRP51, mitochondrial

Chain A:



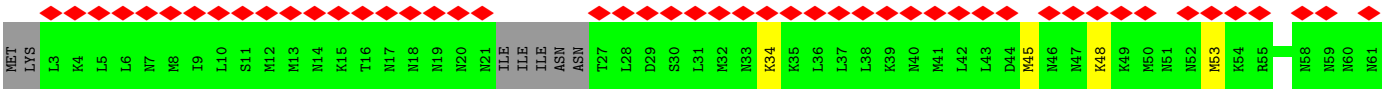
- Molecule 2: 37S ribosomal protein MRP4, mitochondrial

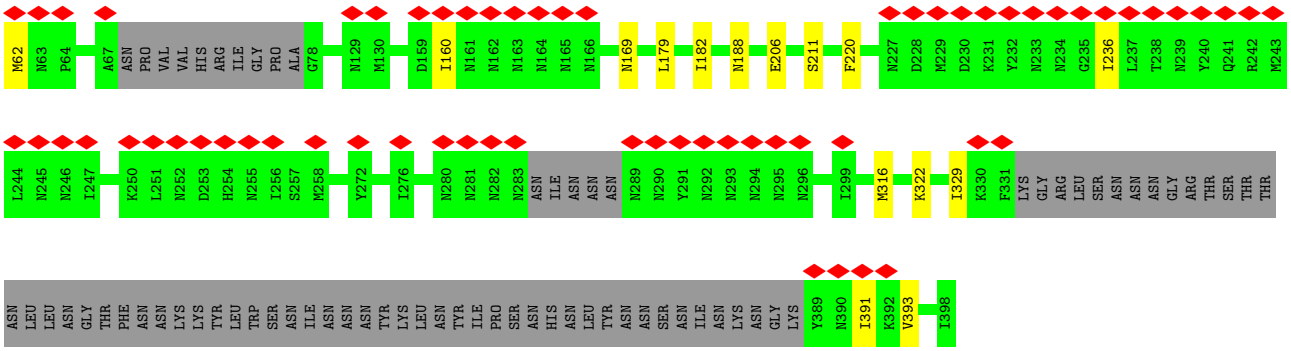
Chain B:



- Molecule 3: Ribosomal protein VAR1, mitochondrial

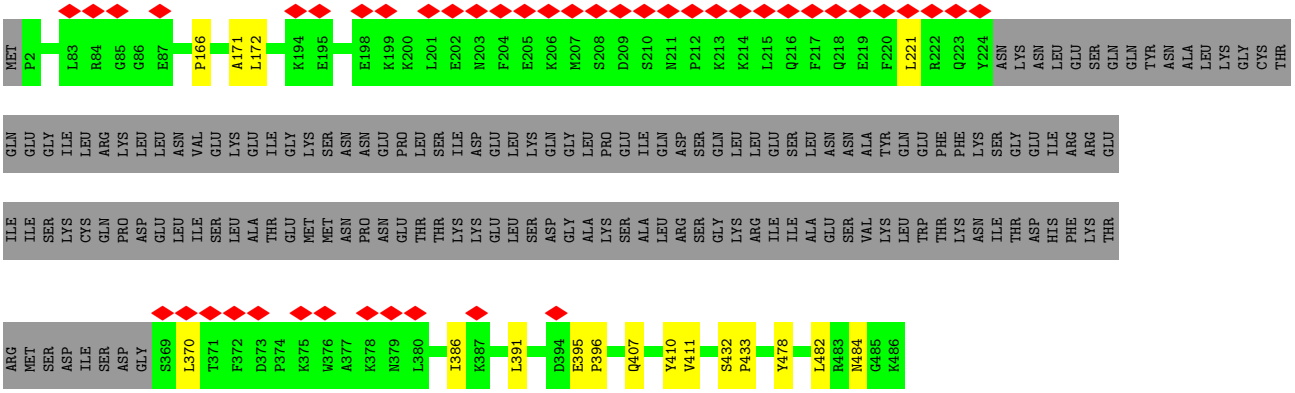
Chain C:





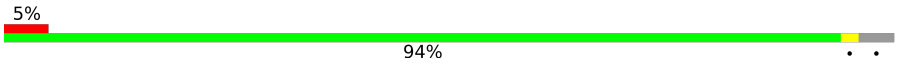
• Molecule 4: 37S ribosomal protein NAM9, mitochondrial

Chain D:



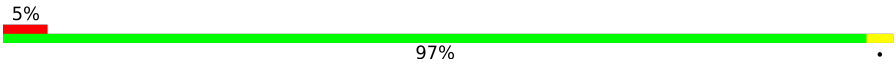
• Molecule 5: 37S ribosomal protein S5, mitochondrial

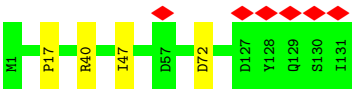
Chain E:



• Molecule 6: 37S ribosomal protein MRP17, mitochondrial

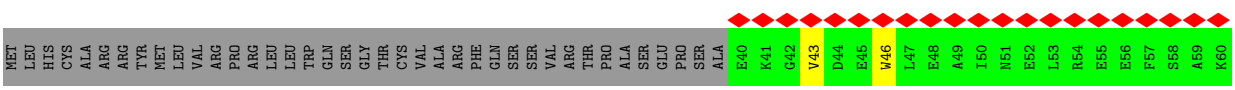
Chain F:

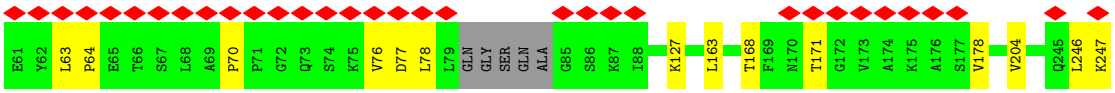




• Molecule 7: 37S ribosomal protein S7, mitochondrial

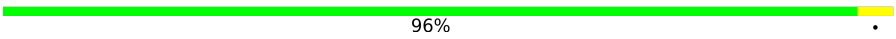
Chain G:

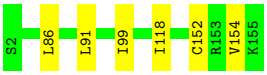




• Molecule 8: 37S ribosomal protein S8, mitochondrial

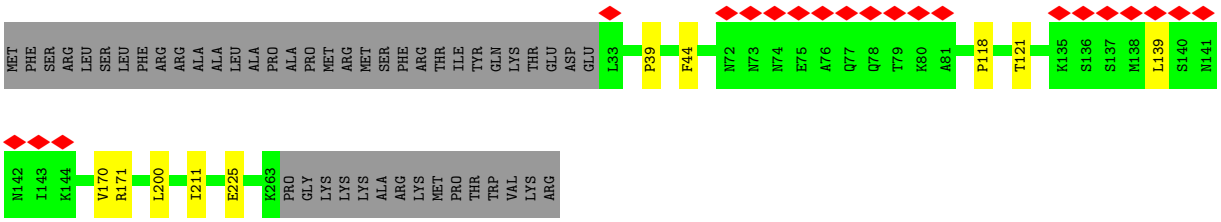
Chain H:





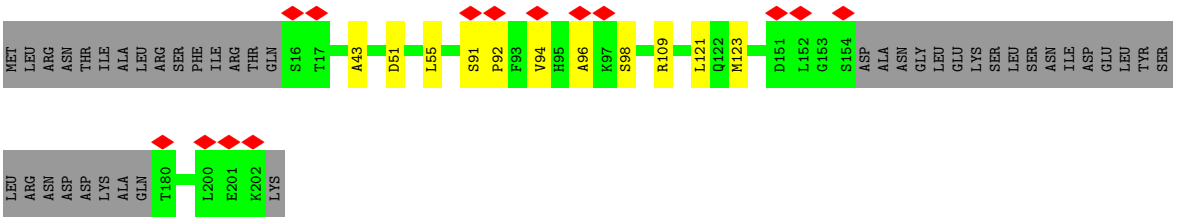
• Molecule 9: 37S ribosomal protein S9, mitochondrial

Chain I:



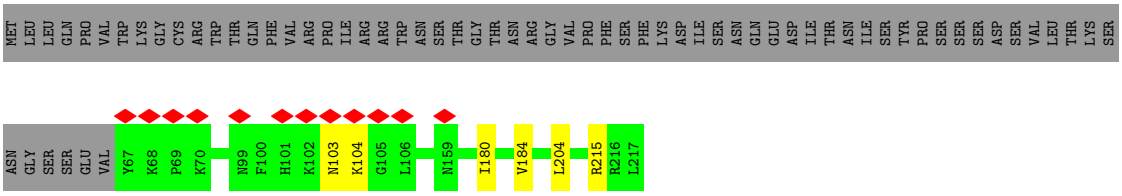
• Molecule 10: 37S ribosomal protein S10, mitochondrial

Chain J:



• Molecule 11: 37S ribosomal protein S18, mitochondrial

Chain K:

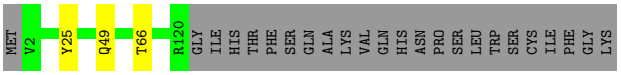


• Molecule 12: 37S ribosomal protein S12, mitochondrial

Chain L:

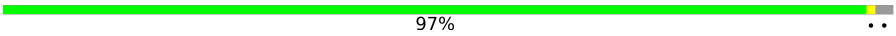
• Molecule 13: 37S ribosomal protein SWS2, mitochondrial

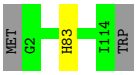
Chain M:



• Molecule 14: 37S ribosomal protein MRP2, mitochondrial

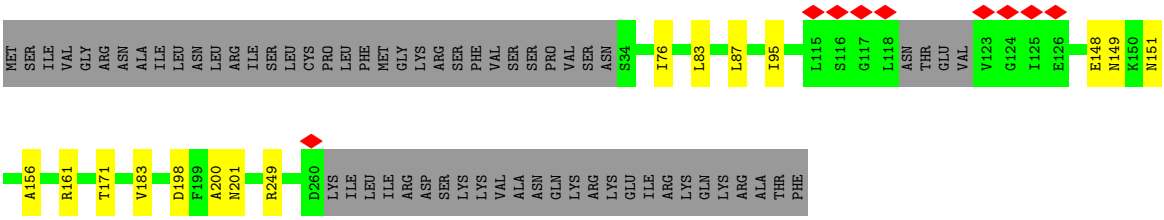
Chain N:





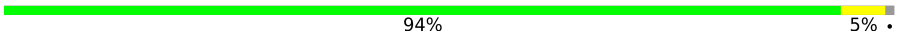
• Molecule 15: 37S ribosomal protein S28, mitochondrial

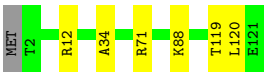
Chain O:



• Molecule 16: 37S ribosomal protein S16, mitochondrial

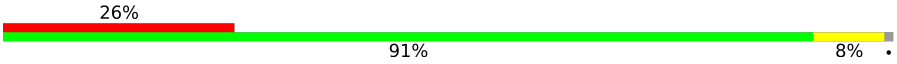
Chain P:

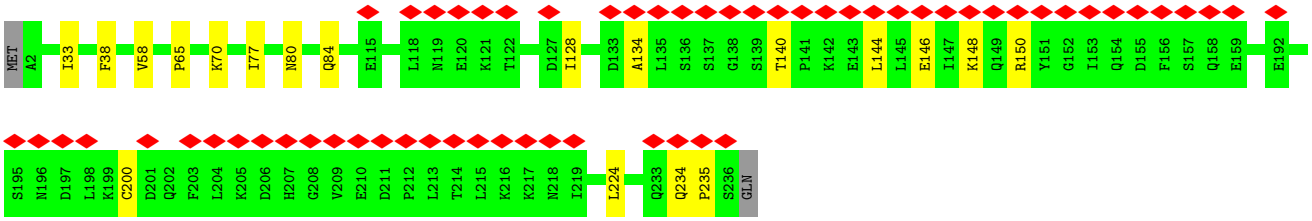




• Molecule 17: 37S ribosomal protein S17, mitochondrial

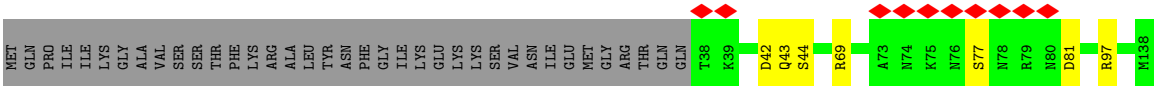
Chain Q:





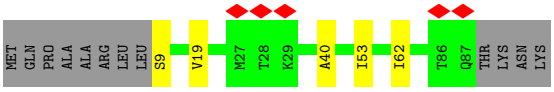
• Molecule 18: 37S ribosomal protein RSM18, mitochondrial

Chain R:



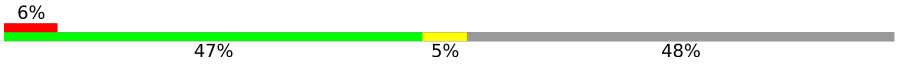
• Molecule 19: 37S ribosomal protein S19, mitochondrial

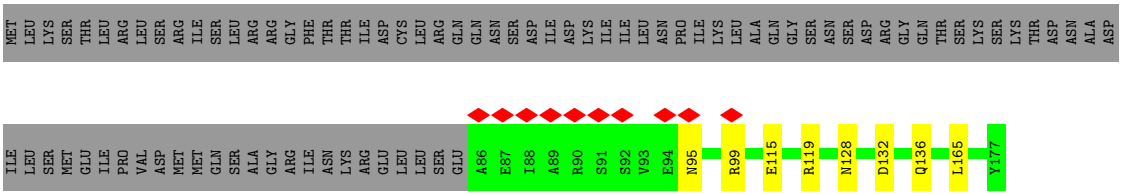
Chain S:



• Molecule 20: 37S ribosomal protein MRP21, mitochondrial

Chain T:



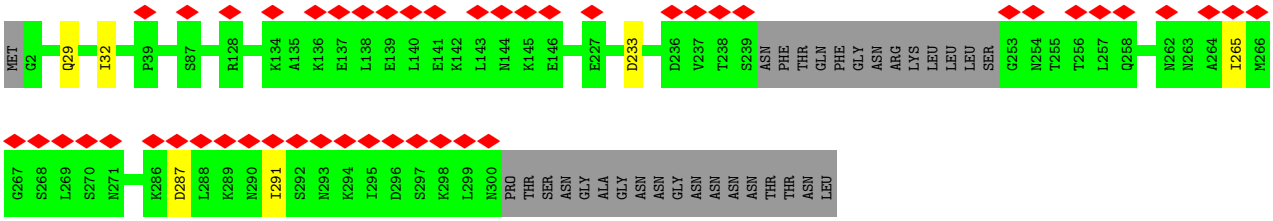


• Molecule 21: 37S ribosomal protein S25, mitochondrial

Chain U:

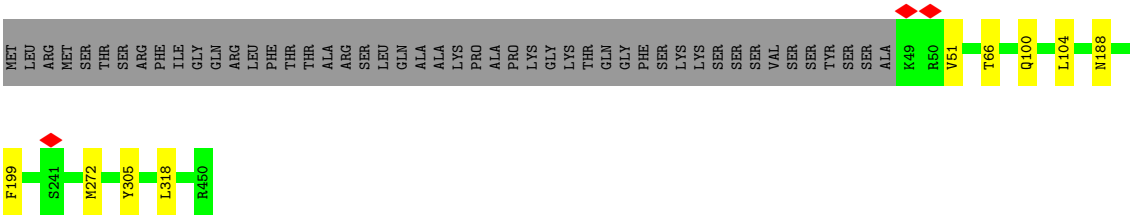
• Molecule 22: 37S ribosomal protein PET123, mitochondrial

Chain V:



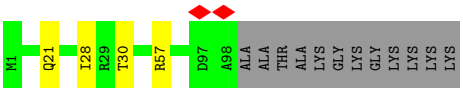
• Molecule 23: 37S ribosomal protein S23, mitochondrial

Chain W:



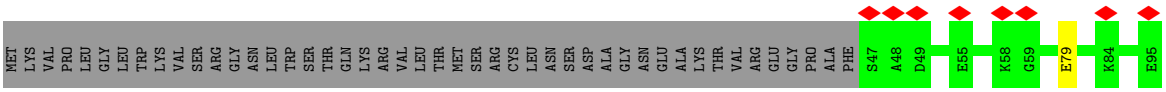
• Molecule 24: Mitochondrial 37S ribosomal protein S27

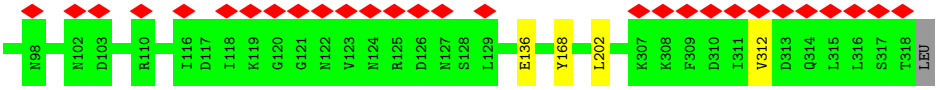
Chain X:



• Molecule 25: 37S ribosomal protein S24, mitochondrial

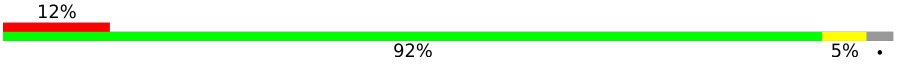
Chain Y:

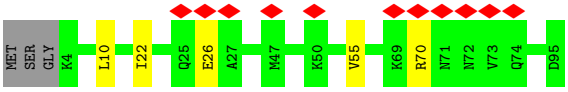




• Molecule 26: 37S ribosomal protein MRP10, mitochondrial

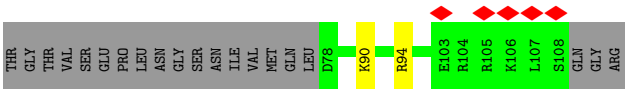
Chain Z:





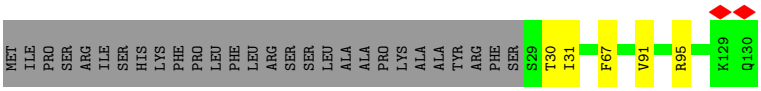
• Molecule 27: Mitochondrial mRNA-processing protein COX24

Chain 1:



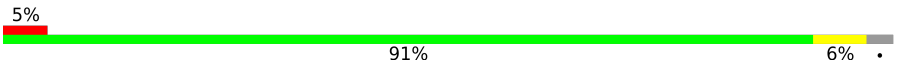
• Molecule 28: Protein FYV4, mitochondrial

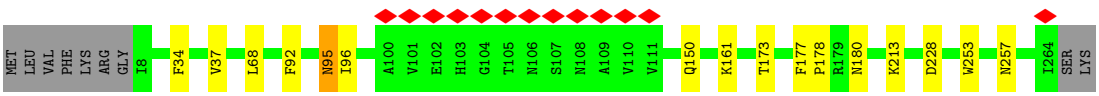
Chain 2:



• Molecule 29: 37S ribosomal protein S26, mitochondrial

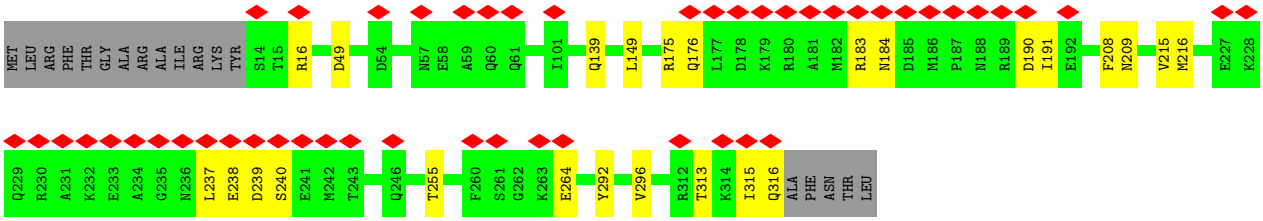
Chain 3:





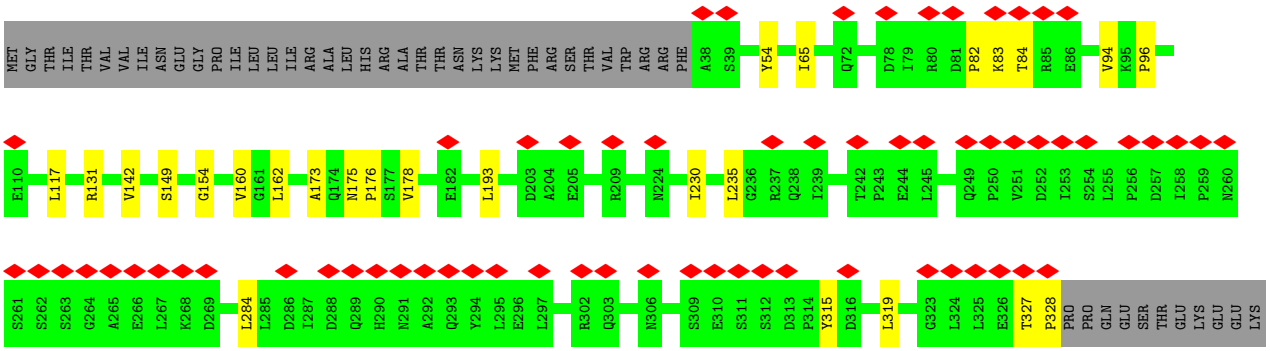
• Molecule 30: 37S ribosomal protein MRP1, mitochondrial

Chain 4:



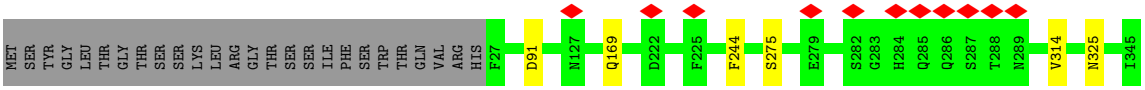
- Molecule 31: 37S ribosomal protein MRP13, mitochondrial

Chain 5:



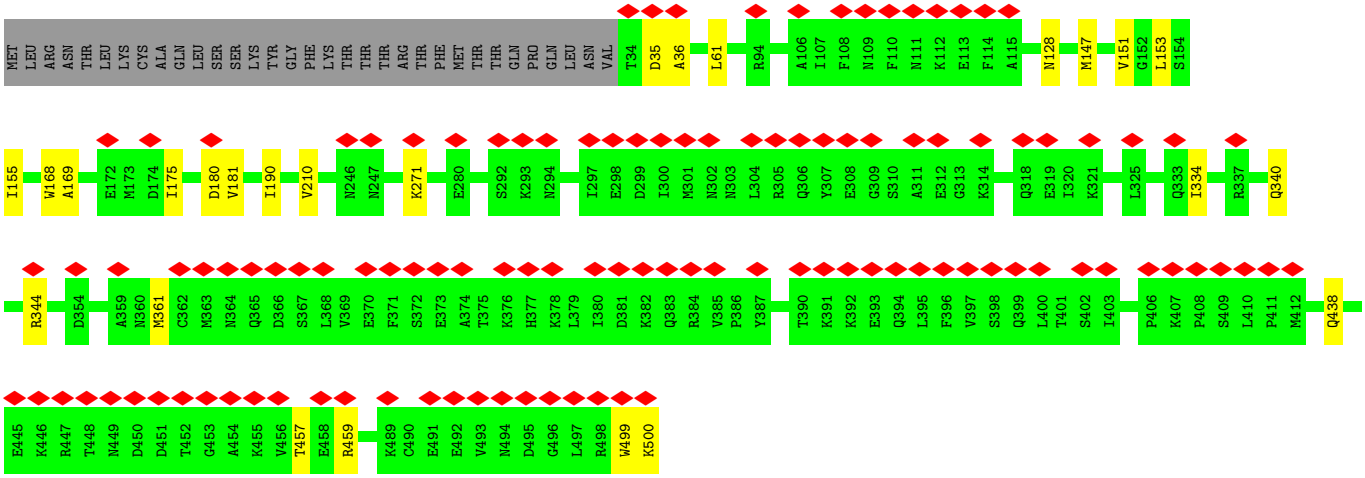
- Molecule 32: 37S ribosomal protein S35, mitochondrial

Chain 6:



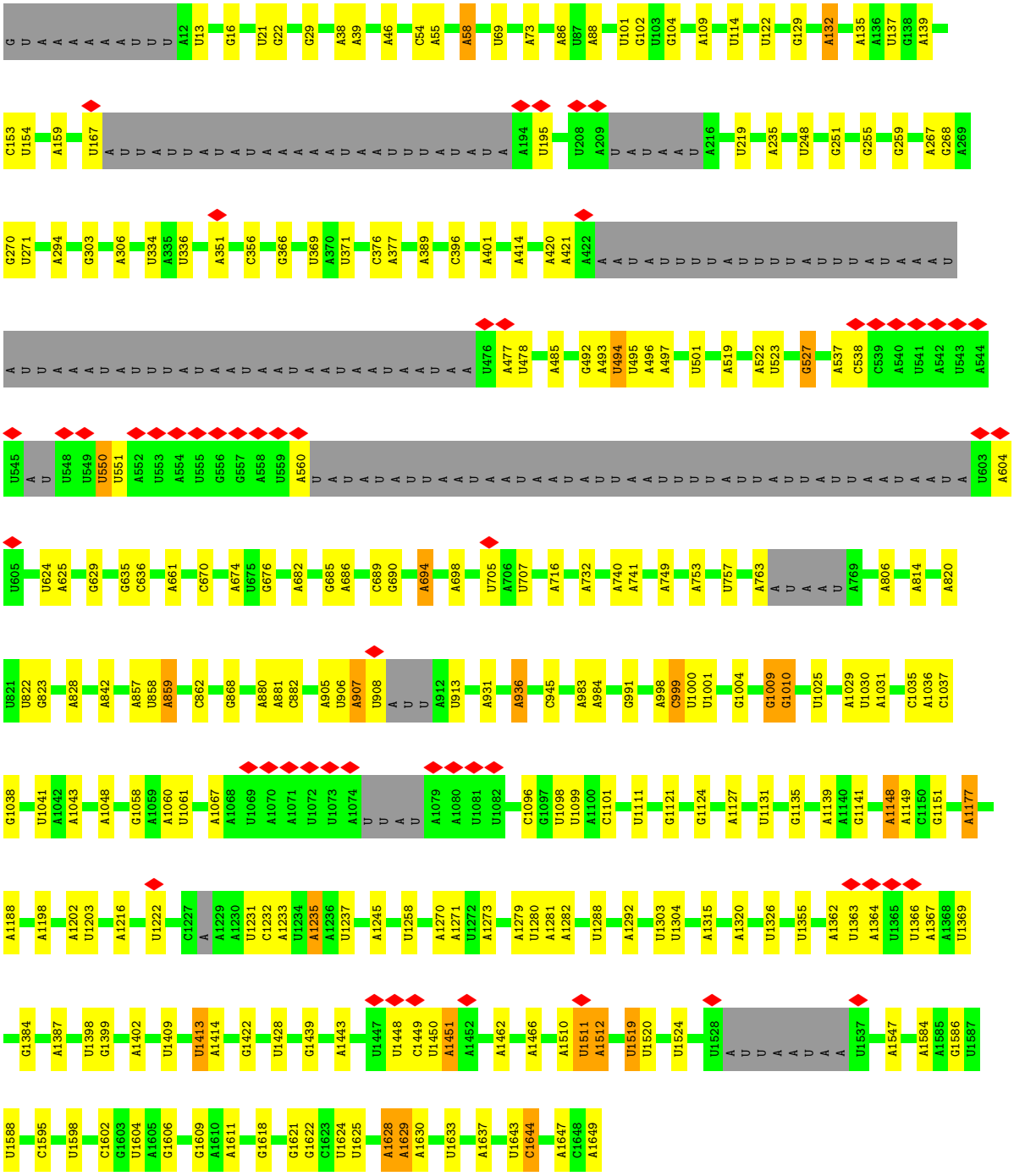
- Molecule 33: 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial

Chain 8:



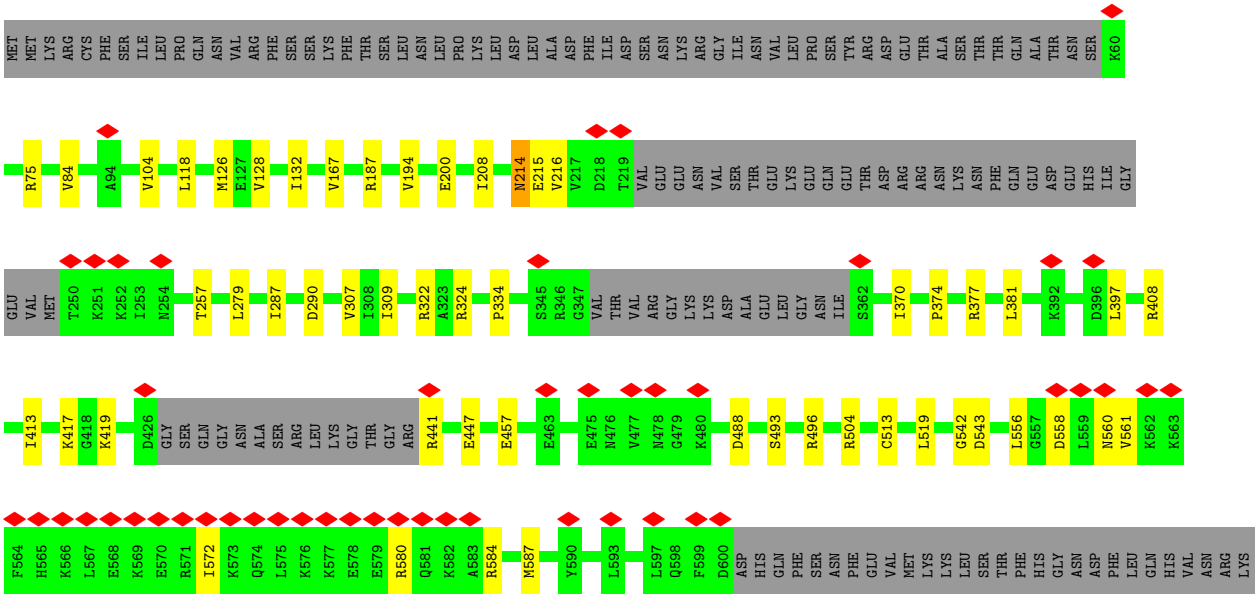
• Molecule 34: 15S mitochondrial rRNA

Chain r: 75% 14% • 10%



• Molecule 35: Probable S-adenosyl-L-methionine-dependent RNA methyltransferase RSM22, mitochondrial

Chain c: 8% 69% 8% 23%


MET MET LYS ARG CYS PHE SER ILE LEU PRO GLN ASN VAL ARG PHE SER SER LYS PHE THR SER LEU ASN LEU PRO LYS LEU ASP LEU ALA ASP PHE ILE ASP SER ASN LYS ARG GLY ILE ASN VAL LEU PRO SER TYR ARG ASP GLU THR ALA SER THR THR GLN ALA THR ASN SER K60
R75 V84 A94 V104 L118 M126 E127 V128 I132 V167 R187 V194 E200 I208 N214 E215 V216 V217 D218 T219 VAL GLU GLU ASN VAL SER THR GLU LYS GLU GLN GLU THR ASP ARG ARG ASN LYS ASN PHE GLN GLU ASP GLU HIS ILE GLY
GLU VAL MET T250 K251 K252 I253 N254 T257 L279 I287 D290 V307 I308 I309 R322 A323 R324 P334 S345 R346 G347 VAL THR VAL ARG GLY LYS LYS ASP ALA GLU LEU GLY ASN ILE S362 I370 P374 R377 L381 K392 D396 L397 R408
I413 K417 G418 K419 D426 GLY SER GLN GLY ASN ALA SER ARG LEU LYS GLY THR GLY ARG R441 E447 E457 E463 E475 N476 V477 N478 G479 K480 D488 S493 R496 R504 C513 L519 G542 D543 L556 G557 D558 L559 N560 V561 K562 K563
F564 H565 K566 L567 E568 K569 E570 R571 I572 K573 Q574 L575 K576 K577 E578 E579 R580 Q581 K582 A583 R584 M587 Y590 L593 L597 Q598 F599 D600 ASP HIS GLN PHE SER ASN PHE GLU VAL MET LYS LYS LEU SER THR PHE HIS GLY ASN ASP PHE LEU GLN HIS VAL ASN ARG LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	283744	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 ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.871	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	398.40192, 398.40192, 398.40192	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.59286, 0.59286, 0.59286	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	A	0.11	0/2483	0.27	0/3345
2	B	0.11	0/2764	0.27	0/3746
3	C	0.09	0/2690	0.25	0/3616
4	D	0.10	0/2913	0.27	0/3923
5	E	0.11	0/2403	0.25	0/3237
6	F	0.09	0/1068	0.24	0/1430
7	G	0.09	0/1641	0.25	0/2216
8	H	0.10	0/1237	0.26	0/1667
9	I	0.09	0/1895	0.24	0/2552
10	J	0.11	0/1355	0.28	0/1834
11	K	0.09	0/1232	0.24	0/1642
12	L	0.11	0/954	0.26	0/1281
13	M	0.10	0/949	0.25	0/1267
14	N	0.13	0/948	0.25	0/1267
15	O	0.10	0/1837	0.22	0/2457
16	P	0.12	0/968	0.30	0/1307
17	Q	0.09	0/1953	0.24	0/2609
18	R	0.09	0/830	0.23	0/1106
19	S	0.12	0/645	0.27	0/872
20	T	0.09	0/784	0.22	0/1035
21	U	0.10	0/1982	0.26	0/2679
22	V	0.10	0/2325	0.21	0/3112
23	W	0.09	0/3292	0.24	0/4449
24	X	0.08	0/801	0.22	0/1070
25	Y	0.08	0/2329	0.23	0/3142
26	Z	0.09	0/745	0.27	0/1004
27	1	0.13	0/279	0.22	0/355
28	2	0.09	0/877	0.26	0/1173
29	3	0.12	0/2114	0.31	1/2872 (0.0%)
30	4	0.10	0/2485	0.28	0/3354
31	5	0.09	0/2417	0.26	0/3275
32	6	0.10	0/2655	0.25	0/3583

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	8	0.08	0/3766	0.24	0/5099
34	r	0.11	0/35387	0.20	0/55053
35	c	0.10	0/4000	0.27	0/5380
All	All	0.10	0/97003	0.24	1/138009 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	95	ASN	CA-CB-CG	8.65	121.25	112.60

There are no chirality outliers.

There are no planarity outliers.

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	A	2427	2481	2480	28	0
2	B	2714	2722	2721	11	0
3	C	2656	2663	2657	17	0
4	D	2833	2896	2895	11	0
5	E	2348	2360	2359	5	0
6	F	1055	1129	1129	2	0
7	G	1612	1660	1658	20	0
8	H	1223	1286	1288	3	0
9	I	1858	1925	1925	7	0
10	J	1321	1334	1332	8	0
11	K	1209	1266	1266	5	0
12	L	939	993	992	4	0
13	M	935	1002	1000	3	0
14	N	931	986	985	1	0
15	O	1815	1853	1851	10	0
16	P	952	1011	1010	5	0
17	Q	1930	2014	2014	14	0
18	R	818	853	852	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	629	648	647	3	0
20	T	769	800	800	5	0
21	U	1939	1929	1929	11	0
22	V	2294	2398	2396	6	0
23	W	3226	3329	3327	7	0
24	X	787	832	832	3	0
25	Y	2273	2241	2240	8	0
26	Z	729	758	757	4	0
27	1	279	334	333	2	0
28	2	858	866	865	3	0
29	3	2063	2040	2039	8	0
30	4	2436	2423	2422	13	0
31	5	2361	2409	2408	15	0
32	6	2593	2615	2613	5	0
33	8	3690	3681	3680	16	0
34	r	31588	15836	15835	86	0
35	c	3924	3983	3977	39	0
36	B	1	0	0	0	0
36	K	1	0	0	0	0
36	W	1	0	0	0	0
36	r	87	0	0	0	0
37	D	1	0	0	0	0
37	M	1	0	0	0	0
37	r	33	0	0	0	0
38	O	13	25	25	2	0
39	W	31	12	12	0	0
40	c	8	0	0	0	0
41	1	9	0	0	0	0
41	2	12	0	0	0	0
41	3	9	0	0	0	0
41	4	2	0	0	0	0
41	5	1	0	0	0	0
41	6	53	0	0	1	0
41	8	11	0	0	0	0
41	A	42	0	0	0	0
41	B	95	0	0	0	0
41	C	12	0	0	0	0
41	D	77	0	0	0	0
41	E	65	0	0	0	0
41	F	5	0	0	0	0
41	G	17	0	0	0	0
41	H	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	I	39	0	0	1	0
41	J	26	0	0	1	0
41	K	10	0	0	0	0
41	L	27	0	0	0	0
41	M	10	0	0	1	0
41	N	42	0	0	0	0
41	O	39	0	0	1	0
41	P	43	0	0	1	0
41	Q	18	0	0	0	0
41	R	7	0	0	0	0
41	S	9	0	0	0	0
41	T	24	0	0	1	0
41	U	55	0	0	0	0
41	V	18	0	0	0	0
41	W	50	0	0	0	0
41	X	6	0	0	0	0
41	Y	28	0	0	0	0
41	Z	11	0	0	0	0
41	c	23	0	0	0	0
41	r	2070	0	0	13	0
All	All	95205	77593	77551	322	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 2.

All (322) 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)
34:r:1151:G:N7	41:r:1911:HOH:O	2.19	0.75
34:r:732:A:OP1	41:r:1902:HOH:O	2.07	0.73
34:r:1151:G:O6	41:r:1903:HOH:O	2.07	0.72
34:r:945:C:OP1	41:r:1904:HOH:O	2.07	0.71
34:r:629:G:N7	41:r:1925:HOH:O	2.25	0.70
34:r:38:A:OP2	41:r:1905:HOH:O	2.09	0.70
34:r:868:G:OP1	41:r:1906:HOH:O	2.10	0.69
16:P:34:ALA:O	41:P:201:HOH:O	2.11	0.68
15:O:200:ALA:O	41:O:401:HOH:O	2.13	0.66
9:I:225:GLU:OE1	41:I:301:HOH:O	2.12	0.66
34:r:1602:C:OP1	41:r:1907:HOH:O	2.13	0.65
9:I:200:LEU:HD11	9:I:211:ILE:HD11	1.78	0.65
34:r:1010:G:N2	34:r:1402:A:O2'	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5:315:TYR:CE2	31:5:319:LEU:HD11	2.33	0.64
4:D:172:LEU:HD21	4:D:391:LEU:CD1	2.28	0.64
1:A:298:LEU:HD13	30:4:255:THR:HG21	1.81	0.63
35:c:104:VAL:HG21	35:c:126:MET:HG2	1.80	0.63
15:O:183:VAL:HG22	38:O:301:LMT:H111	1.80	0.62
34:r:21:U:OP2	35:c:584:ARG:NH1	2.33	0.62
35:c:104:VAL:HG21	35:c:126:MET:CG	2.30	0.62
28:2:67:PHE:O	28:2:95:ARG:NH2	2.32	0.62
34:r:1588:U:P	35:c:287:ILE:HG21	2.40	0.62
18:R:77:SER:O	18:R:81:ASP:N	2.35	0.60
33:8:155:ILE:HD11	33:8:190:ILE:HD11	1.83	0.60
34:r:1288:U:OP2	41:r:1909:HOH:O	2.16	0.60
7:G:168:THR:HG22	7:G:178:VAL:HG22	1.84	0.60
35:c:118:LEU:HD11	35:c:279:LEU:HD23	1.85	0.59
1:A:143:LEU:O	1:A:147:THR:OG1	2.15	0.58
33:8:180:ASP:O	33:8:181:VAL:HG22	2.04	0.58
34:r:1409:U:OP1	35:c:441:ARG:NH2	2.37	0.58
2:B:89:LEU:HD12	7:G:43:VAL:HG13	1.85	0.58
34:r:999:C:H2'	34:r:1000:U:O4'	2.04	0.57
35:c:307:VAL:HG12	35:c:309:ILE:HD11	1.85	0.57
1:A:38:THR:HG1	1:A:42:THR:HG1	1.50	0.57
33:8:334:ILE:HD13	33:8:361:MET:HE2	1.87	0.57
27:1:94:ARG:NH2	34:r:1606:G:N7	2.50	0.57
34:r:881:A:OP1	34:r:1618:G:O2'	2.21	0.57
7:G:204:VAL:HG21	23:W:51:VAL:HG22	1.86	0.56
11:K:204:LEU:O	34:r:740:A:O2'	2.17	0.56
19:S:9:SER:N	34:r:1387:A:HO2'	2.04	0.56
11:K:215[A]:ARG:NH1	34:r:757:U:OP1	2.39	0.56
3:C:48:LYS:HG3	25:Y:312:VAL:HG11	1.86	0.56
31:5:84:THR:HG22	31:5:84:THR:O	2.05	0.56
1:A:195:LYS:CG	21:U:166:VAL:HG21	2.37	0.55
30:4:176:GLN:HG2	30:4:313:THR:HG21	1.87	0.55
2:B:85:LYS:O	7:G:43:VAL:HG11	2.06	0.55
33:8:35:ASP:OD1	33:8:36:ALA:N	2.39	0.55
6:F:17:PRO:HB2	6:F:47:ILE:HD11	1.89	0.55
9:I:200:LEU:HD11	9:I:211:ILE:CD1	2.37	0.54
34:r:1588:U:OP1	35:c:287:ILE:HG21	2.07	0.54
20:T:115:GLU:OE2	20:T:119:ARG:NE	2.40	0.54
7:G:76:VAL:HG12	7:G:77:ASP:N	2.22	0.54
21:U:220:TRP:O	21:U:224:VAL:HG23	2.08	0.54
14:N:83:HIS:NE2	34:r:1235:A:OP2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:OG1	1:A:42:THR:OG1	2.24	0.54
34:r:492:G:O2'	34:r:497:A:N1	2.35	0.54
34:r:1198:A:N6	34:r:1202:A:H61	2.06	0.54
13:M:49:GLN:NE2	41:M:302:HOH:O	2.41	0.53
1:A:161:LEU:HD21	1:A:176:LEU:HD22	1.91	0.53
10:J:123:MET:HE1	25:Y:168:TYR:CD2	2.43	0.53
12:L:44:LYS:NZ	34:r:670:C:OP1	2.40	0.53
7:G:246:LEU:O	7:G:247:LYS:CB	2.57	0.53
34:r:159:A:OP2	41:r:1910:HOH:O	2.18	0.53
10:J:51:ASP:O	41:J:301:HOH:O	2.18	0.53
34:r:1643:U:O2'	34:r:1644:C:O4'	2.26	0.53
29:3:68:LEU:O	29:3:213:LYS:NZ	2.42	0.53
34:r:1399:G:O6	41:r:1908:HOH:O	2.15	0.52
35:c:397:LEU:HD21	35:c:561:VAL:HG11	1.92	0.52
35:c:381:LEU:HD21	35:c:519:LEU:HD11	1.90	0.52
34:r:1448:U:H2'	34:r:1449:C:O4'	2.10	0.52
13:M:66:THR:O	13:M:66:THR:HG23	2.09	0.52
35:c:128:VAL:HG21	35:c:200:GLU:HB2	1.92	0.52
7:G:64:PRO:HB2	7:G:78:LEU:HD11	1.91	0.52
29:3:173:THR:O	29:3:180:ASN:ND2	2.43	0.52
5:E:153:ARG:NE	35:c:587:MET:SD	2.77	0.51
29:3:150:GLN:NE2	29:3:228:ASP:OD2	2.43	0.51
23:W:272:MET:HE3	23:W:272:MET:HA	1.91	0.51
11:K:215[A]:ARG:NE	34:r:862:C:OP1	2.44	0.51
34:r:1121:G:O2'	34:r:1148:A:N1	2.34	0.51
31:5:131:ARG:NH2	31:5:173:ALA:O	2.44	0.51
15:O:87:LEU:HD13	15:O:95:ILE:HD13	1.92	0.51
34:r:1511:U:H3'	34:r:1512:A:C5'	2.41	0.51
3:C:45:MET:HG2	25:Y:312:VAL:HG13	1.92	0.50
1:A:195:LYS:HG3	21:U:166:VAL:HG21	1.94	0.50
4:D:407:GLN:NE2	4:D:410:TYR:O	2.45	0.50
35:c:187:ARG:NH2	35:c:216:VAL:O	2.45	0.50
28:2:30:THR:HG22	28:2:31:ILE:N	2.26	0.50
32:6:91:ASP:OD1	32:6:91:ASP:N	2.43	0.50
35:c:381:LEU:HD23	35:c:558:ASP:HB2	1.94	0.50
4:D:221:LEU:HD13	4:D:370:LEU:HD22	1.94	0.49
7:G:64:PRO:CB	7:G:78:LEU:HD11	2.41	0.49
7:G:246:LEU:HD11	21:U:233:ALA:HB1	1.94	0.49
34:r:1384:G:N1	34:r:1387:A:OP2	2.43	0.49
23:W:188:ASN:OD1	23:W:305:TYR:OH	2.28	0.49
1:A:206:LEU:CD2	1:A:291:VAL:HG21	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLU:HB2	1:A:298:LEU:HD11	1.95	0.49
5:E:153:ARG:HE	35:c:587:MET:CG	2.25	0.49
10:J:96:ALA:O	10:J:98:SER:N	2.44	0.49
32:6:325:ASN:O	41:6:401:HOH:O	2.19	0.49
1:A:234:VAL:O	1:A:234:VAL:HG22	2.12	0.49
26:Z:22:ILE:HG23	26:Z:22:ILE:O	2.12	0.49
33:8:175:ILE:O	33:8:175:ILE:HG22	2.11	0.49
34:r:248:U:OP2	41:r:1912:HOH:O	2.19	0.49
34:r:22:G:OP2	35:c:580:ARG:NE	2.44	0.49
24:X:21:GLN:NE2	34:r:1315:A:OP1	2.45	0.49
34:r:1124:G:N2	34:r:1127:A:OP2	2.43	0.49
17:Q:200:CYS:SG	17:Q:224:LEU:HD11	2.53	0.49
7:G:127:LYS:NZ	34:r:1443:A:OP1	2.37	0.49
34:r:1004:G:N2	34:r:1413:U:O4	2.46	0.49
1:A:63:LEU:C	1:A:63:LEU:HD12	2.38	0.48
1:A:184:LEU:HD11	22:V:265:ILE:HD11	1.94	0.48
35:c:413:ILE:HG22	35:c:417:LYS:HE3	1.95	0.48
33:8:169:ALA:HB2	33:8:210:VAL:HG22	1.94	0.48
17:Q:38:PHE:O	34:r:694:A:O2'	2.20	0.48
29:3:34:PHE:HA	29:3:37:VAL:HG12	1.96	0.48
30:4:190:ASP:OD1	30:4:191:ILE:N	2.47	0.48
35:c:408:ARG:HE	35:c:447:GLU:HG2	1.79	0.48
5:E:172:VAL:HG22	5:E:201:ALA:HB1	1.95	0.48
6:F:40:ARG:NE	6:F:72:ASP:OD2	2.46	0.48
34:r:1098:U:OP1	35:c:504:ARG:NH2	2.41	0.48
19:S:19:VAL:HG21	19:S:40:ALA:HB2	1.96	0.48
35:c:167:VAL:HG22	35:c:194:VAL:HB	1.95	0.48
3:C:329:ILE:HD12	3:C:329:ILE:N	2.29	0.47
10:J:43:ALA:HB2	10:J:121:LEU:HD21	1.95	0.47
15:O:83:LEU:HD11	15:O:156:ALA:HB2	1.96	0.47
29:3:92:PHE:CZ	29:3:96:ILE:HD13	2.49	0.47
18:R:97:ARG:NH1	22:V:233:ASP:OD1	2.47	0.47
21:U:61:VAL:O	21:U:61:VAL:HG13	2.15	0.47
17:Q:65:PRO:O	34:r:268:G:O2'	2.30	0.47
20:T:136:GLN:OE1	41:T:201:HOH:O	2.20	0.47
1:A:121:LYS:HB2	1:A:181:VAL:HG21	1.97	0.46
4:D:386:ILE:HG23	4:D:391:LEU:HD21	1.97	0.46
23:W:66:THR:HG22	23:W:66:THR:O	2.15	0.46
35:c:556:LEU:HB3	35:c:560:ASN:HB2	1.97	0.46
1:A:168:GLU:OE1	1:A:168:GLU:N	2.46	0.46
7:G:246:LEU:O	7:G:247:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:315:ILE:O	30:4:316:GLN:C	2.58	0.46
31:5:149:SER:O	31:5:154:GLY:N	2.49	0.46
1:A:180:VAL:HG13	22:V:265:ILE:HD13	1.98	0.46
34:r:1035:C:OP2	35:c:408:ARG:NH2	2.44	0.46
7:G:70:PRO:HD3	7:G:76:VAL:HG22	1.98	0.46
30:4:215:VAL:HG13	30:4:216:MET:N	2.30	0.46
31:5:160:VAL:HG12	31:5:160:VAL:O	2.14	0.46
3:C:169:ASN:O	5:E:91:ARG:NH2	2.49	0.46
3:C:211:SER:OG	25:Y:136:GLU:OE1	2.16	0.46
16:P:12:ARG:NH2	34:r:396:C:OP1	2.46	0.46
25:Y:202:LEU:C	25:Y:202:LEU:HD23	2.41	0.46
12:L:94:TYR:OH	34:r:636:C:OP2	2.27	0.46
35:c:214:ASN:N	35:c:214:ASN:OD1	2.49	0.46
2:B:89:LEU:CD1	7:G:43:VAL:HG13	2.46	0.45
17:Q:146:GLU:OE2	17:Q:150:ARG:NH2	2.49	0.45
32:6:169:GLN:NE2	32:6:275:SER:OG	2.49	0.45
35:c:215:GLU:OE2	35:c:257:THR:OG1	2.34	0.45
17:Q:234:GLN:HB2	17:Q:235:PRO:HD3	1.98	0.45
19:S:53:ILE:HD12	19:S:62:ILE:HD12	1.97	0.45
2:B:85:LYS:C	7:G:43:VAL:HG11	2.41	0.45
7:G:171:THR:HA	34:r:1449:C:H4'	1.98	0.45
15:O:148:GLU:OE1	15:O:151:ASN:ND2	2.49	0.45
34:r:1628:A:H2'	34:r:1629:A:H5'	1.98	0.45
8:H:86:LEU:CD1	8:H:154:VAL:HG13	2.47	0.45
17:Q:140:THR:HA	17:Q:144:LEU:HD12	1.99	0.45
5:E:286:LEU:HD11	32:6:244:PHE:CE2	2.51	0.45
17:Q:134:ALA:CB	17:Q:144:LEU:HD11	2.47	0.45
11:K:180:ILE:O	11:K:184:VAL:HG22	2.17	0.45
28:2:67:PHE:CD1	28:2:91:VAL:HG13	2.52	0.45
29:3:177:PHE:CG	29:3:178:PRO:HD3	2.52	0.45
30:4:292:TYR:O	30:4:296:VAL:HG23	2.16	0.45
35:c:381:LEU:HD21	35:c:519:LEU:CD1	2.46	0.45
20:T:95:ASN:O	20:T:99:ARG:N	2.50	0.45
20:T:165:LEU:HD12	26:Z:10:LEU:HD12	1.98	0.45
34:r:377:A:O2'	34:r:522:A:N7	2.50	0.45
34:r:998:A:H2'	34:r:999:C:C6	2.52	0.45
33:8:340:GLN:O	33:8:344:ARG:NH1	2.49	0.44
34:r:1148:A:H4'	34:r:1149:A:O5'	2.16	0.44
3:C:206:GLU:HG3	3:C:206:GLU:O	2.16	0.44
4:D:478:TYR:CE2	4:D:482:LEU:HD11	2.51	0.44
15:O:161:ARG:HD2	15:O:171:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:119:THR:OG1	16:P:120:LEU:N	2.50	0.44
31:5:96:PRO:O	34:r:1524:U:O2'	2.35	0.44
2:B:257:ARG:NH2	2:B:261:GLU:OE2	2.50	0.44
1:A:237:GLU:HB2	1:A:240:ASP:HB2	1.99	0.44
17:Q:144:LEU:O	17:Q:148:LYS:N	2.45	0.44
34:r:857:A:O2'	34:r:859:A:N7	2.47	0.44
4:D:172:LEU:HD11	4:D:391:LEU:CD1	2.48	0.44
17:Q:80:ASN:OD1	17:Q:84:GLN:NE2	2.51	0.44
34:r:366:G:N2	34:r:369:U:OP2	2.51	0.44
3:C:34:LYS:HD3	7:G:46:TRP:CD2	2.53	0.44
34:r:132:A:N3	34:r:267:A:O2'	2.46	0.44
35:c:374:PRO:HG3	35:c:513:CYS:O	2.17	0.44
1:A:194:LYS:HA	34:r:907:A:H5"	1.99	0.44
1:A:234:VAL:HB	1:A:268:GLY:O	2.18	0.44
13:M:25:TYR:CE2	34:r:1398:U:H4'	2.52	0.44
26:Z:26:GLU:O	26:Z:70:ARG:NH2	2.51	0.44
30:4:16:ARG:NH2	30:4:49:ASP:OD1	2.51	0.44
33:8:438:GLN:OE1	33:8:438:GLN:N	2.49	0.44
34:r:1048:A:O2'	34:r:1096:C:O2	2.32	0.44
8:H:99:ILE:HG21	8:H:118:ILE:HD11	1.99	0.43
27:1:90:LYS:NZ	34:r:1604:U:OP2	2.46	0.43
34:r:822:U:H2'	34:r:823:G:O4'	2.17	0.43
2:B:106:LEU:HD12	3:C:53:MET:HE2	2.00	0.43
31:5:54:TYR:HB2	31:5:94:VAL:HG21	2.00	0.43
1:A:7:LEU:HA	2:B:189:MET:HE1	1.99	0.43
7:G:247:LYS:OXT	7:G:247:LYS:HG2	2.19	0.43
10:J:92:PRO:O	10:J:94:VAL:HG13	2.18	0.43
15:O:198:ASP:OD2	15:O:201:ASN:ND2	2.51	0.43
34:r:493:A:C2'	34:r:494:U:H5'	2.49	0.43
34:r:1362:A:H2'	34:r:1363:U:O4'	2.18	0.43
1:A:10:SER:HB3	2:B:189:MET:CE	2.47	0.43
1:A:126:LYS:O	1:A:130:GLY:N	2.49	0.43
1:A:172:ASN:OD1	1:A:173:SER:N	2.52	0.43
1:A:43:LEU:HD22	1:A:61:ARG:HG2	2.01	0.43
3:C:391:ILE:HG22	3:C:393:VAL:HG23	2.00	0.43
12:L:31:LEU:HD11	17:Q:33:ILE:HB	2.00	0.43
31:5:65:ILE:HG22	31:5:65:ILE:O	2.17	0.43
16:P:71:ARG:HG2	32:6:314:VAL:HG21	2.01	0.43
17:Q:128:ILE:O	17:Q:128:ILE:HG22	2.18	0.43
31:5:142:VAL:HG11	31:5:178:VAL:CG1	2.48	0.43
15:O:249:ARG:NE	34:r:828:A:OP1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:129:ASP:OD1	33:8:271:LYS:NZ	2.52	0.43
34:r:303:G:N2	34:r:306:A:OP2	2.49	0.43
34:r:983:A:H2'	34:r:984:A:O4'	2.19	0.43
15:O:149:ASN:ND2	34:r:806:A:OP1	2.51	0.43
17:Q:70:LYS:NZ	34:r:259:G:OP1	2.52	0.43
31:5:117:LEU:HD23	31:5:162:LEU:HD12	2.01	0.43
34:r:522:A:H61	34:r:527:G:H5'	1.84	0.43
35:c:290:ASP:OD2	35:c:322:ARG:NH2	2.51	0.43
35:c:307:VAL:HG12	35:c:309:ILE:CD1	2.49	0.43
10:J:55:LEU:HD21	10:J:109:ARG:HG2	2.00	0.43
16:P:88:LYS:NZ	34:r:523:U:O5'	2.52	0.43
30:4:139:GLN:CD	30:4:149:LEU:HD11	2.44	0.43
30:4:175:ARG:NH2	30:4:184:ASN:OD1	2.52	0.43
35:c:496:ARG:NH1	35:c:542:GLY:O	2.50	0.43
34:r:689:C:H2'	34:r:690:G:O4'	2.19	0.43
34:r:1009:G:O3'	34:r:1010:G:H8	2.02	0.43
35:c:84:VAL:HG13	35:c:208:ILE:HG23	2.00	0.43
3:C:236:ILE:HG13	3:C:236:ILE:O	2.19	0.42
8:H:91:LEU:HD23	8:H:152:CYS:HB3	2.01	0.42
23:W:100:GLN:O	23:W:104:LEU:HD13	2.18	0.42
4:D:395:GLU:N	4:D:396:PRO:HD2	2.34	0.42
33:8:499:TRP:O	33:8:500:LYS:C	2.62	0.42
34:r:814:A:N7	41:r:1985:HOH:O	2.36	0.42
1:A:238:ASN:O	1:A:239:ASN:HB2	2.20	0.42
7:G:63:LEU:HD12	7:G:64:PRO:HD2	2.00	0.42
23:W:199:PHE:HB2	23:W:318:LEU:HD23	2.01	0.42
3:C:160:ILE:HG22	3:C:160:ILE:O	2.19	0.42
24:X:57:ARG:NH1	34:r:1061:U:OP1	2.51	0.42
34:r:69:U:OP1	34:r:389:A:O2'	2.31	0.42
35:c:75:ARG:NH2	35:c:543:ASP:OD2	2.40	0.42
35:c:132:ILE:O	35:c:132:ILE:HG22	2.19	0.42
35:c:324:ARG:NH1	35:c:377:ARG:O	2.50	0.42
3:C:179:LEU:O	3:C:182:ILE:HG13	2.18	0.42
9:I:39:PRO:HB3	9:I:44:PHE:CG	2.55	0.42
17:Q:58:VAL:HG12	17:Q:77:ILE:HD13	2.01	0.42
31:5:327:THR:HB	31:5:328:PRO:HD3	2.01	0.42
4:D:172:LEU:HD11	4:D:391:LEU:HD13	2.00	0.42
31:5:82:PRO:O	31:5:83:LYS:HB2	2.19	0.42
34:r:1450:U:H5'	34:r:1451:A:P	2.60	0.42
3:C:45:MET:CG	25:Y:312:VAL:HG13	2.50	0.42
9:I:170:VAL:HG22	9:I:171:ARG:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:8:128:ASN:HD21	33:8:181:VAL:HG12	1.83	0.42
33:8:180:ASP:O	33:8:181:VAL:CG2	2.68	0.42
34:r:1519:U:H2'	34:r:1520:U:O4'	2.20	0.42
4:D:166:PRO:HB2	4:D:171:ALA:HB2	2.01	0.42
21:U:236:SER:O	21:U:237:ASN:C	2.63	0.42
4:D:432:SER:N	4:D:433:PRO:HD2	2.35	0.42
29:3:253:TRP:O	29:3:257:ASN:ND2	2.52	0.42
2:B:354:LEU:HD21	21:U:1:MET:HE1	2.02	0.41
24:X:28:ILE:O	24:X:30:THR:HG23	2.20	0.41
34:r:1363:U:H2'	34:r:1364:A:O4'	2.19	0.41
15:O:76:ILE:HA	38:O:301:LMT:H121	2.03	0.41
1:A:184:LEU:HD11	22:V:265:ILE:CD1	2.50	0.41
3:C:188:ASN:ND2	25:Y:79:GLU:OE2	2.54	0.41
34:r:740:A:H2'	34:r:741:A:O4'	2.20	0.41
4:D:171:ALA:HB1	4:D:411:VAL:HG12	2.02	0.41
12:L:93:ALA:HB1	12:L:125:VAL:HG13	2.02	0.41
34:r:998:A:H2'	34:r:999:C:C5	2.55	0.41
34:r:1510:A:O2'	34:r:1512:A:O5'	2.37	0.41
7:G:163:LEU:HD11	26:Z:55:VAL:HG13	2.02	0.41
22:V:287:ASP:O	22:V:291:ILE:HG22	2.20	0.41
33:8:61:LEU:HD11	33:8:153:LEU:HD11	2.02	0.41
34:r:1177:A:N3	34:r:1177:A:H2'	2.35	0.41
35:c:334:PRO:O	35:c:377:ARG:NH2	2.49	0.41
7:G:246:LEU:CD1	21:U:233:ALA:HB1	2.49	0.41
34:r:550:U:H2'	34:r:551:U:O4'	2.21	0.41
2:B:136:ALA:O	29:3:161:LYS:NZ	2.54	0.41
21:U:125:ASN:O	21:U:126:GLU:HG3	2.21	0.41
35:c:370:ILE:HD11	35:c:457:GLU:HB2	2.03	0.41
1:A:113:ARG:HB3	1:A:114:PRO:HD2	2.02	0.41
1:A:176:LEU:O	1:A:180:VAL:HG23	2.21	0.41
3:C:62:MET:HE1	9:I:139:LEU:HD22	2.03	0.41
3:C:220:PHE:CD2	3:C:393:VAL:HG11	2.55	0.41
18:R:42:ASP:OD1	18:R:43:GLN:N	2.54	0.41
34:r:153:C:N4	34:r:154:U:O4	2.54	0.41
34:r:936:A:H2'	34:r:936:A:N3	2.36	0.41
35:c:104:VAL:HG21	35:c:126:MET:HG3	2.02	0.41
35:c:309:ILE:HD12	35:c:309:ILE:N	2.36	0.41
10:J:123:MET:HE1	25:Y:168:TYR:CG	2.55	0.41
18:R:44:SER:O	18:R:69:ARG:NH2	2.54	0.41
30:4:208:PHE:O	30:4:209:ASN:HB3	2.20	0.41
30:4:237:LEU:O	30:4:238:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:r:58:A:N7	34:r:114:U:O2'	2.52	0.41
35:c:488:ASP:OD1	35:c:493:SER:OG	2.31	0.41
11:K:103:ASN:OD1	11:K:104:LYS:N	2.53	0.40
20:T:128:ASN:ND2	20:T:132:ASP:OD1	2.54	0.40
22:V:29:GLN:OE1	22:V:32:ILE:HD12	2.21	0.40
23:W:66:THR:HG23	34:r:1355:U:H5'	2.03	0.40
31:5:175:ASN:N	31:5:176:PRO:HD3	2.37	0.40
33:8:151:VAL:HG13	33:8:168:TRP:HE1	1.86	0.40
3:C:316:MET:O	3:C:322:LYS:NZ	2.54	0.40
30:4:183:ARG:NH1	30:4:264:GLU:OE1	2.52	0.40
31:5:193:LEU:HD21	31:5:235:LEU:HA	2.03	0.40
34:r:1001:U:H4'	35:c:419:LYS:NZ	2.36	0.40
10:J:91:SER:N	10:J:92:PRO:HD2	2.35	0.40
17:Q:134:ALA:HB1	17:Q:144:LEU:HD11	2.02	0.40
33:8:147:MET:HG2	33:8:169:ALA:HB3	2.03	0.40
34:r:1362:A:O2'	34:r:1363:U:O5'	2.27	0.40
2:B:336:ILE:HG23	21:U:6:ASN:HB3	2.04	0.40
9:I:118:PRO:O	9:I:121:THR:HG22	2.22	0.40
31:5:230:ILE:HG22	31:5:284:LEU:HD22	2.03	0.40
33:8:457:THR:HG22	33:8:459:ARG:H	1.86	0.40
1:A:119:HIS:HB3	1:A:122:LEU:HB3	2.03	0.40
30:4:239:ASP:OD1	30:4:240:SER:N	2.54	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	A	299/344 (87%)	285 (95%)	14 (5%)	0	100	100
2	B	338/394 (86%)	329 (97%)	9 (3%)	0	100	100
3	C	309/398 (78%)	301 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	337/486 (69%)	333 (99%)	4 (1%)	0	100	100
5	E	292/307 (95%)	283 (97%)	9 (3%)	0	100	100
6	F	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
7	G	199/247 (81%)	196 (98%)	3 (2%)	0	100	100
8	H	153/154 (99%)	151 (99%)	2 (1%)	0	100	100
9	I	230/278 (83%)	226 (98%)	4 (2%)	0	100	100
10	J	158/203 (78%)	154 (98%)	4 (2%)	0	100	100
11	K	150/217 (69%)	146 (97%)	4 (3%)	0	100	100
12	L	121/153 (79%)	119 (98%)	2 (2%)	0	100	100
13	M	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
14	N	111/115 (96%)	111 (100%)	0	0	100	100
15	O	219/286 (77%)	217 (99%)	2 (1%)	0	100	100
16	P	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
17	Q	234/237 (99%)	232 (99%)	2 (1%)	0	100	100
18	R	99/138 (72%)	98 (99%)	1 (1%)	0	100	100
19	S	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
20	T	91/177 (51%)	90 (99%)	1 (1%)	0	100	100
21	U	235/264 (89%)	230 (98%)	5 (2%)	0	100	100
22	V	282/318 (89%)	279 (99%)	3 (1%)	0	100	100
23	W	400/450 (89%)	390 (98%)	10 (2%)	0	100	100
24	X	96/110 (87%)	96 (100%)	0	0	100	100
25	Y	270/319 (85%)	266 (98%)	4 (2%)	0	100	100
26	Z	90/95 (95%)	86 (96%)	4 (4%)	0	100	100
27	1	29/111 (26%)	29 (100%)	0	0	100	100
28	2	100/130 (77%)	98 (98%)	2 (2%)	0	100	100
29	3	255/266 (96%)	246 (96%)	9 (4%)	0	100	100
30	4	301/321 (94%)	288 (96%)	13 (4%)	0	100	100
31	5	289/339 (85%)	282 (98%)	7 (2%)	0	100	100
32	6	317/345 (92%)	310 (98%)	7 (2%)	0	100	100
33	8	465/500 (93%)	450 (97%)	15 (3%)	0	100	100
35	c	475/628 (76%)	465 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7385/8816 (84%)	7217 (98%)	168 (2%)	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	A	270/309 (87%)	270 (100%)	0	100	100
2	B	307/350 (88%)	307 (100%)	0	100	100
3	C	312/385 (81%)	312 (100%)	0	100	100
4	D	306/437 (70%)	305 (100%)	1 (0%)	86	94
5	E	253/266 (95%)	253 (100%)	0	100	100
6	F	120/120 (100%)	120 (100%)	0	100	100
7	G	174/211 (82%)	174 (100%)	0	100	100
8	H	141/140 (101%)	141 (100%)	0	100	100
9	I	205/245 (84%)	205 (100%)	0	100	100
10	J	146/183 (80%)	146 (100%)	0	100	100
11	K	131/192 (68%)	131 (100%)	0	100	100
12	L	102/131 (78%)	102 (100%)	0	100	100
13	M	100/121 (83%)	100 (100%)	0	100	100
14	N	101/103 (98%)	101 (100%)	0	100	100
15	O	192/250 (77%)	192 (100%)	0	100	100
16	P	105/106 (99%)	105 (100%)	0	100	100
17	Q	217/218 (100%)	217 (100%)	0	100	100
18	R	89/121 (74%)	89 (100%)	0	100	100
19	S	68/78 (87%)	68 (100%)	0	100	100
20	T	82/159 (52%)	82 (100%)	0	100	100
21	U	212/236 (90%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	V	260/287 (91%)	260 (100%)	0	100	100
23	W	369/409 (90%)	369 (100%)	0	100	100
24	X	85/92 (92%)	85 (100%)	0	100	100
25	Y	249/289 (86%)	249 (100%)	0	100	100
26	Z	83/85 (98%)	83 (100%)	0	100	100
27	1	30/98 (31%)	30 (100%)	0	100	100
28	2	93/117 (80%)	93 (100%)	0	100	100
29	3	232/240 (97%)	231 (100%)	1 (0%)	84	92
30	4	267/281 (95%)	267 (100%)	0	100	100
31	5	259/303 (86%)	259 (100%)	0	100	100
32	6	289/312 (93%)	289 (100%)	0	100	100
33	8	413/444 (93%)	413 (100%)	0	100	100
35	c	433/564 (77%)	431 (100%)	2 (0%)	81	91
All	All	6695/7882 (85%)	6691 (100%)	4 (0%)	87	96

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

Mol	Chain	Res	Type
4	D	484	ASN
29	3	95	ASN
35	c	214	ASN
35	c	572	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	46	GLN
2	B	255	GLN
2	B	381	GLN
3	C	103	ASN
4	D	43	GLN
4	D	66	GLN
5	E	15	HIS
5	E	51	ASN
5	E	114	ASN
7	G	144	GLN

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Mol	Chain	Res	Type
8	H	34	GLN
8	H	122	GLN
8	H	134	ASN
9	I	247	HIS
11	K	79	HIS
12	L	77	GLN
13	M	48	HIS
13	M	49	GLN
13	M	103	HIS
15	O	54	GLN
17	Q	4	GLN
18	R	110	GLN
20	T	128	ASN
22	V	98	GLN
22	V	215	GLN
23	W	201	GLN
25	Y	109	HIS
25	Y	246	GLN
28	2	64	ASN
28	2	80	ASN
28	2	96	ASN
29	3	159	ASN
29	3	170	ASN
29	3	180	ASN
30	4	38	GLN
30	4	69	HIS
30	4	79	HIS
30	4	135	ASN
31	5	143	GLN
31	5	305	GLN
32	6	169	GLN
32	6	260	HIS
32	6	325	ASN
33	8	128	ASN
33	8	464	HIS
35	c	81	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	r	1474/1647 (89%)	165 (11%)	0

All (165) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	r	13	U
34	r	16	G
34	r	29	G
34	r	39	A
34	r	46	A
34	r	54	C
34	r	55	A
34	r	58	A
34	r	73	A
34	r	86	A
34	r	88	A
34	r	101	U
34	r	102	G
34	r	104	G
34	r	109	A
34	r	122	U
34	r	129	G
34	r	132	A
34	r	135	A
34	r	137	U
34	r	139	A
34	r	167	U
34	r	195	U
34	r	219	U
34	r	235	A
34	r	251	G
34	r	255	G
34	r	270	G
34	r	271	U
34	r	294	A
34	r	334	U
34	r	336	U
34	r	351	A
34	r	356	C
34	r	371	U
34	r	376	C
34	r	401	A
34	r	414	A
34	r	420	A
34	r	421	A
34	r	477	A
34	r	478	U

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Mol	Chain	Res	Type
34	r	485	A
34	r	494	U
34	r	495	U
34	r	496	A
34	r	501	U
34	r	519	A
34	r	527	G
34	r	537	A
34	r	538	C
34	r	550	U
34	r	560	A
34	r	604	A
34	r	624	U
34	r	625	A
34	r	635	G
34	r	661	A
34	r	674	A
34	r	676	G
34	r	682	A
34	r	685	G
34	r	686	A
34	r	694	A
34	r	698	A
34	r	705	U
34	r	707	U
34	r	716	A
34	r	749	A
34	r	753	A
34	r	763	A
34	r	820	A
34	r	842	A
34	r	858	U
34	r	859	A
34	r	880	A
34	r	882	C
34	r	905	A
34	r	906	U
34	r	907	A
34	r	908	U
34	r	913	U
34	r	931	A
34	r	936	A

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Mol	Chain	Res	Type
34	r	991	G
34	r	999	C
34	r	1009	G
34	r	1010	G
34	r	1025	U
34	r	1029	A
34	r	1030	U
34	r	1031	A
34	r	1036	A
34	r	1037	C
34	r	1038	G
34	r	1041	U
34	r	1043	A
34	r	1058	G
34	r	1060	A
34	r	1067	A
34	r	1099	U
34	r	1101	C
34	r	1111	U
34	r	1131	U
34	r	1135	G
34	r	1139	A
34	r	1141	G
34	r	1148	A
34	r	1177	A
34	r	1188	A
34	r	1203	U
34	r	1216	A
34	r	1222	U
34	r	1231	U
34	r	1232	C
34	r	1233	A
34	r	1235	A
34	r	1237	U
34	r	1245	A
34	r	1258	U
34	r	1270	A
34	r	1271	A
34	r	1273	A
34	r	1279	A
34	r	1280	U
34	r	1281	A

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Mol	Chain	Res	Type
34	r	1282	A
34	r	1292	A
34	r	1303	U
34	r	1304	U
34	r	1320	A
34	r	1326	U
34	r	1366	U
34	r	1367	A
34	r	1369	U
34	r	1413	U
34	r	1414	A
34	r	1422	G
34	r	1428	U
34	r	1439	G
34	r	1451	A
34	r	1462	A
34	r	1466	A
34	r	1511	U
34	r	1512	A
34	r	1519	U
34	r	1547	A
34	r	1584	A
34	r	1586	G
34	r	1595	C
34	r	1598	U
34	r	1609	G
34	r	1611	A
34	r	1621	G
34	r	1622	G
34	r	1624	U
34	r	1625	U
34	r	1628	A
34	r	1629	A
34	r	1630	A
34	r	1633	U
34	r	1637	A
34	r	1644	C
34	r	1647	A
34	r	1649	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SAC	H	2	8	7,8,9	0.22	0	8,9,11	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SAC	H	2	8	-	0/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 128 ligands modelled in this entry, 125 are monoatomic - leaving 3 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	LMT	O	301	-	12,12,36	0.15	0	11,11,47	0.19	0
40	SF4	c	701	35	0,12,12	-	-	-		
39	ATP	W	501	36	29,33,33	0.49	0	44,52,52	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LMT	O	301	-	-	0/10/10/61	-
40	SF4	c	701	35	-	-	0/6/5/5
39	ATP	W	501	36	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

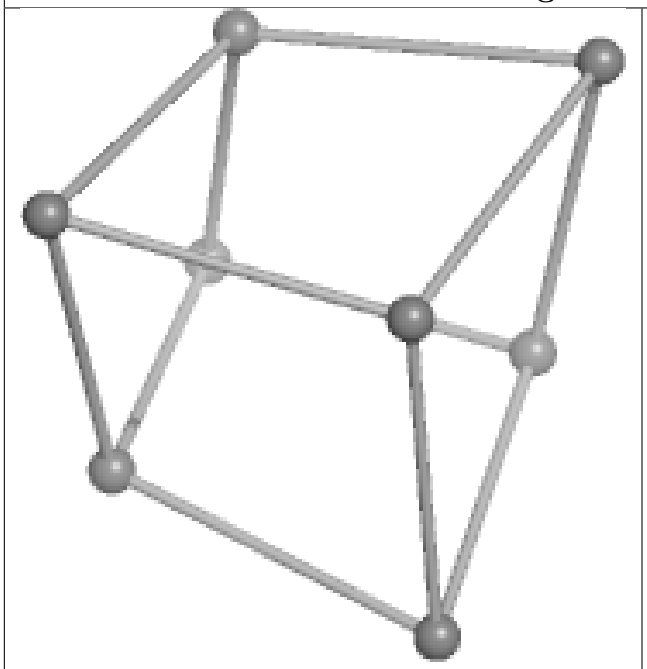
There are no ring outliers.

1 monomer is involved in 2 short contacts:

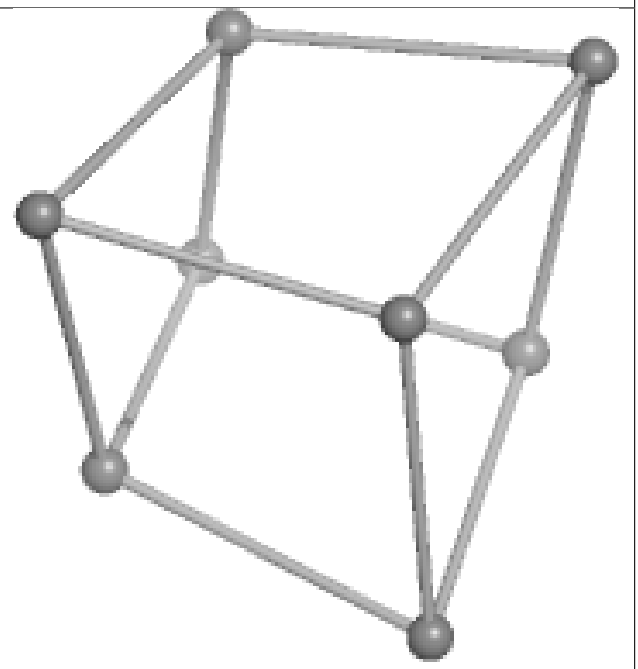
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	O	301	LMT	2	0

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 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.

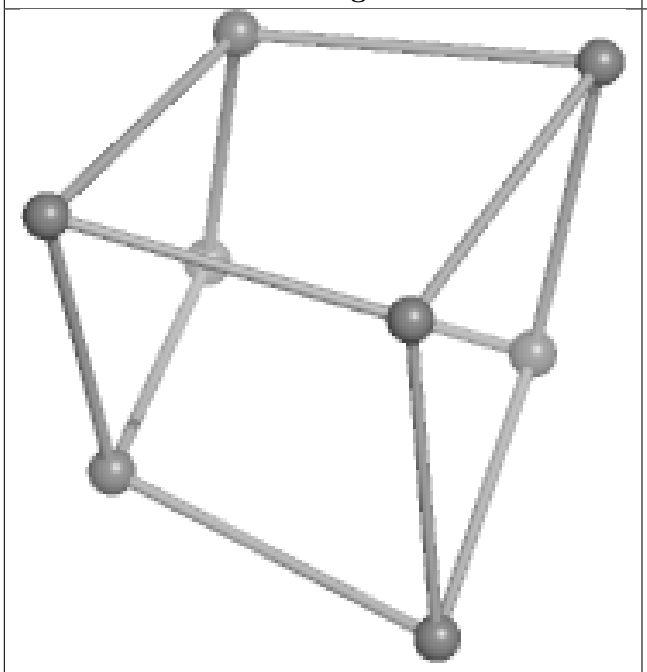
Ligand SF4 c 701



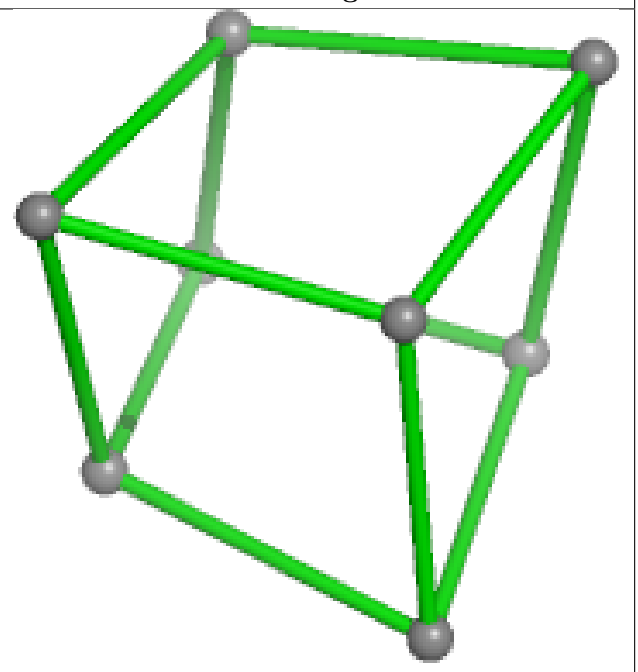
Bond lengths



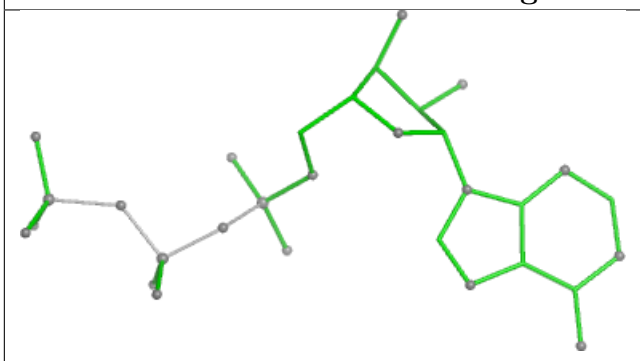
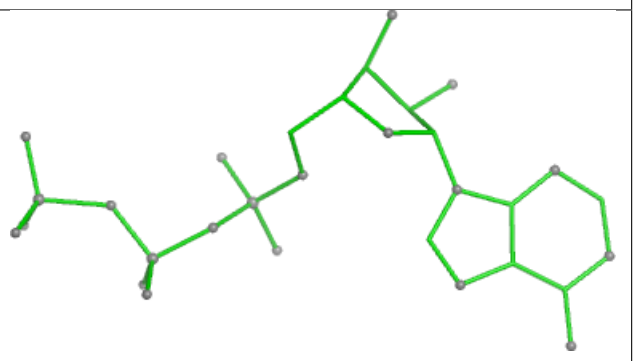
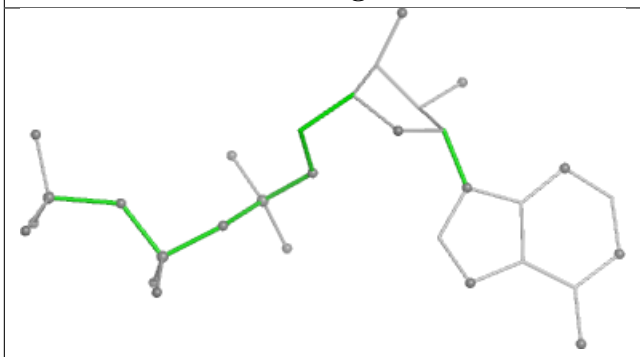
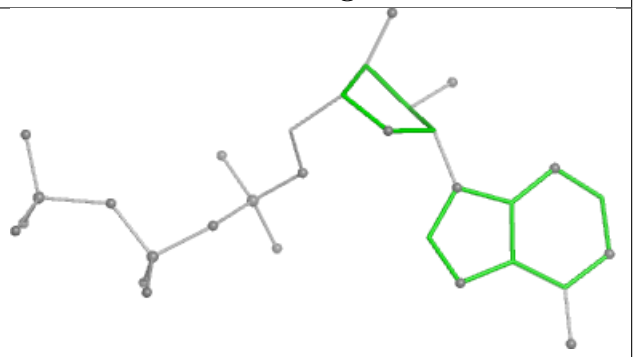
Bond angles



Torsions



Rings

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)

There are no chain breaks in this entry.

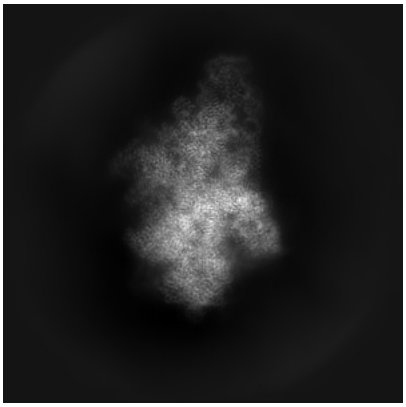
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16966. These allow visual inspection of the internal detail of the map and identification of artifacts.

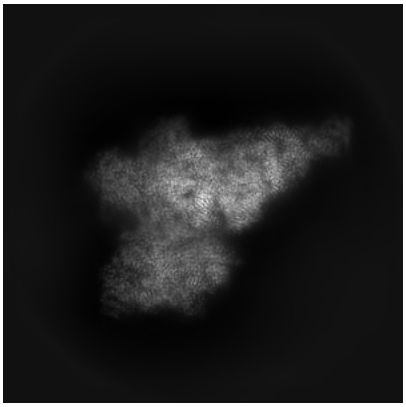
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

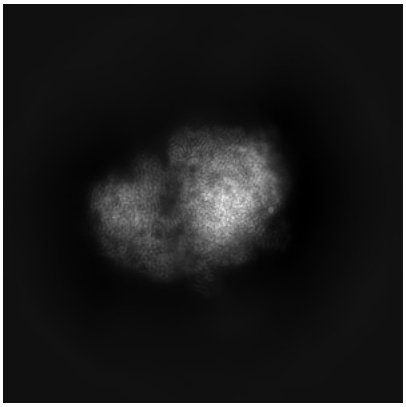
6.1.1 Primary map



X



Y



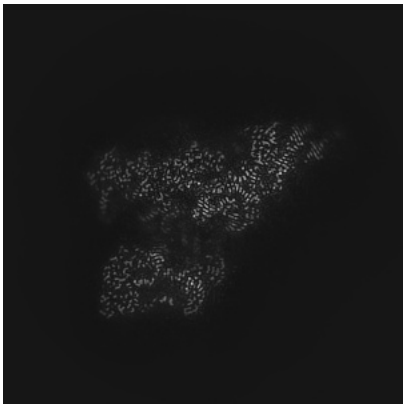
Z

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

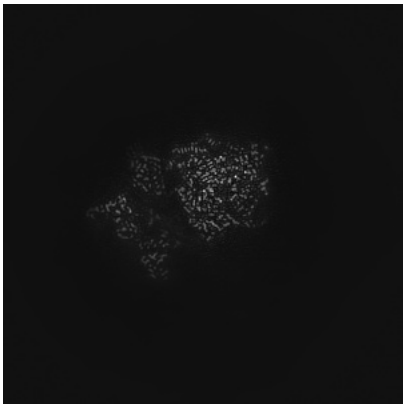
6.2 Central slices (i)

6.2.1 Primary map

X Index: 336



Y Index: 336

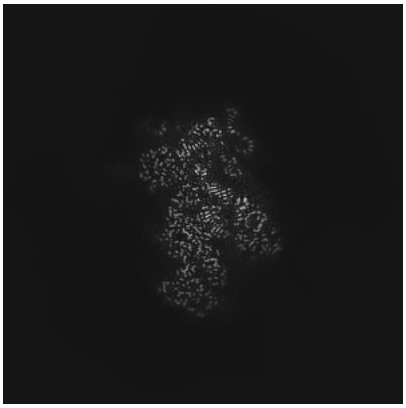


Z Index: 336

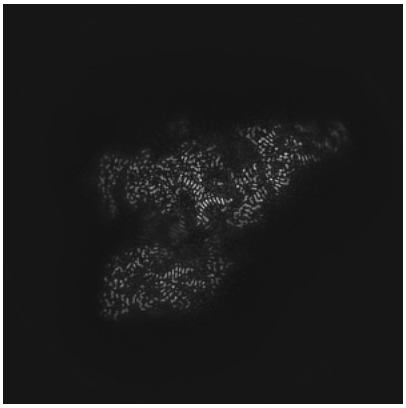
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

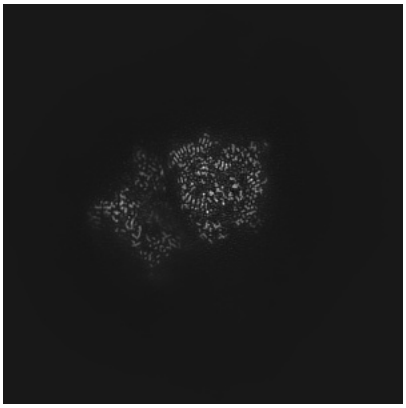
6.3.1 Primary map



X Index: 369



Y Index: 345

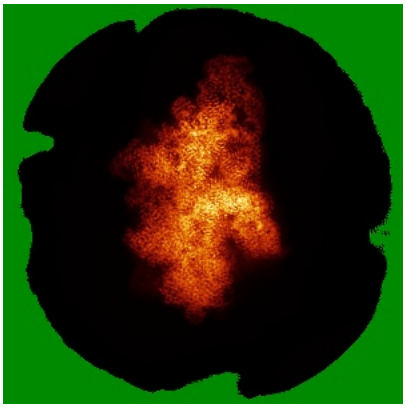


Z Index: 329

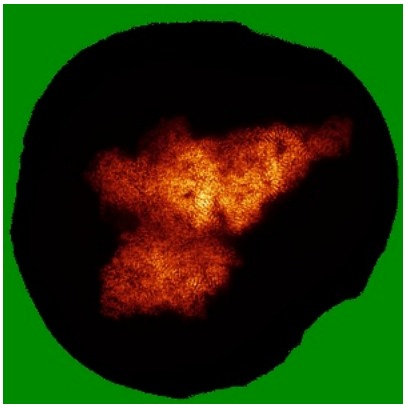
The images above show the largest variance slices of the map in three orthogonal directions.

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

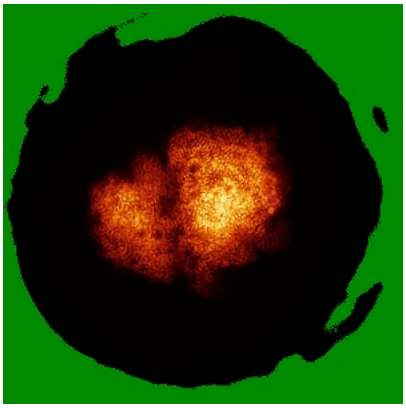
6.4.1 Primary map



X



Y

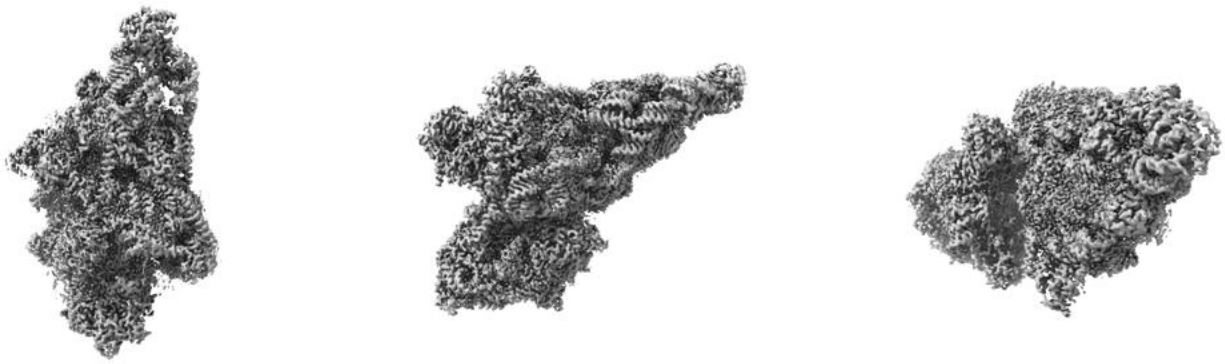


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

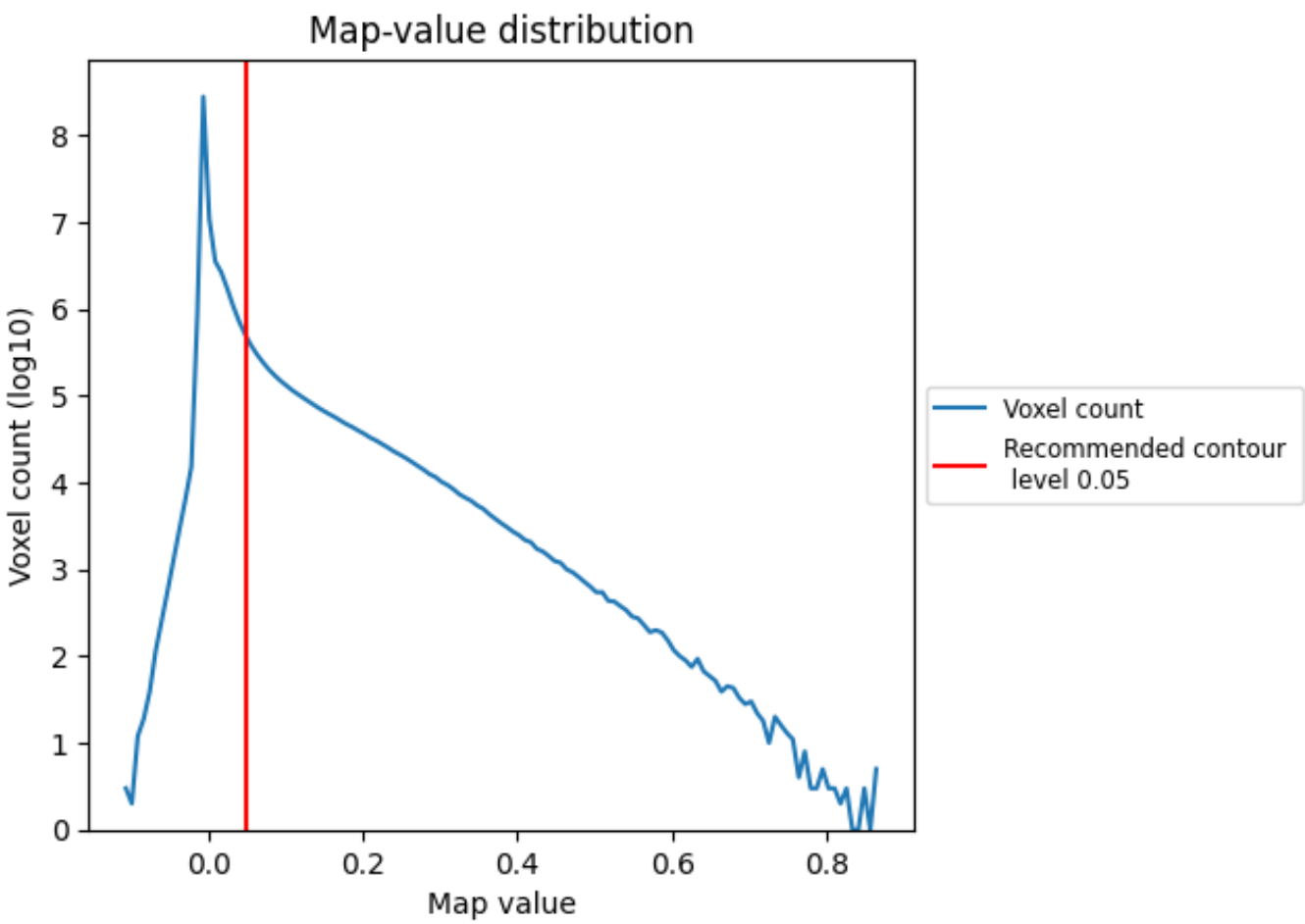
6.6 Mask visualisation (i)

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

7 Map analysis (i)

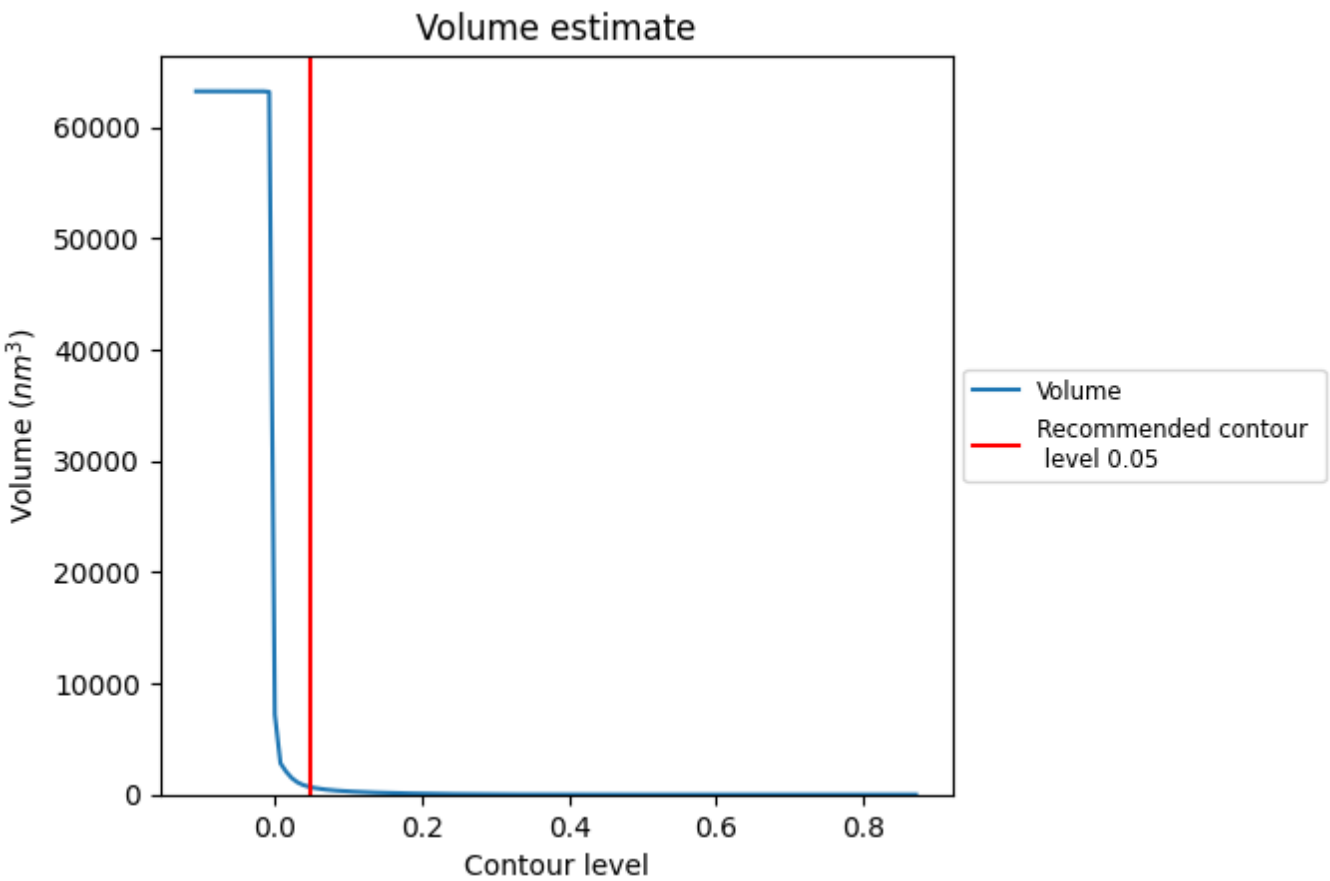
This section contains the results of statistical analysis of the map.

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.

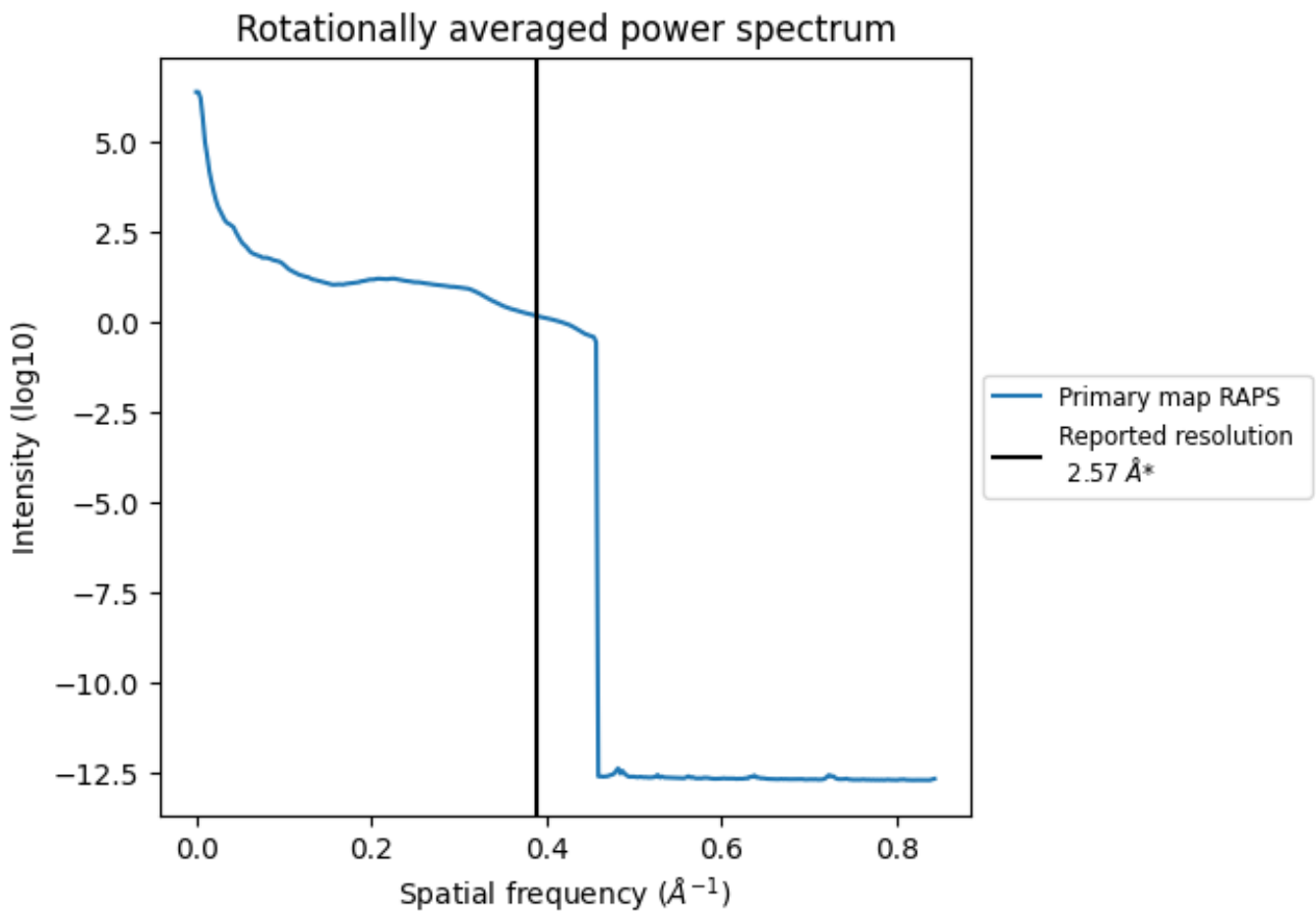
7.2 Volume estimate (i)



The volume at the recommended contour level is 661 nm^3; this corresponds to an approximate mass of 597 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 0.389 Å^{-1}

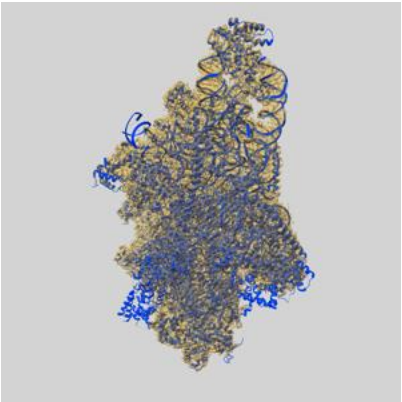
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

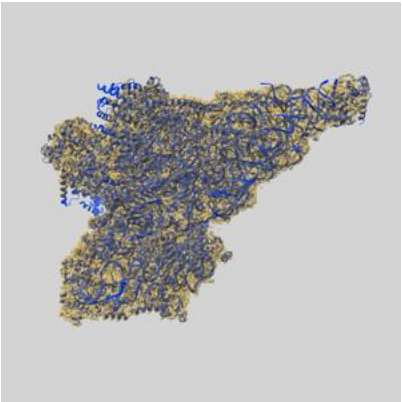
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16966 and PDB model 8OM2. Per-residue inclusion information can be found in section 3 on page 15.

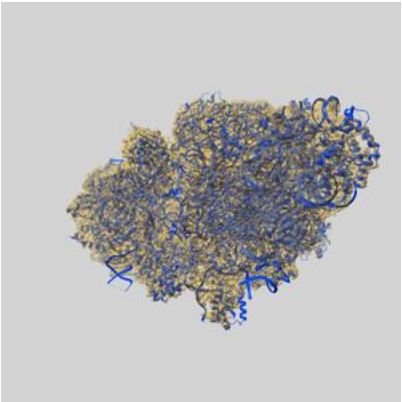
9.1 Map-model overlay (i)



X



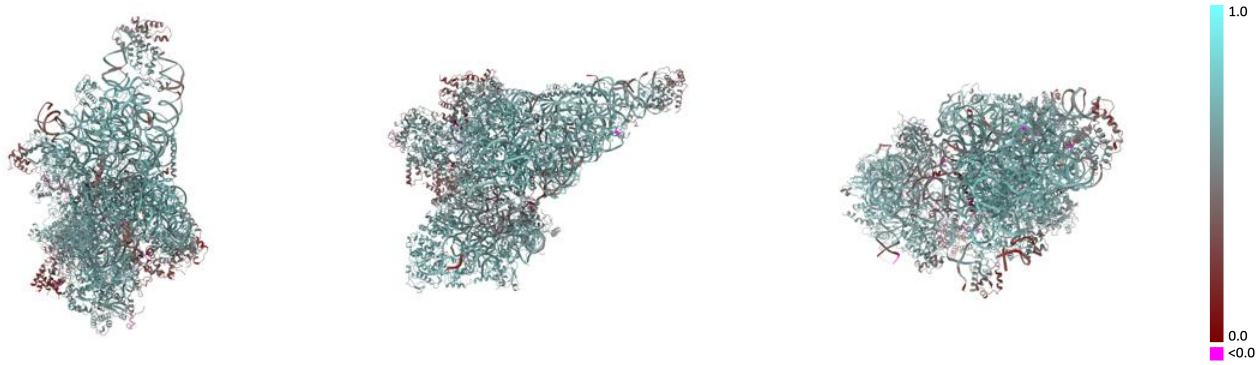
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

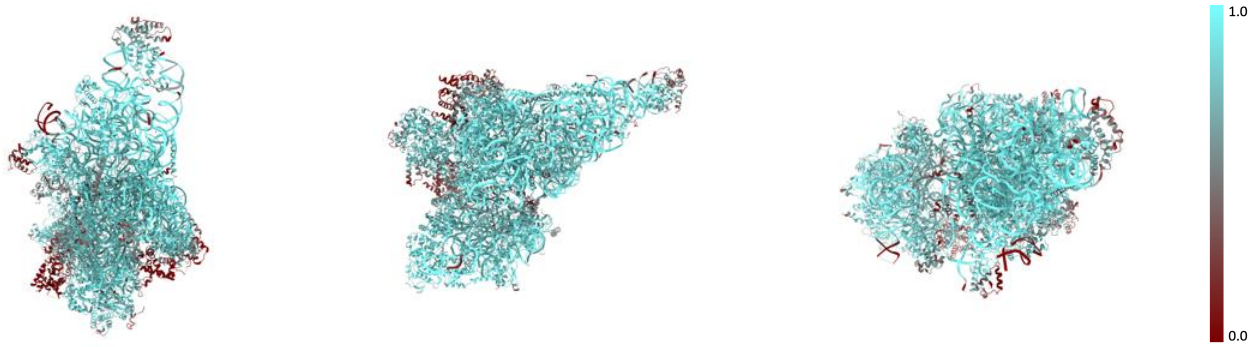
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

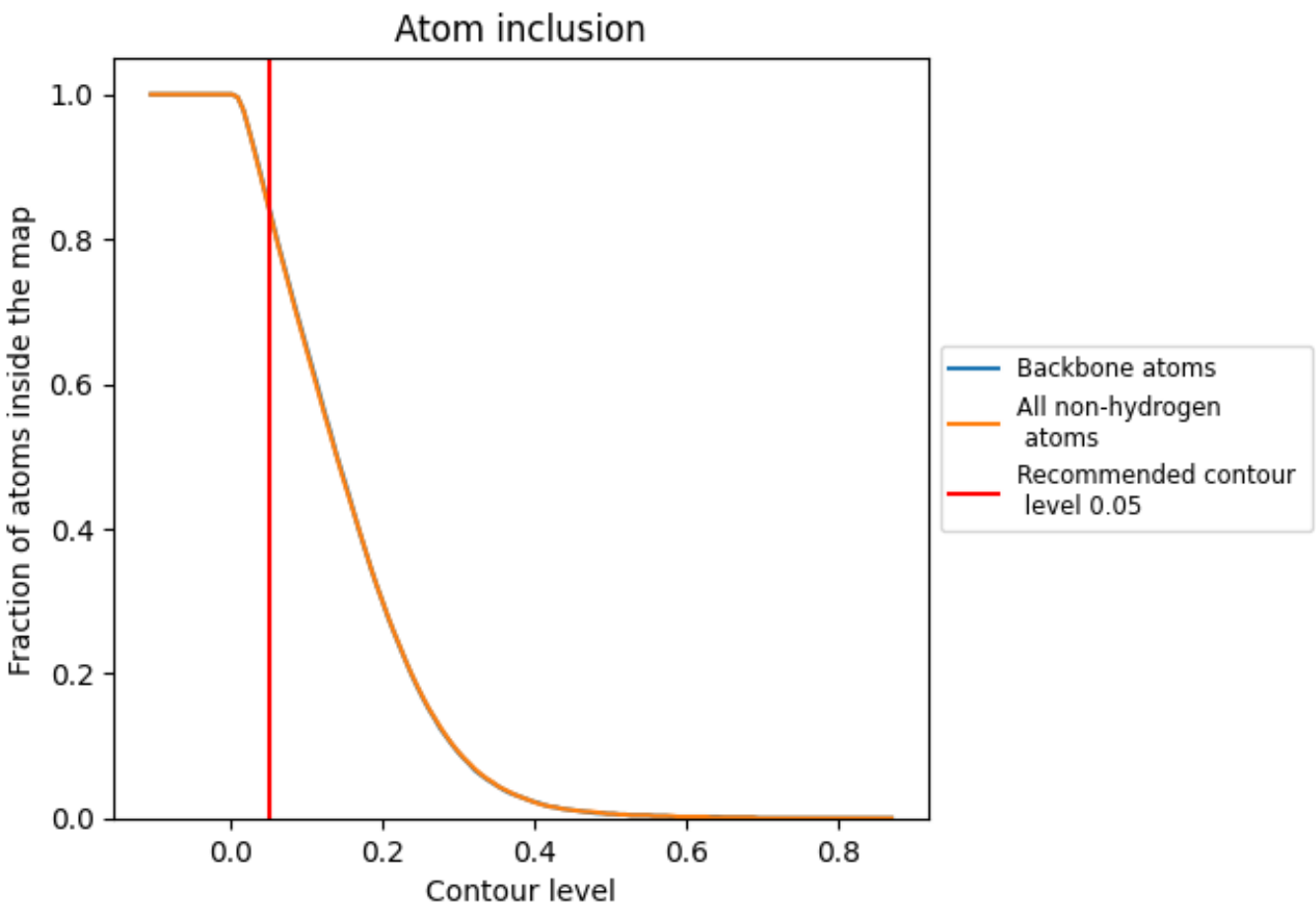
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.6020
1	0.8100	0.6080
2	0.9120	0.6400
3	0.8750	0.6140
4	0.7200	0.5230
5	0.6470	0.4900
6	0.8900	0.6260
8	0.6220	0.5810
A	0.6220	0.5210
B	0.7440	0.5920
C	0.5890	0.4970
D	0.8220	0.6110
E	0.8970	0.6540
F	0.8870	0.6260
G	0.6720	0.5370
H	0.9690	0.7000
I	0.8810	0.6300
J	0.8760	0.6350
K	0.8290	0.5890
L	0.9730	0.6820
M	0.9290	0.6520
N	0.9590	0.6720
O	0.8860	0.6450
P	0.9240	0.6630
Q	0.6720	0.5270
R	0.8730	0.6140
S	0.8790	0.6130
T	0.8390	0.5920
U	0.9210	0.6540
V	0.7520	0.5690
W	0.9200	0.6590
X	0.8830	0.5970
Y	0.7710	0.5910
Z	0.7630	0.5590
c	0.7770	0.5280
r	0.9290	0.6220