Full wwPDB EM Validation Report (i)

Apr 17, 2024 – 07:21 pm BST

PDB ID	:	7PO2
EMDB ID	:	EMD-13560
Title	:	Initiation complex of human mitochondrial ribosome small subunit with IF2, fMet-tRNAMet and mRNA
Authors	:	Itoh, Y.; Khawaja, A.; Rorbach, J.; Amunts, A.
Deposited on	:	2021-09-08
Resolution	:	3.09 Å(reported)
Based on initial model	:	6RW4

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 (1)) were used in the production of this report:

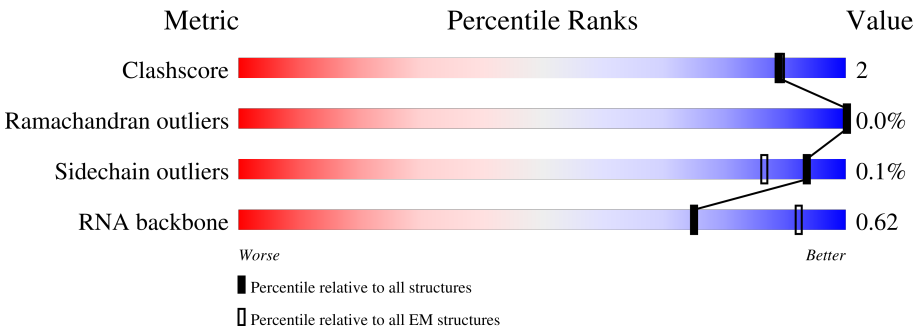
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.09 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	A	955	80% 19%
2	B	296	74% 24%
3	C	167	75% 21%
4	D	430	76% 20%
5	E	125	97%
6	F	242	5% 82% 14%
7	G	396	6% 79% 17%

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Mol	Chain	Length	Quality of chain
8	H	201	64% 6% 30%
9	I	194	65% 5% 29%
10	J	138	72% 6% 22%
11	K	128	75% 21%
12	L	257	7% 64% 32%
13	M	137	5% 85% 13%
14	N	130	78% 6% 15%
15	O	258	73% 25%
16	P	142	65% 32%
17	Q	86	98%
18	R	360	79% 18%
19	S	190	6% 68% 29%
20	T	173	94%
21	U	205	5% 85% 14%
22	V	414	6% 83% 5% 13%
23	W	187	53% 47%
24	X	398	84% 5% 12%
25	Y	395	7% 36% 62%
26	Z	106	6% 92% 6%
27	0	218	92% 6%
28	1	323	6% 83% 14%
29	2	117	96%
30	3	199	34% 64%
31	4	689	23% 81% 5% 14%
32	5	71	49% 79% 18%

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Mol	Chain	Length	Quality of chain
33	6	31	32% 45% 45% 10%
34	7	727	27% 72% 6% 21%
35	t	198	36% 36% 64%

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 139146 atoms, of which 63971 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 RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	955	30595	9098	10313	3652	6577	955	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	132	2172	699	1089	195	185	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	343	5536	1713	2805	518	487	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	122	1973	614	1001	177	177	4	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	208	3495	1104	1770	312	298	11	0	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	327	5378	1710	2690	477	487	14	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	140	2336	745	1184	194	210	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	137	2081	642	1061	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	108	1727	521	888	169	143	6	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	101	1748	537	886	179	141	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	174	2994	925	1541	270	251	7	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	N	110	1797	562	929	156	147	3	0	0

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	O	193	3149	1014	1557	294	277	7	0	0

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 17 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	Q	86	1502	460	758	150	126	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	ARG	CYS	variant	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	R	295	4838	1533	2429	413	455	8	0	0

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	S	135	2227	716	1116	198	196	1	0	0

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	T	168	2765	877	1394	239	244	11	0	0

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	U	176	2988	916	1500	301	267	4	0	0

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	V	362	5933	1904	2964	495	558	12	0	0

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	W	100	1592	498	803	141	146	4	0	0

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	X	352	5694	1822	2845	499	517	11	0	0

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	Y	149	2444	801	1198	207	234	4	0	0

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	Z	100	1699	534	860	153	148	4	0	0

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	0	215	3584	1130	1797	339	313	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	1	278	4545	1430	2289	386	429	11	0	0

- Molecule 29 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	2	117	1904	579	969	182	166	8	0	0

- Molecule 30 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	3	71	1331	403	702	135	90	1	0	0

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	4	592	9593	3070	4798	812	885	28	0	0

- Molecule 32 is a RNA chain called fMet-tRNAMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
32	5	71	2268	674	764	264	495	71	0	0

- Molecule 33 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
33	6	31	978	290	330	104	223	31	0	0

- Molecule 34 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	7	571	8938	2785	4506	779	851	17	0	0

- Molecule 35 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
35	t	71	1147	352	600	93	102	0	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	A	67	67	67	0
36	B	1	1	1	0
36	X	1	1	1	0
36	3	1	1	1	0
36	6	1	1	1	0
36	7	1	1	1	0

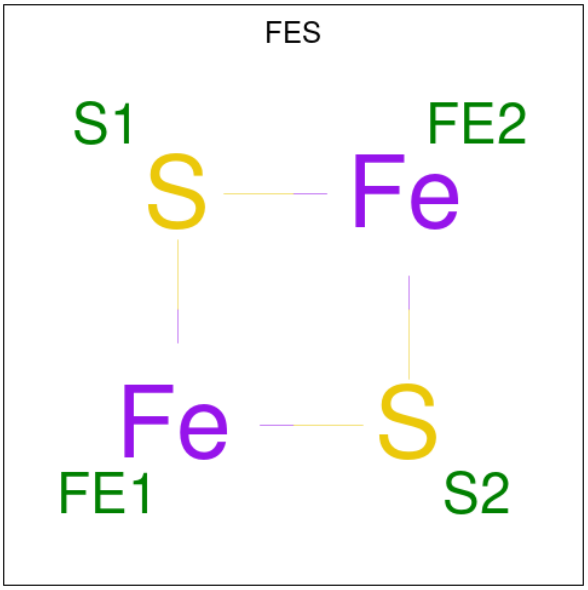
- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
37	A	19	19	19	0
37	7	1	1	1	0

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

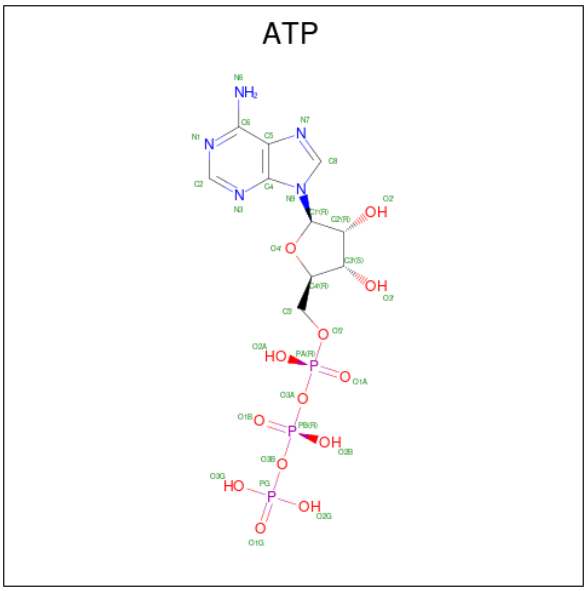
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
38	O	1	1	1	0

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



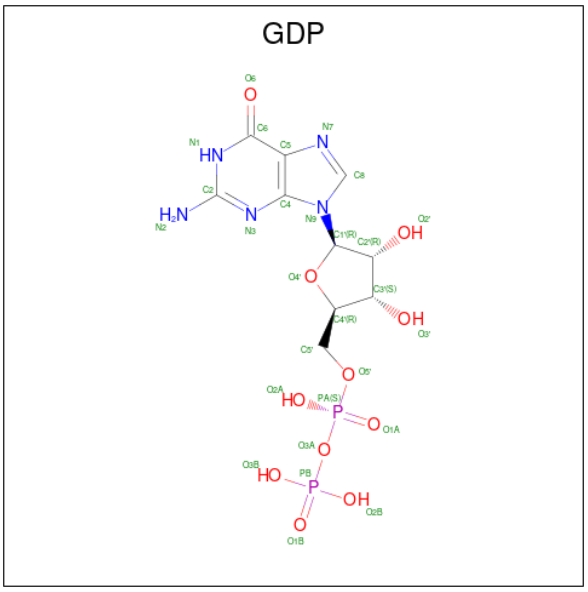
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
39	P	1	4	2	2	0
			Total	Fe	S	
39	T	1	4	2	2	0

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



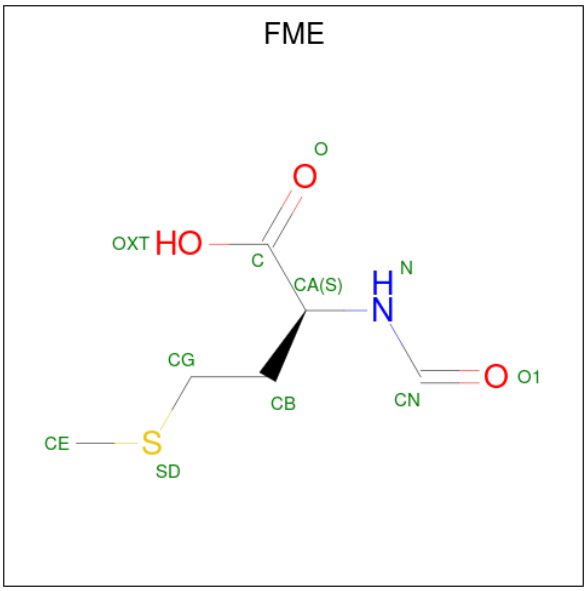
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
40	X	1	43	10	12	5	13	3	0

- Molecule 41 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



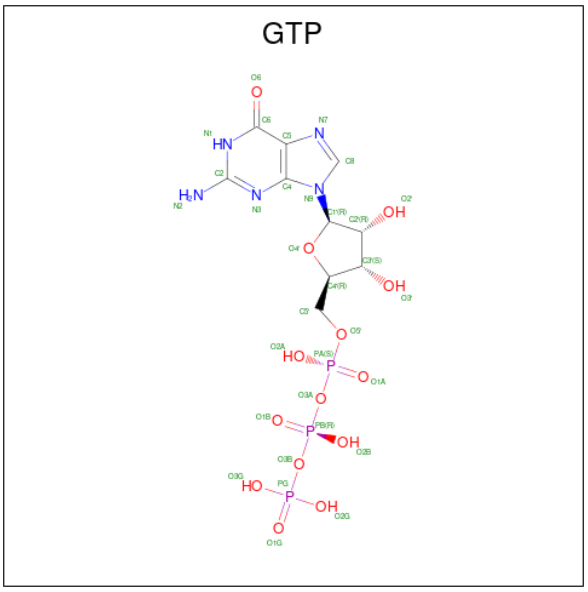
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
41	X	1	40	10	12	5	11	2	0

- Molecule 42 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
42	5	1	20	6	10	1	2	1	0

- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
43	7	1	44	10	12	5	14	3	0

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
44	A	580	580	580	0
44	B	27	27	27	0
44	C	9	9	9	0
44	D	19	19	19	0
44	E	6	6	6	0
44	F	4	4	4	0
44	G	11	11	11	0
44	H	14	14	14	0
44	I	7	7	7	0
44	J	2	2	2	0
44	K	17	17	17	0
44	L	6	6	6	0
44	M	6	6	6	0
44	N	7	7	7	0
44	O	8	8	8	0
44	P	2	2	2	0
44	Q	9	9	9	0
44	R	4	4	4	0
44	S	10	10	10	0
44	T	1	1	1	0
44	U	3	3	3	0
44	V	2	2	2	0

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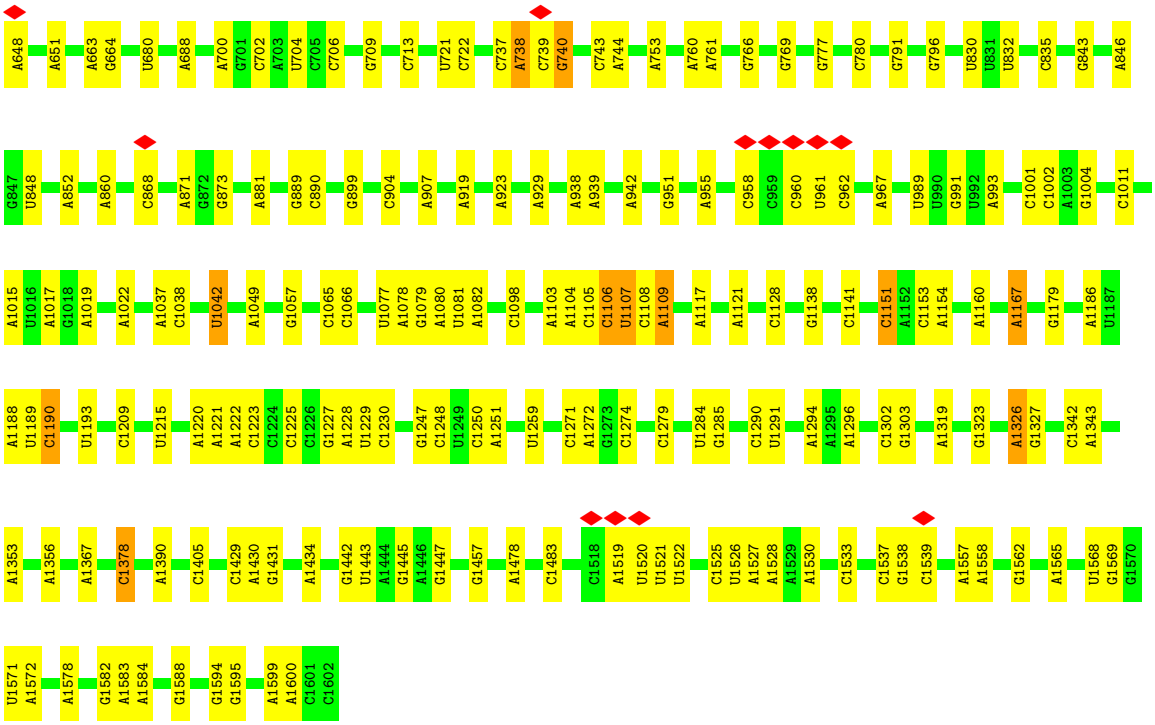
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
44	W	5	5	5	0
			Total	O	
44	Z	5	5	5	0
			Total	O	
44	0	13	13	13	0
			Total	O	
44	1	5	5	5	0
			Total	O	
44	2	8	8	8	0
			Total	O	
44	3	3	3	3	0
			Total	O	
44	5	6	6	6	0
			Total	O	
44	6	7	7	7	0
			Total	O	
44	7	1	1	1	0

3 Residue-property plots (i)

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

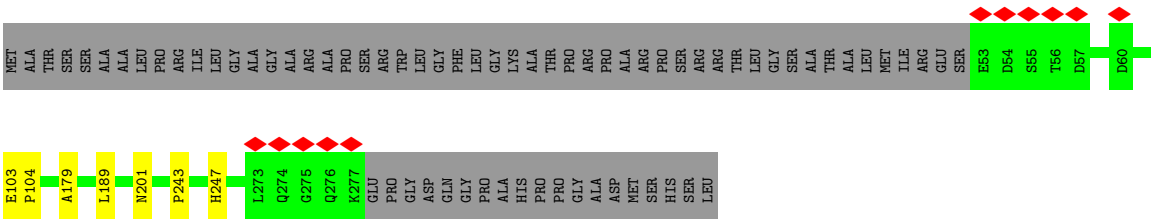
• Molecule 1: 12S mitochondrial rRNA

Chain A:



• Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:

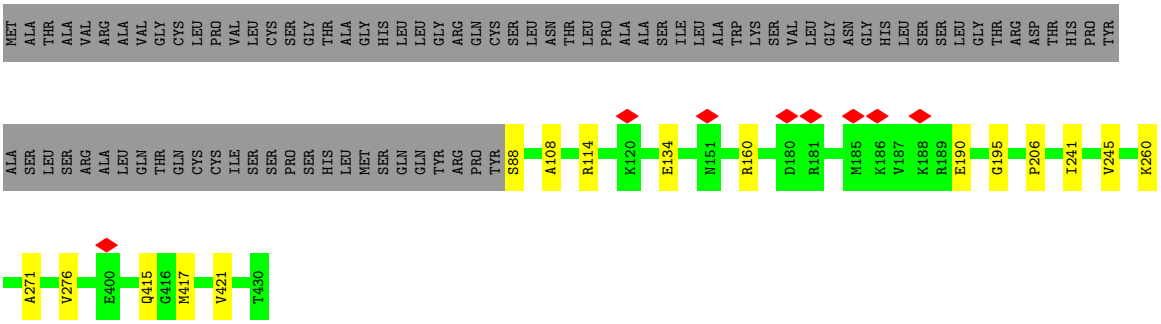


• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:

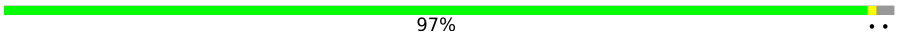
- Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain D:



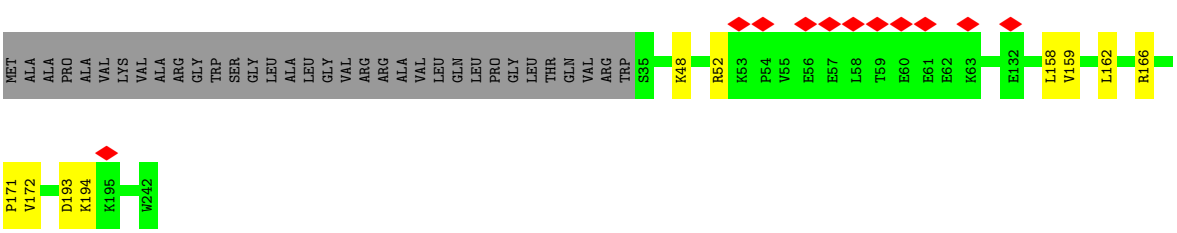
- Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain E:



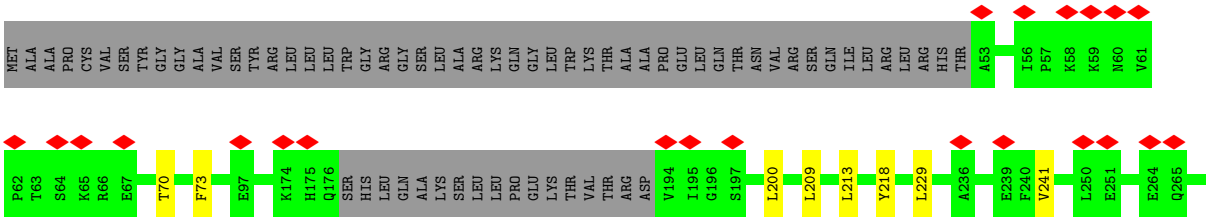
- Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:



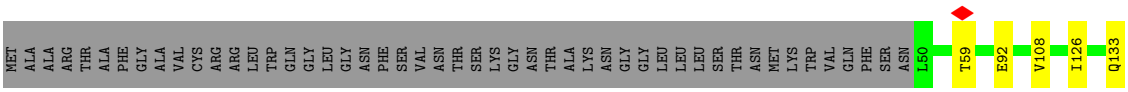
- Molecule 7: 28S ribosomal protein S9, mitochondrial

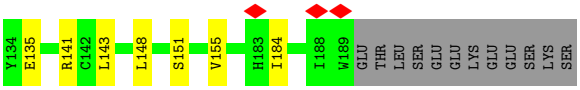
Chain G:



• Molecule 8: 28S ribosomal protein S10, mitochondrial

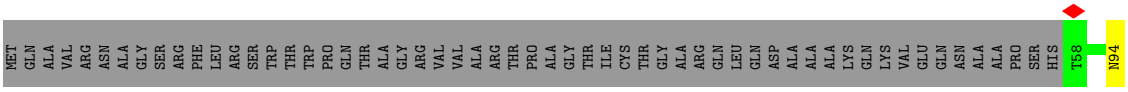
Chain H:





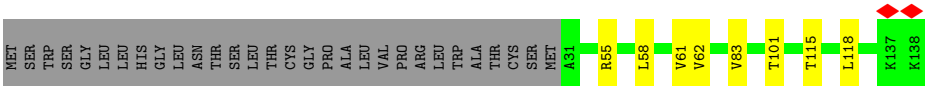
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:

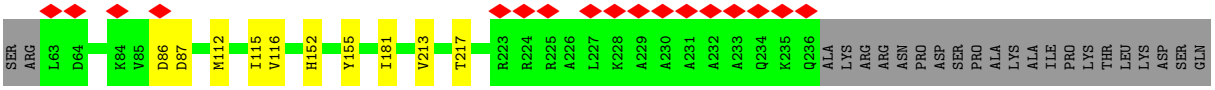


• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:

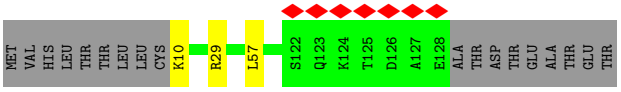
• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L:



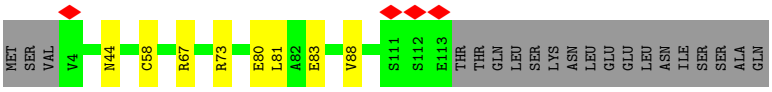
• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain M:



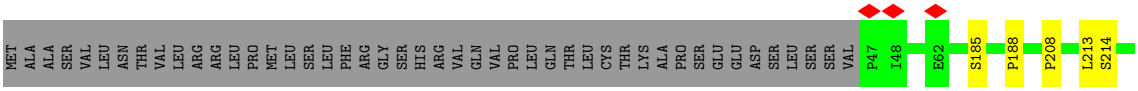
• Molecule 14: 28S ribosomal protein S17, mitochondrial

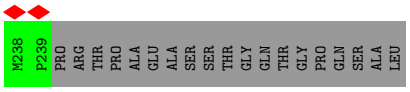
Chain N:



• Molecule 15: 28S ribosomal protein S18b, mitochondrial

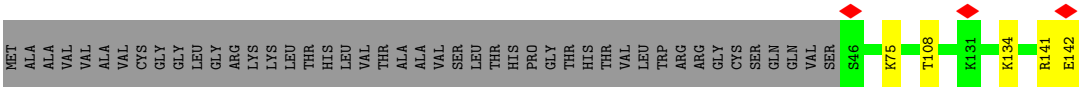
Chain O:





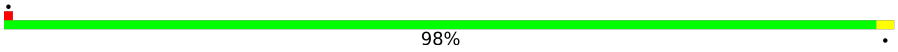
• Molecule 16: 28S ribosomal protein S18c, mitochondrial

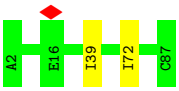
Chain P:



• Molecule 17: 28S ribosomal protein S21, mitochondrial

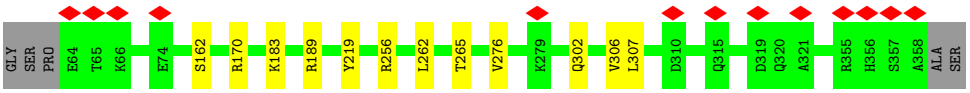
Chain Q:





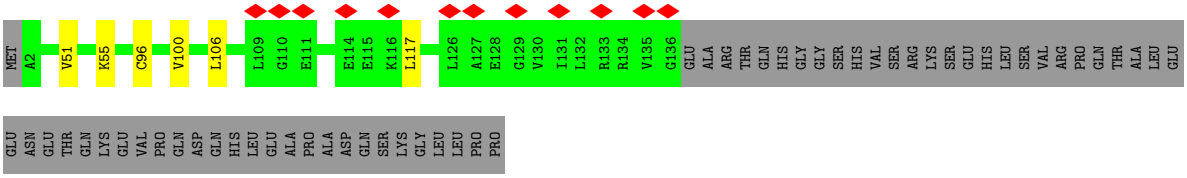
• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:



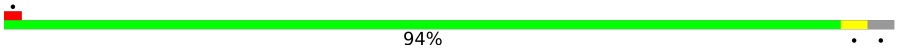
• Molecule 19: 28S ribosomal protein S23, mitochondrial

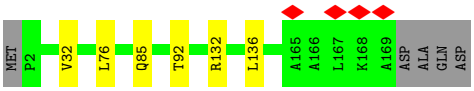
Chain S:



• Molecule 20: 28S ribosomal protein S25, mitochondrial

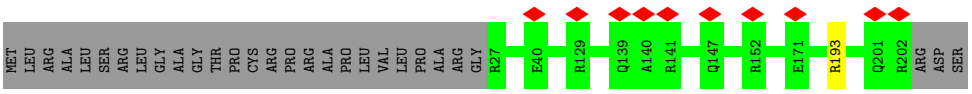
Chain T:





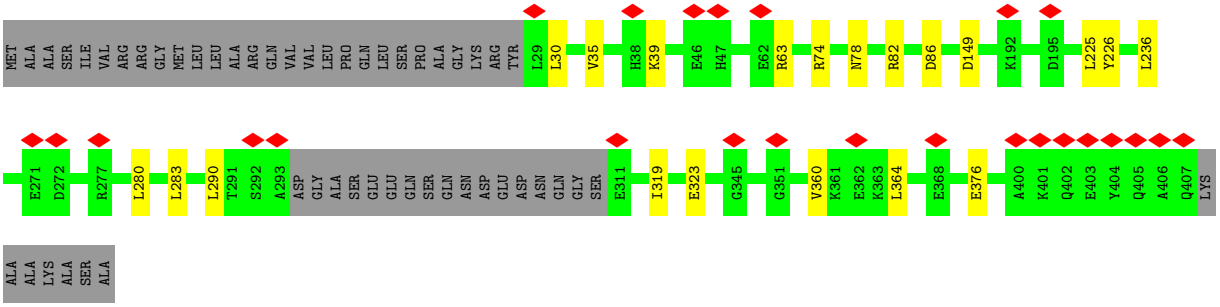
• Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U:



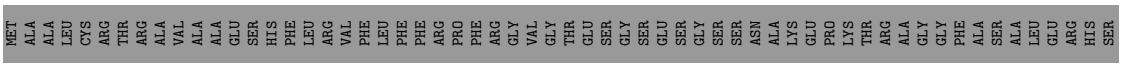
• Molecule 22: 28S ribosomal protein S27, mitochondrial

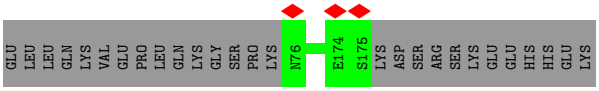
Chain V:



• Molecule 23: 28S ribosomal protein S28, mitochondrial

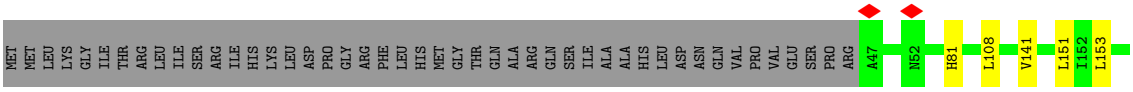
Chain W:





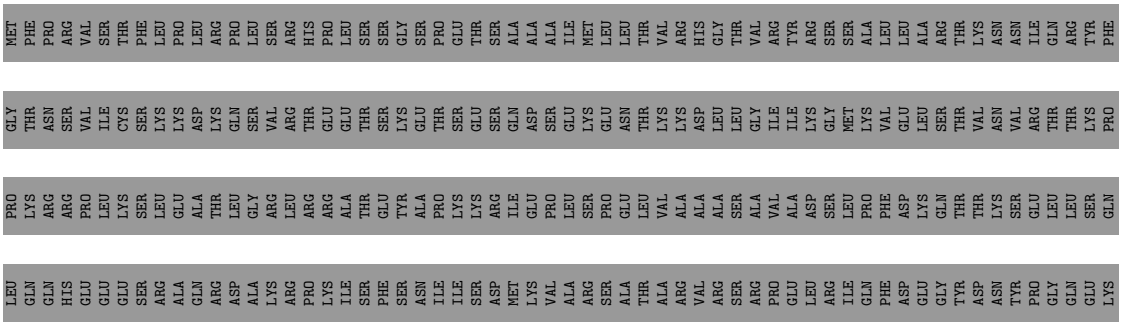
• Molecule 24: 28S ribosomal protein S29, mitochondrial

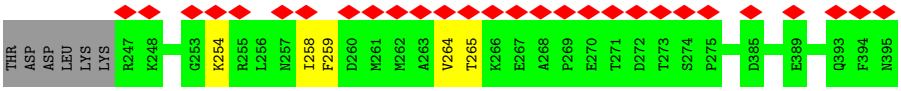
Chain X:



• Molecule 25: 28S ribosomal protein S31, mitochondrial

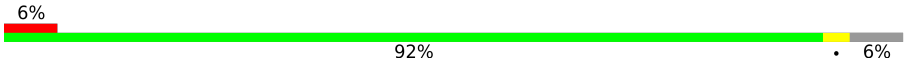
Chain Y:

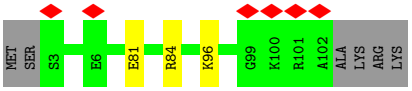




• Molecule 26: 28S ribosomal protein S33, mitochondrial

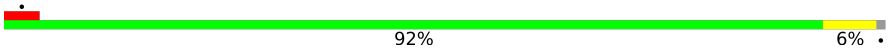
Chain Z:

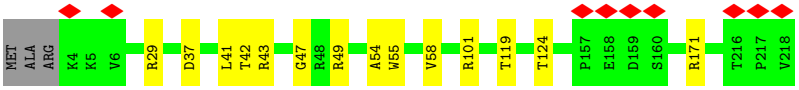




• Molecule 27: 28S ribosomal protein S34, mitochondrial

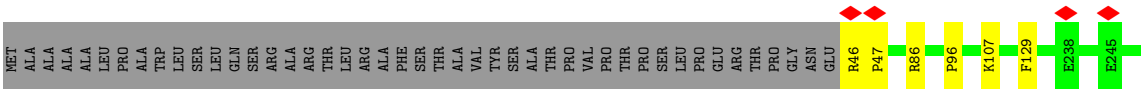
Chain 0:

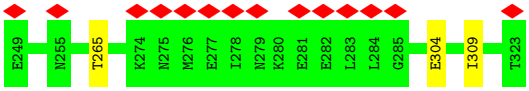




• Molecule 28: 28S ribosomal protein S35, mitochondrial

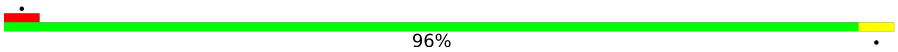
Chain 1:

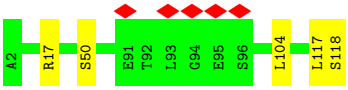




• Molecule 29: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

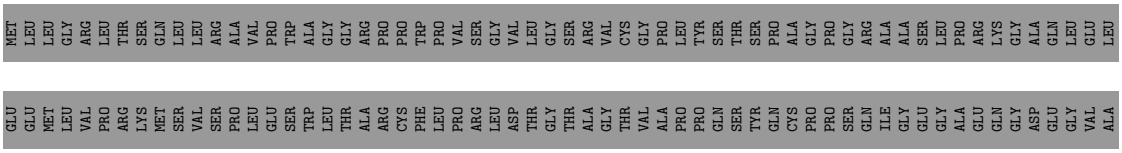
Chain 2:

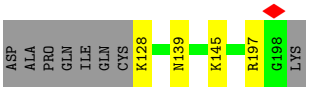




• Molecule 30: Aurora kinase A-interacting protein

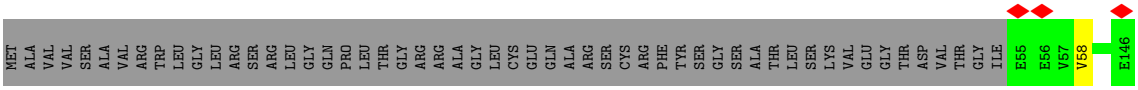
Chain 3:

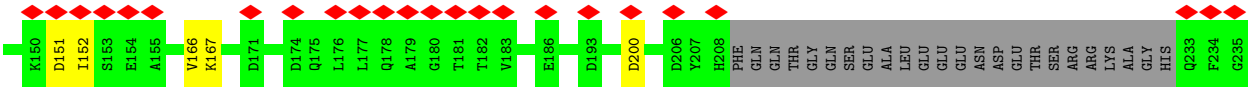


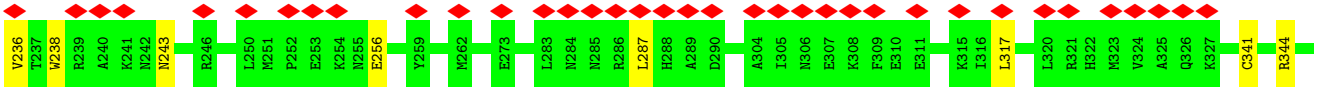


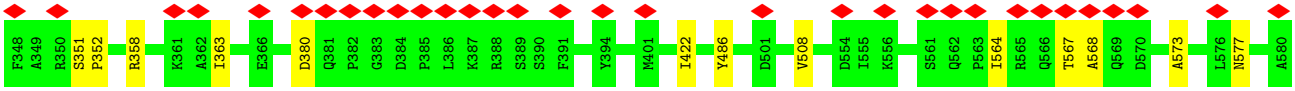
• Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

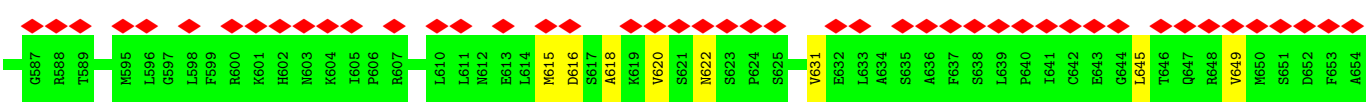
Chain 4:

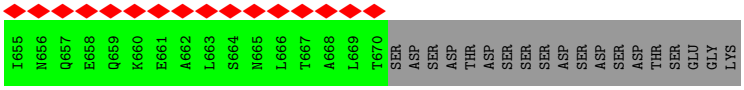






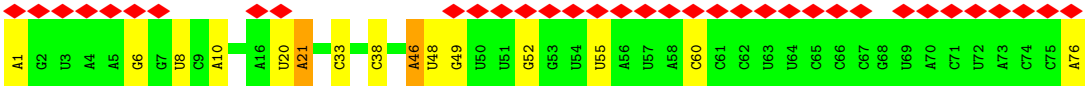






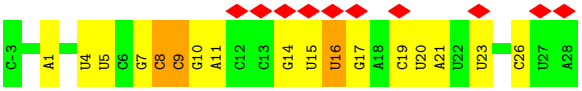
• Molecule 32: fMet-tRNAMet

Chain 5:



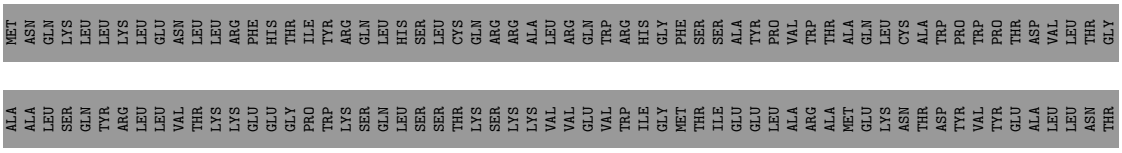
• Molecule 33: mRNA

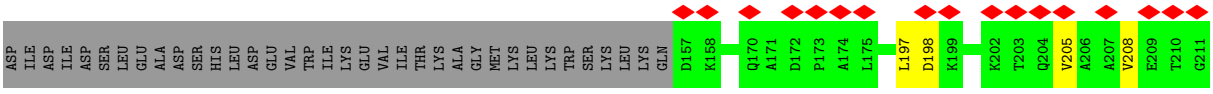
Chain 6:

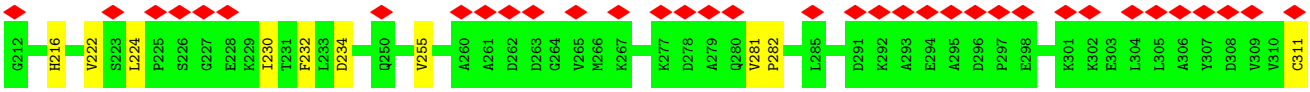


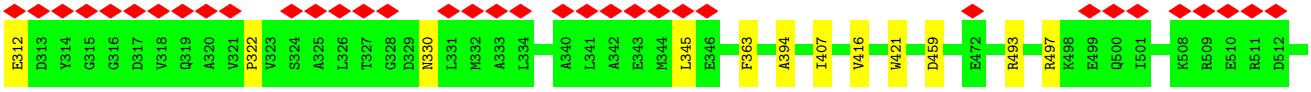
• Molecule 34: Translation initiation factor IF-2, mitochondrial

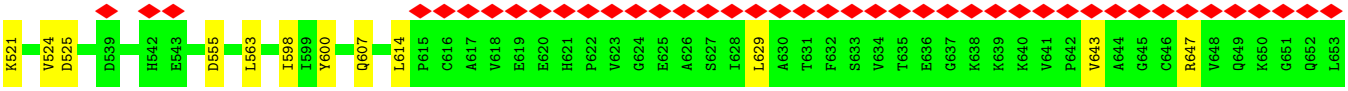
Chain 7:

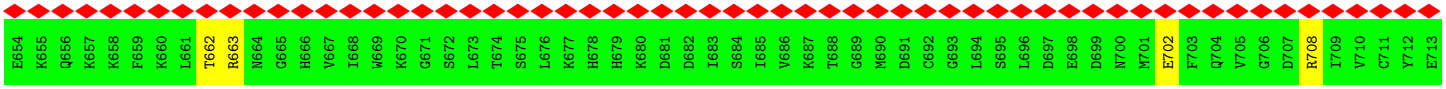


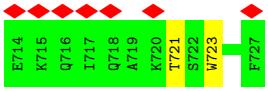












• Molecule 35: 39S ribosomal protein L12, mitochondrial

Chain t:

MET LEU PRO ALA ALA ALA ARG PRO LEU TRP GLY PRO CYS LEU GLY LEU ARG ALA ALA ALA PHE ARG LEU ALA ARG ARG GLN VAL PRO CYS VAL CYS ALA VAL ARG HIS MET ARG SER SER GLY HIS GLN ARG CYS GLU ALA LEU ALA GLY ALA PRO LEU ASP ASN ALA PRO LYS GLU TYR

PRO PRO LYS ILE GLN GLN LEU VAL GLN ASP ILE ALA SER LEU THR LEU LEU GLU ILE SER ASP LEU ASN GLU LEU LEU LYS LYS THR LEU LYS ILE GLN ASP VAL GLY LEU VAL PRO MET GLY GLY VAL MET SER GLY ALA VAL PRO ALA ALA ALA ALA GLN GLU ALA VAL GLU GLU ASP

ILE PRO ILE ALA LYS GLU ARG T128 H129 F130 T131 V132 R133 L134 T135 E136 A137 K138 P139 V140 D141 K142 V143 K144 L145 I146 K147 E148 I149 K150 N151 Y152 I153 Q154 G155 I156 N157 L158 V159 Q160 A161 K162 K163 L164 V165 E166 S167 L168 P169 Q170 E171 I172 K173 A174 N175 V176 A177 K178 A179 E180

A181 E182 K183 I184 K185 A186 A187 L188 E189 A190 V191 G192 G193 T194 V195 V196 L197 E198

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19601	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 ($e^-/Å^2$)	31	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.586	Depositor
Minimum map value	-0.800	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.675, 0.675, 0.675	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: RSQ, 5MU, MG, K, 5MC, GDP, MA6, ATP, 5F0, AYA, FES, GTP, B8T, FME, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.26	0/22562	0.67	0/35124
2	B	0.25	0/1871	0.41	0/2531
3	C	0.26	0/1113	0.41	0/1505
4	D	0.25	0/2783	0.42	0/3724
5	E	0.25	0/989	0.42	0/1335
6	F	0.24	0/1767	0.37	0/2373
7	G	0.25	0/2746	0.39	0/3681
8	H	0.25	0/1178	0.41	0/1598
9	I	0.25	0/1030	0.44	0/1386
10	J	0.26	0/855	0.46	0/1148
11	K	0.23	0/880	0.41	0/1182
12	L	0.24	0/1477	0.36	0/1974
13	M	0.25	0/963	0.42	0/1295
14	N	0.25	0/886	0.44	0/1199
15	O	0.25	0/1648	0.39	0/2243
16	P	0.26	0/798	0.41	0/1070
17	Q	0.25	0/748	0.38	0/994
18	R	0.24	0/2456	0.37	0/3317
19	S	0.26	0/1138	0.39	0/1533
20	T	0.25	0/1402	0.40	0/1883
21	U	0.24	0/1510	0.37	0/2025
22	V	0.23	0/3030	0.35	0/4093
23	W	0.25	0/801	0.42	0/1079
24	X	0.24	0/2921	0.38	0/3954
25	Y	0.24	0/1280	0.37	0/1725
26	Z	0.25	0/857	0.39	0/1141
27	0	0.24	0/1834	0.41	0/2484
28	1	0.24	0/2304	0.38	0/3117
29	2	0.24	0/941	0.40	0/1257
30	3	0.24	0/640	0.38	0/844
31	4	0.23	0/4904	0.35	0/6636
32	5	0.30	1/1654 (0.1%)	0.66	0/2568

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	6	0.17	0/720	0.68	0/1117
34	7	0.23	0/4502	0.41	0/6073
35	t	0.24	0/551	0.40	0/740
All	All	0.25	1/77739 (0.0%)	0.51	0/109948

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	1	A	OP3-P	-10.58	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	184	5F0	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20282	10313	10298	63	0
2	B	1828	1816	1815	4	0
3	C	1083	1089	1088	5	0
4	D	2731	2805	2804	10	0
5	E	972	1001	1000	1	0
6	F	1725	1770	1769	6	0
7	G	2688	2690	2687	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1152	1184	1183	11	0
9	I	1020	1061	1053	9	0
10	J	839	888	887	5	0
11	K	862	886	885	3	0
12	L	1453	1541	1540	6	0
13	M	942	966	965	2	0
14	N	868	929	928	6	0
15	O	1592	1557	1557	4	0
16	P	781	807	806	4	0
17	Q	744	758	758	2	0
18	R	2409	2429	2428	8	0
19	S	1111	1116	1115	4	0
20	T	1371	1394	1393	4	0
21	U	1488	1500	1499	1	0
22	V	2969	2964	2961	14	0
23	W	789	803	802	0	0
24	X	2849	2845	2843	13	0
25	Y	1246	1198	1197	4	0
26	Z	839	860	858	2	0
27	0	1787	1797	1796	10	0
28	1	2256	2289	2288	8	0
29	2	935	969	973	6	0
30	3	629	702	702	4	0
31	4	4795	4798	4796	23	0
32	5	1504	764	764	4	0
33	6	648	330	331	3	0
34	7	4432	4506	4502	27	0
35	t	547	600	599	0	0
36	3	1	0	0	0	0
36	6	1	0	0	0	0
36	7	1	0	0	0	0
36	A	67	0	0	0	0
36	B	1	0	0	0	0
36	X	1	0	0	0	0
37	7	1	0	0	0	0
37	A	19	0	0	0	0
38	O	1	0	0	0	0
39	P	4	0	0	0	0
39	T	4	0	0	0	0
40	X	31	12	12	0	0
41	X	28	12	12	0	0
42	5	10	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	7	32	12	12	0	0
44	0	13	0	0	0	0
44	1	5	0	0	0	0
44	2	8	0	0	1	0
44	3	3	0	0	0	0
44	5	6	0	0	0	0
44	6	7	0	0	0	0
44	7	1	0	0	0	0
44	A	580	0	0	5	0
44	B	27	0	0	0	0
44	C	9	0	0	0	0
44	D	19	0	0	1	0
44	E	6	0	0	0	0
44	F	4	0	0	0	0
44	G	11	0	0	0	0
44	H	14	0	0	1	0
44	I	7	0	0	1	0
44	J	2	0	0	0	0
44	K	17	0	0	0	0
44	L	6	0	0	0	0
44	M	6	0	0	1	0
44	N	7	0	0	0	0
44	O	8	0	0	0	0
44	P	2	0	0	0	0
44	Q	9	0	0	0	0
44	R	4	0	0	0	0
44	S	10	0	0	0	0
44	T	1	0	0	0	0
44	U	3	0	0	0	0
44	V	2	0	0	0	0
44	W	5	0	0	0	0
44	Z	5	0	0	0	0
All	All	75175	63971	63916	230	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 (230) 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:A:1294:A:OP1	2:B:201:ASN:ND2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1353:A:N1	44:A:1802:HOH:O	2.21	0.72
1:A:700:A:N1	1:A:709:G:O2'	2.24	0.71
1:A:1078:A:OP1	32:5:38:C:O2'	2.09	0.70
34:7:493:ARG:O	34:7:497:ARG:N	2.26	0.69
1:A:1342:C:OP2	26:Z:96:LYS:NZ	2.26	0.69
12:L:112:MET:O	12:L:116:VAL:HG22	1.93	0.67
31:4:200:ASP:OD2	31:4:243:ASN:N	2.27	0.67
15:O:185:SER:O	18:R:183:LYS:NZ	2.30	0.65
34:7:407:ILE:HD11	34:7:416:VAL:HG23	1.78	0.64
1:A:843:G:N2	1:A:846:A:OP2	2.31	0.64
1:A:1272:A:N1	1:A:1303:G:O2'	2.26	0.64
34:7:322:PRO:O	34:7:330:ASN:ND2	2.30	0.63
1:A:899:G:O2'	1:A:907:A:N1	2.26	0.61
24:X:299:ASN:ND2	28:1:265:THR:OG1	2.34	0.60
27:0:41:LEU:HD13	27:0:55:TRP:CG	2.37	0.60
20:T:132:ARG:NH1	20:T:136:LEU:O	2.34	0.60
3:C:84:GLU:N	3:C:84:GLU:OE1	2.32	0.60
22:V:39:LYS:NZ	22:V:376:GLU:OE2	2.35	0.60
1:A:1104:A:OP2	44:A:1801:HOH:O	2.17	0.58
34:7:282:PRO:HG2	34:7:345:LEU:HD21	1.86	0.58
6:F:159:VAL:HG23	6:F:172:VAL:HG21	1.85	0.57
1:A:1530:A:OP1	27:0:29:ARG:NH2	2.37	0.56
1:A:1259:U:H6	1:A:1326:A:HO2'	1.52	0.56
7:G:229:LEU:HD21	7:G:241:VAL:HG11	1.87	0.56
12:L:86:ASP:OD1	12:L:87:ASP:N	2.38	0.56
1:A:1319:A:N3	44:A:1817:HOH:O	2.33	0.56
27:0:42:THR:HG22	27:0:49:ARG:HG2	1.88	0.56
1:A:1279:C:O2'	1:A:1296:A:N1	2.32	0.55
18:R:276:VAL:HG11	18:R:307:LEU:HD12	1.88	0.55
24:X:108:LEU:HD23	24:X:141:VAL:HG21	1.87	0.55
33:6:8:C:O2'	33:6:9:C:O5'	2.24	0.55
31:4:573:ALA:O	31:4:577:ASN:ND2	2.41	0.54
34:7:663:ARG:NH2	34:7:702:GLU:O	2.41	0.54
1:A:1077:U:O2'	1:A:1079:G:N7	2.30	0.54
34:7:222:VAL:HG22	34:7:230:ILE:O	2.08	0.53
34:7:614:LEU:HD11	34:7:721:THR:HA	1.88	0.53
22:V:74:ARG:O	22:V:78:ASN:ND2	2.41	0.53
1:A:760:A:N1	1:A:780:C:O2'	2.38	0.53
9:I:126:ILE:HD11	29:2:50:SER:HB2	1.90	0.53
24:X:151:LEU:HD23	24:X:247:LEU:HD22	1.90	0.53
31:4:631:VAL:HG21	31:4:649:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:G:OP2	14:N:73:ARG:NH2	2.40	0.53
31:4:151:ASP:OD1	31:4:152:ILE:N	2.40	0.53
34:7:222:VAL:HG21	34:7:232:PHE:CE2	2.44	0.53
1:A:1478:A:N1	1:A:1565:A:O2'	2.36	0.53
31:4:615:MET:CE	31:4:649:VAL:HG22	2.39	0.53
34:7:208:VAL:O	34:7:208:VAL:HG12	2.09	0.53
17:Q:72:ILE:HD13	29:2:104:LEU:HD21	1.91	0.53
29:2:118:SER:OXT	44:2:201:HOH:O	2.19	0.52
28:1:46:ARG:NH1	33:6:16:U:OP2	2.42	0.52
19:S:51:VAL:HG13	29:2:117:LEU:HD11	1.92	0.52
7:G:396:ARG:NH2	32:5:33:C:OP2	2.41	0.52
1:A:1138:G:O2'	1:A:1167:A:N1	2.38	0.52
1:A:1378:C:O2	24:X:389:SER:OG	2.28	0.52
1:A:1584:MA6:OP1	30:3:145:LYS:NZ	2.39	0.52
11:K:120:LEU:HB3	11:K:123:ILE:HD12	1.92	0.52
34:7:198:ASP:OD1	34:7:205:VAL:HG22	2.10	0.52
18:R:162:SER:O	18:R:170:ARG:NH2	2.42	0.52
1:A:1221:A:OP2	1:A:1222:A:O2'	2.22	0.52
24:X:151:LEU:CD2	24:X:247:LEU:HD22	2.40	0.51
22:V:236:LEU:HD21	22:V:323:GLU:HB3	1.93	0.51
31:4:615:MET:HG3	31:4:645:LEU:HD11	1.91	0.51
8:H:148:LEU:HD23	8:H:148:LEU:H	1.76	0.51
1:A:1227:G:OP2	1:A:1228:A:O2'	2.19	0.51
1:A:989:U:OP1	9:I:94:ASN:ND2	2.43	0.51
9:I:126:ILE:HD11	29:2:50:SER:CB	2.41	0.51
22:V:35:VAL:HG12	22:V:35:VAL:O	2.10	0.51
31:4:618:ALA:O	31:4:622:ASN:N	2.44	0.51
1:A:1004:G:O2'	9:I:98:GLN:NE2	2.44	0.50
1:A:1528:A:OP1	27:0:101:ARG:NH1	2.44	0.50
22:V:360:VAL:HG13	22:V:364:LEU:HD22	1.93	0.50
1:A:951:G:OP1	14:N:44:ASN:ND2	2.44	0.50
1:A:1434:A:N7	44:A:1821:HOH:O	2.34	0.50
22:V:236:LEU:HD12	22:V:290:LEU:HD13	1.93	0.50
34:7:629:LEU:HD11	34:7:647:ARG:HB2	1.92	0.50
1:A:713:C:HO2'	1:A:852:A:HO2'	1.59	0.50
31:4:631:VAL:CG2	31:4:649:VAL:HG21	2.41	0.50
34:7:311:CYS:SG	34:7:312:GLU:N	2.85	0.50
25:Y:259:PHE:HB2	31:4:363:ILE:HD11	1.94	0.49
28:1:304:GLU:OE1	28:1:309:ILE:HD11	2.12	0.49
31:4:564:ILE:HG22	31:4:564:ILE:O	2.12	0.49
27:0:54:ALA:O	27:0:58:VAL:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:208:PRO:HG2	15:O:213:LEU:HD21	1.95	0.49
3:C:96:MET:HB2	3:C:108:LEU:HD11	1.94	0.49
31:4:380:ASP:HB2	31:4:422:ILE:HD11	1.93	0.49
34:7:363:PHE:HB3	34:7:524:VAL:HG12	1.94	0.49
34:7:598:ILE:HG21	34:7:600:TYR:CE2	2.48	0.49
4:D:245:VAL:HG22	4:D:271:ALA:HB1	1.94	0.49
24:X:108:LEU:HD21	24:X:307:VAL:CG1	2.42	0.49
19:S:106:LEU:HB2	19:S:117:LEU:HD11	1.93	0.49
1:A:929:A:O4'	4:D:421:VAL:HG13	2.13	0.49
10:J:61:VAL:HG21	34:7:563:LEU:HD21	1.95	0.48
22:V:30:LEU:HD12	22:V:149:ASP:HB2	1.95	0.48
1:A:929:A:H1'	4:D:421:VAL:HG22	1.96	0.48
1:A:1057:G:H4'	1:A:1578:A:H4'	1.95	0.48
31:4:58:VAL:HG23	31:4:58:VAL:O	2.14	0.48
32:5:76:A:O4'	34:7:643:VAL:HG11	2.14	0.48
1:A:1583:MA6:H102	1:A:1584:MA6:H103	1.95	0.48
7:G:200:LEU:O	7:G:218:TYR:OH	2.18	0.48
18:R:262:LEU:O	18:R:265:THR:OG1	2.22	0.48
1:A:991:G:O6	9:I:122:LYS:NZ	2.46	0.47
31:4:567:THR:HG22	31:4:568:ALA:N	2.29	0.47
26:Z:81:GLU:OE1	26:Z:84:ARG:NH2	2.42	0.47
1:A:1141:C:OP1	30:3:139:ASN:ND2	2.45	0.47
1:A:1429:C:OP1	7:G:388:ARG:NH2	2.47	0.47
25:Y:264:VAL:HG12	25:Y:265:THR:N	2.29	0.47
6:F:162:LEU:HD12	6:F:166:ARG:O	2.14	0.47
25:Y:258:ILE:HD11	31:4:317:LEU:HD22	1.96	0.47
1:A:702:C:OP1	1:A:848:U:O2'	2.25	0.47
22:V:236:LEU:HD21	22:V:323:GLU:CB	2.44	0.47
2:B:243:PRO:O	2:B:247:HIS:ND1	2.48	0.47
7:G:318:HIS:NE2	24:X:379:GLU:OE2	2.49	0.46
27:0:43:ARG:O	27:0:47:GLY:N	2.41	0.46
27:0:119:THR:OG1	27:0:124:THR:HG22	2.16	0.46
31:4:256:GLU:HG3	31:4:287:LEU:HD22	1.96	0.46
24:X:153:LEU:HD21	24:X:244:LEU:HD22	1.97	0.46
31:4:615:MET:HE1	31:4:649:VAL:HG22	1.96	0.46
1:A:1017:A:O2'	16:P:108:THR:OG1	2.23	0.46
7:G:70:THR:HG23	7:G:73:PHE:H	1.80	0.46
27:0:37:ASP:O	27:0:41:LEU:N	2.46	0.46
34:7:607:GLN:NE2	34:7:723:TRP:O	2.48	0.46
8:H:108:VAL:HG22	8:H:143:LEU:HD23	1.97	0.46
9:I:189:ARG:NH2	44:I:202:HOH:O	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:616:ASP:O	31:4:620:VAL:HG23	2.16	0.46
1:A:1431:G:O2'	1:A:1457:G:O6	2.26	0.46
18:R:302:GLN:O	18:R:306:VAL:HG23	2.16	0.46
24:X:276:ARG:NH2	24:X:286:GLU:OE1	2.49	0.46
18:R:170:ARG:O	18:R:189:ARG:NH1	2.47	0.45
20:T:32:VAL:HG22	20:T:76:LEU:HD22	1.97	0.45
24:X:206:GLU:OE2	24:X:249:ARG:NH2	2.46	0.45
31:4:341:CYS:O	31:4:344:ARG:NH2	2.49	0.45
14:N:67:ARG:NH1	14:N:80:GLU:OE1	2.50	0.45
4:D:415:GLN:NE2	4:D:417:MET:SD	2.87	0.45
11:K:34:MET:O	11:K:38:VAL:HG23	2.17	0.45
34:7:255:VAL:HG23	34:7:281:VAL:HG21	1.97	0.45
1:A:1098:C:OP1	1:A:1151:C:N4	2.49	0.45
6:F:193:ASP:OD1	6:F:194:LYS:N	2.50	0.45
8:H:148:LEU:HD23	8:H:148:LEU:N	2.31	0.45
18:R:162:SER:O	18:R:170:ARG:NH1	2.50	0.45
2:B:103:GLU:N	2:B:104:PRO:CD	2.80	0.45
24:X:273:THR:HG23	24:X:316:LEU:HD13	1.97	0.45
34:7:197:LEU:HD22	34:7:234:ASP:HB2	1.99	0.45
1:A:1106:C:O2'	1:A:1108:C:OP2	2.31	0.45
28:1:86:ARG:NH1	28:1:96:PRO:O	2.47	0.45
1:A:1108:C:H4'	1:A:1109:A:OP2	2.17	0.44
12:L:213:VAL:O	12:L:217:THR:HG23	2.17	0.44
9:I:179:THR:HG21	17:Q:39:ILE:HD13	1.99	0.44
18:R:219:TYR:O	18:R:256:ARG:NH1	2.50	0.44
19:S:96:CYS:O	19:S:100:VAL:HG23	2.18	0.44
1:A:1066:C:O2'	9:I:187:ARG:O	2.35	0.44
2:B:179:ALA:CB	2:B:189:LEU:HD21	2.47	0.44
31:4:166:VAL:HG23	31:4:167:LYS:N	2.33	0.44
34:7:394:ALA:HB2	34:7:421:TRP:HA	1.98	0.44
8:H:92:GLU:OE1	8:H:141:ARG:NH1	2.43	0.44
8:H:155:VAL:HG21	28:1:129:PHE:CB	2.47	0.44
15:O:214:SER:OG	22:V:319:ILE:HG23	2.18	0.44
1:A:1302:C:OP1	3:C:165:LYS:NZ	2.46	0.44
1:A:1037:A:O2'	12:L:152:HIS:NE2	2.15	0.44
8:H:184:ILE:O	8:H:184:ILE:HG22	2.18	0.44
1:A:1230:C:OP2	1:A:1442:G:O2'	2.33	0.44
16:P:141:ARG:O	16:P:142:GLU:C	2.56	0.44
24:X:380:LEU:HD21	24:X:398:LEU:CD1	2.47	0.44
14:N:58:CYS:SG	14:N:81:LEU:HD22	2.57	0.43
28:1:46:ARG:N	28:1:47:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:C:HO2'	12:L:155:TYR:HH	1.65	0.43
1:A:1569:G:OP2	1:A:1572:A:O2'	2.37	0.43
13:M:10:LYS:N	44:M:201:HOH:O	2.51	0.43
20:T:92:THR:O	20:T:92:THR:HG22	2.18	0.43
4:D:134:GLU:OE2	4:D:160:ARG:NH1	2.45	0.43
1:A:1107:U:O4	30:3:128:LYS:NZ	2.50	0.43
4:D:241:ILE:O	4:D:260:LYS:HA	2.19	0.43
8:H:59:THR:HG23	8:H:59:THR:O	2.18	0.43
1:A:648:A:N3	1:A:929:A:H2'	2.34	0.43
8:H:135:GLU:HB3	11:K:126:ALA:HB2	2.00	0.43
10:J:101:THR:HG21	34:7:459:ASP:HB3	2.00	0.43
34:7:216:HIS:HD2	34:7:524:VAL:HG21	1.84	0.43
1:A:738:A:H2'	1:A:740:G:C5	2.53	0.43
13:M:29:ARG:CD	13:M:57:LEU:HD12	2.49	0.43
1:A:663:A:H2'	1:A:664:G:C8	2.54	0.43
8:H:151:SER:O	8:H:155:VAL:HG23	2.19	0.42
9:I:153:GLY:O	9:I:158:ARG:NH2	2.44	0.42
24:X:108:LEU:HD21	24:X:307:VAL:HG13	2.01	0.42
1:A:955:A:O4'	1:A:1042:U:H1'	2.18	0.42
31:4:236:VAL:HG12	31:4:238:TRP:H	1.83	0.42
1:A:1186:A:HO2'	1:A:1190:C:H5	1.64	0.42
22:V:225:LEU:HD11	22:V:283:LEU:HD22	2.02	0.42
34:7:521:LYS:NZ	34:7:555:ASP:O	2.53	0.42
6:F:158:LEU:HD23	6:F:171:PRO:HA	2.02	0.42
5:E:65:LEU:HD11	16:P:75:LYS:CD	2.49	0.42
1:A:706:C:OP1	27:0:43:ARG:NE	2.47	0.42
1:A:1153:C:O2'	30:3:197:ARG:NH1	2.53	0.41
34:7:598:ILE:HG21	34:7:600:TYR:CZ	2.55	0.41
6:F:48:LYS:NZ	7:G:321:ASP:OD1	2.36	0.41
14:N:83:GLU:OE1	20:T:85:GLN:NE2	2.44	0.41
1:A:1588:G:N2	44:A:1889:HOH:O	2.50	0.41
4:D:206:PRO:HG2	4:D:276:VAL:HG11	2.01	0.41
8:H:133:GLN:NE2	44:H:304:HOH:O	2.54	0.41
10:J:62:VAL:HA	10:J:83:VAL:HG12	2.03	0.41
22:V:225:LEU:HD21	22:V:280:LEU:HD23	2.02	0.41
34:7:407:ILE:HD11	34:7:416:VAL:CG2	2.48	0.41
10:J:55:ARG:HD3	10:J:58:LEU:HD21	2.02	0.41
6:F:52:ARG:NH1	7:G:321:ASP:OD2	2.53	0.41
16:P:134:LYS:O	21:U:193:ARG:NE	2.54	0.41
34:7:224:LEU:HD11	34:7:230:ILE:HD12	2.02	0.41
19:S:55:LYS:HG2	19:S:55:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:254:LYS:O	31:4:358:ARG:NH1	2.54	0.41
33:6:8:C:HO2'	33:6:9:C:P	2.44	0.41
1:A:743:C:H2'	1:A:744:A:O4'	2.21	0.41
1:A:1022:A:OP2	29:2:17:ARG:NE	2.50	0.41
1:A:1443:U:O2'	1:A:1445:G:N7	2.30	0.41
3:C:54:GLU:OE2	28:1:107:LYS:NZ	2.49	0.41
4:D:88:SER:N	44:D:504:HOH:O	2.54	0.41
22:V:82:ARG:NH2	22:V:86:ASP:OD1	2.54	0.41
31:4:508:VAL:O	31:4:508:VAL:HG12	2.21	0.41
14:N:88:VAL:O	14:N:88:VAL:HG13	2.21	0.41
34:7:662:THR:N	34:7:708:ARG:O	2.43	0.41
1:A:881:A:OP1	4:D:195:GLY:N	2.54	0.40
1:A:1220:A:O2'	7:G:395:LYS:O	2.38	0.40
1:A:1323:G:N7	3:C:36:LYS:NZ	2.58	0.40
15:O:188:PRO:O	27:0:171:ARG:NH1	2.50	0.40
7:G:209:LEU:HD12	7:G:213:LEU:HD11	2.04	0.40
10:J:115:THR:HG21	10:J:118:LEU:HD12	2.03	0.40
1:A:1521:U:O2'	22:V:63:ARG:NH2	2.55	0.40
8:H:155:VAL:HG21	28:1:129:PHE:HB3	2.04	0.40
12:L:115:ILE:HG21	12:L:181:ILE:HD13	2.02	0.40
22:V:30:LEU:HD12	22:V:149:ASP:CB	2.52	0.40
31:4:351:SER:HB3	31:4:352:PRO:HD3	2.03	0.40
4:D:108:ALA:O	4:D:114:ARG:NH1	2.49	0.40
32:5:21:A:N6	32:5:46:A:O2'	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
2	B	223/296 (75%)	221 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
4	D	341/430 (79%)	333 (98%)	8 (2%)	0	100	100
5	E	120/125 (96%)	120 (100%)	0	0	100	100
6	F	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
7	G	323/396 (82%)	316 (98%)	7 (2%)	0	100	100
8	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	22	57
9	I	134/194 (69%)	133 (99%)	1 (1%)	0	100	100
10	J	106/138 (77%)	103 (97%)	3 (3%)	0	100	100
11	K	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
12	L	172/257 (67%)	172 (100%)	0	0	100	100
13	M	117/137 (85%)	117 (100%)	0	0	100	100
14	N	108/130 (83%)	108 (100%)	0	0	100	100
15	O	191/258 (74%)	189 (99%)	2 (1%)	0	100	100
16	P	95/142 (67%)	95 (100%)	0	0	100	100
17	Q	84/86 (98%)	84 (100%)	0	0	100	100
18	R	293/360 (81%)	287 (98%)	6 (2%)	0	100	100
19	S	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
20	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	U	174/205 (85%)	174 (100%)	0	0	100	100
22	V	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
23	W	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
24	X	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
25	Y	147/395 (37%)	146 (99%)	1 (1%)	0	100	100
26	Z	98/106 (92%)	97 (99%)	1 (1%)	0	100	100
27	0	213/218 (98%)	212 (100%)	1 (0%)	0	100	100
28	1	276/323 (85%)	273 (99%)	3 (1%)	0	100	100
29	2	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
30	3	69/199 (35%)	68 (99%)	1 (1%)	0	100	100
31	4	588/689 (85%)	581 (99%)	7 (1%)	0	100	100
34	7	569/727 (78%)	558 (98%)	11 (2%)	0	100	100
35	t	69/198 (35%)	67 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6303/8226 (77%)	6228 (99%)	74 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	126	ILE

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	
2	B	198/249 (80%)	198 (100%)	0	100	100
3	C	115/143 (80%)	115 (100%)	0	100	100
4	D	286/357 (80%)	285 (100%)	1 (0%)	92	96
5	E	104/107 (97%)	104 (100%)	0	100	100
6	F	185/209 (88%)	185 (100%)	0	100	100
7	G	285/342 (83%)	284 (100%)	1 (0%)	91	96
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	104/146 (71%)	104 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	158/226 (70%)	158 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	174/230 (76%)	174 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100
17	Q	78/78 (100%)	78 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100
19	S	116/164 (71%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	V	325/364 (89%)	324 (100%)	1 (0%)	92	96
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	310 (100%)	1 (0%)	92	96
25	Y	137/357 (38%)	137 (100%)	0	100	100
26	Z	90/95 (95%)	90 (100%)	0	100	100
27	0	188/190 (99%)	188 (100%)	0	100	100
28	1	256/291 (88%)	256 (100%)	0	100	100
29	2	100/100 (100%)	100 (100%)	0	100	100
30	3	65/166 (39%)	65 (100%)	0	100	100
31	4	529/609 (87%)	528 (100%)	1 (0%)	93	97
34	7	481/621 (78%)	480 (100%)	1 (0%)	93	97
35	t	59/158 (37%)	59 (100%)	0	100	100
All	All	5595/7122 (79%)	5589 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	190	GLU
7	G	389	ARG
22	V	226	TYR
24	X	81	HIS
31	4	486	TYR
34	7	525	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	113	GLN
6	F	146	HIS
9	I	98	GLN
22	V	78	ASN
22	V	134	GLN
25	Y	290	ASN
29	2	109	GLN

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Mol	Chain	Res	Type
31	4	295	ASN
34	7	649	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	951/955 (99%)	111 (11%)	0
32	5	69/71 (97%)	11 (15%)	0
33	6	30/31 (96%)	17 (56%)	0
All	All	1050/1057 (99%)	139 (13%)	0

All (139) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	651	A
1	A	680	U
1	A	688	A
1	A	704	U
1	A	721	U
1	A	722	C
1	A	737	C
1	A	738	A
1	A	739	C
1	A	740	G
1	A	753	A
1	A	761	A
1	A	766	G
1	A	777	G
1	A	791	G
1	A	796	G
1	A	830	U
1	A	832	U
1	A	835	C
1	A	860	A
1	A	868	C
1	A	871	A
1	A	873	G
1	A	889	G
1	A	890	C
1	A	904	C
1	A	919	A

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Mol	Chain	Res	Type
1	A	923	A
1	A	938	A
1	A	939	A
1	A	942	A
1	A	958	C
1	A	960	C
1	A	961	U
1	A	962	C
1	A	967	A
1	A	993	A
1	A	1001	C
1	A	1002	C
1	A	1011	C
1	A	1015	A
1	A	1019	A
1	A	1042	U
1	A	1049	A
1	A	1065	C
1	A	1080	A
1	A	1081	U
1	A	1082	A
1	A	1103	A
1	A	1105	C
1	A	1106	C
1	A	1107	U
1	A	1109	A
1	A	1117	A
1	A	1121	A
1	A	1128	C
1	A	1151	C
1	A	1154	A
1	A	1160	A
1	A	1167	A
1	A	1179	G
1	A	1188	A
1	A	1189	U
1	A	1190	C
1	A	1193	U
1	A	1209	C
1	A	1215	U
1	A	1223	C
1	A	1225	C

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Mol	Chain	Res	Type
1	A	1229	U
1	A	1247	G
1	A	1248	C
1	A	1250	C
1	A	1251	A
1	A	1271	C
1	A	1274	C
1	A	1284	U
1	A	1285	G
1	A	1290	C
1	A	1291	U
1	A	1326	A
1	A	1327	G
1	A	1343	A
1	A	1356	A
1	A	1367	A
1	A	1378	C
1	A	1390	A
1	A	1405	C
1	A	1430	A
1	A	1447	G
1	A	1483	C
1	A	1519	A
1	A	1520	U
1	A	1522	U
1	A	1525	C
1	A	1526	U
1	A	1527	A
1	A	1533	C
1	A	1537	C
1	A	1538	G
1	A	1539	C
1	A	1557	A
1	A	1558	A
1	A	1562	G
1	A	1568	U
1	A	1571	U
1	A	1582	G
1	A	1594	G
1	A	1595	G
1	A	1599	A
1	A	1600	A

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Mol	Chain	Res	Type
32	5	6	G
32	5	8	U
32	5	10	A
32	5	20	U
32	5	21	A
32	5	46	A
32	5	48	U
32	5	49	G
32	5	52	G
32	5	55	U
32	5	60	C
33	6	1	A
33	6	4	U
33	6	5	U
33	6	7	G
33	6	8	C
33	6	9	C
33	6	10	G
33	6	11	A
33	6	14	G
33	6	15	U
33	6	16	U
33	6	17	G
33	6	19	C
33	6	20	U
33	6	21	A
33	6	23	U
33	6	26	C

There are no RNA pucker outliers to report.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	AYA	Q	2	17	6,7,8	0.75	0	5,8,10	0.58	0
32	RSQ	5	34	33,32	20,23,24	0.32	0	26,33,36	0.34	0
1	B8T	A	1486	36,1	19,22,23	0.30	0	26,31,34	0.36	0
1	5MC	A	1488	1	18,22,23	0.32	0	26,32,35	0.43	0
1	MA6	A	1583	1	18,26,27	0.75	0	19,38,41	0.54	0
29	AYA	2	2	29	6,7,8	0.80	0	5,8,10	0.49	0
1	MA6	A	1584	1	18,26,27	0.75	0	19,38,41	0.58	0
1	5MU	A	1076	1	19,22,23	0.29	0	28,32,35	0.31	0
9	5F0	I	184	9	8,8,9	0.55	0	7,9,11	1.07	1 (14%)

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
17	AYA	Q	2	17	-	0/4/6/8	-
32	RSQ	5	34	33,32	-	2/9/27/28	0/2/2/2
1	B8T	A	1486	36,1	-	3/7/27/28	0/2/2/2
1	5MC	A	1488	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1583	1	-	0/7/29/30	0/3/3/3
29	AYA	2	2	29	-	0/4/6/8	-
1	MA6	A	1584	1	-	1/7/29/30	0/3/3/3
1	5MU	A	1076	1	-	0/7/25/26	0/2/2/2
9	5F0	I	184	9	-	1/9/9/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	184	5F0	O-C-CB	-2.49	118.17	125.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	5	34	RSQ	O30-C10-C5-C4
32	5	34	RSQ	O30-C10-C5-C6
1	A	1486	B8T	C3'-C4'-C5'-O5'
1	A	1486	B8T	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
9	I	184	5F0	OD1-C1-CA-CB
1	A	1584	MA6	C4'-C5'-O5'-P
1	A	1486	B8T	C2'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1583	MA6	1	0
1	A	1584	MA6	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 99 ligands modelled in this entry, 93 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
40	ATP	X	501	36	26,33,33	0.75	0	31,52,52	0.66	0
42	FME	5	101	32	8,9,10	0.53	0	7,9,11	0.31	0
41	GDP	X	502	-	24,30,30	0.86	1 (4%)	30,47,47	0.63	0
39	FES	T	201	13,20	0,4,4	-	-	-		
39	FES	P	201	16,5	0,4,4	-	-	-		
43	GTP	7	801	36,37	26,34,34	0.88	1 (3%)	32,54,54	0.69	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
40	ATP	X	501	36	-	0/18/38/38	0/3/3/3
42	FME	5	101	32	-	0/7/9/11	-
41	GDP	X	502	-	-	0/12/32/32	0/3/3/3
39	FES	T	201	13,20	-	-	0/1/1/1
39	FES	P	201	16,5	-	-	0/1/1/1
43	GTP	7	801	36,37	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	502	GDP	C5-C6	-2.10	1.43	1.47
43	7	801	GTP	C5-C6	-2.06	1.43	1.47

There are no bond angle outliers.

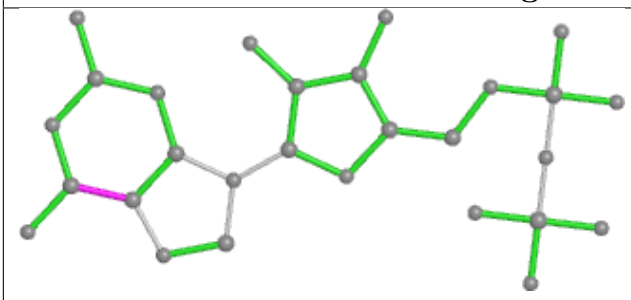
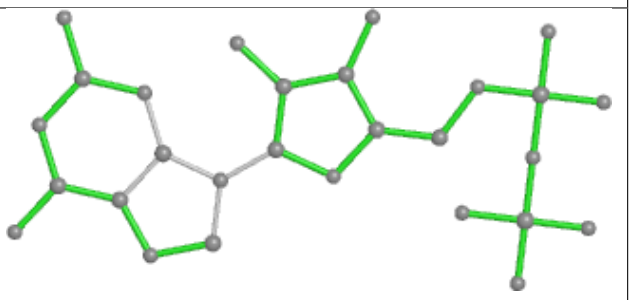
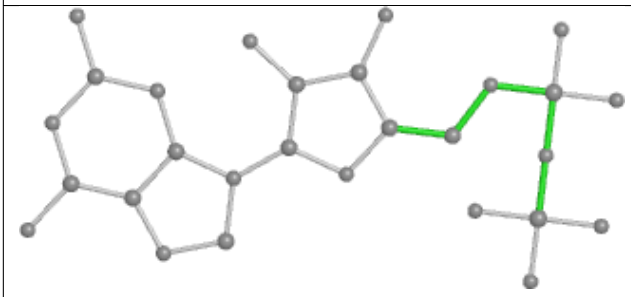
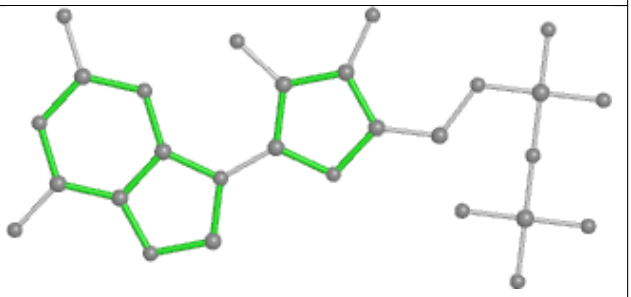
There are no chirality outliers.

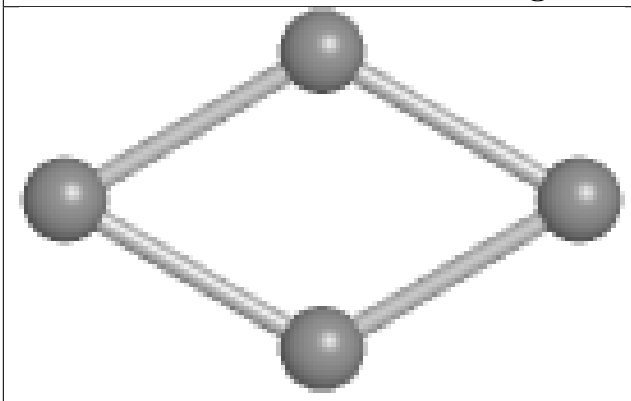
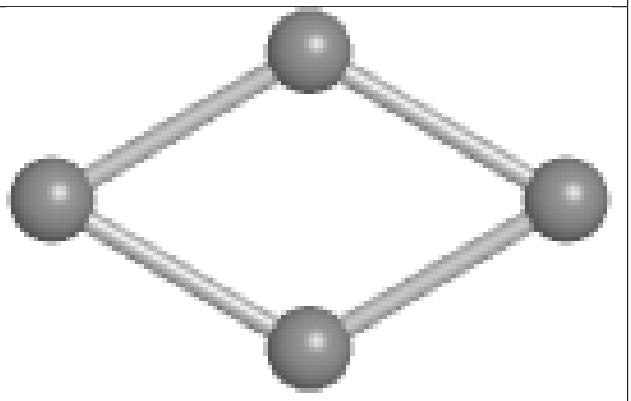
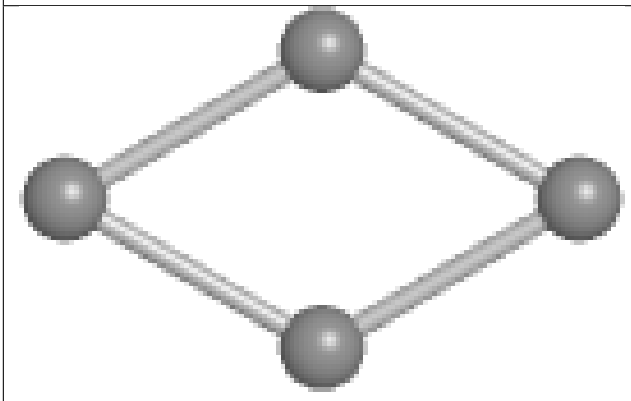
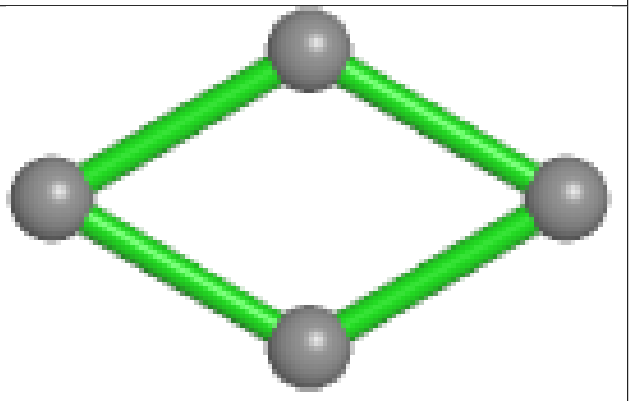
There are no torsion outliers.

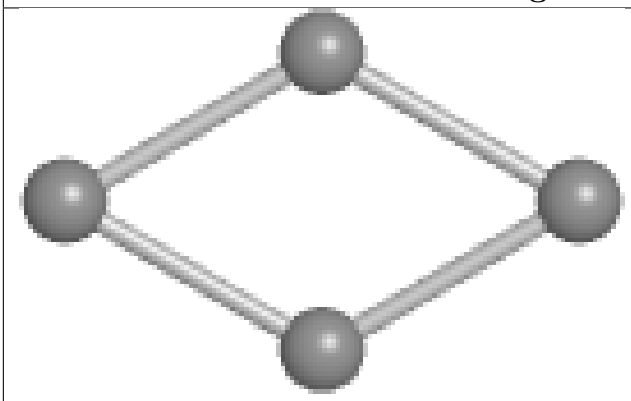
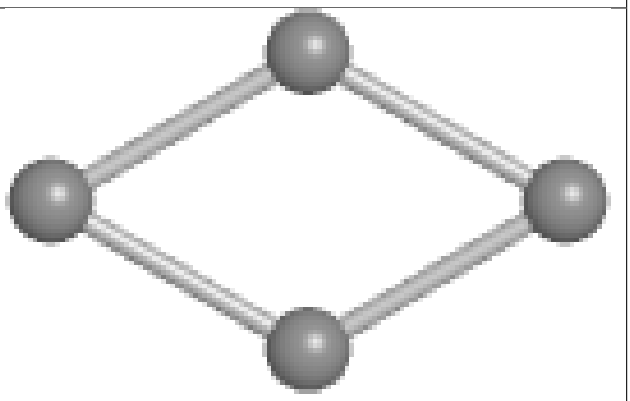
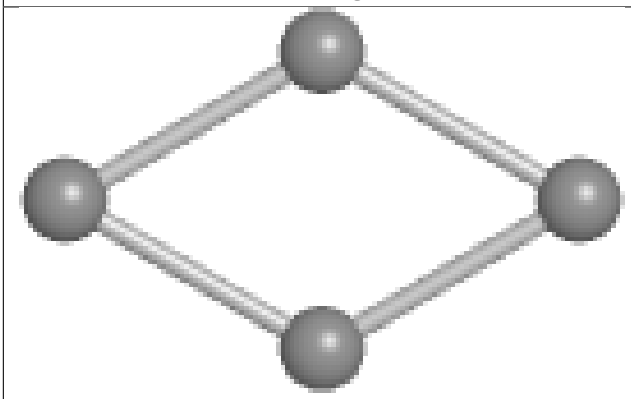
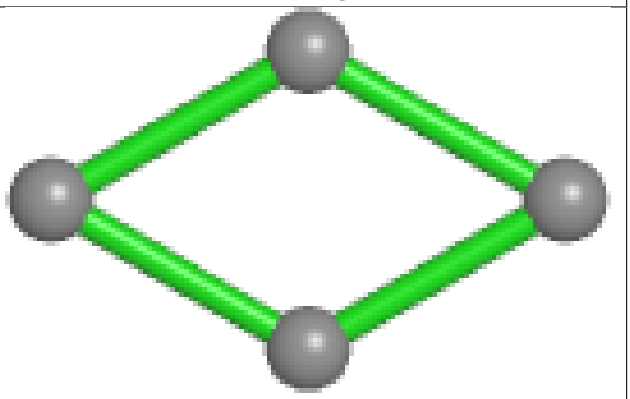
There are no ring outliers.

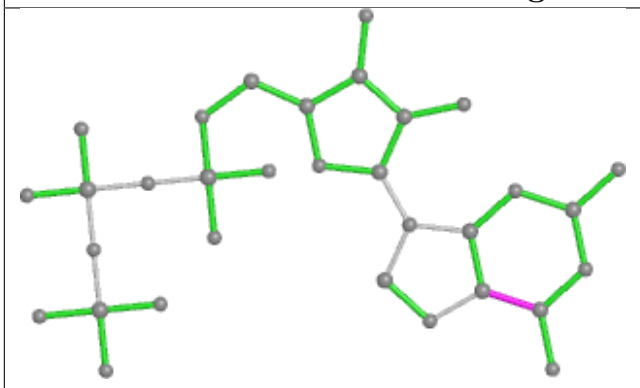
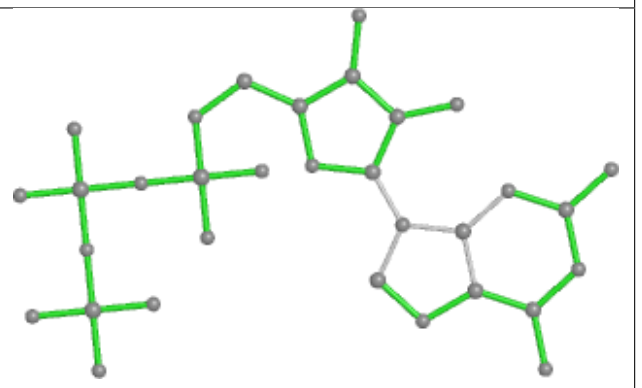
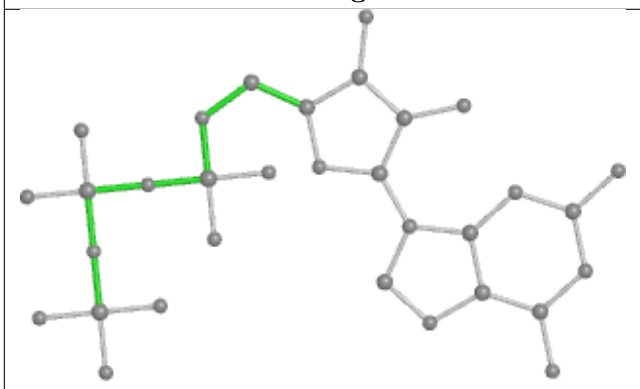
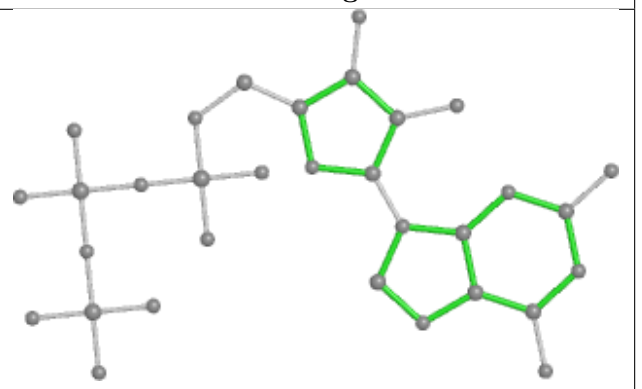
No monomer is involved in short contacts.

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 GDP X 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES T 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES P 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP 7 801	
 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.

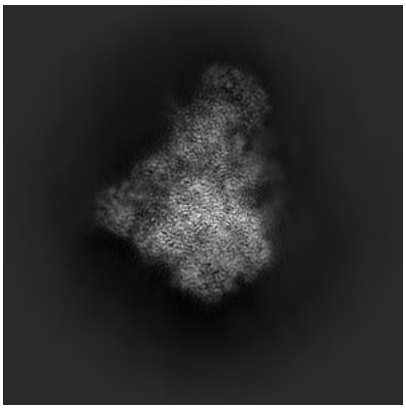
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13560. These allow visual inspection of the internal detail of the map and identification of artifacts.

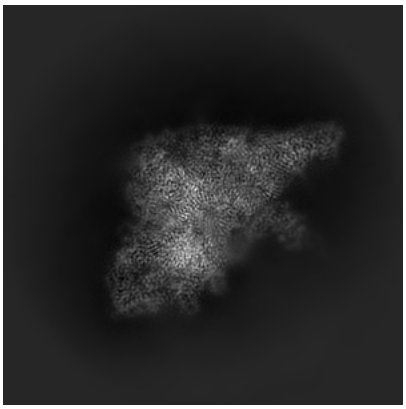
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

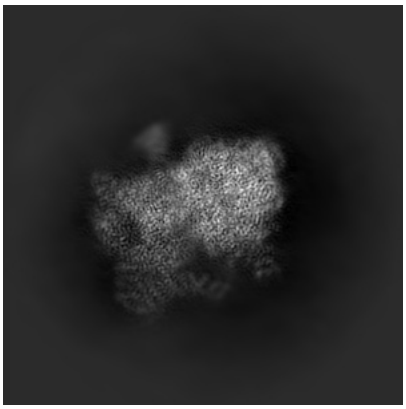
6.1.1 Primary map



X

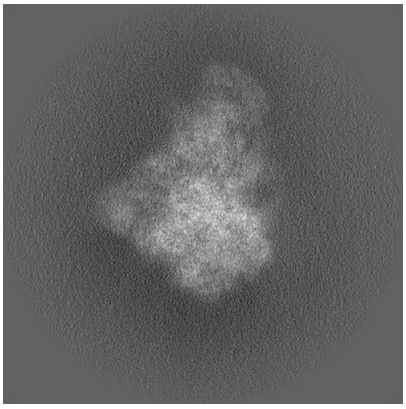


Y

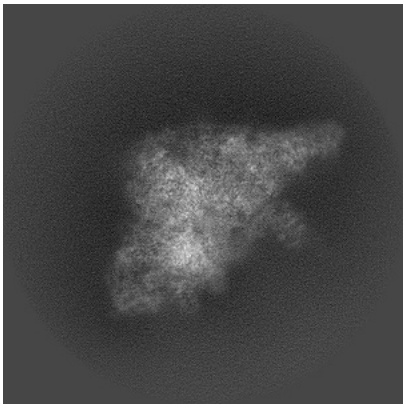


Z

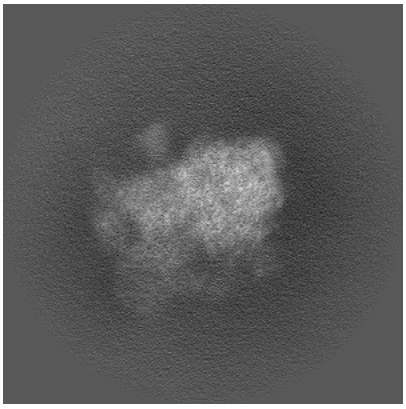
6.1.2 Raw map



X



Y



Z

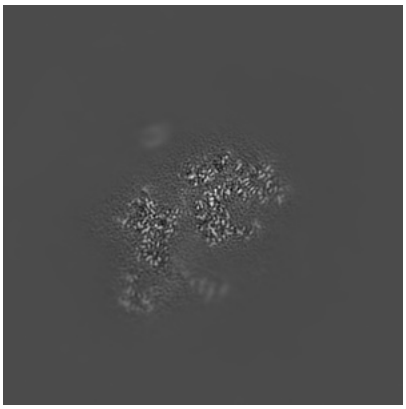
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

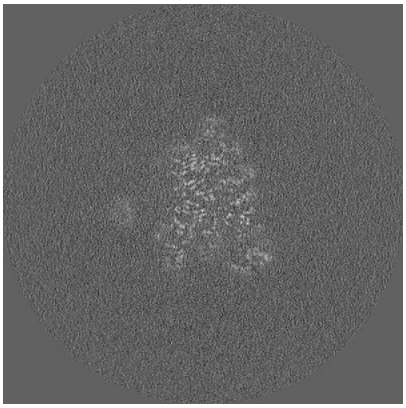
6.2.1 Primary map

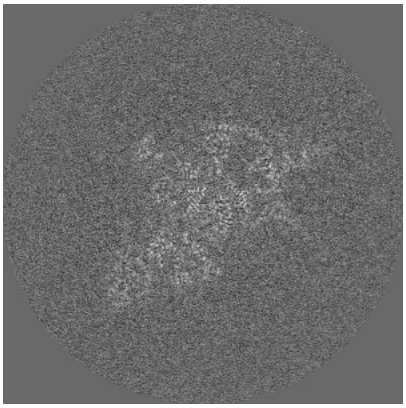
X Index: 288

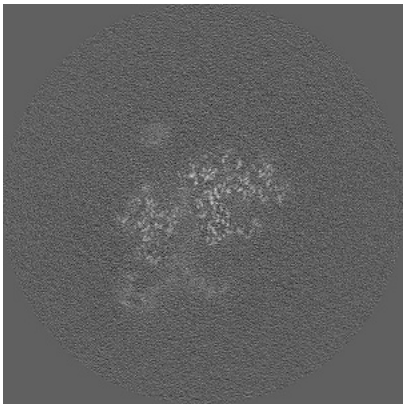
Y Index: 288


Z Index: 288

6.2.2 Raw map


X Index: 240

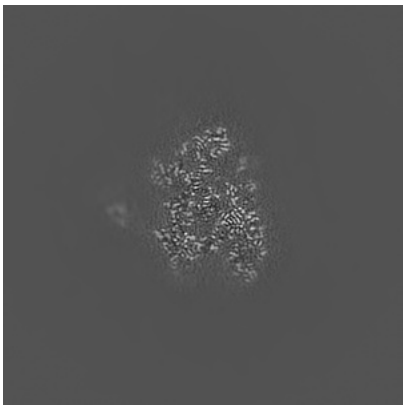

Y Index: 240

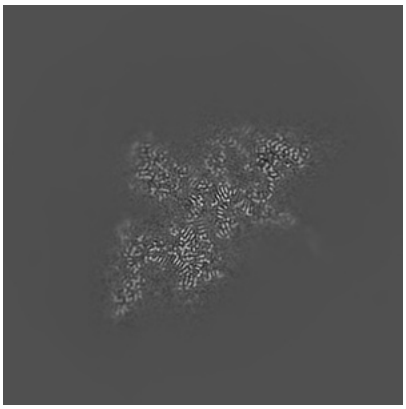

Z Index: 240

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

6.3 Largest variance slices (i)

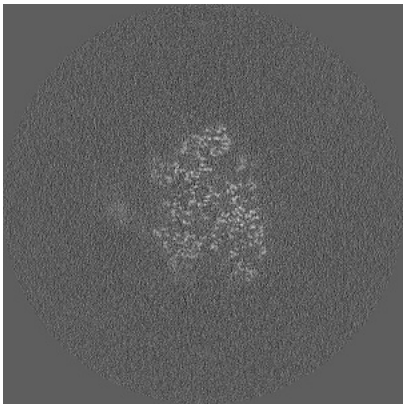
6.3.1 Primary map

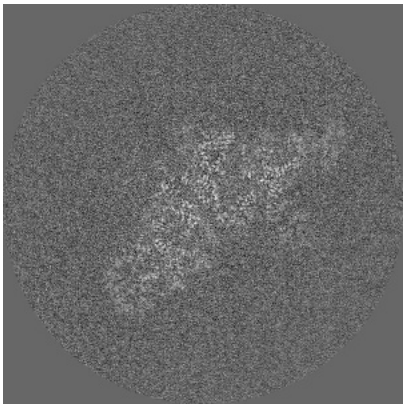

X Index: 303

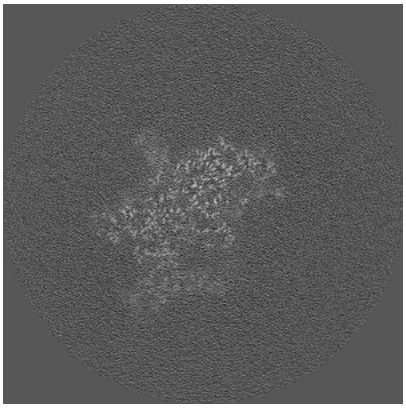

Y Index: 279

Z Index: 264

6.3.2 Raw map


X Index: 253

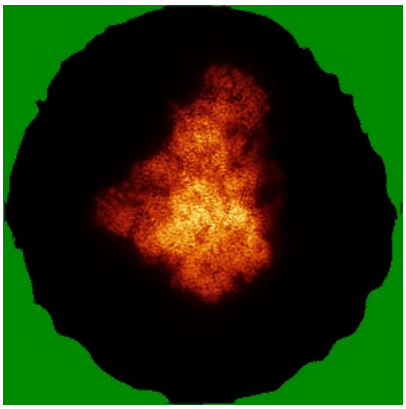

Y Index: 254

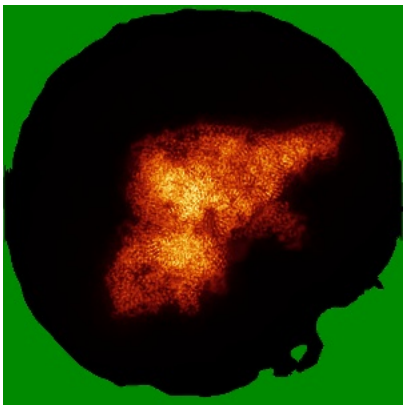

Z Index: 222

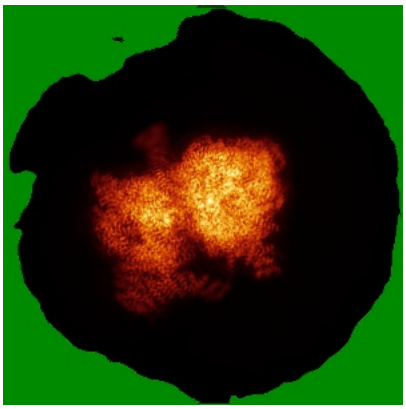
The images above show the largest variance slices of the map in three orthogonal directions.

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

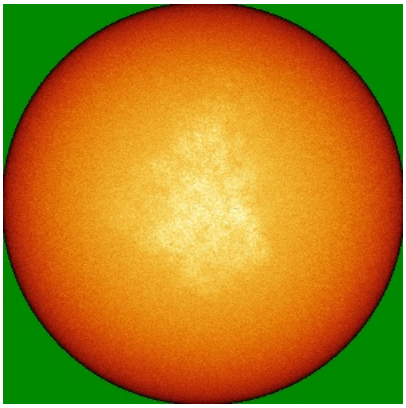
6.4.1 Primary map

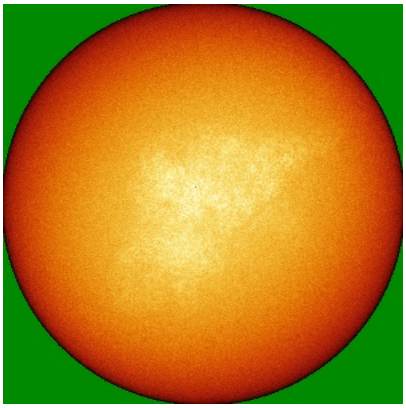

X

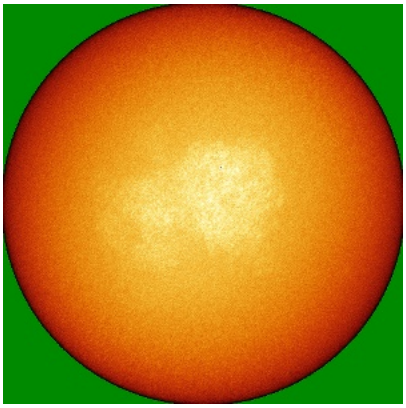

Y


Z

6.4.2 Raw map


X


Y


Z

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

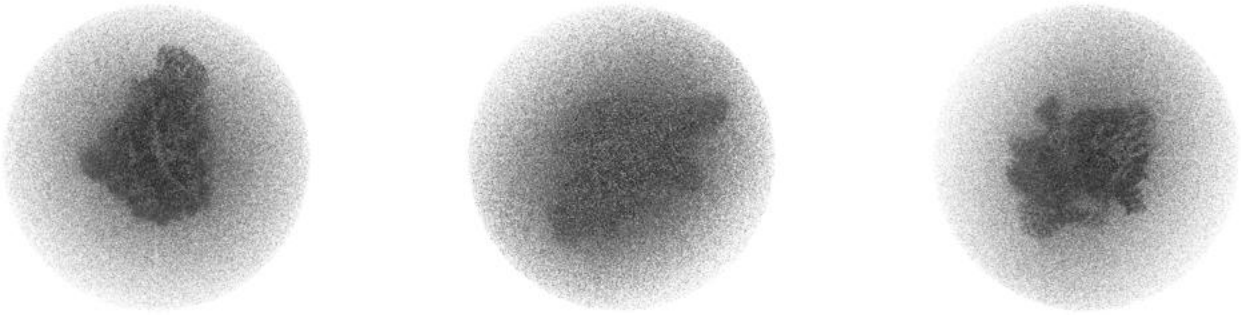
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

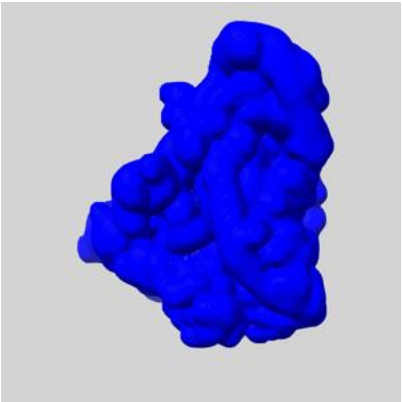
6.6 Mask visualisation (i)

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

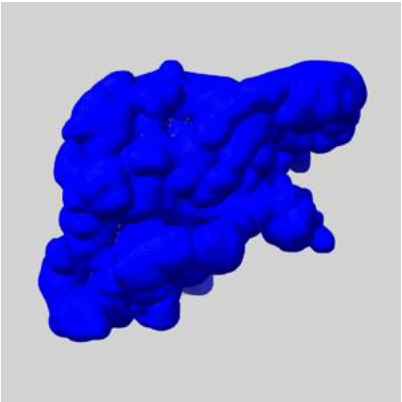
A mask typically either:

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

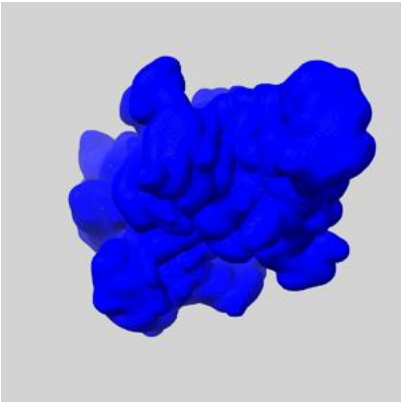
6.6.1 emd_13560_msk_1.map (i)



X



Y

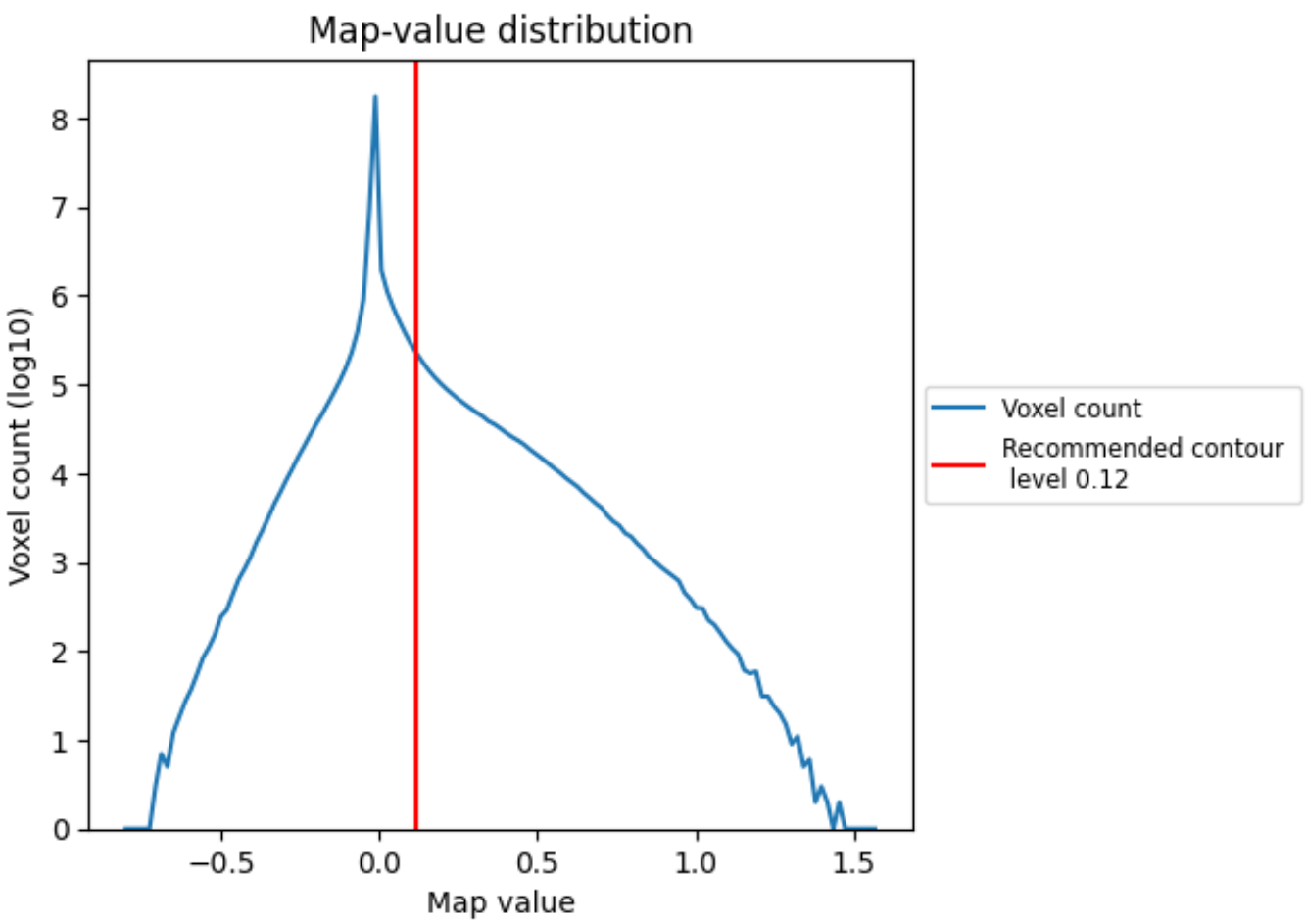


Z

7 Map analysis (i)

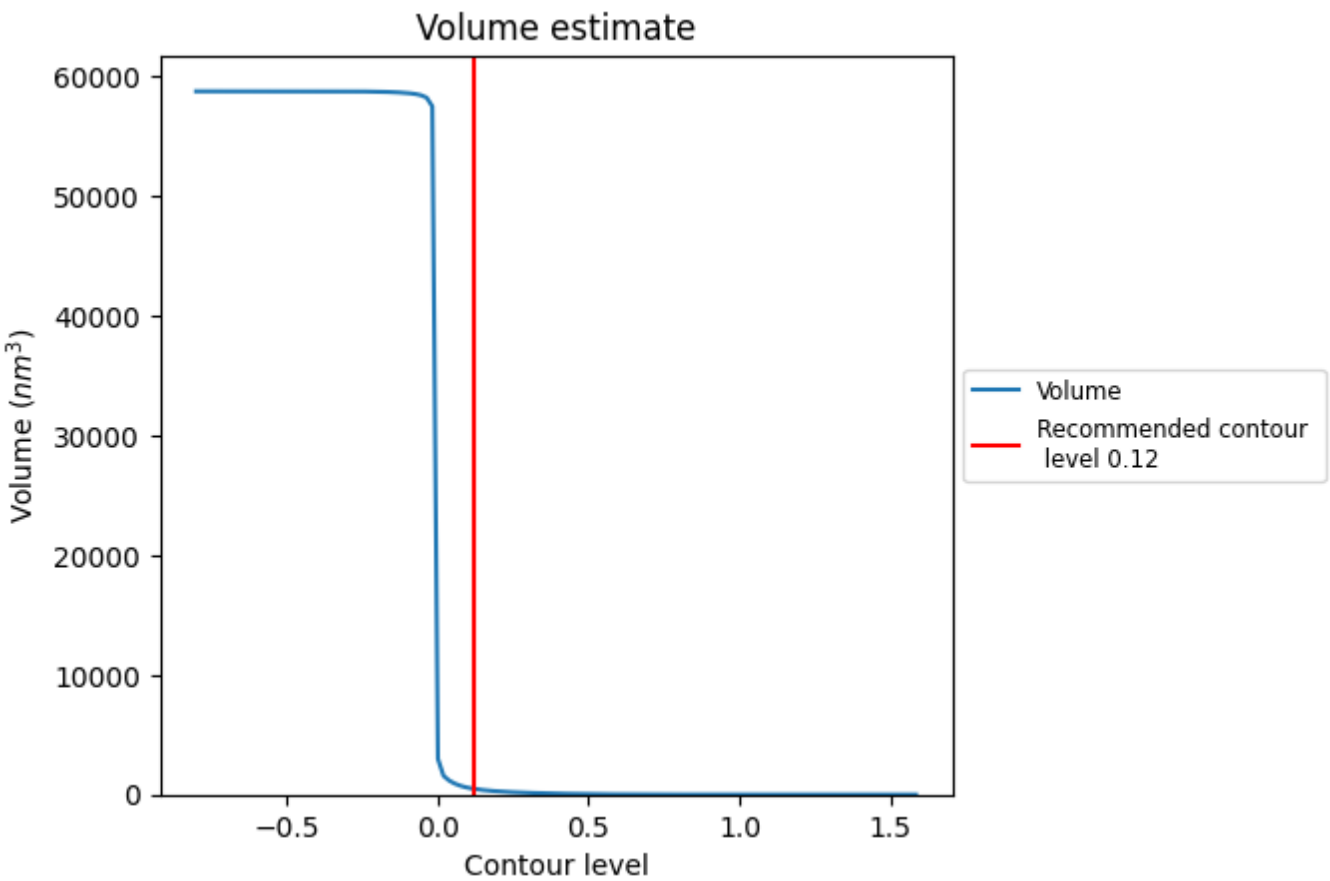
This section contains the results of statistical analysis of the map.

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.

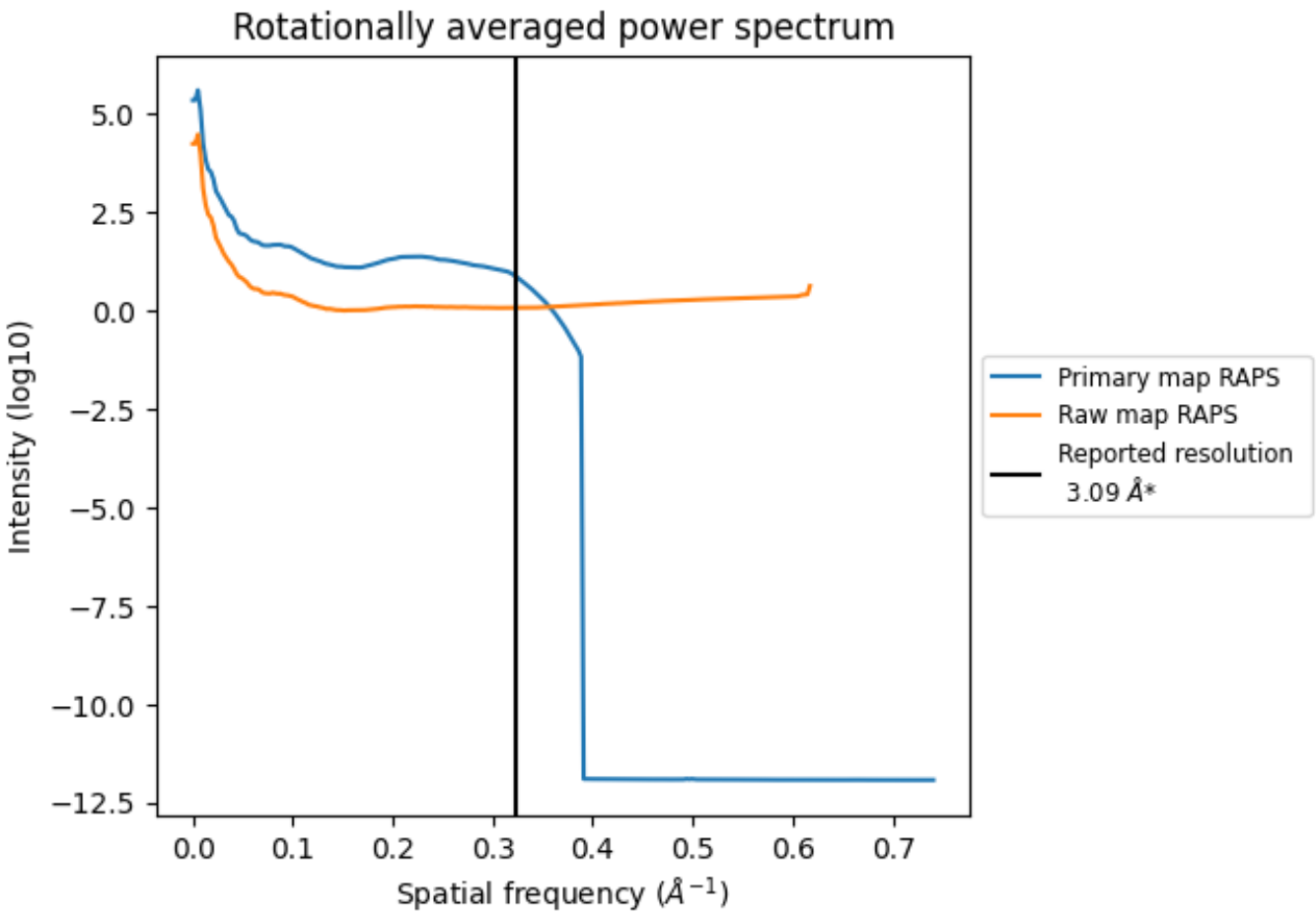
7.2 Volume estimate (i)



The volume at the recommended contour level is 483 nm^3; this corresponds to an approximate mass of 436 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)

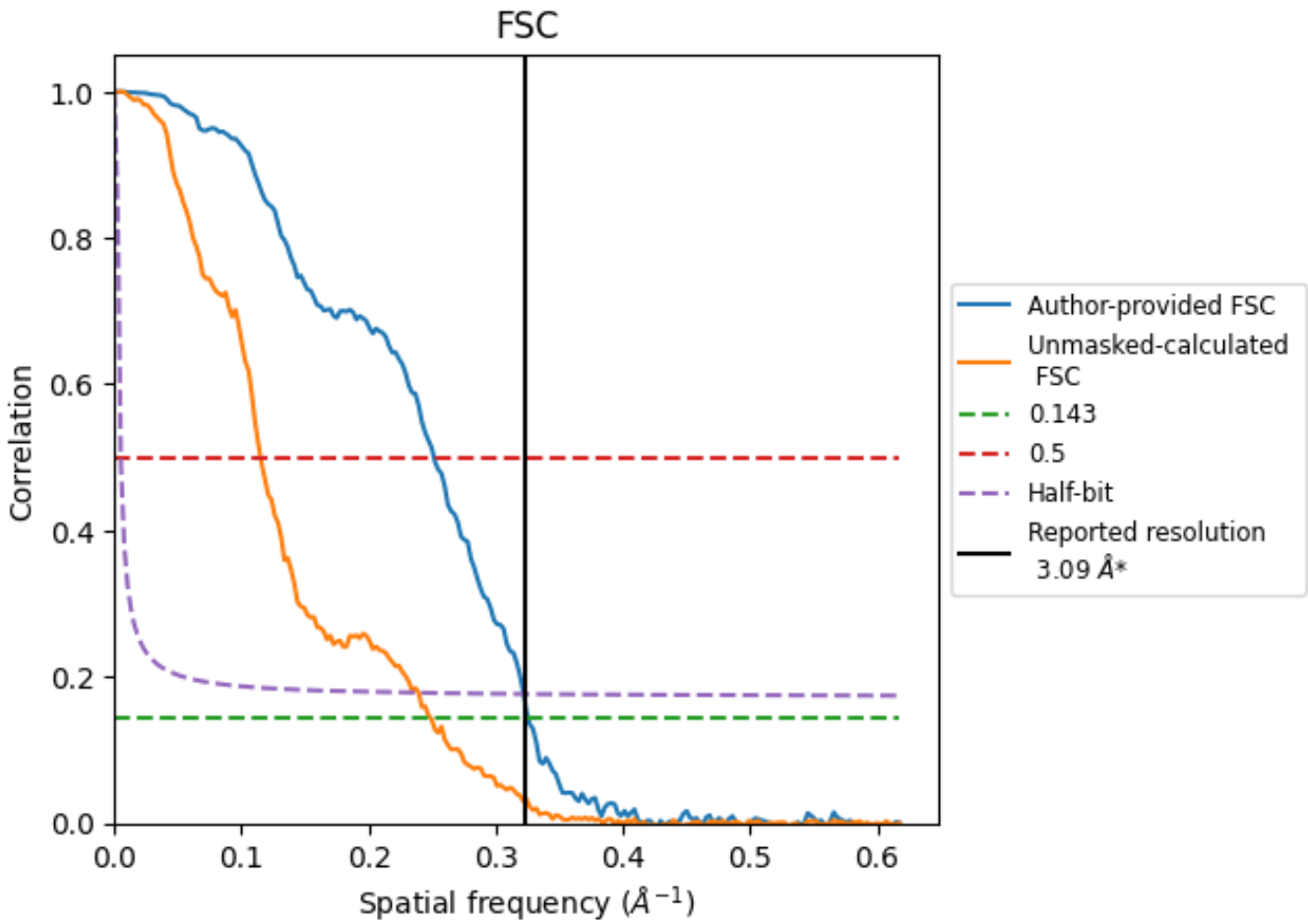


*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

8.2 Resolution estimates (i)

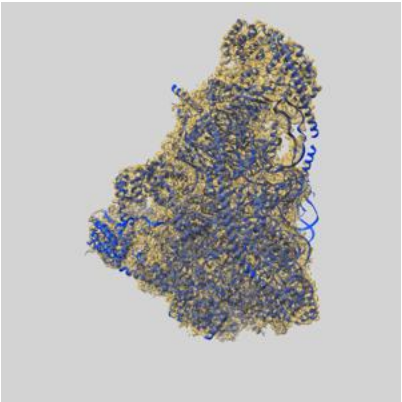
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.07	3.98	3.11
Unmasked-calculated*	4.02	8.70	4.18

*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 4.02 differs from the reported value 3.09 by more than 10 %

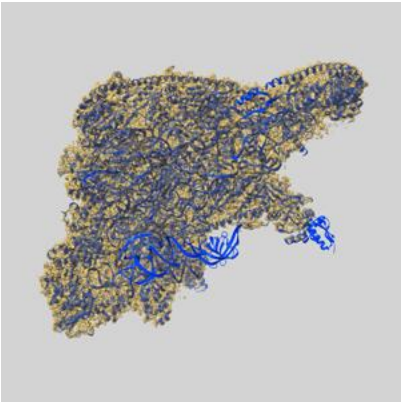
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13560 and PDB model 7PO2. Per-residue inclusion information can be found in section 3 on page 16.

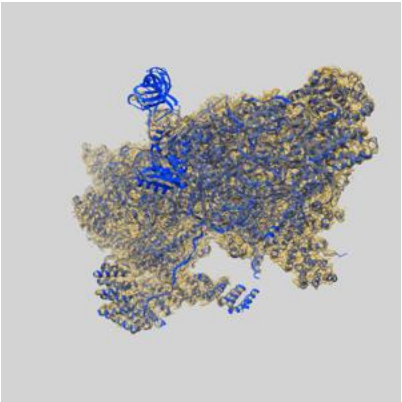
9.1 Map-model overlay (i)



X



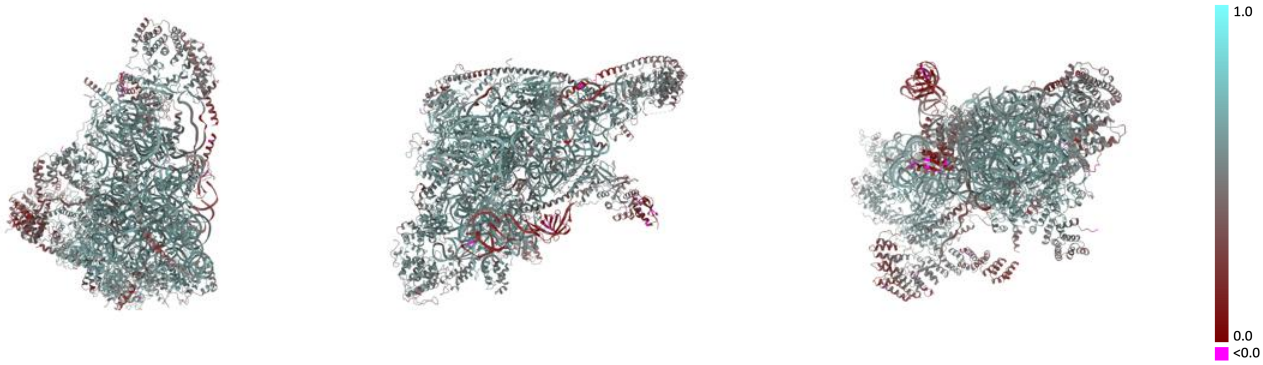
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

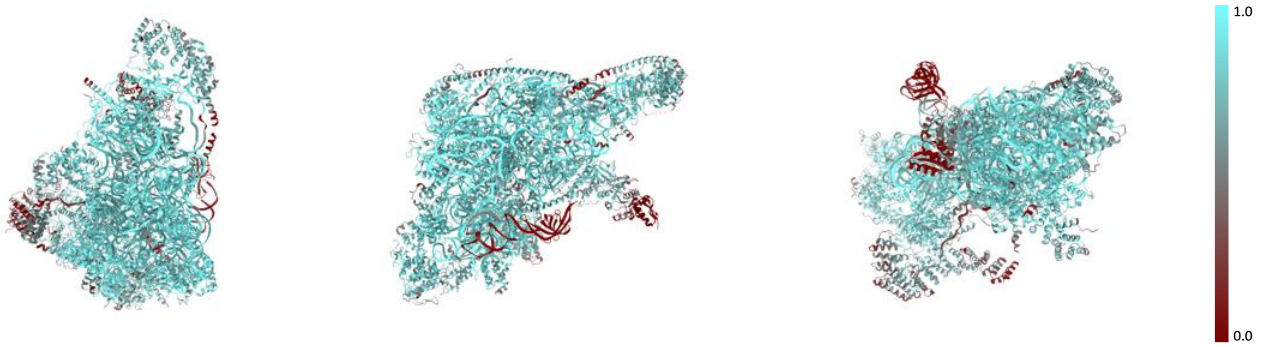
9.2 Q-score mapped to coordinate model (i)



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.

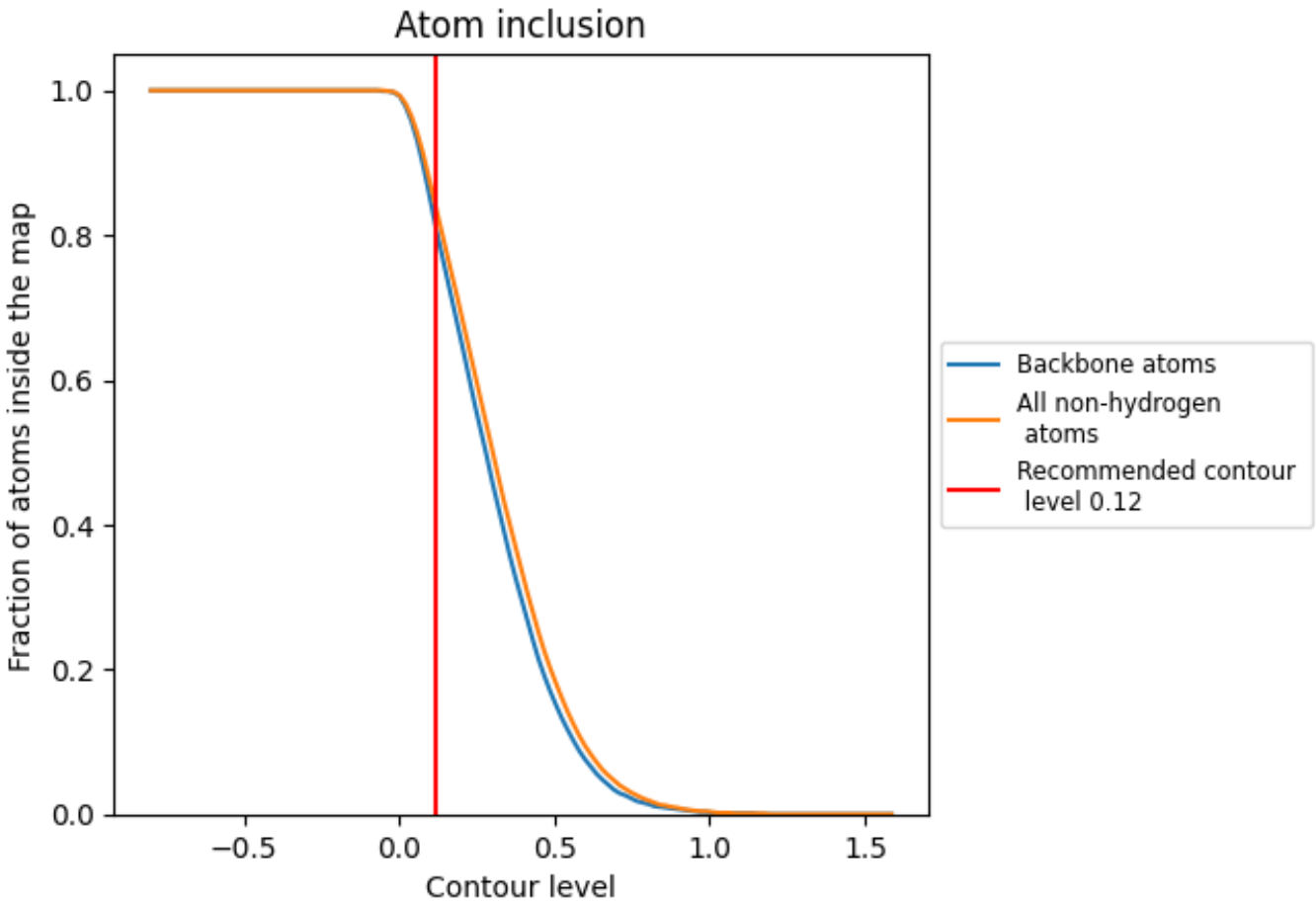
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 81% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5390
0	0.8560	0.5320
1	0.7760	0.5240
2	0.8140	0.5250
3	0.8620	0.5550
4	0.5820	0.4010
5	0.4510	0.3320
6	0.5220	0.3910
7	0.5220	0.4160
A	0.9640	0.6110
B	0.9090	0.5920
C	0.9490	0.6220
D	0.8890	0.5740
E	0.8680	0.5630
F	0.8380	0.5430
G	0.8290	0.5500
H	0.8730	0.5750
I	0.8920	0.5740
J	0.9300	0.5970
K	0.9460	0.6290
L	0.8000	0.5320
M	0.8960	0.5910
N	0.9140	0.5920
O	0.8910	0.5710
P	0.9120	0.5830
Q	0.9490	0.6140
R	0.8000	0.5130
S	0.7980	0.5070
T	0.8840	0.5740
U	0.7530	0.4890
V	0.7200	0.4590
W	0.8940	0.5640
X	0.8230	0.5400
Y	0.6830	0.4780
Z	0.8600	0.5630
t	0.0000	0.1710