Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 07:12 am BST

PDB ID	:	7PNX / pdb_00007pnx
EMDB ID	:	EMD-13555
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit without mS37 in complex with RBFA and METTL15 conformation a
Authors	:	Itoh, Y.; Khawaja, A.; Rorbach, J.; Amunts, A.
Deposited on	:	2021-09-08
Resolution	:	2.76 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 (i)) were used in the production of this report:

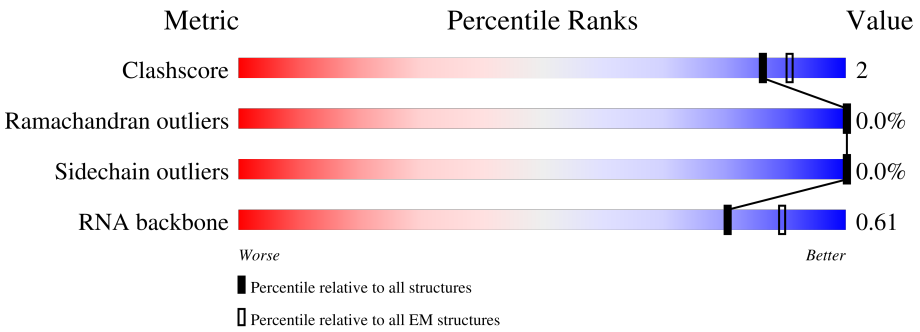
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

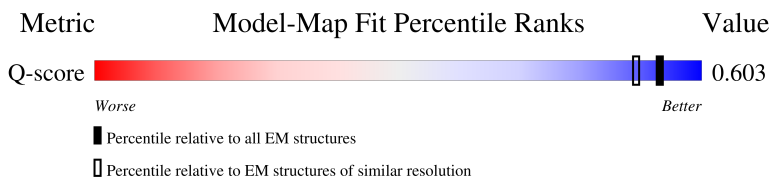
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.76 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	10642 (2.26 - 3.26)

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	79% 20%
2	B	296	72% 24%
3	C	167	72% 7% 21%

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Mol	Chain	Length	Quality of chain
4	D	430	76% 20%
5	E	125	90% 6%
6	F	242	81% 15%
7	G	396	5% 78% 5% 17%
8	H	201	64% 6% 30%
9	I	194	64% 6% 29%
10	J	138	76% 22%
11	K	128	70% 9% 21%
12	L	257	5% 63% 32%
13	M	137	85% 13%
14	N	130	82% 15%
15	O	258	73% 25%
16	P	142	65% 32%
17	Q	86	92% 8%
18	R	360	77% 5% 18%
19	S	190	66% 5% 29%
20	T	173	91% 6%
21	U	205	83% 14%
22	V	414	82% 5% 13%
23	W	187	52% 47%
24	X	398	84% 12%
25	Y	395	5% 36% 62%
26	Z	106	5% 93% 6%
27	0	218	93% 6%
28	1	323	84% 14%

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Mol	Chain	Length	Quality of chain
29	3	199	35% 64%
30	4	689	8% 80% 6% 14%
31	a	343	26% 54% 7% 39%
32	b	407	17% 72% 8% 20%

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 133745 atoms, of which 61111 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	951	30467	9060	10269	3636	6551	951	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	118	1891	592	955	168	172	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	205	3673	1158	1869	324	311	11	15	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 Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	3	71	1331	403	702	135	90	1	0	0

- Molecule 30 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	4	590	9556	3056	4781	809	882	28	0	0

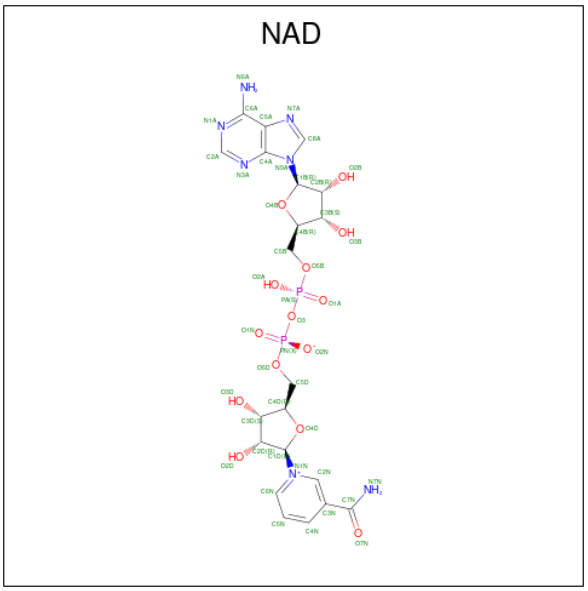
- Molecule 31 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	a	210	3347	1046	1672	297	323	9	0	0

- Molecule 32 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	b	326	5167	1610	2621	456	466	14	0	0

- Molecule 33 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	A	61	61	61	0
34	B	1	1	1	0
34	X	1	1	1	0
34	3	1	1	1	0

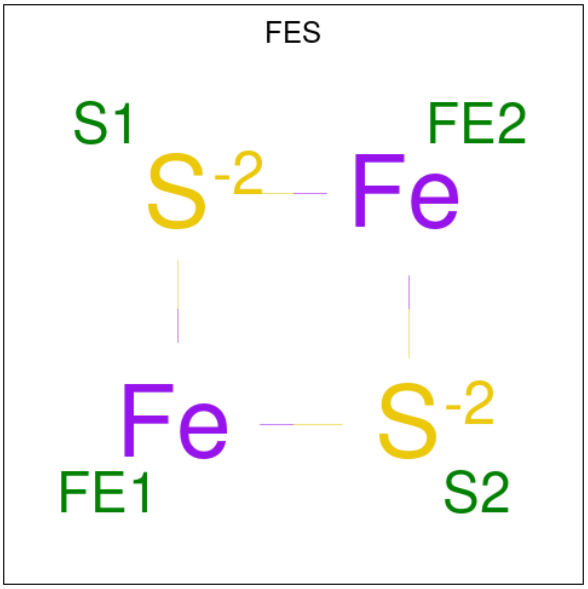
- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
35	A	16	16	16	0

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

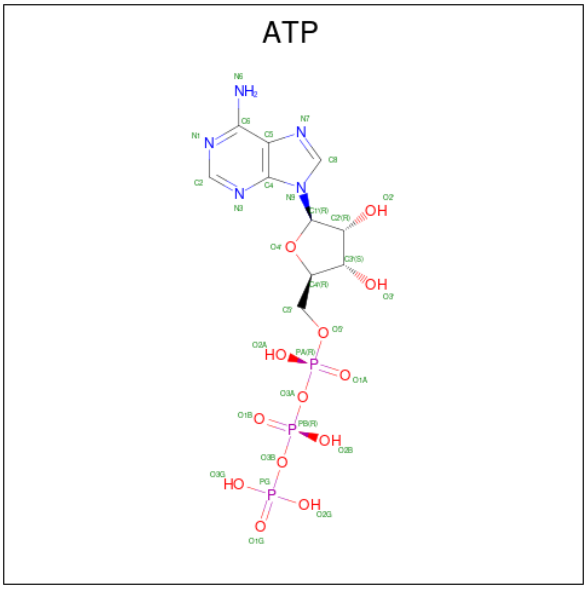
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
36	O	1	1	1	0

- Molecule 37 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



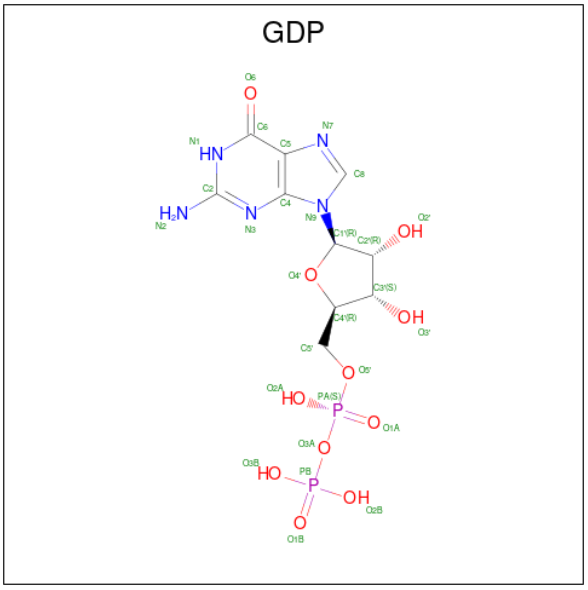
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
37	P	1	4	2	2	0
			Total	Fe	S	
37	T	1	4	2	2	0

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



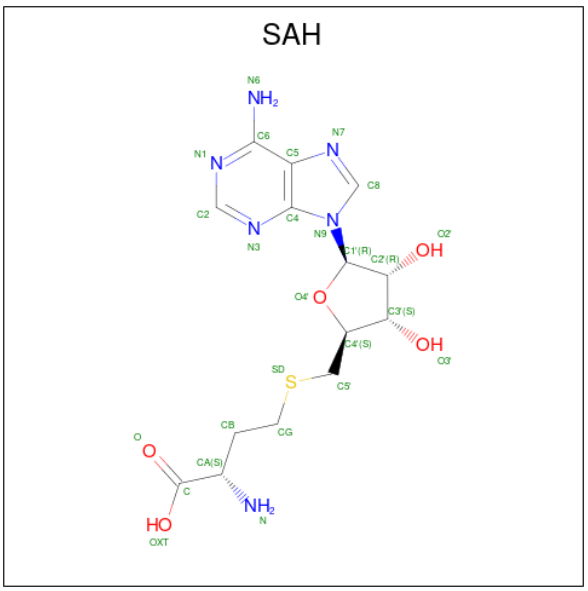
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
38	X	1	43	10	12	5	13	3	0

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



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

- Molecule 40 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
40	b	1	46	14	20	6	5	1	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
41	A	1296	1296	1296	0
41	B	81	81	81	0
41	C	60	60	60	0
41	D	72	72	72	0
41	E	4	4	4	0
41	F	24	24	24	0
41	G	60	60	60	0
41	H	32	32	32	0
41	I	14	14	14	0
41	J	28	28	28	0
41	K	45	45	45	0
41	L	23	23	23	0
41	M	44	44	44	0
41	N	28	28	28	0
41	O	56	56	56	0
41	P	9	9	9	0
41	Q	14	14	14	0
41	R	45	45	45	0
41	S	25	25	25	0

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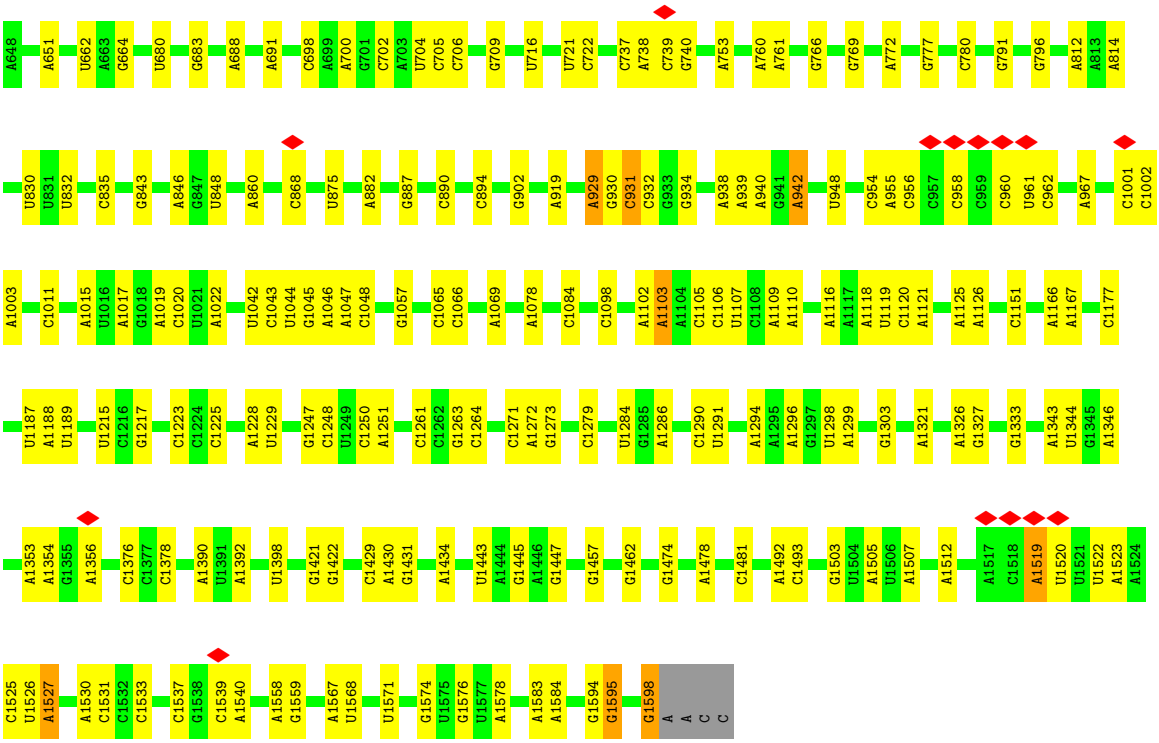
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
41	T	40	40	40	0
			Total	O	
41	U	15	15	15	0
			Total	O	
41	V	2	2	2	0
			Total	O	
41	W	13	13	13	0
			Total	O	
41	X	32	32	32	0
			Total	O	
41	Y	3	3	3	0
			Total	O	
41	Z	19	19	19	0
			Total	O	
41	0	26	26	26	0
			Total	O	
41	1	26	26	26	0
			Total	O	
41	3	9	9	9	0
			Total	O	
41	4	7	7	7	0
			Total	O	
41	a	4	4	4	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.

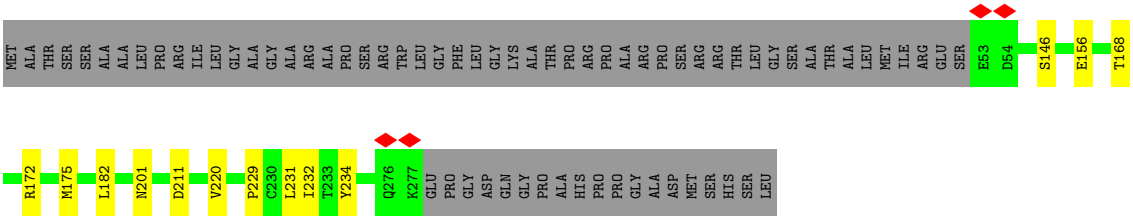
• Molecule 1: 12S mitochondrial rRNA

Chain A:



• Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:



• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C: 72% 7% 21%

MET ALA ALA SER VAL CYS SER GLY LEU LEU GLY PRO ARG VAL LEU SER TRP SER ARG GLU LEU PRO CYS ALA TRP ARG ALA LEU HIS THR SER PRO VAL CYS ALA K36 A58 P59 D89 V90 M96 L108 R112 N115 Y132 V136 T157 L167

- Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain D: 76% 20%

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

ALA SER LEU SER ARG ALA LEU GLN THR GLN CYS CYS ILE SER SER PRO SER HIS LEU MET SER GLN GLN TYR ARG PRO TYR S88 D96 L103 G115 K116 R117 T118 K119 K120 R123 K184 M185 W198 Y215 K234 V243 L244 V245 K260 F268 A271

V276 Y285 L296 S339 Q347 E372 E398 D399 E400 R419 S420 V421 T430

- Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain E: 90% 6%

MET P2 R15 E40 L65 V94 L117 Y118 S119 THR LYS LYS ARG LYS LYS

- Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F: 81% 15%

MET ALA ALA PRO ALA VAL LYS VAL ALA ARG GLY TRP SER GLY LEU ALA LEU GLY VAL ARG ARG ALA VAL LEU GLN LEU PRO GLY LEU THR GLN VAL ARG TRP S35 K48 E56 E57 L158 L162 K163 G164 G165 R166 V170 P171 D193 K194 A230 A237 H238 Y239

ARG TRP TRP

- Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G: 5% 78% 5% 17%

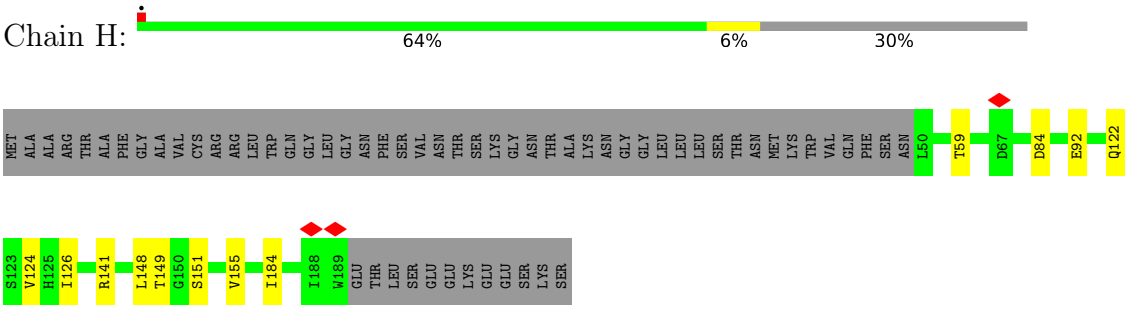
MET ALA ALA PRO CYS VAL SER TYR GLY GLY ALA VAL SER TYR ARG LEU LEU LEU TRP GLY ARG GLY SER LEU ALA ARG LYS GLN GLY LEU TRP LYS THR ALA ALA PRO GLU LEU GLN THR ASN VAL ARG SER GLN ILE LEU ARG LEU ARG HIS THR A53 F54 V55 I56 P57 K58 K59 N60

V61 P62 T63 S64 K65 R66 E67 T70 F73 G115 A137 I138 H163 H175 Q176 SER HIS LEU GLN ALA LYS SER LEU LEU PRO GLU LYS THR VAL THR ARG ASP V194 I195 L200 V210 Y218 L229 V241 V248 T249 L250 E251 Q312 H318

D321 V356 V361 R388 R389 R396

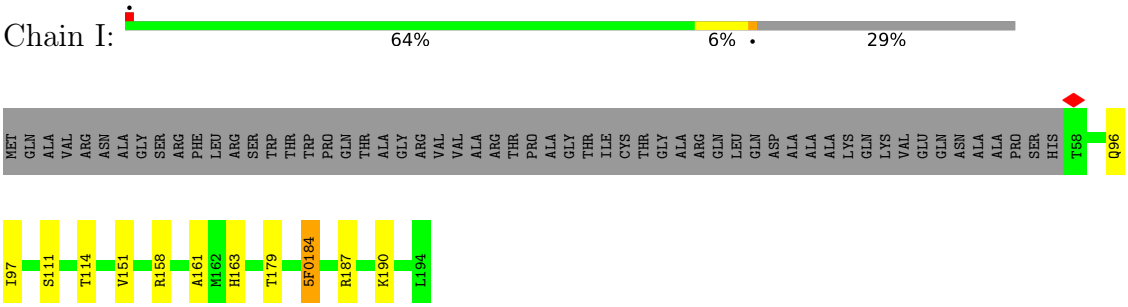
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



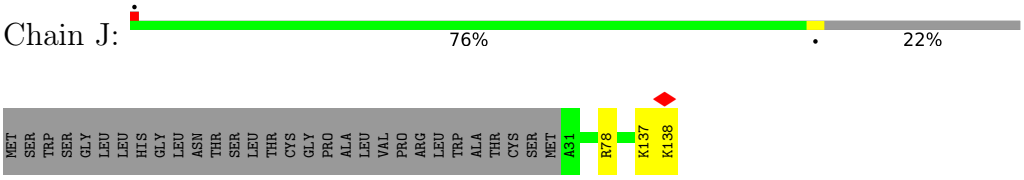
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



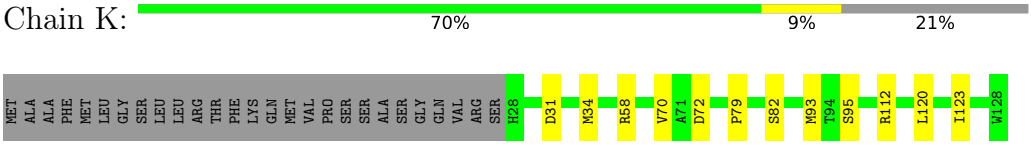
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:



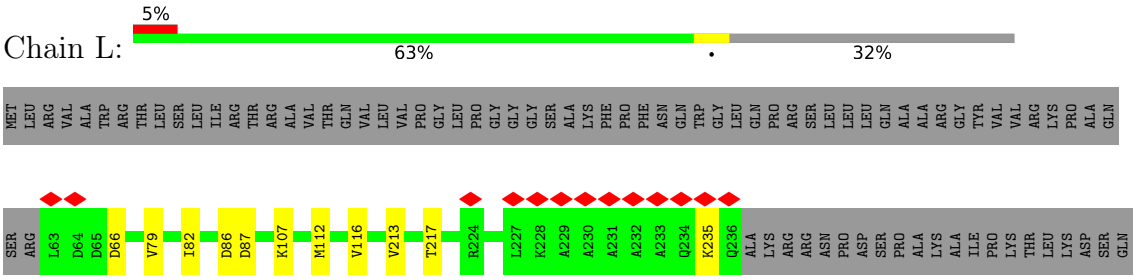
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:



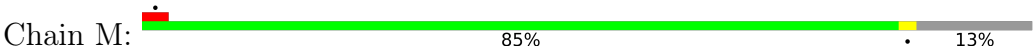
• Molecule 12: 28S ribosomal protein S15, mitochondrial

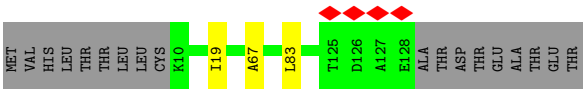
Chain L:



• Molecule 13: 28S ribosomal protein S16, mitochondrial

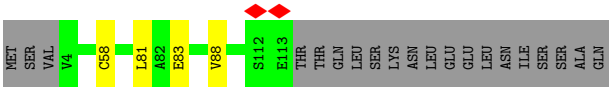
Chain M:





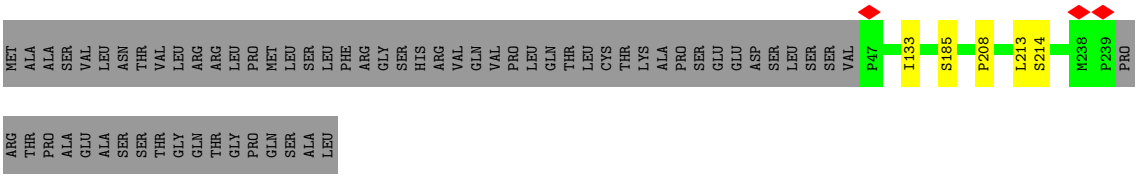
• Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain N:



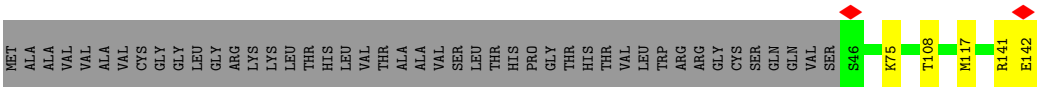
• Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain O:



• Molecule 16: 28S ribosomal protein S18c, mitochondrial

Chain P:

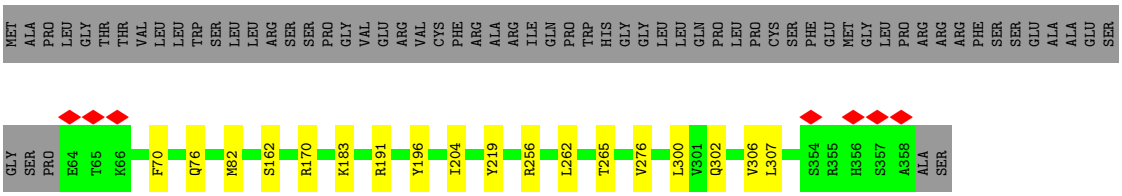


• Molecule 17: 28S ribosomal protein S21, mitochondrial

Chain Q:

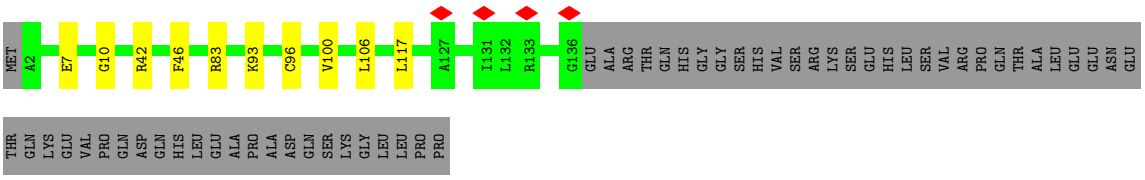
• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:



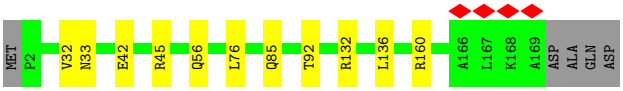
• Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S:



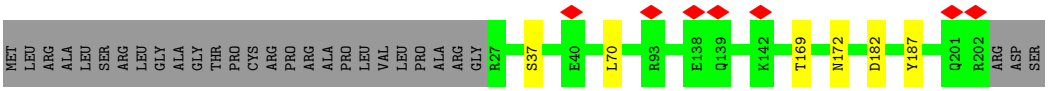
• Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T:



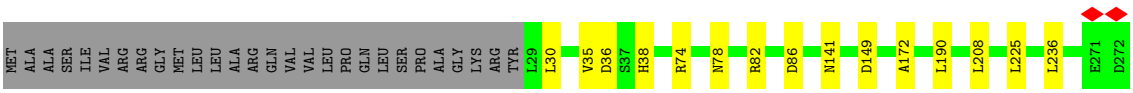
• Molecule 21: 28S ribosomal protein S26, mitochondrial

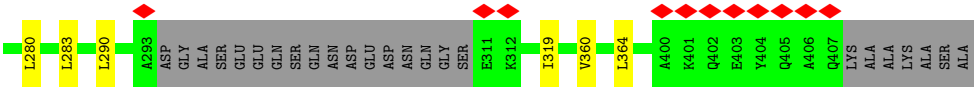
Chain U:



• Molecule 22: 28S ribosomal protein S27, mitochondrial

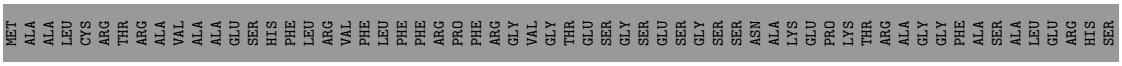
Chain V:

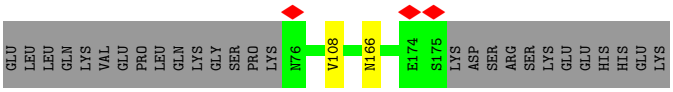




• Molecule 23: 28S ribosomal protein S28, mitochondrial

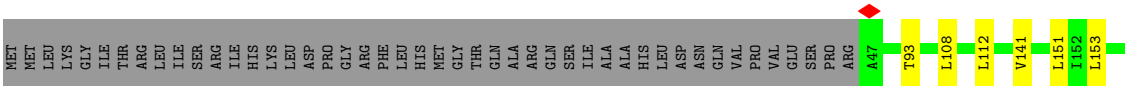
Chain W:

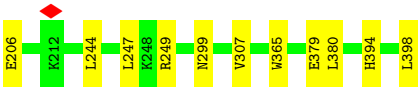




• Molecule 24: 28S ribosomal protein S29, mitochondrial

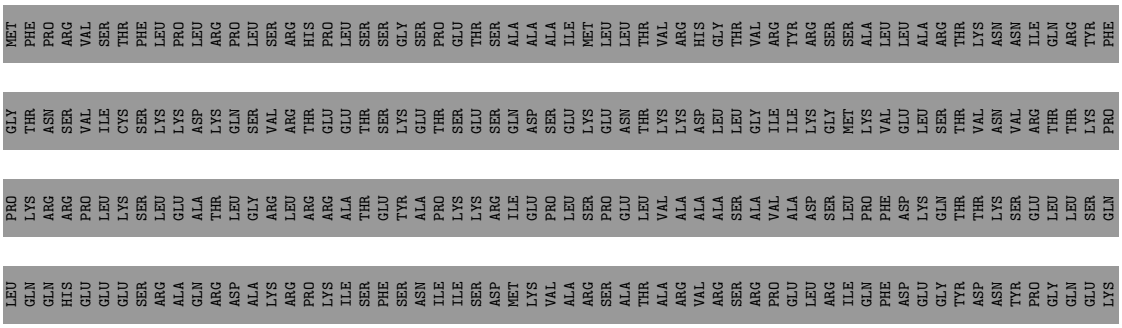
Chain X:

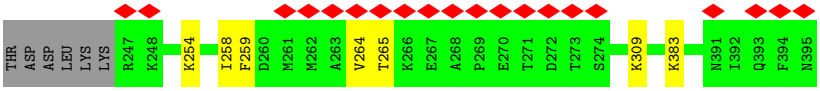




• Molecule 25: 28S ribosomal protein S31, mitochondrial

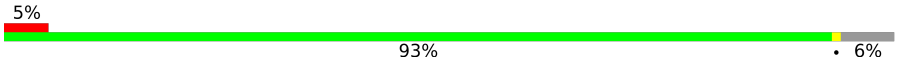
Chain Y:

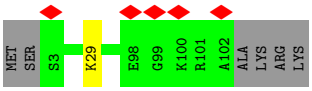




• Molecule 26: 28S ribosomal protein S33, mitochondrial

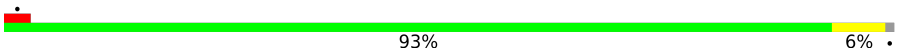
Chain Z:

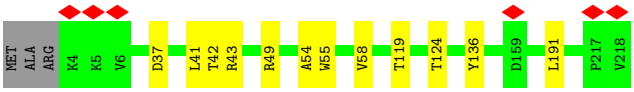




• Molecule 27: 28S ribosomal protein S34, mitochondrial

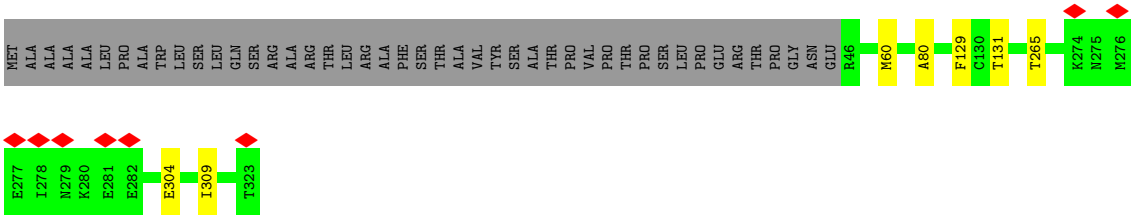
Chain 0:





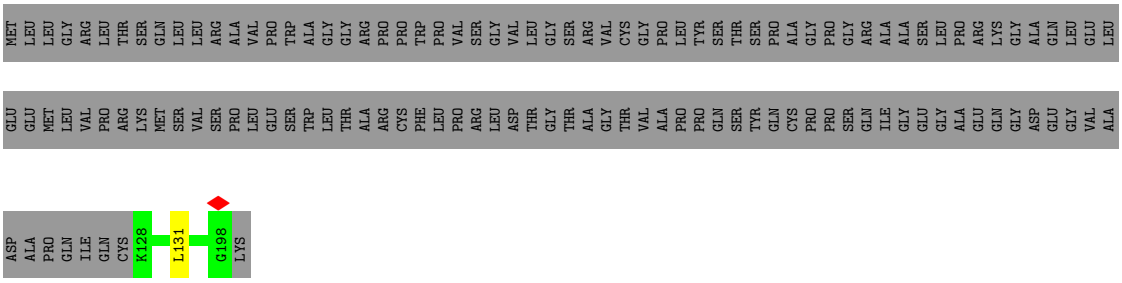
• Molecule 28: 28S ribosomal protein S35, mitochondrial

Chain 1:



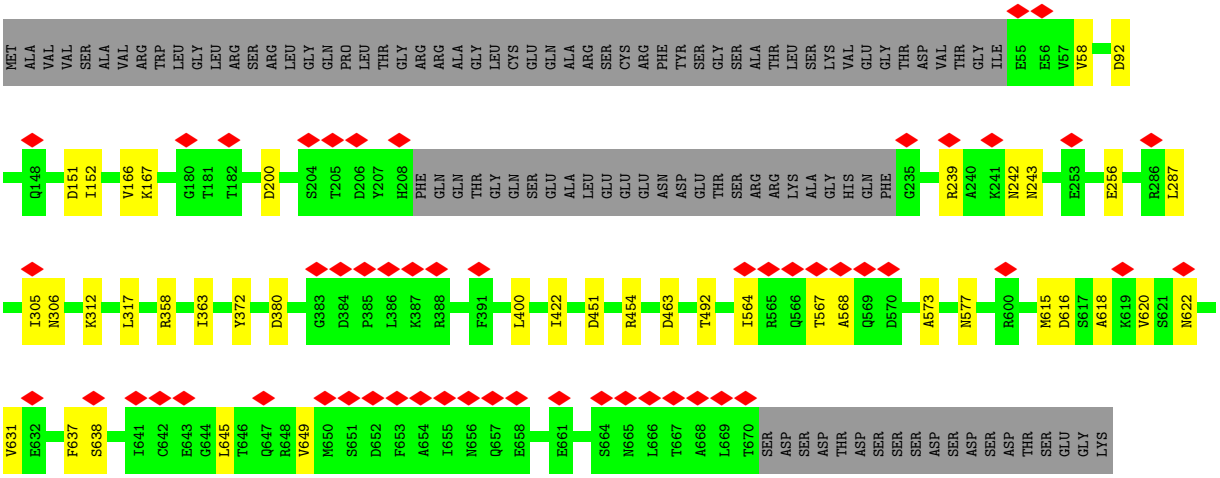
• Molecule 29: Aurora kinase A-interacting protein

Chain 3:



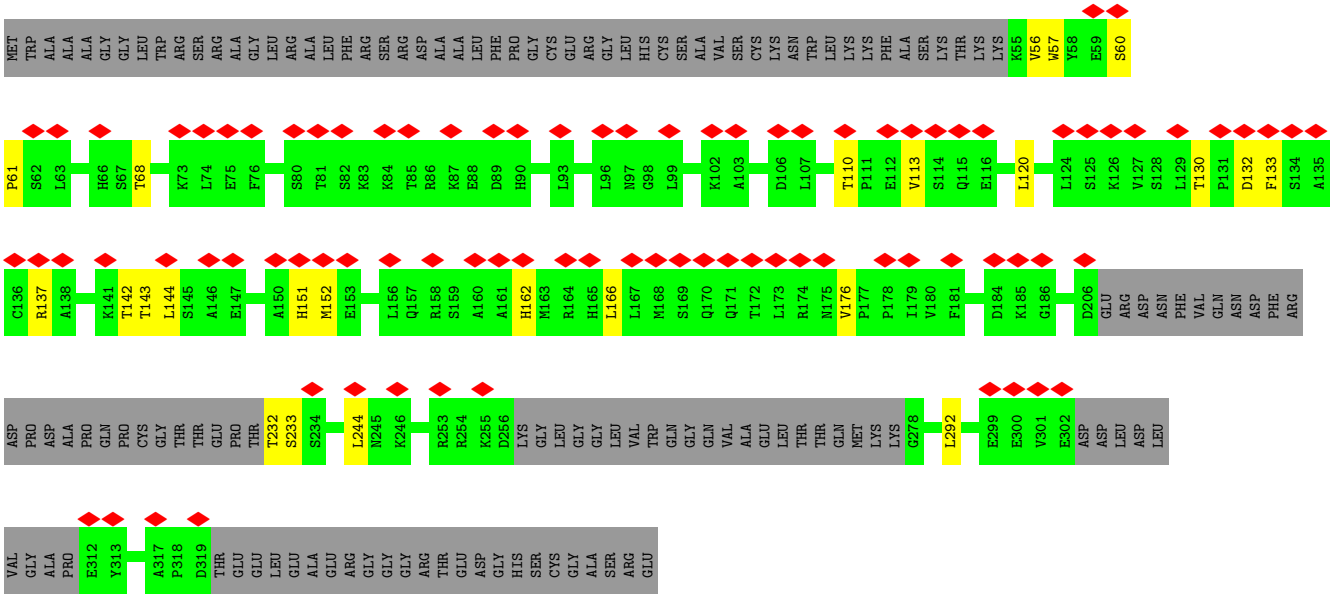
• Molecule 30: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain 4:



• Molecule 31: Putative ribosome-binding factor A, mitochondrial

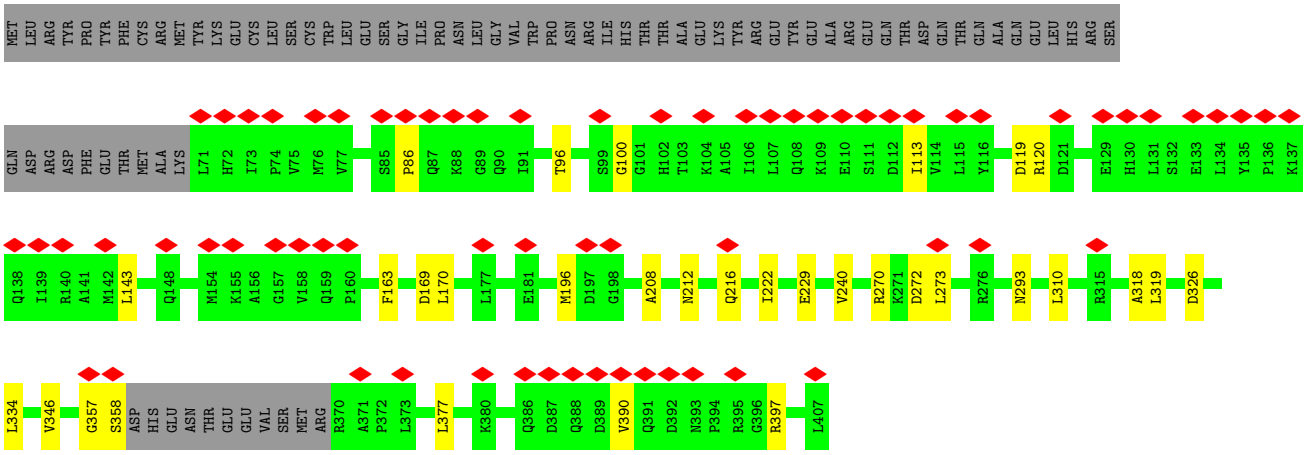
Chain a:



• Molecule 32: 12S rRNA N4-methylcytidine (m4C) methyltransferase

Chain b:

17%
72%
8%
20%


MET LEU ARG TYR PRO TYR PHE CYS ARG MET TYR LYS GLU CYS LEU SER CYS TRP LEU GLU SER GLY ILE PRO ASN LEU GLY VAL TRP PRO ASN ARG ILE HIS THR THR ALA GLU LYS TYR ARG GLU TYR GLU ALA ARG GLU GLN THR ASP GLN THR GLN ALA GLN GLU LEU HIS ARG SER
GLN ASP ARG ASP PHE GLU THR MET ALA LYS L71 H72 I73 P74 V75 M76 V77 S85 P86 Q87 K88 G89 Q90 I91 T96 S99 G100 G101 H102 T103 K104 A105 I106 L107 Q108 K109 E110 S111 D112 I113 V114 L115 Y116 D119 R120 D121 E129 H130 L131 S132 E133 L134 Y135 P136 K137
Q138 I139 R140 A141 M142 L143 Q148 M154 K155 A156 G157 V158 Q159 P160 F163 D169 L170 L177 E181 M196 D197 G198 A208 N212 Q216 I222 E229 V240 R270 K271 D272 L273 R276 N293 L310 R315 A318 L319 D326
L334 V346 G357 S358 ASP HIS GLU ASN THR GLU GLU VAL SER MET ARG R370 A371 P372 L373 L377 K380 Q386 D387 Q388 D389 V390 Q391 D392 N393 P394 R395 G396 R397 L407

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	119673	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	1.898	Depositor
Minimum map value	-0.947	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6, 0.6, 0.6	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: 5MC, 5F0, MA6, AYA, MG, K, NAD, 5MU, GDP, ATP, B8T, FES, SAH, 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	0.12	0/22468	0.21	0/34978
2	B	0.13	0/1871	0.30	0/2531
3	C	0.12	0/1113	0.27	0/1505
4	D	0.12	0/2783	0.28	0/3724
5	E	0.11	0/953	0.27	0/1289
6	F	0.11	0/1846	0.25	0/2482
7	G	0.12	0/2746	0.28	0/3681
8	H	0.13	0/1178	0.28	0/1598
9	I	0.11	0/1030	0.27	0/1386
10	J	0.14	0/855	0.31	0/1148
11	K	0.14	0/880	0.32	0/1182
12	L	0.11	0/1477	0.25	0/1974
13	M	0.13	0/963	0.30	0/1295
14	N	0.12	0/886	0.28	0/1199
15	O	0.11	0/1648	0.27	0/2243
16	P	0.13	0/798	0.30	0/1070
17	Q	0.12	0/748	0.31	0/994
18	R	0.11	0/2456	0.24	0/3317
19	S	0.13	0/1138	0.26	0/1533
20	T	0.11	0/1402	0.28	0/1883
21	U	0.12	0/1510	0.27	0/2025
22	V	0.09	0/3030	0.22	0/4093
23	W	0.12	0/801	0.26	0/1079
24	X	0.12	0/2921	0.28	0/3954
25	Y	0.10	0/1280	0.25	0/1725
26	Z	0.11	0/857	0.26	0/1141
27	0	0.12	0/1834	0.31	0/2484
28	1	0.11	0/2304	0.25	0/3117
29	3	0.13	0/640	0.32	0/844
30	4	0.10	0/4883	0.24	0/6608
31	a	0.09	0/1703	0.27	0/2292
32	b	0.10	0/2590	0.27	0/3492

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.11	0/73592	0.25	0/103866

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

There are no bond length outliers.

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	20198	10269	10253	62	0
2	B	1828	1816	1815	9	0
3	C	1083	1089	1088	8	0
4	D	2731	2805	2804	13	0
5	E	936	955	954	6	0
6	F	1804	1869	1868	5	0
7	G	2688	2690	2687	16	0
8	H	1152	1184	1183	11	0
9	I	1020	1061	1053	8	0
10	J	839	888	887	2	0
11	K	862	886	885	8	0
12	L	1453	1541	1540	6	0
13	M	942	966	965	2	0
14	N	868	929	928	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	1592	1557	1557	4	0
16	P	781	807	806	4	0
17	Q	744	758	758	7	0
18	R	2409	2429	2428	11	0
19	S	1111	1116	1115	8	0
20	T	1371	1394	1393	8	0
21	U	1488	1500	1499	6	0
22	V	2969	2964	2961	12	0
23	W	789	803	802	2	0
24	X	2849	2845	2843	14	0
25	Y	1246	1198	1197	6	0
26	Z	839	860	858	1	0
27	0	1787	1797	1796	9	0
28	1	2256	2289	2288	5	0
29	3	629	702	702	1	0
30	4	4775	4781	4779	27	0
31	a	1675	1672	1668	23	0
32	b	2546	2621	2615	22	0
33	A	44	26	26	0	0
34	3	1	0	0	0	0
34	A	61	0	0	0	0
34	B	1	0	0	0	0
34	X	1	0	0	0	0
35	A	16	0	0	0	0
36	O	1	0	0	0	0
37	P	4	0	0	0	0
37	T	4	0	0	0	0
38	X	31	12	12	0	0
39	X	28	12	12	0	0
40	b	26	20	19	1	0
41	0	26	0	0	0	0
41	1	26	0	0	0	0
41	3	9	0	0	0	0
41	4	7	0	0	0	0
41	A	1296	0	0	11	0
41	B	81	0	0	1	0
41	C	60	0	0	1	0
41	D	72	0	0	2	0
41	E	4	0	0	0	0
41	F	24	0	0	0	0
41	G	60	0	0	2	0
41	H	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	I	14	0	0	1	0
41	J	28	0	0	0	0
41	K	45	0	0	1	0
41	L	23	0	0	0	0
41	M	44	0	0	0	0
41	N	28	0	0	0	0
41	O	56	0	0	0	0
41	P	9	0	0	0	0
41	Q	14	0	0	1	0
41	R	45	0	0	0	0
41	S	25	0	0	2	0
41	T	40	0	0	2	0
41	U	15	0	0	0	0
41	V	2	0	0	0	0
41	W	13	0	0	0	0
41	X	32	0	0	0	0
41	Y	3	0	0	0	0
41	Z	19	0	0	0	0
41	a	4	0	0	0	0
All	All	72634	61111	61044	271	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 (271) 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)
12:L:112:MET:O	12:L:116:VAL:HG22	1.82	0.79
1:A:1353:A:N1	41:A:1805:HOH:O	2.18	0.76
30:4:200:ASP:OD2	30:4:243:ASN:N	2.20	0.75
30:4:451:ASP:OD1	30:4:454:ARG:NH1	2.22	0.72
1:A:1217:G:O6	41:A:1801:HOH:O	2.07	0.72
1:A:1217:G:N7	41:A:1820:HOH:O	2.27	0.66
5:E:117:LEU:HD13	31:a:56:VAL:CG2	2.28	0.64
19:S:42:ARG:NH2	41:S:202:HOH:O	2.32	0.63
1:A:1294:A:OP1	2:B:201:ASN:ND2	2.32	0.62
32:b:163:PHE:O	32:b:310:LEU:HD12	2.00	0.62
17:Q:87:CYS:O	41:Q:101:HOH:O	2.16	0.62
19:S:10:GLY:O	41:S:201:HOH:O	2.16	0.62
1:A:700:A:N1	1:A:709:G:O2'	2.32	0.61
2:B:211:ASP:OD2	41:B:401:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:0:41:LEU:HD13	27:0:55:TRP:CG	2.35	0.61
1:A:1443:U:O2'	1:A:1445:G:N7	2.33	0.61
24:X:153:LEU:HD21	24:X:244:LEU:HD22	1.83	0.61
1:A:1346:A:OP2	41:A:1804:HOH:O	2.16	0.60
31:a:56:VAL:HG12	31:a:57:TRP:H	1.67	0.60
20:T:33:ASN:OD1	41:T:301:HOH:O	2.17	0.60
1:A:1321:A:OP2	41:A:1803:HOH:O	2.16	0.60
4:D:420:SER:O	41:D:501:HOH:O	2.17	0.60
32:b:86:PRO:HB3	32:b:113:ILE:HD12	1.84	0.60
1:A:1078:A:O2'	32:b:326:ASP:OD2	2.18	0.60
21:U:70:LEU:CD2	27:0:191:LEU:HD11	2.33	0.59
1:A:942:A:N6	1:A:1047:A:OP2	2.33	0.59
18:R:70:PHE:O	18:R:76:GLN:NE2	2.36	0.59
24:X:151:LEU:HD23	24:X:247:LEU:HD22	1.85	0.58
28:1:304:GLU:OE1	28:1:309:ILE:HD11	2.04	0.58
5:E:94:VAL:CG1	16:P:117:MET:HE1	2.34	0.58
7:G:312:GLN:NE2	41:G:404:HOH:O	2.36	0.57
31:a:130:THR:HG22	31:a:137:ARG:NH1	2.20	0.57
1:A:702:C:OP1	1:A:848:U:O2'	2.22	0.57
1:A:843:G:N2	1:A:846:A:OP2	2.35	0.56
4:D:347:GLN:NE2	41:D:505:HOH:O	2.38	0.56
1:A:1272:A:N1	1:A:1303:G:O2'	2.30	0.56
20:T:132:ARG:NH1	20:T:136:LEU:O	2.39	0.56
31:a:56:VAL:HG12	31:a:57:TRP:N	2.20	0.56
22:V:236:LEU:HD12	22:V:290:LEU:HD13	1.86	0.56
1:A:1066:C:O2'	9:I:187:ARG:O	2.23	0.56
25:Y:258:ILE:HD11	30:4:317:LEU:HD22	1.88	0.55
32:b:318:ALA:C	32:b:319:LEU:HD12	2.32	0.55
4:D:285:TYR:OH	4:D:372:GLU:OE2	2.17	0.55
32:b:196:MET:SD	32:b:293:ASN:ND2	2.80	0.55
30:4:151:ASP:OD1	30:4:152:ILE:N	2.40	0.55
15:O:208:PRO:HG2	15:O:213:LEU:HD21	1.89	0.55
3:C:90:VAL:HG21	11:K:93:MET:HE1	1.88	0.55
17:Q:83:PRO:HA	23:W:108:VAL:HG21	1.89	0.55
12:L:86:ASP:OD1	12:L:87:ASP:N	2.39	0.54
25:Y:259:PHE:HB2	30:4:363:ILE:HD11	1.89	0.54
32:b:119:ASP:O	32:b:143:LEU:HD12	2.07	0.54
1:A:1084:C:H1'	32:b:346:VAL:HG11	1.89	0.54
31:a:130:THR:HG22	31:a:137:ARG:CZ	2.37	0.54
1:A:1434:A:OP1	7:G:389:ARG:NE	2.41	0.54
30:4:631:VAL:HG21	30:4:649:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:G:N7	41:A:1830:HOH:O	2.33	0.53
3:C:115:ASN:ND2	25:Y:309:LYS:O	2.39	0.53
9:I:163:HIS:CE1	31:a:144:LEU:HD22	2.43	0.53
31:a:113:VAL:HG13	31:a:166:LEU:HD13	1.90	0.53
32:b:229:GLU:OE1	32:b:270:ARG:NH1	2.40	0.53
1:A:1598:G:OP2	17:Q:57:TYR:OH	2.26	0.53
6:F:158[A]:LEU:HD23	6:F:171[A]:PRO:HA	1.90	0.53
7:G:229:LEU:HD21	7:G:241:VAL:HG11	1.90	0.53
24:X:151:LEU:CD2	24:X:247:LEU:HD22	2.39	0.53
31:a:120:LEU:HD22	31:a:152:MET:CG	2.39	0.53
7:G:115:GLY:O	41:G:401:HOH:O	2.18	0.52
19:S:106:LEU:HB2	19:S:117:LEU:HD11	1.90	0.52
30:4:615:MET:HG3	30:4:645:LEU:HD11	1.92	0.52
32:b:318:ALA:O	32:b:319:LEU:HD12	2.09	0.52
15:O:185:SER:O	18:R:183:LYS:NZ	2.41	0.52
24:X:380:LEU:HD23	24:X:394:HIS:CD2	2.45	0.52
27:0:42:THR:HG22	27:0:49:ARG:HG2	1.92	0.52
1:A:875:U:O2'	1:A:882:A:N1	2.39	0.52
1:A:948:U:OP2	1:A:1045:G:N1	2.37	0.52
1:A:934:G:O2'	1:A:940:A:N1	2.43	0.52
27:0:54:ALA:O	27:0:58:VAL:HG23	2.10	0.51
1:A:1431:G:O2'	1:A:1457:G:O6	2.26	0.51
1:A:1530:A:N1	1:A:1531:C:N4	2.59	0.51
11:K:120:LEU:HB3	11:K:123:ILE:HD12	1.92	0.51
28:1:60:MET:HE1	28:1:80:ALA:O	2.10	0.51
1:A:664:G:O2'	1:A:1166:A:N1	2.41	0.51
31:a:120:LEU:HD21	31:a:151:HIS:ND1	2.26	0.51
17:Q:77:ARG:NH1	23:W:166:ASN:OD1	2.43	0.51
30:4:239:ARG:O	30:4:242:ASN:ND2	2.44	0.51
1:A:760:A:N1	1:A:780:C:O2'	2.36	0.50
6:F:48:LYS:NZ	7:G:321:ASP:OD1	2.36	0.50
21:U:70:LEU:HD21	27:0:191:LEU:HD11	1.93	0.50
32:b:208:ALA:O	32:b:212:ASN:ND2	2.44	0.50
18:R:276:VAL:HG11	18:R:307:LEU:HD12	1.94	0.49
32:b:390:VAL:HG13	32:b:397:ARG:HB2	1.93	0.49
1:A:1046:A:O2'	1:A:1048:C:OP2	2.17	0.49
1:A:1057:G:H4'	1:A:1578:A:H4'	1.93	0.49
3:C:89:ASP:OD1	3:C:112:ARG:NH2	2.42	0.49
32:b:216:GLN:CG	32:b:240:VAL:HG21	2.42	0.49
4:D:198:TRP:CD2	31:a:292:LEU:HD13	2.47	0.49
24:X:108:LEU:HD23	24:X:141:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:35:VAL:HG12	22:V:35:VAL:O	2.12	0.49
31:a:120:LEU:HD22	31:a:152:MET:HG2	1.94	0.49
22:V:360:VAL:HG13	22:V:364:LEU:HD22	1.95	0.49
1:A:930:G:O2'	1:A:931:C:OP2	2.26	0.48
30:4:567:THR:HG22	30:4:568:ALA:N	2.28	0.48
1:A:1392:A:N7	41:A:1837:HOH:O	2.35	0.48
9:I:190:LYS:NZ	41:I:202:HOH:O	2.47	0.48
1:A:1279:C:O2'	1:A:1296:A:N1	2.47	0.48
11:K:79:PRO:O	11:K:82:SER:OG	2.26	0.48
24:X:380:LEU:HD21	24:X:398:LEU:CD1	2.44	0.48
22:V:74:ARG:O	22:V:78:ASN:ND2	2.46	0.48
6:F:170[B]:VAL:HG13	6:F:237:ALA:HA	1.94	0.48
27:0:119:THR:OG1	27:0:124:THR:HG22	2.14	0.48
9:I:179:THR:HG21	17:Q:39:ILE:HD13	1.95	0.48
18:R:162:SER:O	18:R:170:ARG:NH2	2.45	0.48
2:B:156:GLU:OE1	7:G:163:HIS:ND1	2.41	0.47
12:L:213:VAL:O	12:L:217:THR:HG23	2.13	0.47
20:T:32:VAL:HG22	20:T:76:LEU:HD22	1.96	0.47
22:V:225:LEU:HD21	22:V:280:LEU:HD23	1.96	0.47
1:A:887:G:N7	41:A:1839:HOH:O	2.35	0.47
7:G:318:HIS:NE2	24:X:379:GLU:OE2	2.47	0.47
30:4:256:GLU:HG3	30:4:287:LEU:HD22	1.96	0.47
30:4:564:ILE:HG22	30:4:564:ILE:O	2.13	0.47
18:R:219:TYR:O	18:R:256:ARG:NH1	2.46	0.47
30:4:618:ALA:O	30:4:622:ASN:N	2.48	0.47
13:M:19:ILE:HB	13:M:83:LEU:HD23	1.96	0.47
17:Q:78:LYS:HG3	31:a:68:THR:HG21	1.96	0.47
24:X:108:LEU:HD21	24:X:307:VAL:CG1	2.44	0.47
5:E:117:LEU:HD13	31:a:56:VAL:HG22	1.95	0.47
7:G:248:VAL:O	7:G:250:LEU:N	2.47	0.47
11:K:58:ARG:NE	11:K:72:ASP:OD1	2.39	0.47
30:4:380:ASP:HB2	30:4:422:ILE:HD11	1.95	0.47
1:A:929:A:O4'	4:D:421:VAL:HG13	2.14	0.47
25:Y:264:VAL:HG12	25:Y:265:THR:N	2.30	0.47
30:4:58:VAL:HG23	30:4:58:VAL:O	2.14	0.47
30:4:372:TYR:CE2	30:4:400:LEU:HD21	2.49	0.47
1:A:662:U:OP2	4:D:339:SER:OG	2.30	0.47
2:B:220:VAL:HG22	2:B:234:TYR:HB2	1.97	0.46
11:K:70:VAL:HG11	25:Y:383:LYS:HE3	1.97	0.46
3:C:157:THR:OG1	30:4:92:ASP:OD2	2.31	0.46
22:V:225:LEU:HD11	22:V:283:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:176:VAL:O	31:a:176:VAL:HG13	2.15	0.46
14:N:58:CYS:SG	14:N:81:LEU:HD22	2.55	0.46
1:A:1044:U:OP1	1:A:1110:A:O2'	2.32	0.46
31:a:244:LEU:HD13	32:b:222:ILE:HD11	1.97	0.46
8:H:148:LEU:HD23	8:H:148:LEU:H	1.79	0.46
31:a:143:THR:HG22	31:a:144:LEU:N	2.31	0.46
14:N:83:GLU:OE1	20:T:85:GLN:NE2	2.42	0.46
18:R:302:GLN:O	18:R:306:VAL:HG23	2.16	0.46
20:T:56:GLN:OE1	41:T:302:HOH:O	2.20	0.46
30:4:631:VAL:CG2	30:4:649:VAL:HG21	2.46	0.46
1:A:706:C:OP1	27:0:43:ARG:NE	2.41	0.46
7:G:137:ALA:O	7:G:138:ILE:C	2.57	0.46
7:G:200:LEU:O	7:G:218:TYR:OH	2.26	0.46
11:K:31:ASP:OD2	41:K:201:HOH:O	2.20	0.46
31:a:110:THR:HG23	31:a:110:THR:O	2.15	0.46
21:U:169:THR:N	21:U:172:ASN:OD1	2.46	0.46
27:0:37:ASP:O	27:0:41:LEU:N	2.47	0.46
24:X:206:GLU:OE2	24:X:249:ARG:NH2	2.47	0.45
32:b:272:ASP:OD1	32:b:273:LEU:N	2.45	0.45
11:K:34:MET:HE3	11:K:95:SER:HB2	1.99	0.45
32:b:120:ARG:NH2	32:b:293:ASN:O	2.49	0.45
1:A:1017:A:O2'	16:P:108:THR:OG1	2.30	0.45
1:A:1102:A:H5'	1:A:1576:G:H4'	1.99	0.45
5:E:15:ARG:NH2	21:U:182:ASP:OD1	2.48	0.45
30:4:615:MET:CE	30:4:649:VAL:HG22	2.46	0.45
1:A:894:C:H41	10:J:78:ARG:NH1	2.15	0.45
2:B:172:ARG:O	2:B:175:MET:HG2	2.15	0.45
32:b:216:GLN:HG3	32:b:240:VAL:HG21	1.99	0.45
1:A:1519:A:N7	12:L:235:LYS:NZ	2.62	0.45
6:F:193:ASP:OD1	6:F:194:LYS:N	2.50	0.45
31:a:132:ASP:O	31:a:133:PHE:HB2	2.17	0.45
1:A:738:A:H2'	1:A:740:G:C4	2.52	0.45
1:A:1429:C:OP1	7:G:388:ARG:NH2	2.45	0.45
7:G:70:THR:HG23	7:G:73:PHE:H	1.82	0.45
18:R:262:LEU:O	18:R:265:THR:OG1	2.23	0.45
1:A:931:C:O2	1:A:931:C:O2'	2.33	0.44
1:A:1263:G:N7	41:A:1847:HOH:O	2.36	0.44
4:D:245:VAL:HG22	4:D:271:ALA:HB1	1.99	0.44
15:O:214:SER:OG	22:V:319:ILE:HG23	2.17	0.44
32:b:357:GLY:O	32:b:358:SER:C	2.59	0.44
1:A:1125:A:N1	41:A:1846:HOH:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:A:O2'	9:I:96:GLN:OE1	2.36	0.44
1:A:1298:U:H2'	1:A:1299:A:C8	2.52	0.44
9:I:97:ILE:HD11	9:I:161:ALA:HB1	2.00	0.44
20:T:92:THR:O	20:T:92:THR:HG22	2.18	0.44
1:A:698:C:OP1	21:U:37:SER:OG	2.31	0.44
3:C:112:ARG:NH1	41:C:205:HOH:O	2.51	0.44
1:A:1478:A:C2	29:3:131:LEU:HD21	2.53	0.44
20:T:42:GLU:OE1	20:T:45:ARG:NH2	2.45	0.44
22:V:30:LEU:HD12	22:V:149:ASP:HB2	1.99	0.44
31:a:232:THR:OG1	31:a:233:SER:N	2.51	0.44
32:b:100:GLY:N	40:b:501:SAH:O	2.46	0.44
5:E:40:GLU:OE1	21:U:187:TYR:OH	2.31	0.44
8:H:149:THR:OG1	28:1:131:THR:OG1	2.27	0.44
25:Y:254:LYS:O	30:4:358:ARG:NH1	2.51	0.44
32:b:169:ASP:OD1	32:b:170:LEU:N	2.51	0.44
2:B:231:LEU:HD21	19:S:46:PHE:HB2	2.00	0.43
4:D:103:LEU:HD11	4:D:123:ARG:HB2	2.00	0.43
1:A:1298:U:O2'	2:B:182:LEU:HD23	2.17	0.43
7:G:210:VAL:HG12	7:G:210:VAL:O	2.19	0.43
8:H:155:VAL:HG21	28:1:129:PHE:CB	2.48	0.43
16:P:141:ARG:O	16:P:142:GLU:C	2.62	0.43
22:V:141:ASN:ND2	22:V:172:ALA:O	2.46	0.43
24:X:299:ASN:ND2	28:1:265:THR:OG1	2.51	0.43
3:C:96:MET:HB2	3:C:108:LEU:HD11	2.00	0.43
32:b:229:GLU:OE2	32:b:270:ARG:NH2	2.52	0.43
19:S:7:GLU:OE1	19:S:7:GLU:N	2.48	0.43
31:a:120:LEU:HD22	31:a:152:MET:HG3	2.01	0.43
5:E:65:LEU:HD21	16:P:75:LYS:HD3	2.01	0.43
8:H:184:ILE:O	8:H:184:ILE:HG22	2.18	0.43
24:X:380:LEU:HD21	24:X:398:LEU:HD12	2.01	0.43
1:A:1177:C:O2'	1:A:1567:A:N1	2.47	0.43
31:a:162:HIS:CD2	31:a:166:LEU:HD11	2.54	0.43
4:D:243:VAL:HG11	4:D:268:PHE:CD1	2.54	0.42
8:H:148:LEU:HD23	8:H:148:LEU:N	2.34	0.42
24:X:112:LEU:CD1	24:X:141:VAL:HG13	2.49	0.42
30:4:637:PHE:O	30:4:638:SER:OG	2.29	0.42
14:N:88:VAL:O	14:N:88:VAL:HG13	2.19	0.42
31:a:60:SER:N	31:a:61:PRO:HD3	2.34	0.42
31:a:142:THR:HG22	31:a:143:THR:N	2.33	0.42
1:A:769:G:N2	1:A:772:A:OP2	2.51	0.42
1:A:1595:G:O6	17:Q:50:ARG:NH2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:PRO:HA	2:B:232:ILE:HD12	2.00	0.42
4:D:215:TYR:CD2	4:D:276:VAL:HG21	2.54	0.42
7:G:356:VAL:HG23	7:G:361:VAL:HG23	2.01	0.42
18:R:162:SER:O	18:R:170:ARG:NH1	2.52	0.42
19:S:96:CYS:O	19:S:100:VAL:HG23	2.20	0.42
1:A:1398:U:OP1	26:Z:29:LYS:NZ	2.30	0.42
7:G:250:LEU:O	7:G:250:LEU:HG	2.19	0.42
30:4:305:ILE:O	30:4:312:LYS:NZ	2.47	0.42
32:b:96:THR:HG21	32:b:169:ASP:O	2.19	0.42
22:V:36:ASP:OD1	22:V:38:HIS:ND1	2.53	0.42
30:4:616:ASP:O	30:4:620:VAL:HG23	2.19	0.42
1:A:705:C:OP2	27:0:136:TYR:OH	2.30	0.42
2:B:146:SER:O	2:B:168:THR:HA	2.20	0.42
4:D:96:ASP:OD1	4:D:123:ARG:NH1	2.51	0.42
8:H:59:THR:O	8:H:59:THR:HG23	2.18	0.42
19:S:83:ARG:NH1	19:S:93:LYS:O	2.53	0.42
9:I:111:SER:OG	9:I:114:THR:HG23	2.20	0.41
1:A:1523:A:O2'	1:A:1527:A:N1	2.39	0.41
10:J:137:LYS:O	10:J:138:LYS:C	2.63	0.41
9:I:151:VAL:HG21	9:I:158:ARG:HG3	2.03	0.41
1:A:691:A:N7	1:A:716:U:O2'	2.49	0.41
22:V:82:ARG:NH2	22:V:86:ASP:OD1	2.52	0.41
22:V:190:LEU:HD11	22:V:208:LEU:HD11	2.03	0.41
30:4:305:ILE:HG22	30:4:306:ASN:N	2.35	0.41
24:X:93:THR:HG21	24:X:365:TRP:CZ3	2.56	0.41
1:A:1264:C:H1'	8:H:124:VAL:HG13	2.02	0.41
3:C:58:ALA:HB1	3:C:59:PRO:CD	2.51	0.41
3:C:132:TYR:O	3:C:136:VAL:HG23	2.21	0.41
8:H:151:SER:O	8:H:155:VAL:HG23	2.21	0.41
13:M:67:ALA:HB2	18:R:196:TYR:CE1	2.56	0.41
30:4:615:MET:HE1	30:4:649:VAL:HG22	2.02	0.41
32:b:334:LEU:HD21	32:b:377:LEU:HD11	2.03	0.41
4:D:243:VAL:HG11	4:D:268:PHE:HD1	1.85	0.41
12:L:66:ASP:OD1	12:L:107:LYS:NZ	2.43	0.41
15:O:133:ILE:HD12	15:O:133:ILE:C	2.46	0.41
1:A:1286:A:OP1	4:D:260:LYS:NZ	2.51	0.40
30:4:573:ALA:O	30:4:577:ASN:ND2	2.53	0.40
1:A:1228:A:N6	41:A:1969:HOH:O	2.52	0.40
12:L:79:VAL:HG21	12:L:82:ILE:HD13	2.03	0.40
18:R:191:ARG:HG3	18:R:204:ILE:HG23	2.03	0.40
19:S:106:LEU:CB	19:S:117:LEU:HD11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:108:LEU:HD21	24:X:307:VAL:HG13	2.03	0.40
6:F:158[A]:LEU:HD21	6:F:230:ALA:HA	2.03	0.40
7:G:115:GLY:N	8:H:84:ASP:OD2	2.54	0.40
8:H:122:GLN:O	11:K:112:ARG:NH1	2.53	0.40
1:A:683:G:OP1	20:T:160:ARG:NH1	2.54	0.40
1:A:812:A:O2'	1:A:814:A:N1	2.52	0.40
1:A:1103:A:N7	1:A:1574:G:O2'	2.42	0.40
8:H:92:GLU:OE1	8:H:141:ARG:NH1	2.49	0.40
18:R:82:MET:HE1	18:R:300:LEU:HD13	2.04	0.40
30:4:166:VAL:HG23	30:4:167:LYS:N	2.36	0.40
30:4:463:ASP:OD1	30:4:492:THR:HG22	2.22	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%)	222 (100%)	1 (0%)	0	100	100
3	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
4	D	341/430 (79%)	334 (98%)	7 (2%)	0	100	100
5	E	116/125 (93%)	116 (100%)	0	0	100	100
6	F	218/242 (90%)	212 (97%)	6 (3%)	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%)	18	34
9	I	134/194 (69%)	131 (98%)	3 (2%)	0	100	100
10	J	106/138 (77%)	104 (98%)	2 (2%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	94 (99%)	1 (1%)	0	100	100
17	Q	84/86 (98%)	84 (100%)	0	0	100	100
18	R	293/360 (81%)	286 (98%)	7 (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%)	353 (99%)	5 (1%)	0	100	100
23	W	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
24	X	350/398 (88%)	345 (99%)	5 (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	3	69/199 (35%)	69 (100%)	0	0	100	100
30	4	586/689 (85%)	579 (99%)	7 (1%)	0	100	100
31	a	202/343 (59%)	195 (96%)	7 (4%)	0	100	100
32	b	322/407 (79%)	316 (98%)	6 (2%)	0	100	100
All	All	6080/7934 (77%)	5998 (99%)	81 (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%)	284 (99%)	2 (1%)	76	86
5	E	100/107 (94%)	100 (100%)	0	100	100
6	F	195/209 (93%)	195 (100%)	0	100	100
7	G	285/342 (83%)	285 (100%)	0	100	100
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
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%)	325 (100%)	0	100	100
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	311 (100%)	0	100	100
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	3	65/166 (39%)	65 (100%)	0	100	100
30	4	527/609 (86%)	527 (100%)	0	100	100
31	a	185/288 (64%)	185 (100%)	0	100	100
32	b	275/350 (79%)	275 (100%)	0	100	100
All	All	5419/6881 (79%)	5417 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	276	VAL
4	D	296	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	37	ASN
3	C	81	HIS
3	C	116	GLN
4	D	356	GLN
4	D	361	GLN
5	E	58	HIS
6	F	113	GLN
6	F	146	HIS
6	F	207	HIS
7	G	77	GLN
7	G	176	GLN
8	H	109	HIS
8	H	122	GLN
9	I	87	HIS
9	I	96	GLN
10	J	105	HIS
18	R	88	GLN
20	T	33	ASN
21	U	31	HIS
22	V	134	GLN
22	V	188	HIS
24	X	69	ASN
24	X	81	HIS
24	X	143	HIS
24	X	180	GLN
24	X	190	ASN
24	X	302	HIS
25	Y	290	ASN
26	Z	82	GLN
27	0	32	GLN
27	0	111	HIS
27	0	192	ASN
28	1	185	HIS
30	4	129	GLN
30	4	453	HIS

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Mol	Chain	Res	Type
30	4	602	HIS
31	a	162	HIS
32	b	212	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	950/955 (99%)	117 (12%)	0

All (117) 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	739	C
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	890	C
1	A	902	G
1	A	919	A
1	A	929	A
1	A	931	C
1	A	932	C
1	A	938	A
1	A	939	A
1	A	942	A
1	A	954	C

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Mol	Chain	Res	Type
1	A	955	A
1	A	956	C
1	A	958	C
1	A	960	C
1	A	961	U
1	A	962	C
1	A	967	A
1	A	1001	C
1	A	1002	C
1	A	1011	C
1	A	1015	A
1	A	1019	A
1	A	1020	C
1	A	1022	A
1	A	1042	U
1	A	1043	C
1	A	1065	C
1	A	1069	A
1	A	1098	C
1	A	1103	A
1	A	1105	C
1	A	1106	C
1	A	1107	U
1	A	1109	A
1	A	1116	A
1	A	1118	A
1	A	1119	U
1	A	1120	C
1	A	1121	A
1	A	1126	A
1	A	1151	C
1	A	1167	A
1	A	1187	U
1	A	1188	A
1	A	1189	U
1	A	1215	U
1	A	1223	C
1	A	1225	C
1	A	1229	U
1	A	1247	G
1	A	1248	C
1	A	1250	C

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Mol	Chain	Res	Type
1	A	1251	A
1	A	1261	C
1	A	1271	C
1	A	1273	G
1	A	1284	U
1	A	1290	C
1	A	1291	U
1	A	1326	A
1	A	1327	G
1	A	1343	A
1	A	1344	U
1	A	1354	A
1	A	1356	A
1	A	1376	C
1	A	1378	C
1	A	1390	A
1	A	1421	G
1	A	1422	G
1	A	1430	A
1	A	1447	G
1	A	1462	G
1	A	1474	G
1	A	1481	C
1	A	1492	A
1	A	1493	C
1	A	1503	G
1	A	1505	A
1	A	1507	A
1	A	1512	A
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	1539	C
1	A	1540	A
1	A	1558	A
1	A	1559	G
1	A	1568	U

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Mol	Chain	Res	Type
1	A	1571	U
1	A	1594	G
1	A	1595	G
1	A	1598	G

There are no RNA pucker outliers to report.

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

7 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	$\#\|Z\| > 2$
1	5MU	A	1076	1	19,22,23	0.30	0	28,32,35	0.37	0
1	5MC	A	1488	1	18,22,23	0.33	0	26,32,35	0.45	0
9	5F0	I	184	9	8,8,9	0.58	0	7,9,11	1.04	1 (14%)
1	MA6	A	1584	1	23,26,27	0.28	0	34,38,41	0.57	1 (2%)
17	AYA	Q	2	17	6,7,8	0.76	0	5,8,10	0.50	0
1	B8T	A	1486	1	19,22,23	0.32	0	26,31,34	0.33	0
1	MA6	A	1583	1	23,26,27	0.31	0	34,38,41	0.57	1 (2%)

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
1	5MU	A	1076	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1488	1	-	0/7/25/26	0/2/2/2
9	5F0	I	184	9	-	0/9/9/10	-
1	MA6	A	1584	1	-	1/11/29/30	0/3/3/3
17	AYA	Q	2	17	-	0/4/6/8	-
1	B8T	A	1486	1	-	0/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1583	1	-	2/11/29/30	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1583	MA6	C2-N1-C6	2.37	117.36	111.75
1	A	1584	MA6	C2-N1-C6	2.35	117.30	111.75
9	I	184	5F0	O-C-CB	-2.33	118.64	125.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1584	MA6	C5-C6-N6-C9
1	A	1583	MA6	O4'-C4'-C5'-O5'
1	A	1583	MA6	C3'-C4'-C5'-O5'

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 87 ligands modelled in this entry, 81 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	$\#\|Z\| > 2$
37	FES	P	201	5,16	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	FES	T	201	20,13	0,4,4	-	-	-		
33	NAD	A	1701	34	45,48,48	0.37	0	63,73,73	0.36	0
40	SAH	b	501	-	27,28,28	0.40	0	38,40,40	0.45	0
38	ATP	X	501	34	29,33,33	0.50	0	44,52,52	0.49	0
39	GDP	X	502	-	28,30,30	0.43	0	44,47,47	0.40	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
37	FES	P	201	5,16	-	-	0/1/1/1
37	FES	T	201	20,13	-	-	0/1/1/1
33	NAD	A	1701	34	-	2/30/62/62	0/5/5/5
40	SAH	b	501	-	-	5/15/31/31	0/3/3/3
38	ATP	X	501	34	-	0/22/38/38	0/3/3/3
39	GDP	X	502	-	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	b	501	SAH	OXT-C-CA-N
40	b	501	SAH	OXT-C-CA-CB
40	b	501	SAH	O-C-CA-CB
40	b	501	SAH	O-C-CA-N
40	b	501	SAH	C2'-C1'-N9-C8
33	A	1701	NAD	PA-O3-PN-O1N
33	A	1701	NAD	PA-O3-PN-O2N

There are no ring outliers.

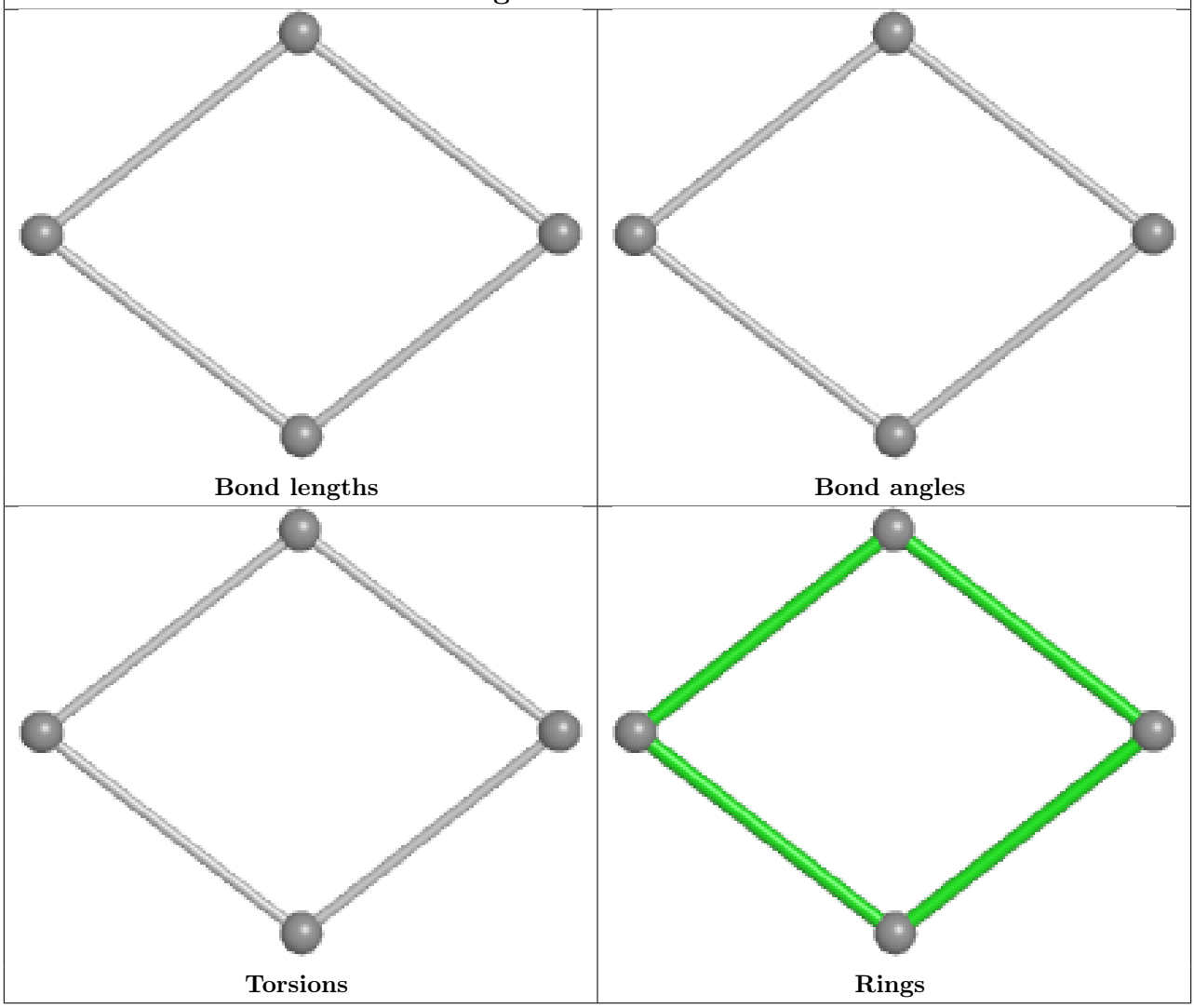
1 monomer is involved in 1 short contact:

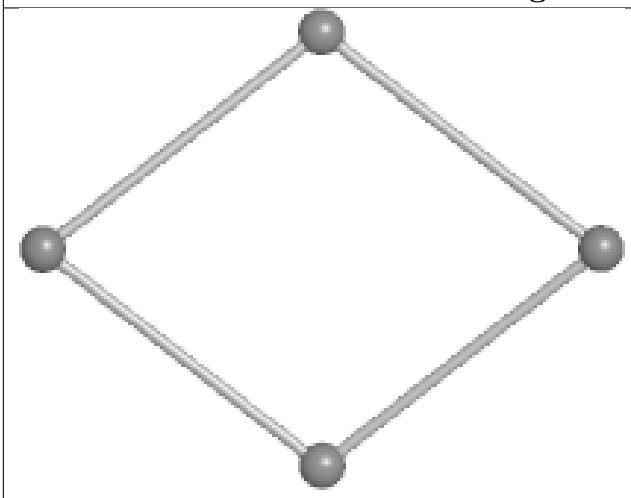
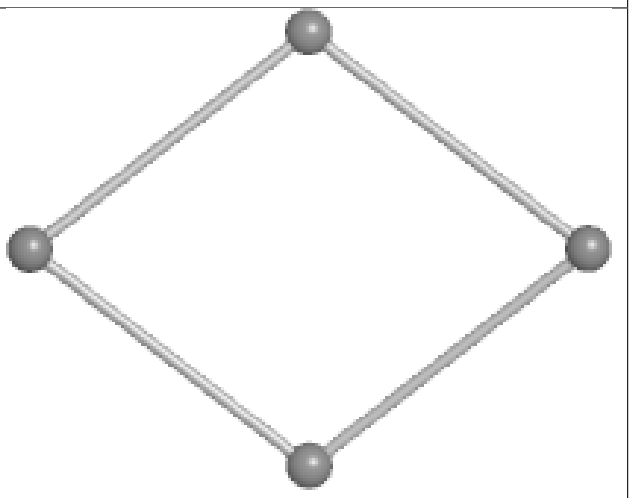
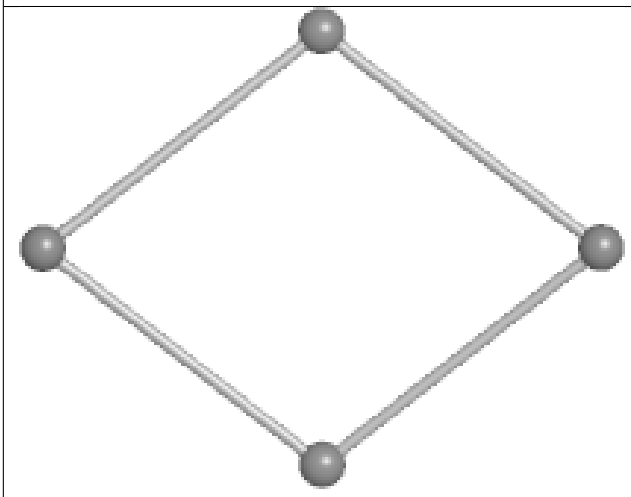
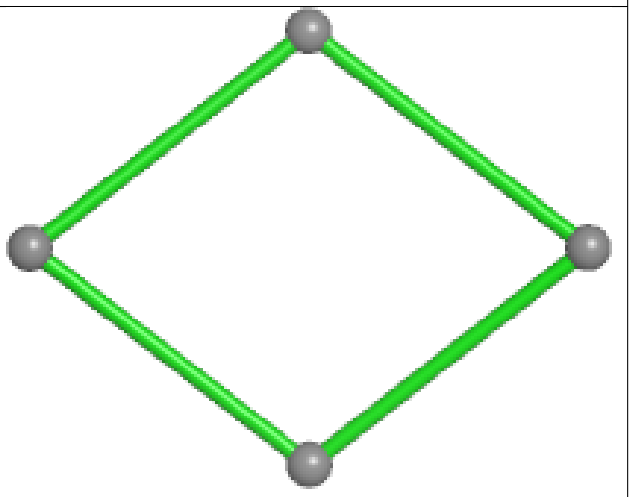
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	b	501	SAH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

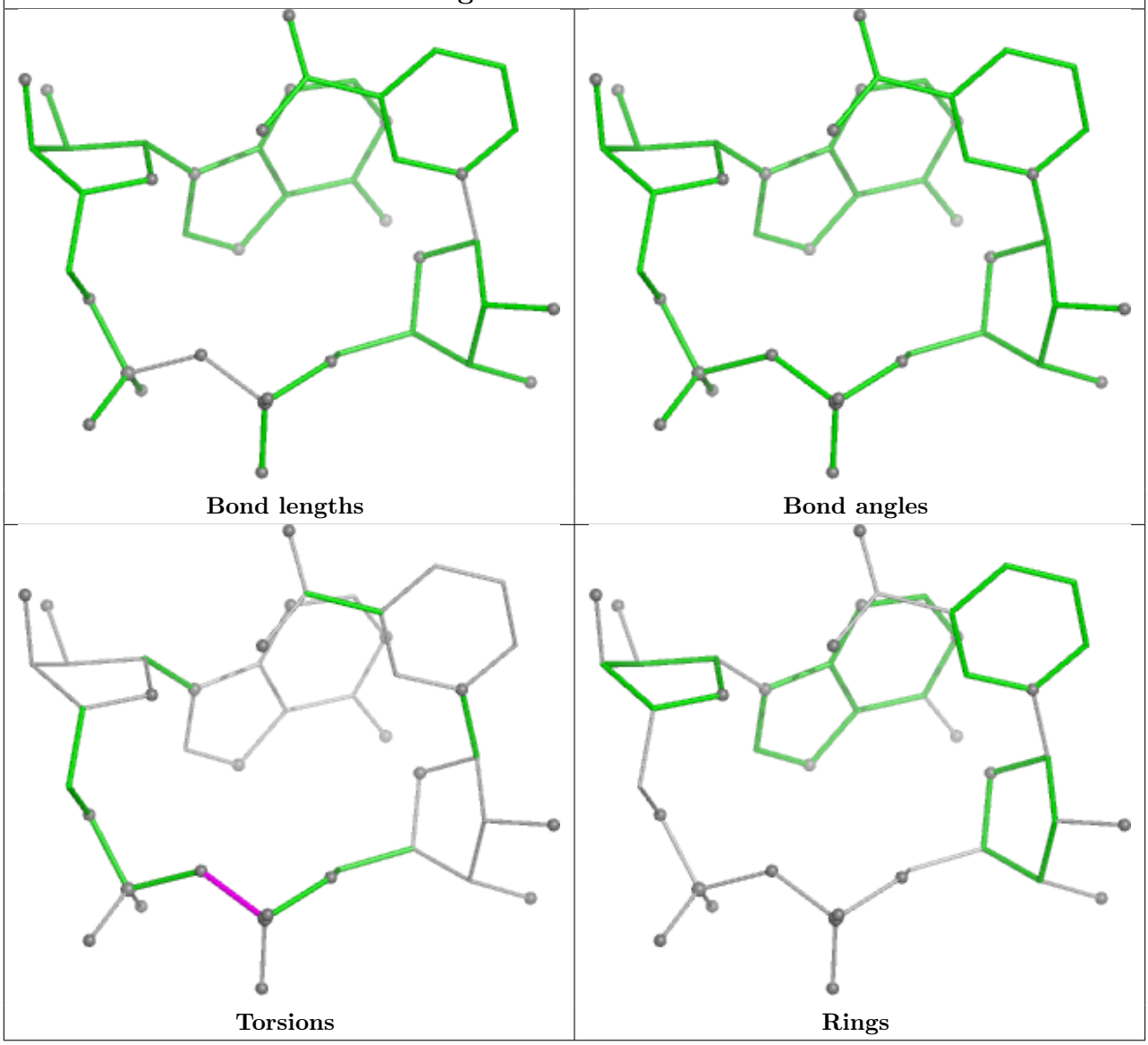
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 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.

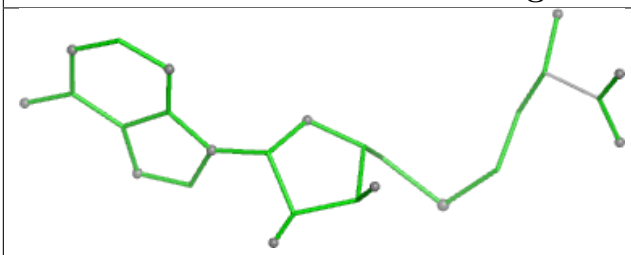
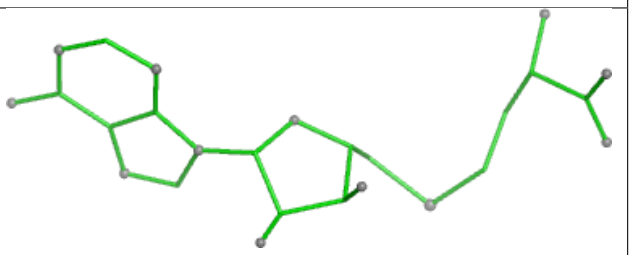
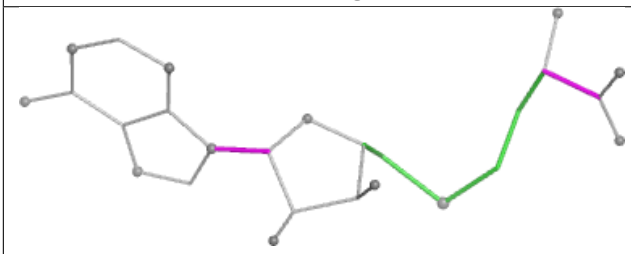
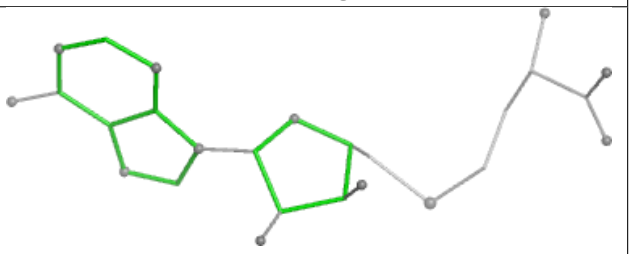
Ligand FES P 201



Ligand FES T 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAD A 1701



Ligand SAH b 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.

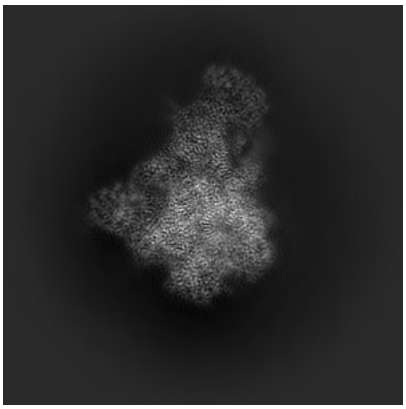
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13555. These allow visual inspection of the internal detail of the map and identification of artifacts.

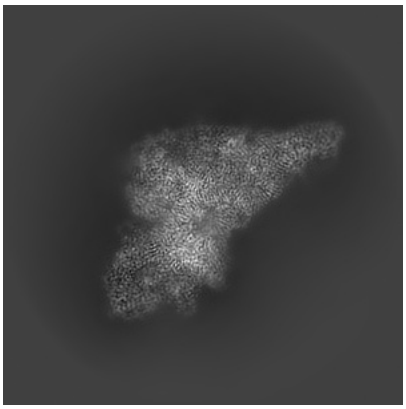
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

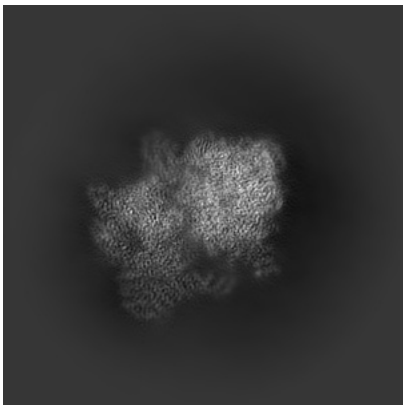
6.1.1 Primary map



X

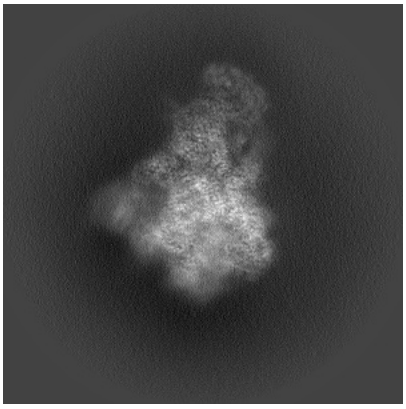


Y

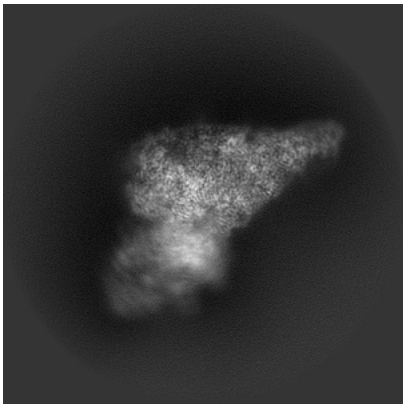


Z

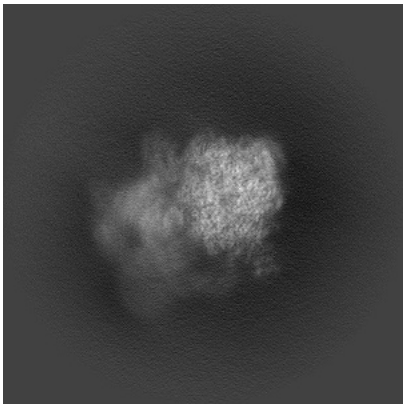
6.1.2 Raw map



X



Y

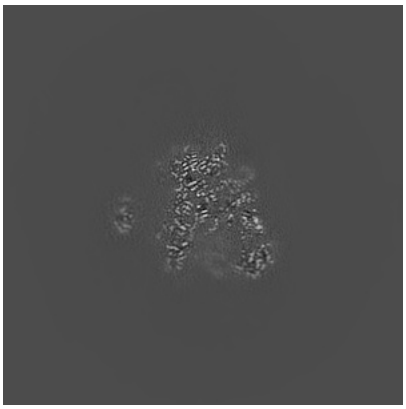


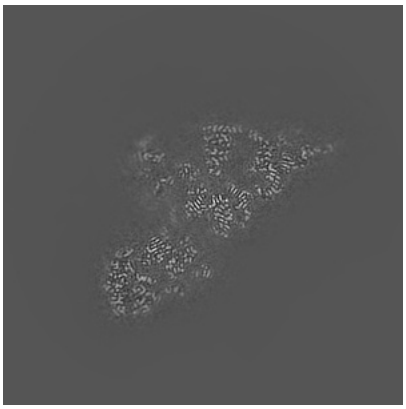
Z

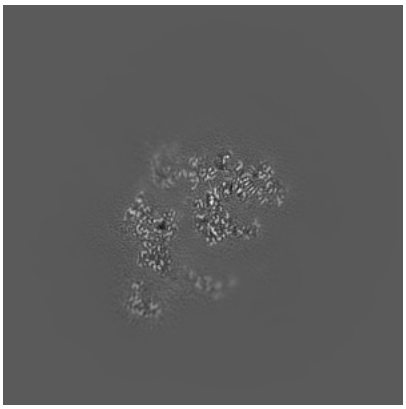
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

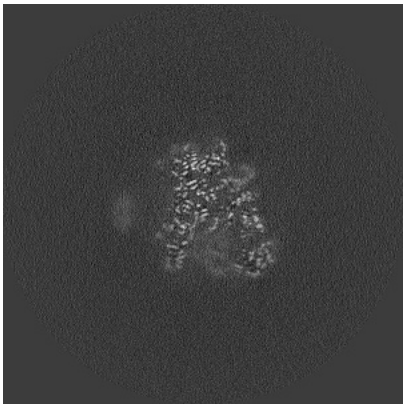
6.2.1 Primary map

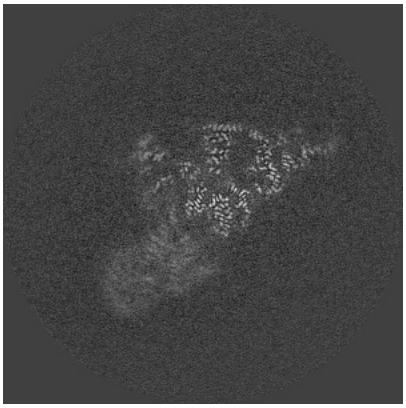

X Index: 324

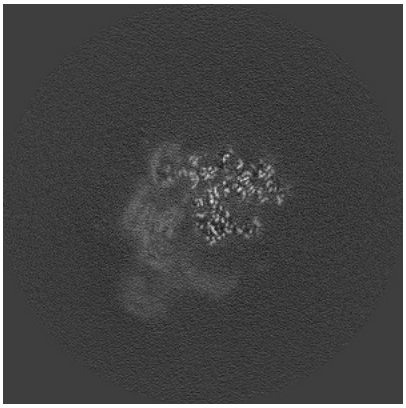

Y Index: 324


Z Index: 324

6.2.2 Raw map


X Index: 240

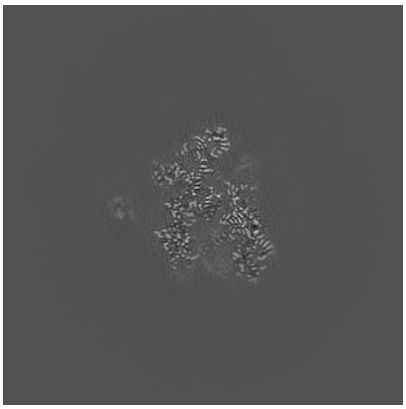

Y Index: 240


Z Index: 240

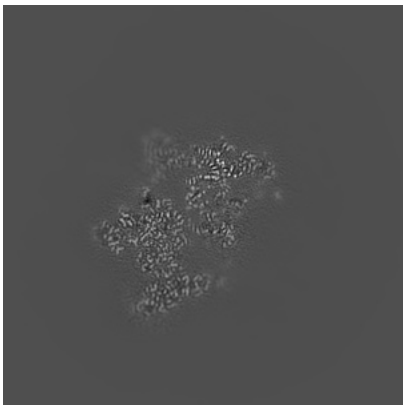
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

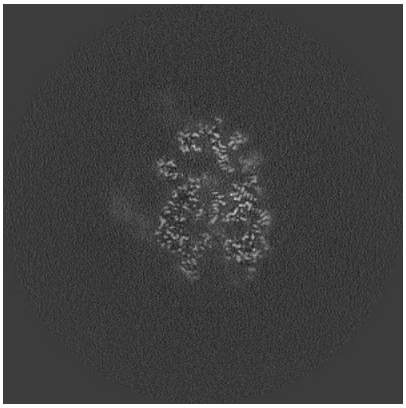
6.3.1 Primary map

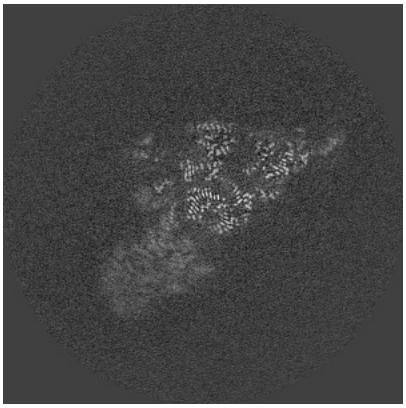

X Index: 341

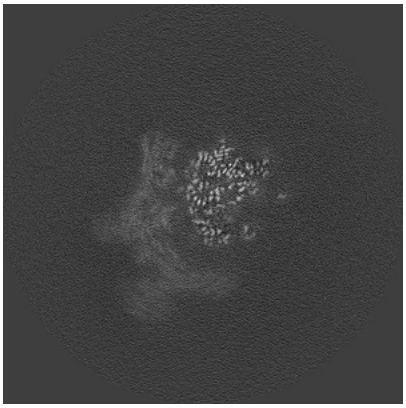
Y Index: 329


Z Index: 298

6.3.2 Raw map


X Index: 265

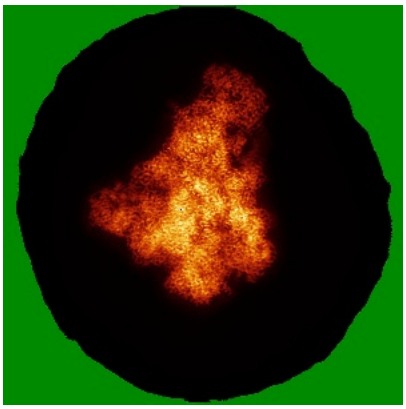

Y Index: 244

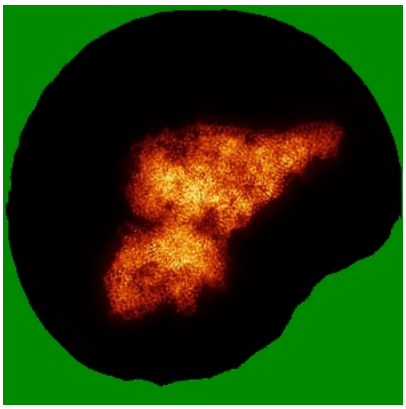

Z Index: 231

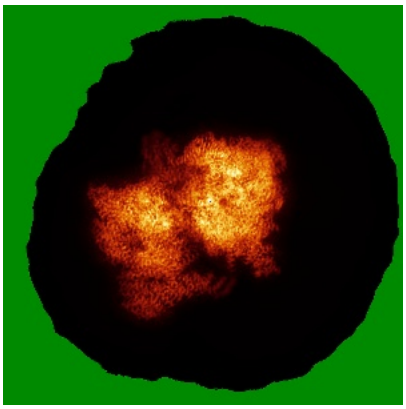
The images above show the largest variance slices of the map in three orthogonal directions.

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

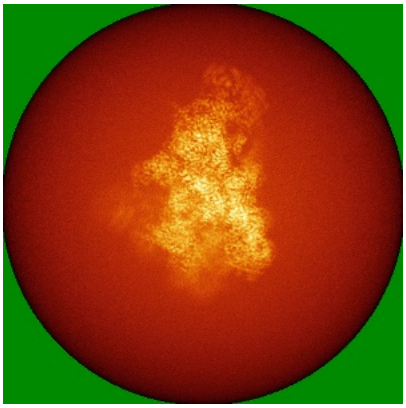
6.4.1 Primary map

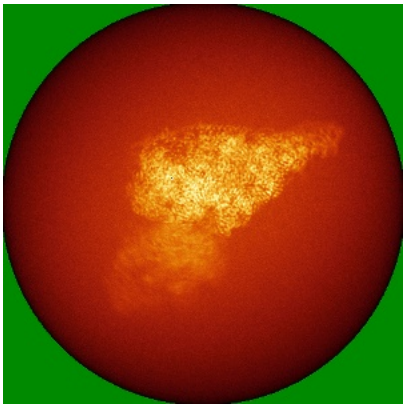

X

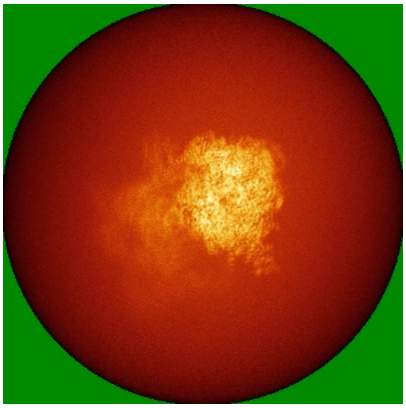

Y


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.

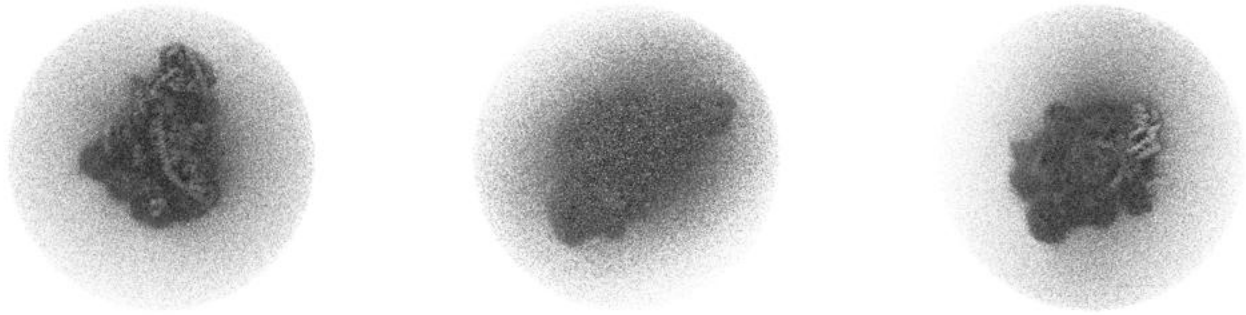
6.5 Orthogonal surface views (i)

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.

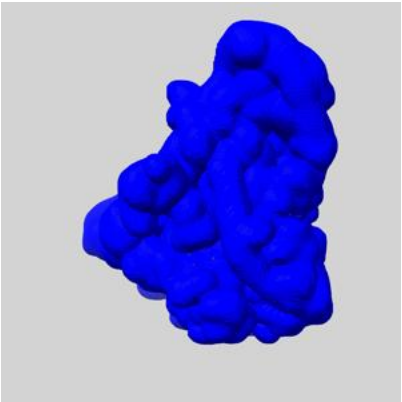
6.6 Mask visualisation (i)

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

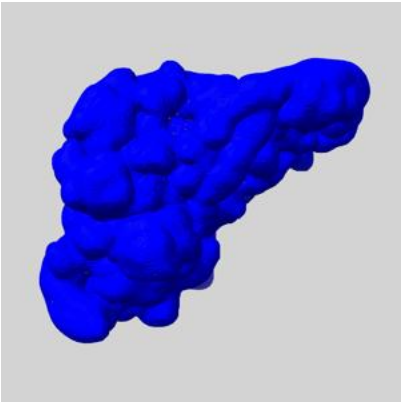
A mask typically either:

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

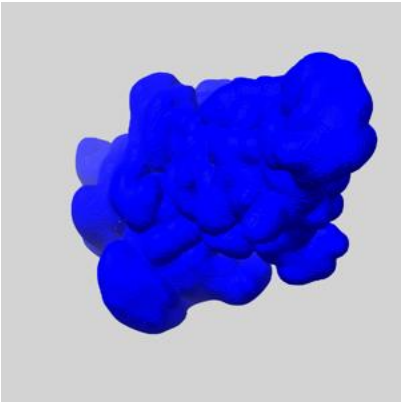
6.6.1 emd_13555_msk_1.map (i)



X



Y

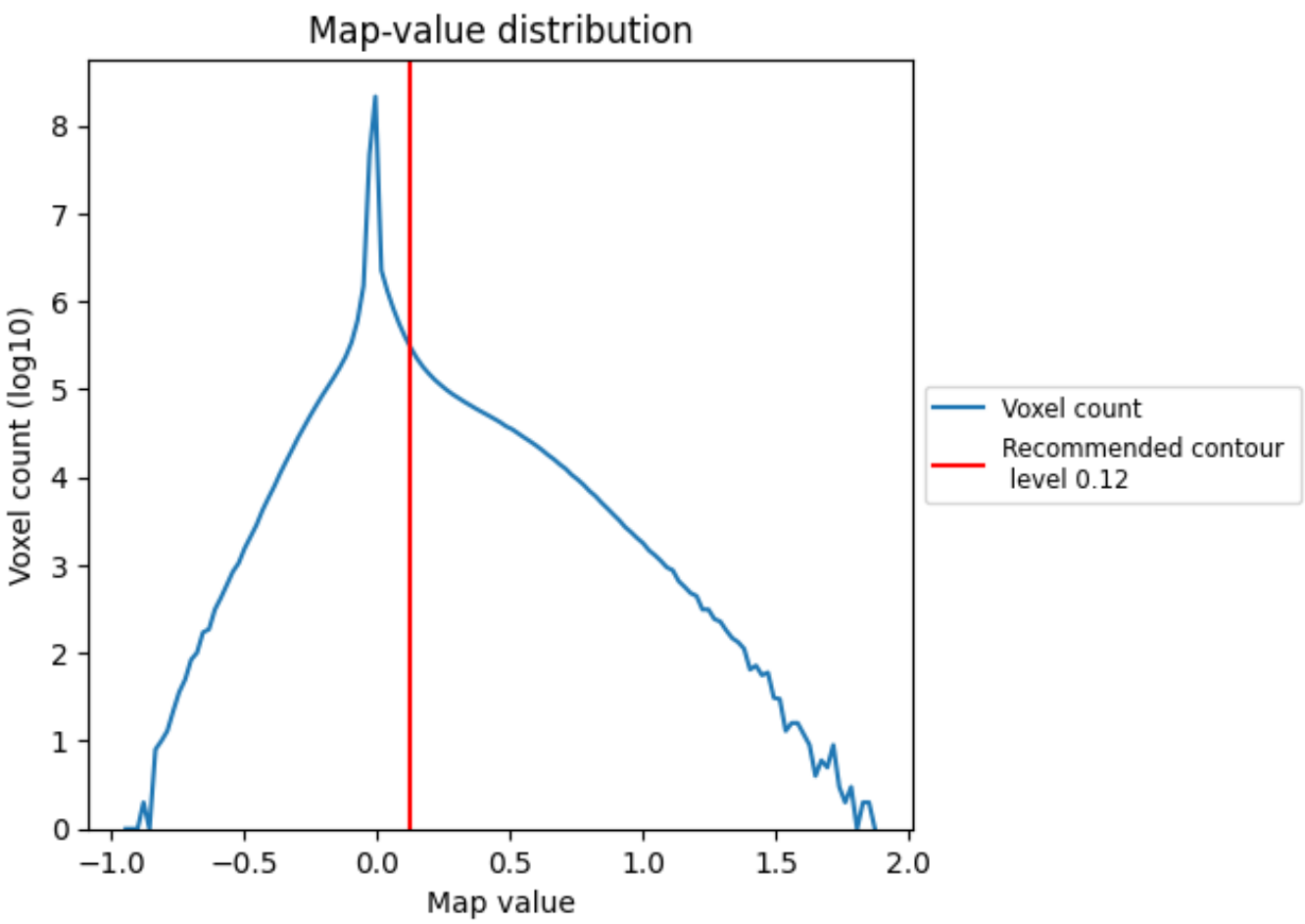


Z

7 Map analysis (i)

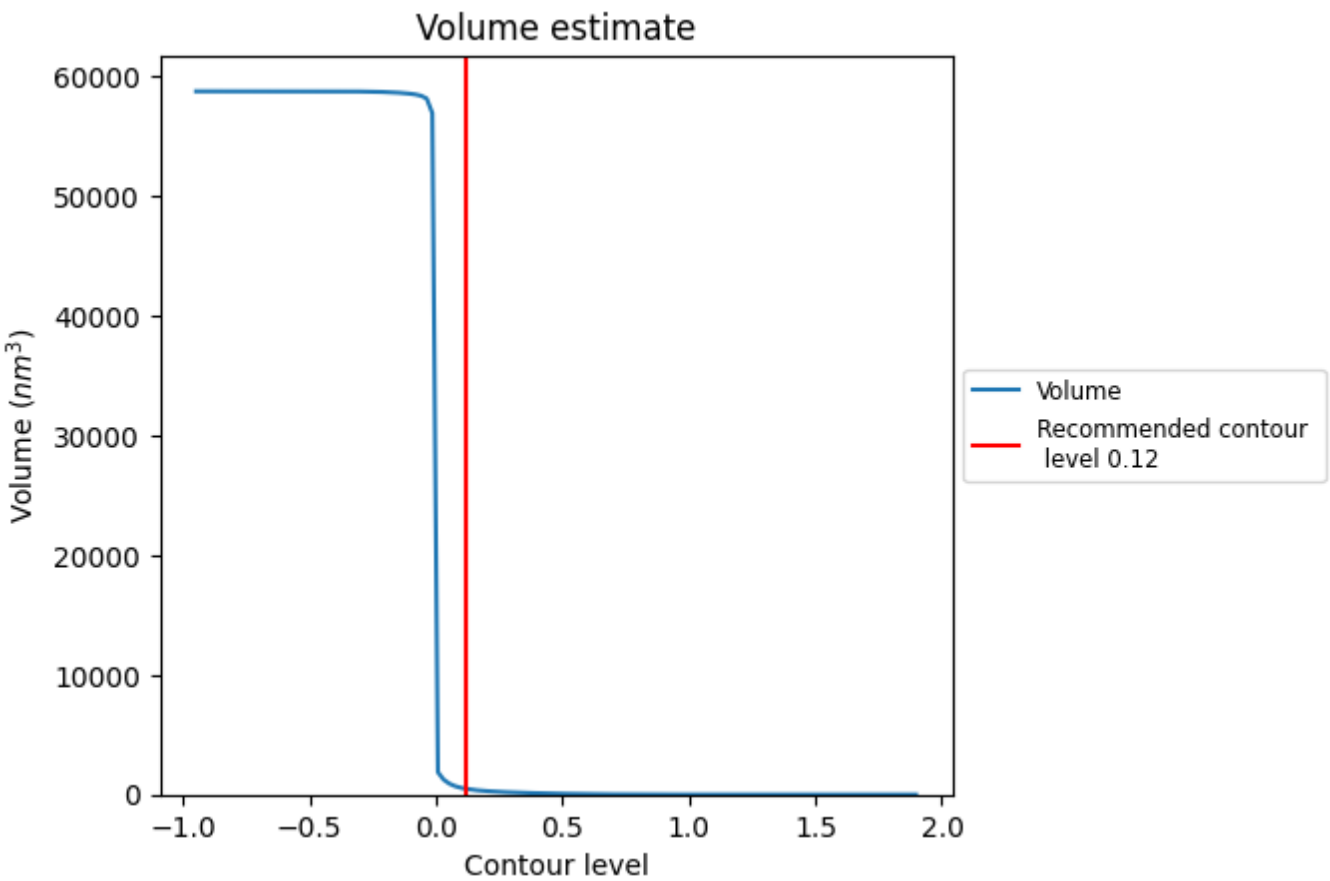
This section contains the results of statistical analysis of the map.

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.

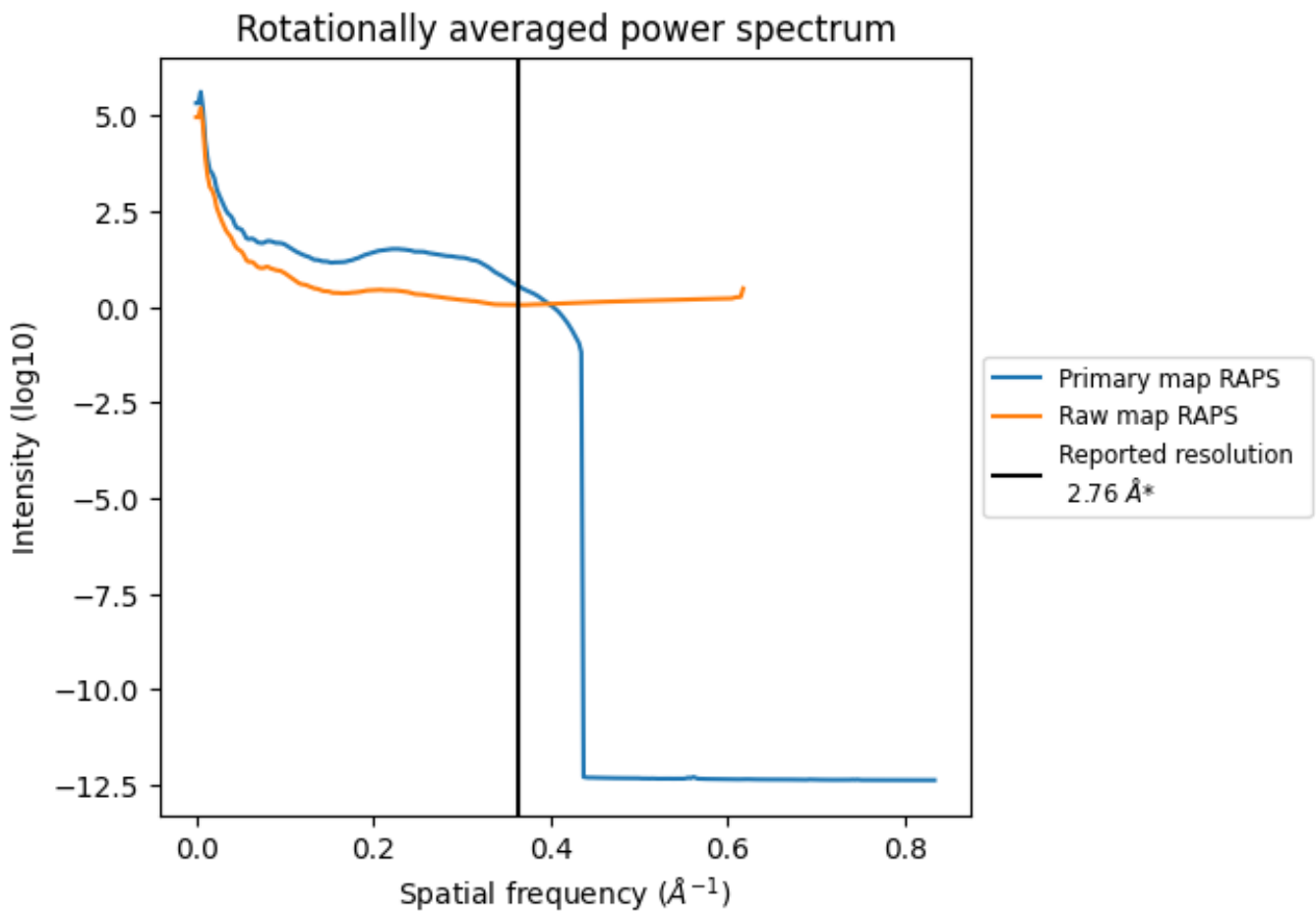
7.2 Volume estimate (i)



The volume at the recommended contour level is 477 nm^3; this corresponds to an approximate mass of 431 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)

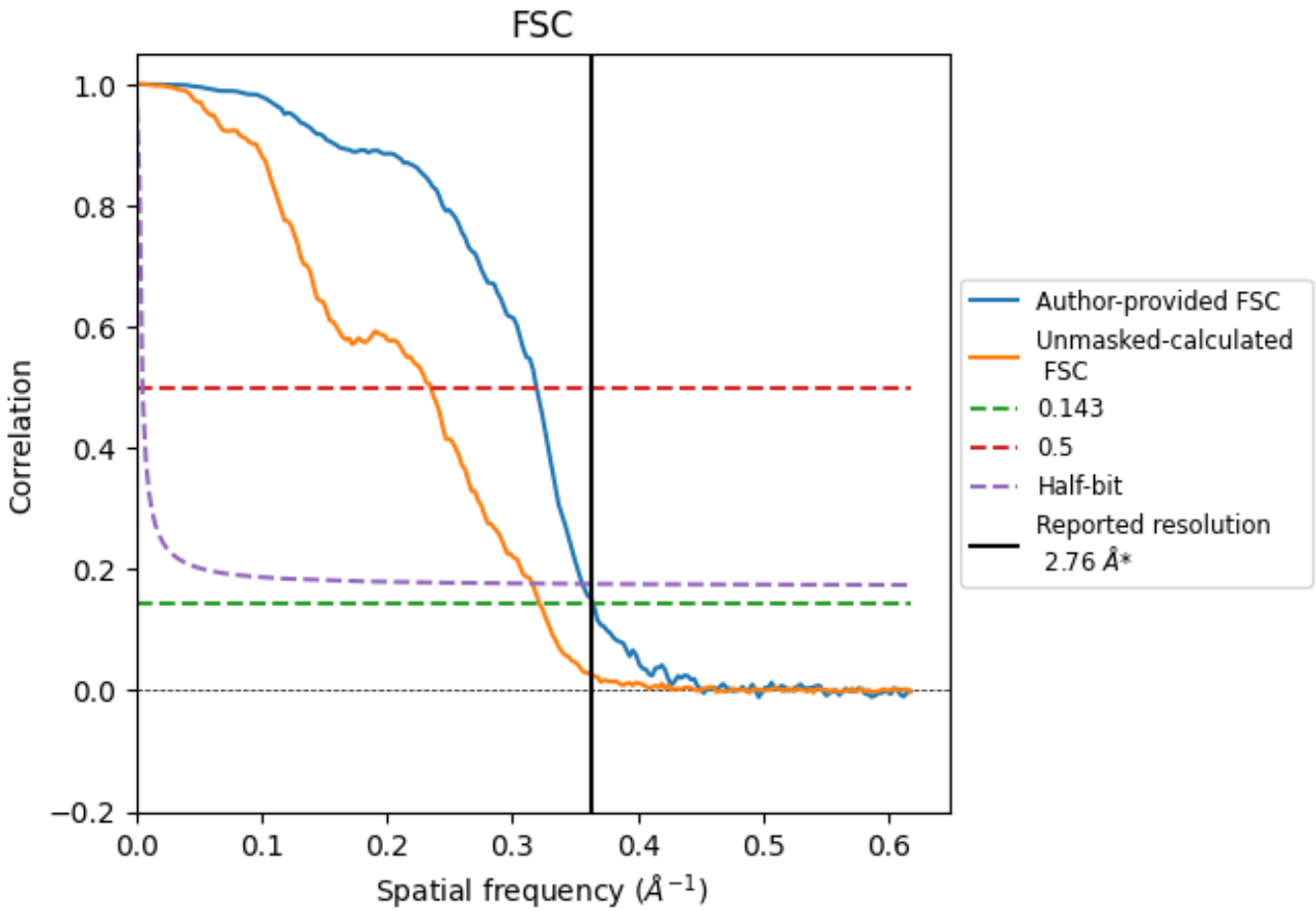


*Reported resolution corresponds to spatial frequency of 0.362 Å^{-1}

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 0.362 Å^{-1}

8.2 Resolution estimates (i)

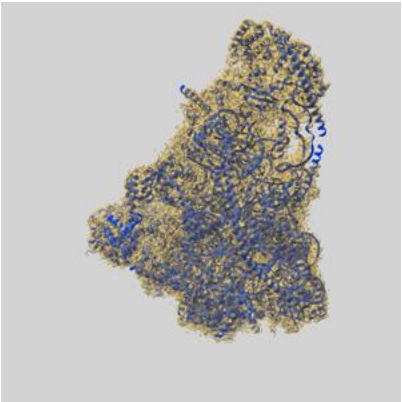
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.74	3.13	2.81
Unmasked-calculated*	3.11	4.26	3.17

*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 3.11 differs from the reported value 2.76 by more than 10 %

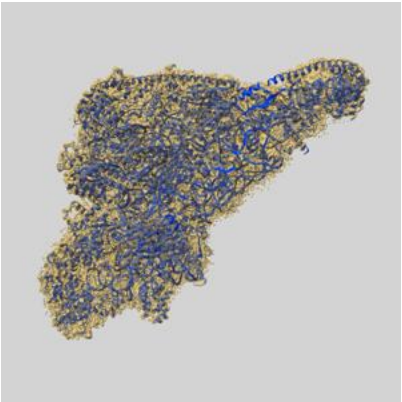
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13555 and PDB model 7PNX. Per-residue inclusion information can be found in section 3 on page 15.

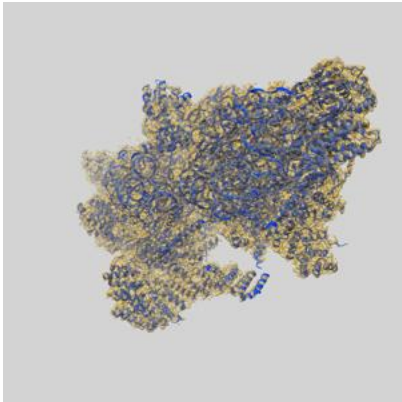
9.1 Map-model overlay (i)



X



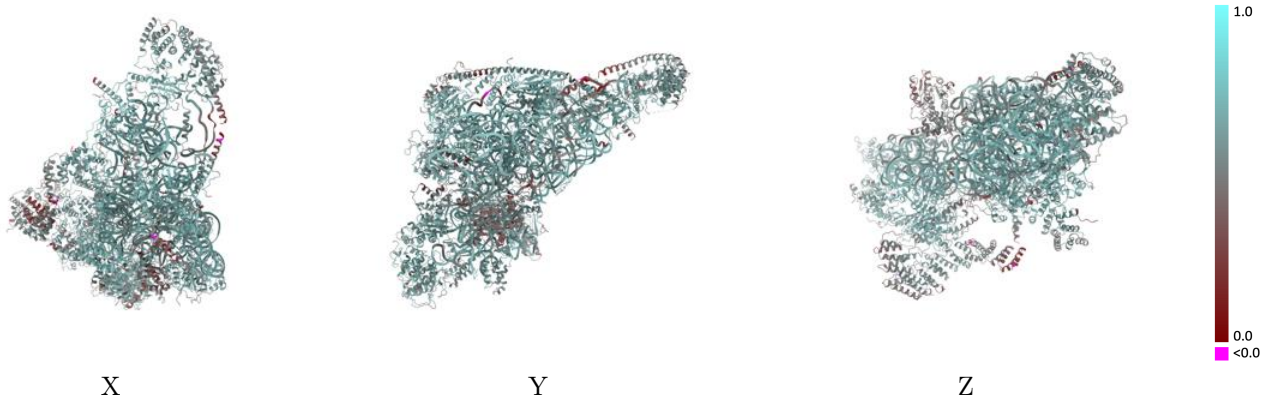
Y



Z

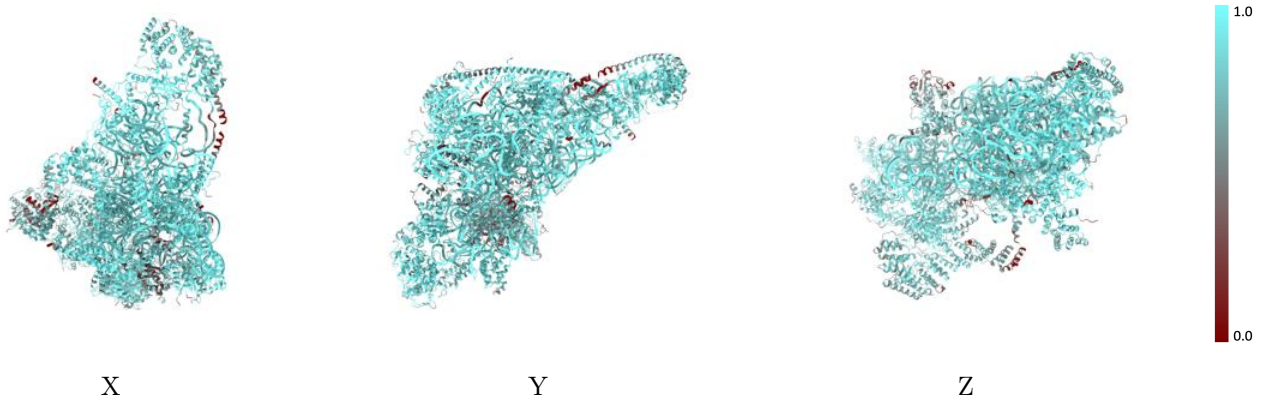
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



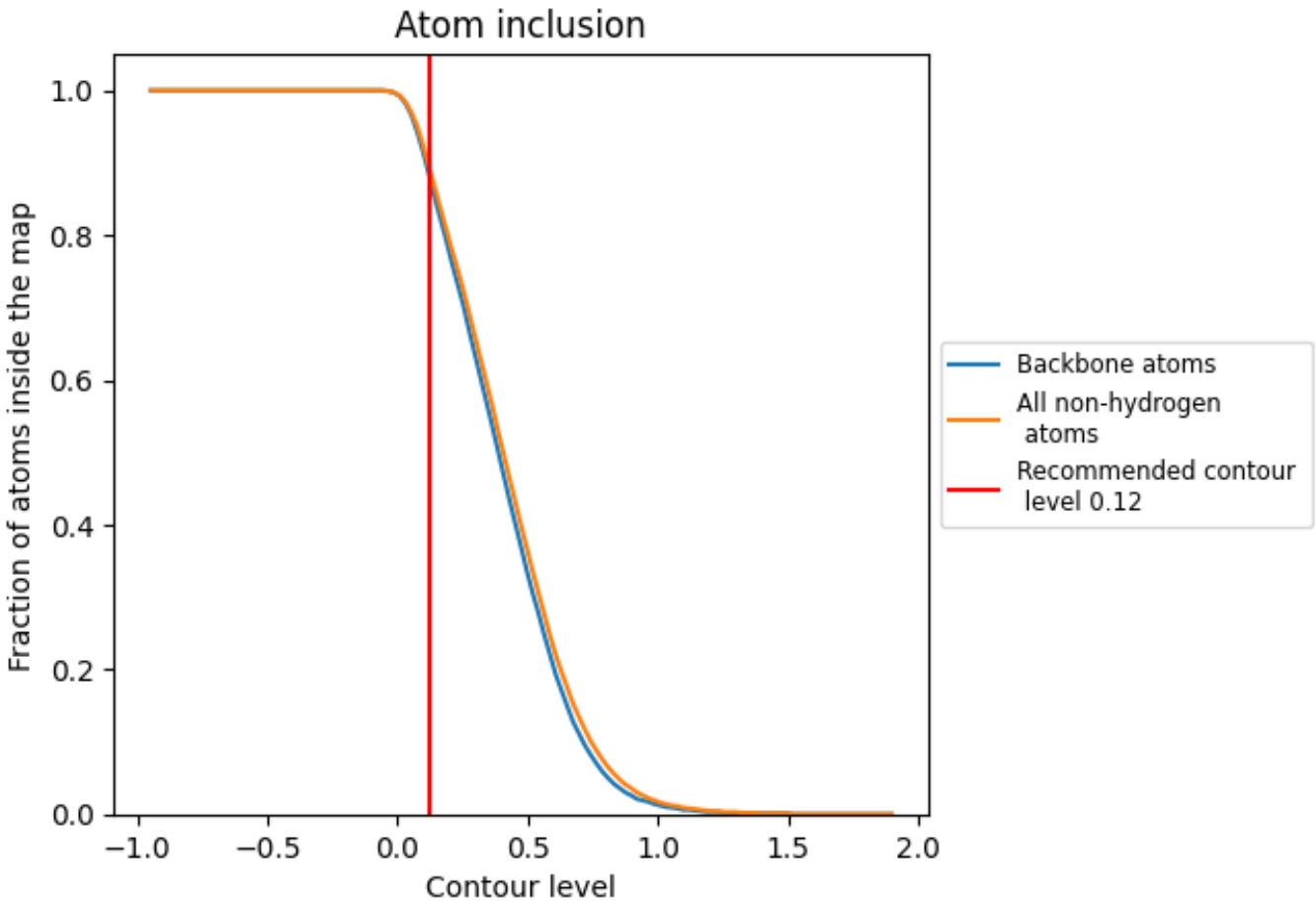
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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, 88% of all backbone atoms, 90% 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	0.8960	0.6030
0	0.9110	0.6180
1	0.8830	0.6030
3	0.9220	0.6210
4	0.7660	0.5070
A	0.9640	0.6430
B	0.9430	0.6590
C	0.9780	0.6870
D	0.9030	0.6180
E	0.9140	0.6150
F	0.8680	0.5820
G	0.8690	0.5940
H	0.9050	0.6360
I	0.9240	0.6190
J	0.9450	0.6410
K	0.9740	0.6810
L	0.8730	0.6030
M	0.9350	0.6640
N	0.9530	0.6690
O	0.9420	0.6470
P	0.9330	0.6290
Q	0.9650	0.6510
R	0.8970	0.6060
S	0.8530	0.5720
T	0.9270	0.6390
U	0.8230	0.5560
V	0.8240	0.5590
W	0.9210	0.6220
X	0.9280	0.6220
Y	0.7850	0.5440
Z	0.9050	0.6220
a	0.4990	0.4140
b	0.6300	0.4260