Full wwPDB EM Validation Report (i)

Apr 16, 2024 – 02:18 pm BST

PDB ID	:	6RW5
EMDB ID	:	EMD-10022
Title	:	Structure of human mitochondrial 28S ribosome in complex with mitochondrial IF2 and IF3
Authors	:	Itoh, Y.; Khawaja, A.; Rorbach, J.; Amunts, A.
Deposited on	:	2019-06-03
Resolution	:	3.14 Å(reported)
Based on initial model	:	3J9M

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:

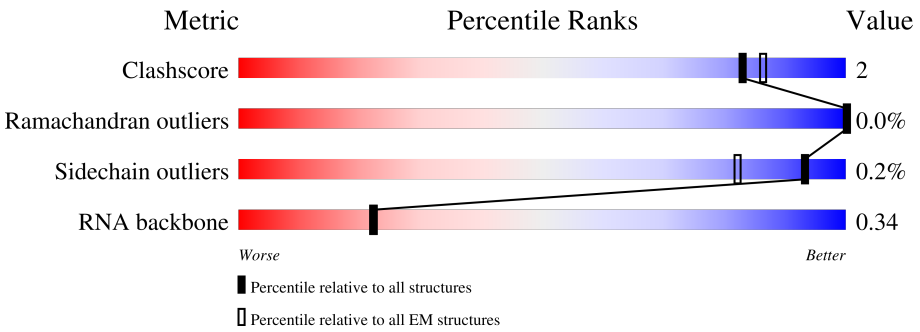
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.14 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	65% 30% 5%
2	B	296	72% • 24%
3	C	167	65% 14% 21%
4	D	430	74% 5% 20%
5	E	125	93% 5% •
6	F	242	80% 6% 14%
7	G	396	73% 10% 17%

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Mol	Chain	Length	Quality of chain
8	H	201	63% 6% 30%
9	I	194	68% 29%
10	J	138	70% 8% 22%
11	K	128	70% 9% 21%
12	L	257	61% 6% 32%
13	M	137	82% 5% 13%
14	N	130	84% 15%
15	O	258	69% 6% 25%
16	P	142	65% 32%
17	Q	86	93% 7%
18	R	360	76% 6% 18%
19	S	190	66% 5% 29%
20	T	173	91% 6%
21	U	205	81% 5% 14%
22	V	414	82% 5% 13%
23	W	187	50% 47%
24	X	398	81% 7% 12%
25	Y	395	36% 62%
26	Z	106	92% 6%
27	0	218	90% 9%
28	1	323	81% 15%
29	2	117	13% 95% 5%
30	3	199	35% 65%
31	4	689	6% 80% 6% 15%
32	7	699	20% 77% 5% 18%

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Mol	Chain	Length	Quality of chain
33	8	285	18% 61% 6% 33%

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 137263 atoms, of which 63928 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	1972	614	1000	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	330	5434	1726	2718	485	491	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	2079	641	1060	193	181	4	0	0

- 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	194	3165	1019	1566	295	278	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	2764	877	1393	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	276	4507	1419	2269	381	427	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	70	1325	401	700	134	89	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	588	9536	3053	4768	808	879	28	0	0

- Molecule 32 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	7	571	8936	2785	4505	779	850	17	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	37	MET	-	initiating methionine	UNP P46199
7	728	LEU	-	expression tag	UNP P46199
7	729	GLU	-	expression tag	UNP P46199
7	730	HIS	-	expression tag	UNP P46199
7	731	HIS	-	expression tag	UNP P46199

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Chain	Residue	Modelled	Actual	Comment	Reference
7	732	HIS	-	expression tag	UNP P46199
7	733	HIS	-	expression tag	UNP P46199
7	734	HIS	-	expression tag	UNP P46199
7	735	HIS	-	expression tag	UNP P46199

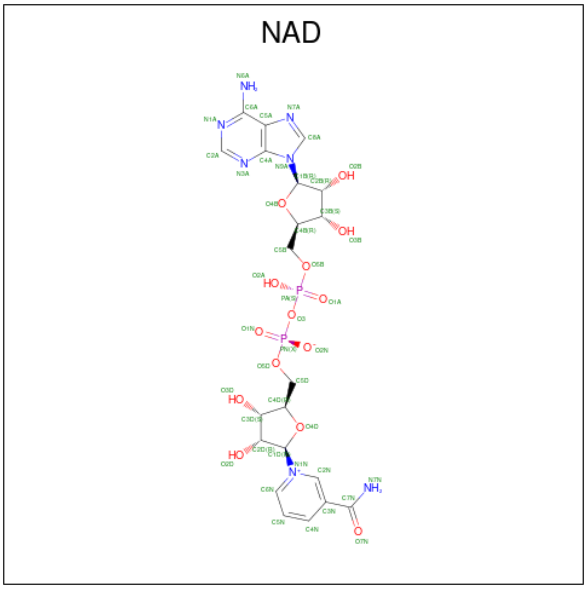
- Molecule 33 is a protein called Translation initiation factor IF-3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	8	191	3131	953	1588	289	293	8	0	0

There are 9 discrepancies between the modelled and reference sequences:

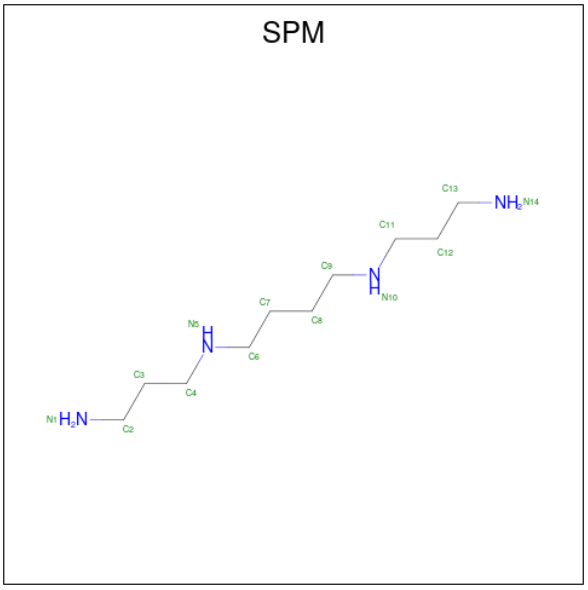
Chain	Residue	Modelled	Actual	Comment	Reference
8	68	ILE	THR	variant	UNP Q9H2K0
8	243	LEU	PHE	variant	UNP Q9H2K0
8	279	GLY	-	expression tag	UNP Q9H2K0
8	280	LEU	-	expression tag	UNP Q9H2K0
8	281	GLU	-	expression tag	UNP Q9H2K0
8	282	VAL	-	expression tag	UNP Q9H2K0
8	283	LEU	-	expression tag	UNP Q9H2K0
8	284	PHE	-	expression tag	UNP Q9H2K0
8	285	GLN	-	expression tag	UNP Q9H2K0

- Molecule 34 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



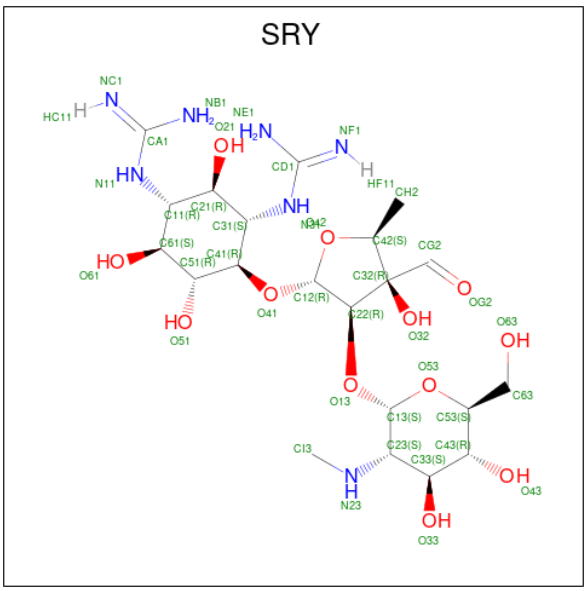
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
34	A	1	70	21	26	7	14	2	0

- Molecule 35 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
35	A	1	39	10	25	4	0

- Molecule 36 is STREPTOMYCIN (three-letter code: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
36	A	1	79	21	39	7	12	0

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
37	A	57	57	57	0
37	B	1	1	1	0
37	X	1	1	1	0
37	3	1	1	1	0
37	7	1	1	1	0

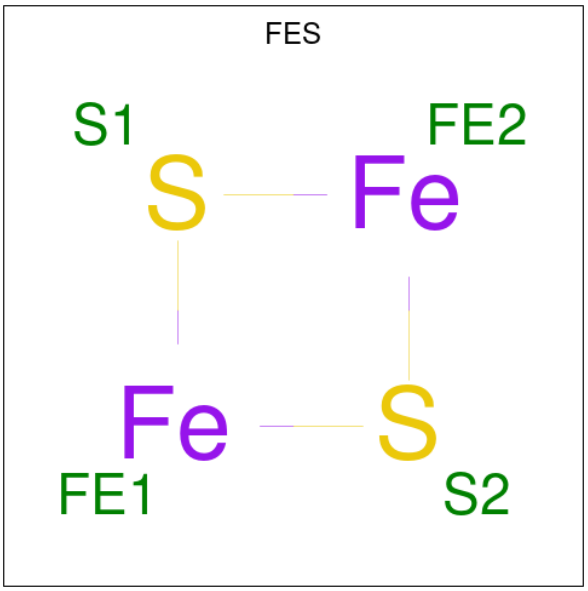
- Molecule 38 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
38	A	17	17	17	0

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

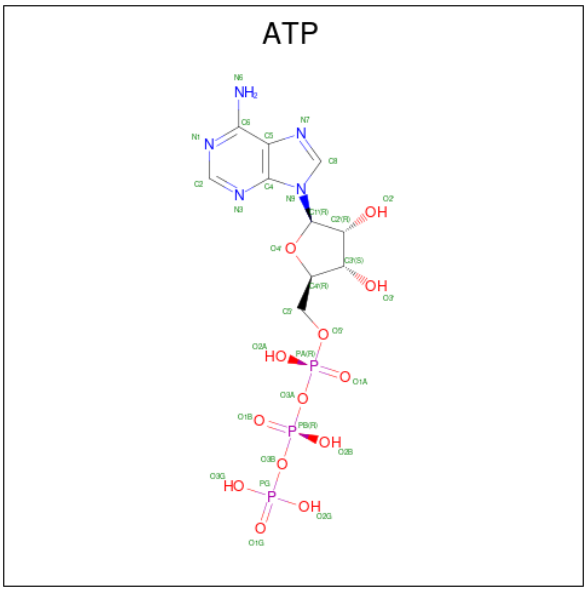
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
39	O	1	1	1	0

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



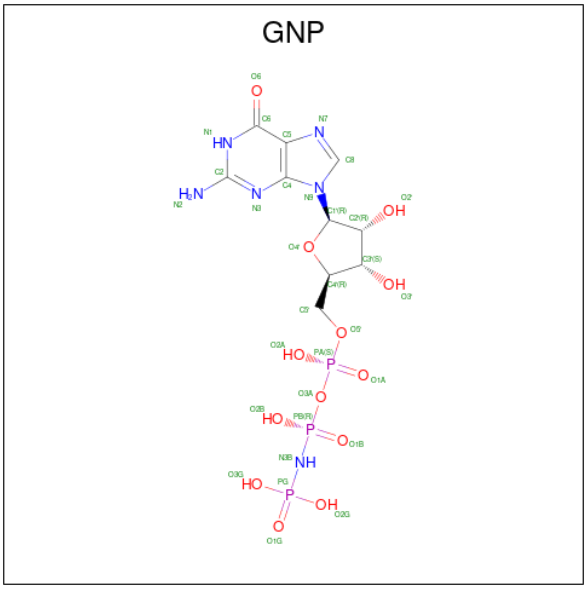
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
40	P	1	4	2	2	0
			Total	Fe	S	
40	T	1	4	2	2	0

- Molecule 41 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	
41	X	1	43	10	12	5	13	3	0

- Molecule 42 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
42	X	1	45	10	13	6	13	3	0
42	7	1	45	10	13	6	13	3	0

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
43	A	47	47	47	0
43	C	2	2	2	0
43	G	1	1	1	0
43	I	2	2	2	0
43	K	1	1	1	0
43	T	1	1	1	0
43	X	3	3	3	0
43	0	1	1	1	0

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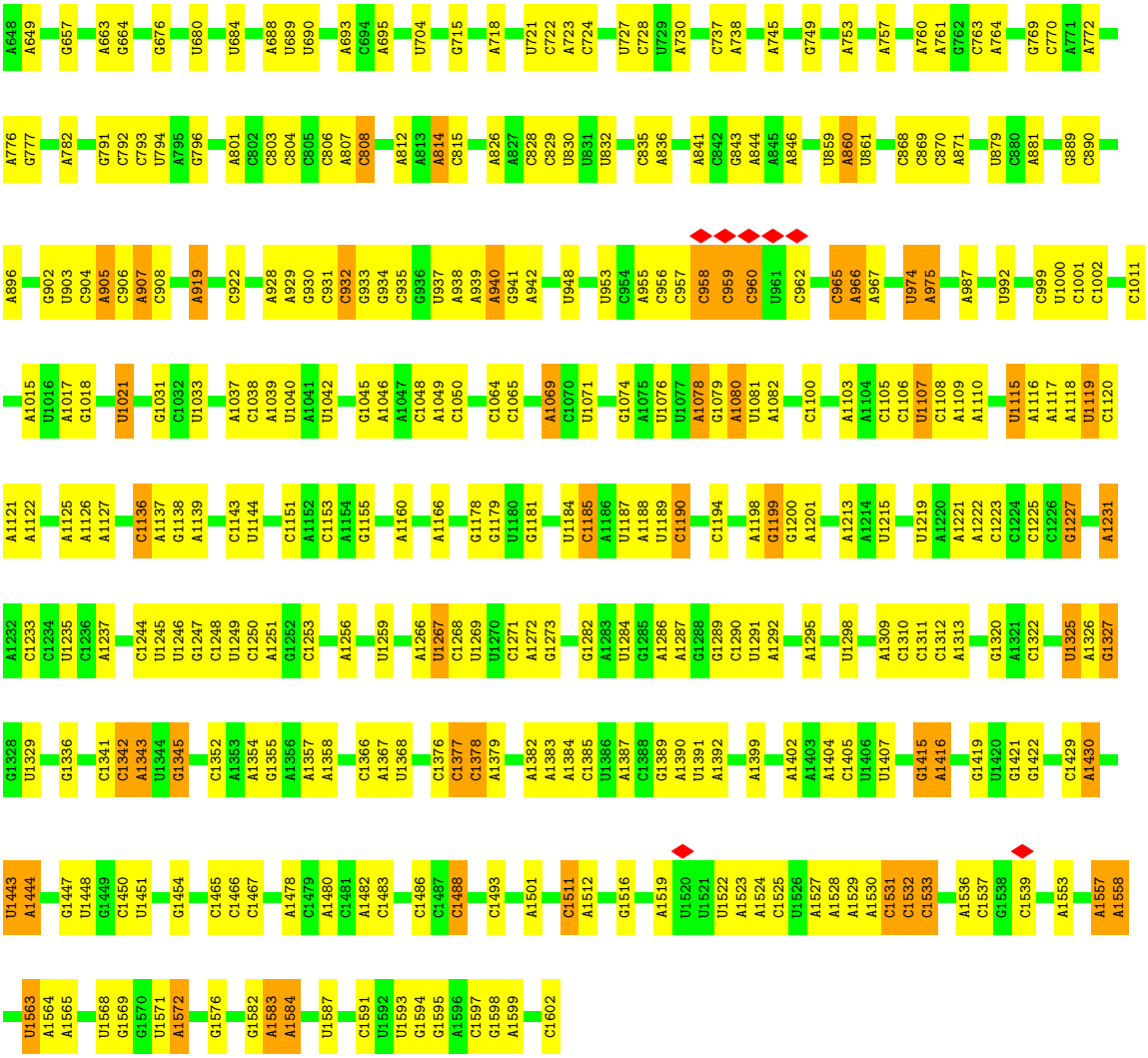
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
43	2	1	1	1	0
			Total	O	
43	7	2	2	2	0

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.

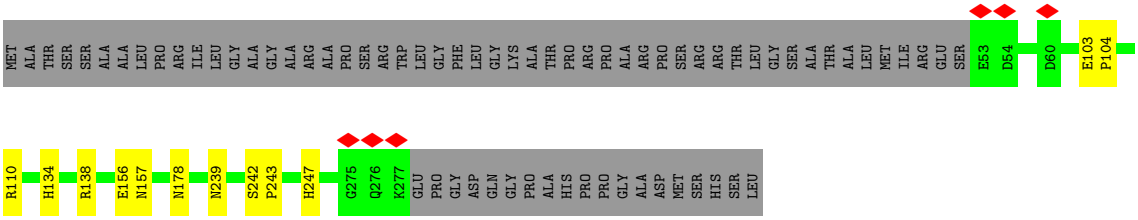
- Molecule 1: 12S mitochondrial rRNA

Chain A: 65% 30% 5%



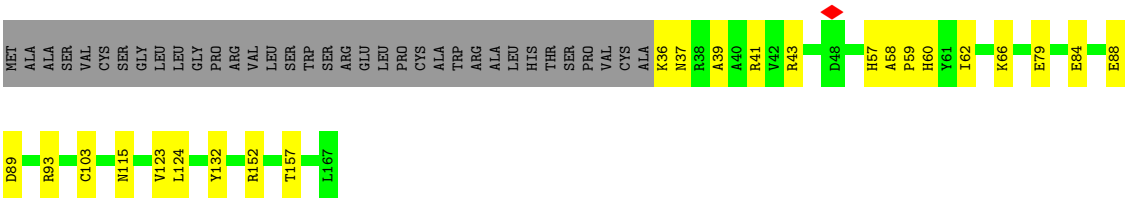
- Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B: 72% 24%



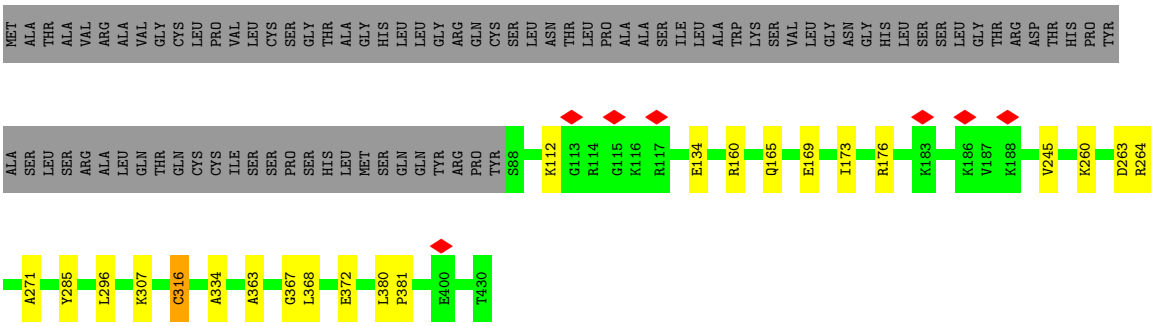
• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:



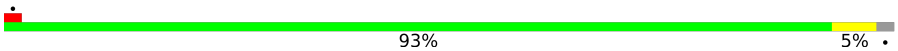
• Molecule 4: 28S ribosomal protein S5, mitochondrial

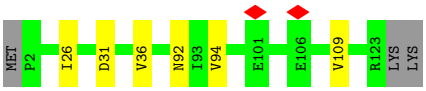
Chain D:



• Molecule 5: 28S ribosomal protein S6, mitochondrial

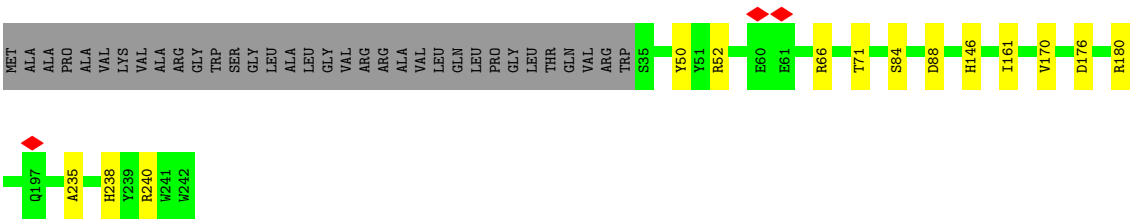
Chain E:





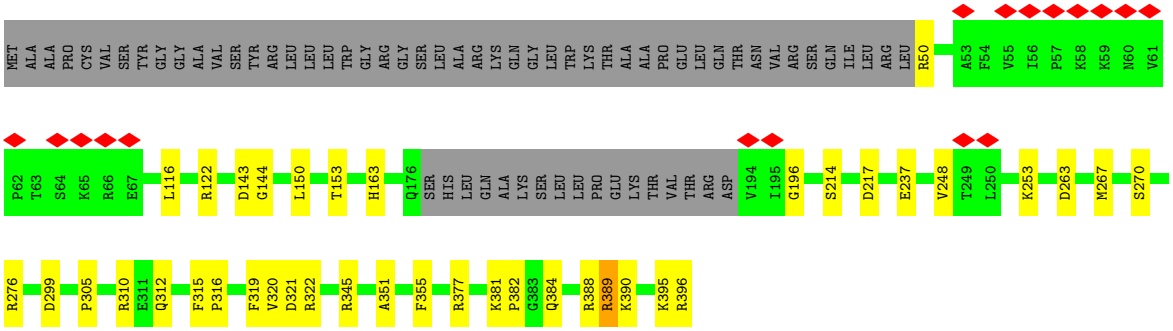
• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:



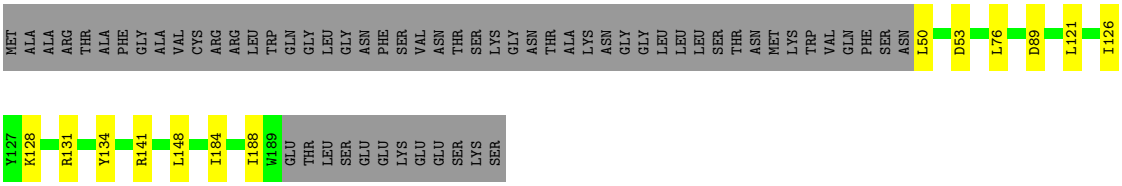
• Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G:



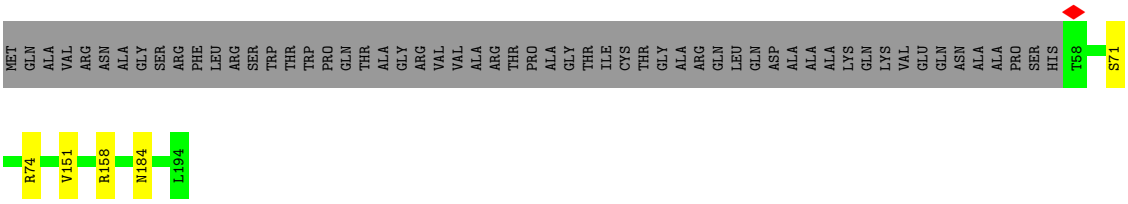
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



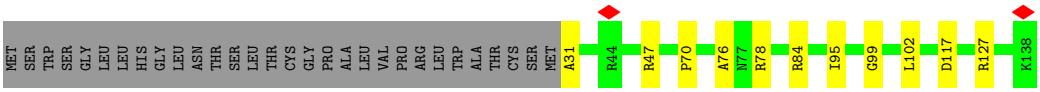
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



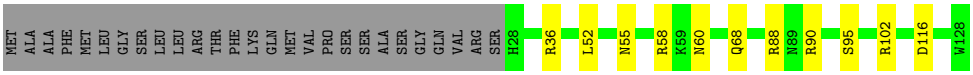
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:



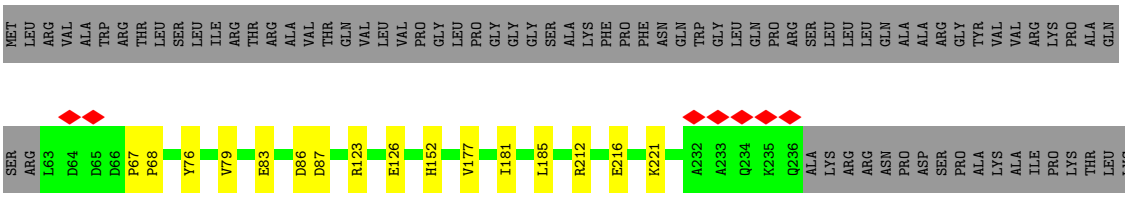
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:



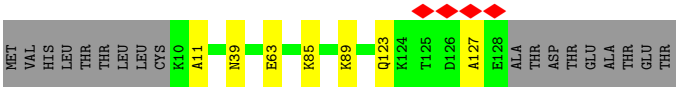
• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L:



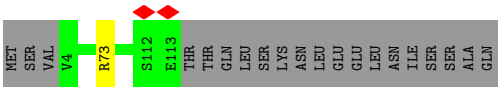
• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain M:



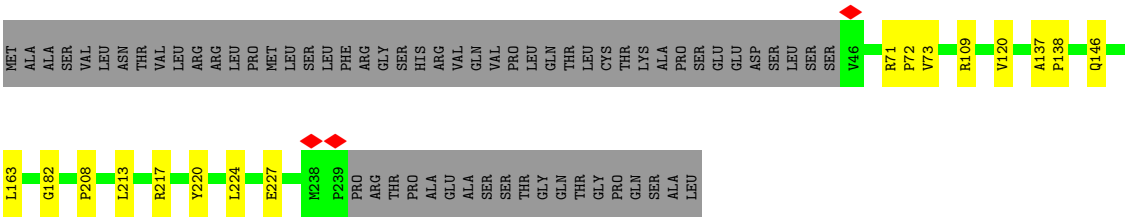
• Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain N:



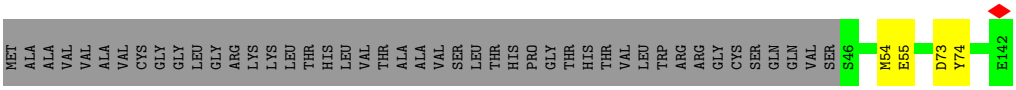
• Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain O:



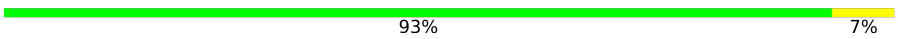
• Molecule 16: 28S ribosomal protein S18c, mitochondrial

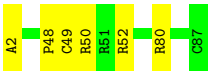
Chain P:



• Molecule 17: 28S ribosomal protein S21, mitochondrial

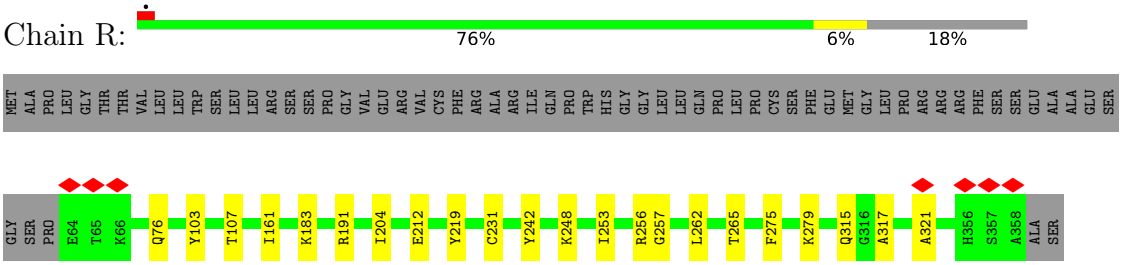
Chain Q:





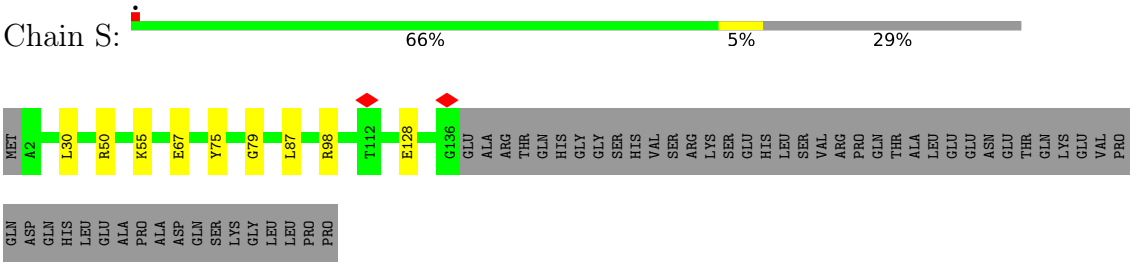
• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:



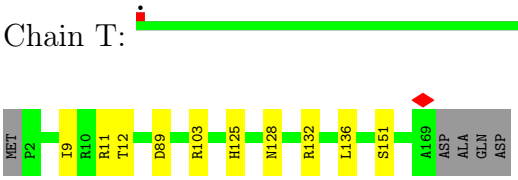
• Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S:



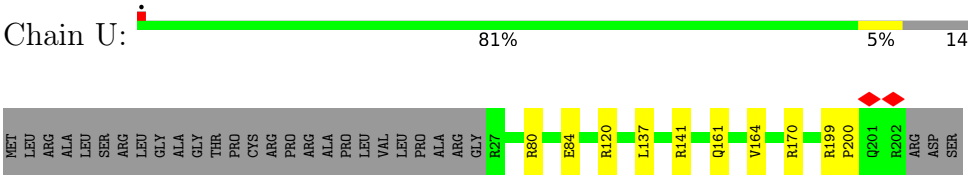
• Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T:



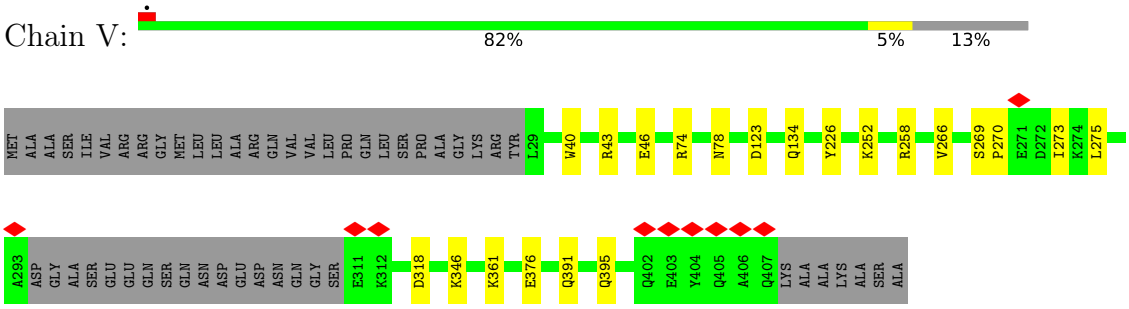
• Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U:



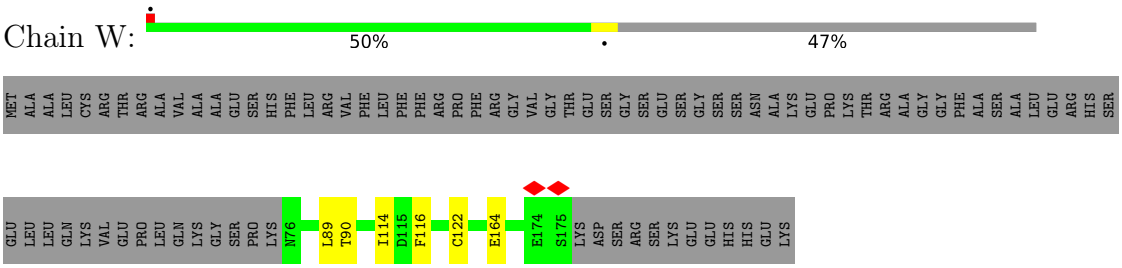
• Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V:



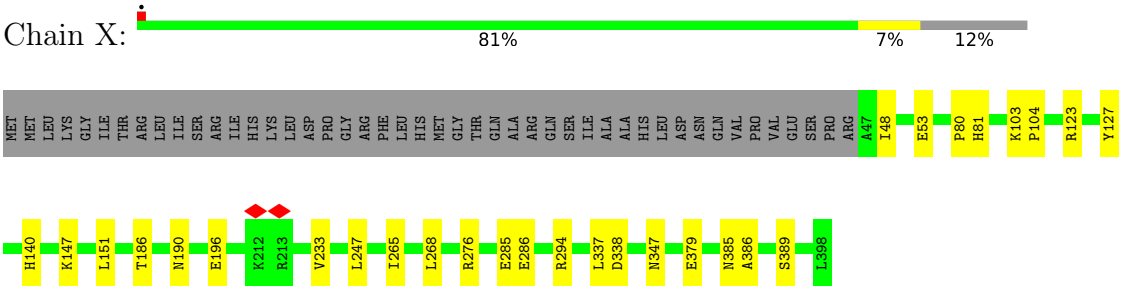
• Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain W:



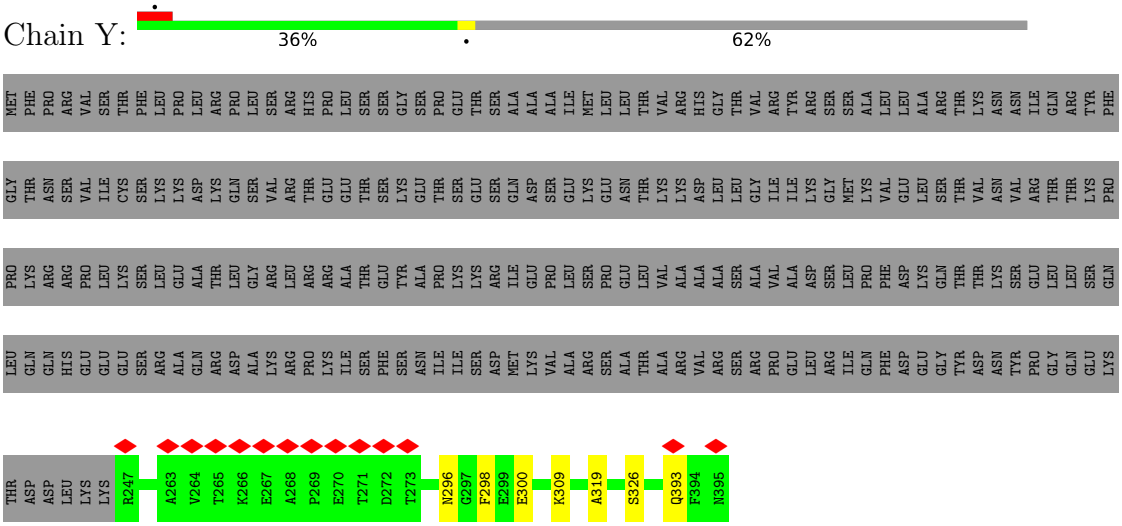
• Molecule 24: 28S ribosomal protein S29, mitochondrial

Chain X:



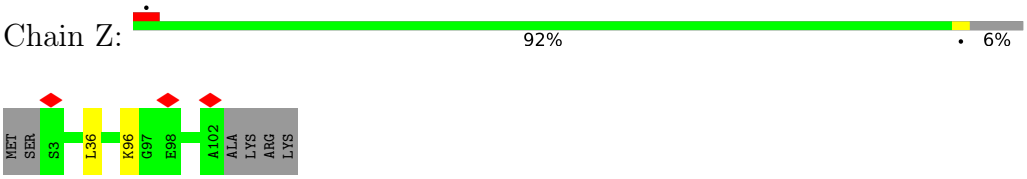
• Molecule 25: 28S ribosomal protein S31, mitochondrial

Chain Y:



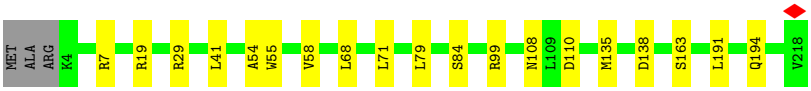
• Molecule 26: 28S ribosomal protein S33, mitochondrial

Chain Z:



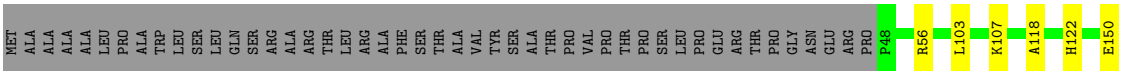
• Molecule 27: 28S ribosomal protein S34, mitochondrial

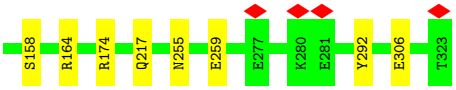
Chain 0:



• Molecule 28: 28S ribosomal protein S35, mitochondrial

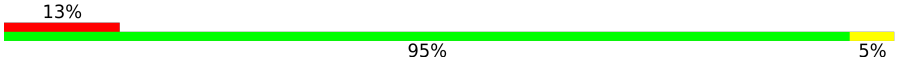
Chain 1:

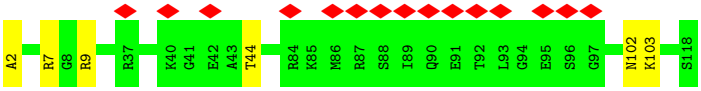




• Molecule 29: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

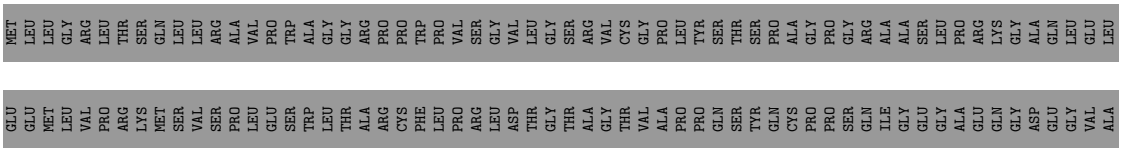
Chain 2:





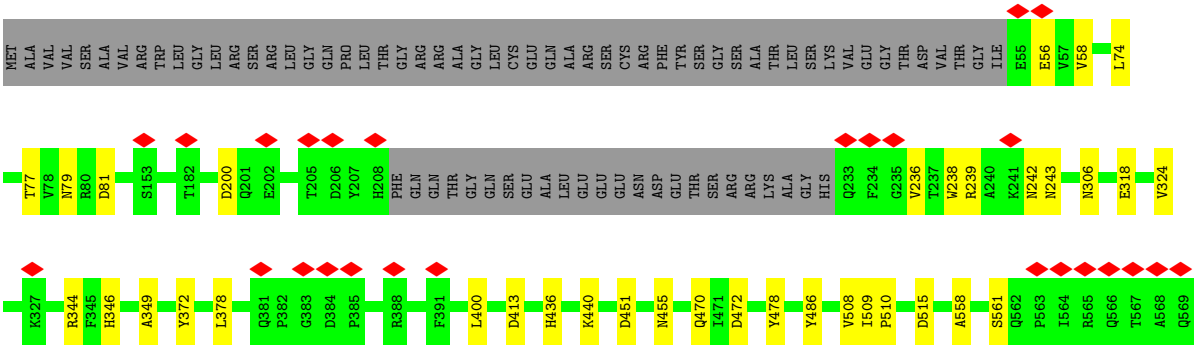
• Molecule 30: Aurora kinase A-interacting protein

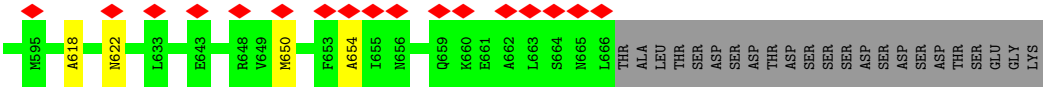
Chain 3:



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

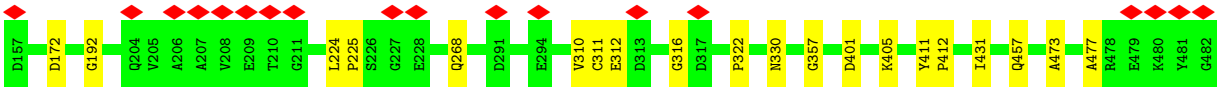
Chain 4:

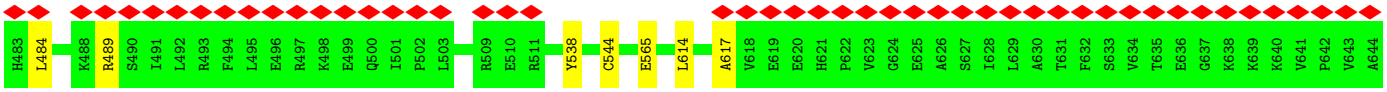


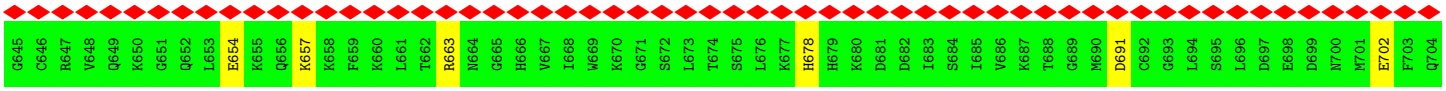


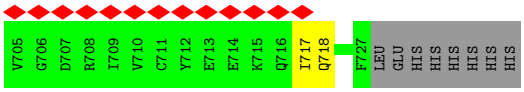
• Molecule 32: Translation initiation factor IF-2, mitochondrial

Chain 7:



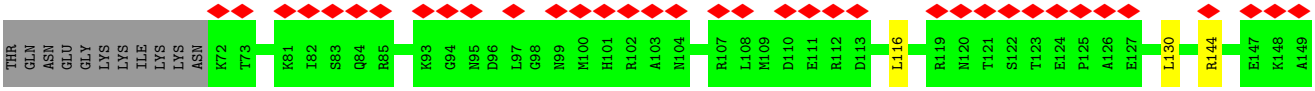


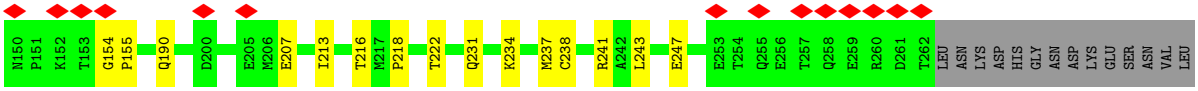


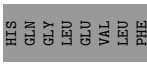


• Molecule 33: Translation initiation factor IF-3, mitochondrial

Chain 8:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103165	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 ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	250	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.414	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	398.4, 398.4, 398.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: SPM, SRY, MG, B8T, K, MA6, ATP, 5MC, NAD, GNP, ZN, 5MU, FES, AYA

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	0.62	0/22562	0.78	0/35124
2	B	0.40	0/1871	0.46	0/2531
3	C	0.49	0/1113	0.48	0/1505
4	D	0.37	0/2783	0.48	0/3724
5	E	0.36	0/989	0.47	0/1335
6	F	0.33	0/1767	0.42	0/2373
7	G	0.37	0/2775	0.44	0/3720
8	H	0.44	0/1178	0.48	0/1598
9	I	0.34	0/1039	0.45	0/1400
10	J	0.42	0/855	0.48	0/1148
11	K	0.44	0/880	0.48	0/1182
12	L	0.37	0/1477	0.41	0/1974
13	M	0.40	0/963	0.48	0/1295
14	N	0.42	0/886	0.47	0/1199
15	O	0.40	0/1655	0.43	0/2254
16	P	0.40	0/798	0.43	0/1070
17	Q	0.41	0/748	0.47	0/994
18	R	0.36	0/2456	0.42	0/3317
19	S	0.37	0/1138	0.45	0/1533
20	T	0.41	0/1402	0.44	0/1883
21	U	0.32	0/1510	0.41	0/2025
22	V	0.28	0/3030	0.39	0/4093
23	W	0.36	0/801	0.48	0/1079
24	X	0.33	0/2921	0.42	0/3954
25	Y	0.35	0/1280	0.40	0/1725
26	Z	0.39	0/857	0.42	0/1141
27	0	0.34	0/1834	0.45	0/2484
28	1	0.38	0/2285	0.43	0/3090
29	2	0.31	0/941	0.44	0/1257
30	3	0.35	0/636	0.45	0/839
31	4	0.30	0/4877	0.40	0/6598
32	7	0.26	0/4501	0.41	0/6073

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	8	0.25	0/1560	0.45	0/2089
All	All	0.45	0/76368	0.57	0/107606

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20282	10313	10297	78	0
2	B	1828	1816	1815	8	0
3	C	1083	1089	1088	15	0
4	D	2731	2805	2804	13	0
5	E	972	1000	1000	4	0
6	F	1725	1770	1769	9	0
7	G	2716	2718	2714	28	0
8	H	1152	1184	1183	10	0
9	I	1019	1060	1059	2	0
10	J	839	888	887	8	0
11	K	862	886	885	8	0
12	L	1453	1541	1540	10	0
13	M	942	966	965	5	0
14	N	868	929	928	1	0
15	O	1599	1566	1565	10	0
16	P	781	807	806	2	0
17	Q	744	758	758	4	0
18	R	2409	2429	2428	15	0
19	S	1111	1116	1115	8	0
20	T	1371	1393	1393	8	0
21	U	1488	1500	1499	7	0
22	V	2969	2964	2961	14	0
23	W	789	803	802	5	0
24	X	2849	2845	2843	21	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y	1246	1198	1197	6	0
26	Z	839	860	858	2	0
27	0	1787	1797	1796	12	0
28	1	2238	2269	2269	10	0
29	2	935	969	969	4	0
30	3	625	700	699	1	0
31	4	4768	4768	4766	24	0
32	7	4431	4505	4502	21	0
33	8	1543	1588	1587	12	0
34	A	44	26	26	1	0
35	A	14	25	26	0	0
36	A	40	39	39	0	0
37	3	1	0	0	0	0
37	7	1	0	0	0	0
37	A	57	0	0	0	0
37	B	1	0	0	0	0
37	X	1	0	0	0	0
38	A	17	0	0	0	0
39	O	1	0	0	0	0
40	P	4	0	0	0	0
40	T	4	0	0	0	0
41	X	31	12	12	0	0
42	7	32	13	13	1	0
42	X	32	13	13	0	0
43	0	1	0	0	0	0
43	2	1	0	0	0	0
43	7	2	0	0	0	0
43	A	47	0	0	2	0
43	C	2	0	0	0	0
43	G	1	0	0	1	0
43	I	2	0	0	0	0
43	K	1	0	0	0	0
43	T	1	0	0	1	0
43	X	3	0	0	1	0
All	All	73335	63928	63876	318	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 (318) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:134:TYR:OH	11:K:116:ASP:OD1	2.01	0.78
1:A:1235:U:OP1	11:K:36:ARG:NH2	2.17	0.78
1:A:1021:U:OP2	29:2:9:ARG:NH2	2.17	0.76
1:A:1071:U:OP2	43:A:1801:HOH:O	2.04	0.75
7:G:214:SER:N	7:G:217:ASP:OD2	2.19	0.75
4:D:285:TYR:OH	4:D:372:GLU:OE2	2.05	0.74
20:T:128:ASN:O	43:T:301:HOH:O	2.06	0.73
20:T:132:ARG:NH1	20:T:136:LEU:O	2.22	0.73
12:L:126:GLU:HG2	12:L:177:VAL:HG11	1.71	0.72
1:A:1322:C:OP2	3:C:36:LYS:NZ	2.23	0.71
32:7:322:PRO:O	32:7:330:ASN:ND2	2.24	0.70
13:M:63:GLU:OE1	18:R:191:ARG:NH1	2.24	0.69
1:A:841:A:OP1	13:M:39:ASN:ND2	2.24	0.69
24:X:268:LEU:O	24:X:294:ARG:NH1	2.26	0.69
7:G:312:GLN:OE1	7:G:345:ARG:NH2	2.25	0.68
1:A:769:G:OP2	14:N:73:ARG:NH2	2.25	0.68
1:A:932:C:N3	20:T:11:ARG:NH1	2.41	0.68
1:A:1511:C:OP1	27:0:7:ARG:NH1	2.27	0.68
3:C:115:ASN:ND2	25:Y:309:LYS:O	2.27	0.68
31:4:306:ASN:OD1	31:4:344:ARG:NH2	2.29	0.66
31:4:200:ASP:OD2	31:4:243:ASN:N	2.30	0.64
32:7:678:HIS:ND1	32:7:691:ASP:O	2.30	0.64
4:D:363:ALA:O	4:D:367:GLY:N	2.30	0.64
31:4:349:ALA:HB3	31:4:378:LEU:HD11	1.80	0.64
3:C:37:ASN:O	3:C:43:ARG:NH2	2.30	0.63
12:L:86:ASP:OD1	12:L:87:ASP:N	2.30	0.63
15:O:182:GLY:O	18:R:183:LYS:NZ	2.28	0.63
31:4:470:GLN:NE2	31:4:472:ASP:OD2	2.31	0.63
1:A:1530:A:OP1	27:0:29:ARG:NH2	2.31	0.63
31:4:74:LEU:O	31:4:77:THR:OG1	2.16	0.63
1:A:1107:U:O4	30:3:128:LYS:NZ	2.31	0.63
18:R:212:GLU:OE1	18:R:248:LYS:NZ	2.25	0.62
22:V:74:ARG:O	22:V:78:ASN:ND2	2.31	0.61
11:K:60:ASN:OD1	11:K:68:GLN:NE2	2.33	0.61
18:R:317:ALA:O	18:R:321:ALA:N	2.32	0.61
1:A:1287:A:OP2	4:D:260:LYS:NZ	2.30	0.61
1:A:808:C:OP1	27:0:19:ARG:NH1	2.34	0.60
2:B:156:GLU:OE1	7:G:163:HIS:ND1	2.35	0.60
17:Q:80:ARG:NH1	23:W:164:GLU:OE1	2.35	0.60
1:A:1569:G:OP2	1:A:1572:A:O2'	2.18	0.60
28:1:56:ARG:NH2	31:4:81:ASP:OD2	2.34	0.60
1:A:1199:G:N1	1:A:1422:G:OP2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:478:TYR:OH	31:4:515:ASP:OD2	2.18	0.59
18:R:161:ILE:O	20:T:125:HIS:NE2	2.36	0.59
31:4:239:ARG:O	31:4:242:ASN:ND2	2.36	0.59
1:A:1231:A:OP1	11:K:88:ARG:NH2	2.27	0.58
1:A:843:G:N2	1:A:846:A:OP2	2.31	0.58
6:F:50:TYR:O	6:F:66:ARG:NH2	2.36	0.58
24:X:140:HIS:ND1	43:X:601:HOH:O	2.20	0.58
1:A:1583:MA6:H93	1:A:1584:MA6:C9	2.34	0.58
31:4:346:HIS:HA	31:4:378:LEU:HD12	1.85	0.58
3:C:124:LEU:O	3:C:132:TYR:OH	2.17	0.57
32:7:473:ALA:O	32:7:477:ALA:N	2.37	0.57
1:A:1528:A:OP1	27:0:99:ARG:NH2	2.37	0.57
3:C:152:ARG:NH1	25:Y:300:GLU:OE2	2.34	0.57
22:V:270:PRO:O	22:V:346:LYS:NZ	2.38	0.57
1:A:1557:A:O2'	1:A:1558:A:O5'	2.18	0.57
7:G:388:ARG:O	7:G:390:LYS:NZ	2.32	0.57
31:4:451:ASP:OD1	31:4:455:ASN:ND2	2.38	0.57
3:C:79:GLU:OE1	28:1:158:SER:OG	2.16	0.57
31:4:372:TYR:CE2	31:4:400:LEU:HD21	2.40	0.57
33:8:213:ILE:O	33:8:216:THR:OG1	2.22	0.57
17:Q:49:CYS:SG	17:Q:50:ARG:NH1	2.79	0.56
28:1:150:GLU:OE1	28:1:174:ARG:NH2	2.38	0.56
33:8:154:GLY:N	33:8:155:PRO:CD	2.69	0.56
24:X:276:ARG:NH2	24:X:286:GLU:OE1	2.38	0.56
31:4:618:ALA:O	31:4:622:ASN:N	2.35	0.56
1:A:769:G:N2	1:A:772:A:OP2	2.38	0.56
15:O:217:ARG:NH2	15:O:227:GLU:OE2	2.39	0.56
4:D:307:LYS:NZ	18:R:103:TYR:OH	2.39	0.55
1:A:1037:A:O2'	12:L:152:HIS:NE2	2.30	0.55
22:V:40:TRP:O	22:V:43:ARG:NH1	2.38	0.55
8:H:89:ASP:OD1	8:H:141:ARG:NH1	2.35	0.54
9:I:71:SER:O	9:I:74:ARG:NH1	2.37	0.54
24:X:147:LYS:HE2	24:X:147:LYS:HA	1.89	0.54
33:8:222:THR:CG2	33:8:243:LEU:HD13	2.37	0.54
1:A:1069:A:O2'	1:A:1587:U:O2	2.24	0.54
6:F:240:ARG:NH2	29:2:44:THR:O	2.41	0.54
1:A:1376:C:H4'	1:A:1377:C:H5'	1.90	0.54
6:F:88:ASP:OD2	6:F:146:HIS:NE2	2.37	0.54
32:7:172:ASP:OD1	32:7:172:ASP:N	2.41	0.54
7:G:322:ARG:NH1	7:G:355:PHE:O	2.41	0.53
31:4:236:VAL:HG12	31:4:238:TRP:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:G:O6	10:J:31:ALA:N	2.41	0.53
1:A:958:C:H4'	1:A:959:C:H5'	1.89	0.53
1:A:1342:C:OP2	26:Z:96:LYS:NZ	2.36	0.53
1:A:1429:C:H4'	1:A:1430:A:H5"	1.89	0.53
1:A:684:U:O2'	20:T:151:SER:OG	2.25	0.53
1:A:1443:U:OP2	11:K:102:ARG:NH2	2.40	0.53
1:A:1532:C:O2'	1:A:1533:C:OP1	2.23	0.53
18:R:219:TYR:O	18:R:256:ARG:NH1	2.42	0.53
1:A:1000:U:OP2	33:8:144:ARG:NH2	2.42	0.53
1:A:860:A:N7	1:A:919:A:O2'	2.41	0.52
1:A:1583:MA6:H93	1:A:1584:MA6:H92	1.92	0.52
7:G:276:ARG:NH1	43:G:2001:HOH:O	2.37	0.52
1:A:1454:G:OP2	7:G:377:ARG:NH2	2.41	0.52
27:0:110:ASP:OD1	27:0:110:ASP:N	2.40	0.52
4:D:134:GLU:OE2	4:D:160:ARG:NH1	2.37	0.52
29:2:102:ASN:OD1	29:2:103:LYS:N	2.42	0.52
33:8:116:LEU:HD12	33:8:116:LEU:O	2.10	0.52
31:4:413:ASP:N	31:4:413:ASP:OD1	2.42	0.52
7:G:263:ASP:OD1	7:G:267:MET:N	2.42	0.52
7:G:237:GLU:OE2	7:G:237:GLU:N	2.41	0.51
13:M:123:GLN:O	13:M:127:ALA:N	2.41	0.51
15:O:73:VAL:O	15:O:109:ARG:NH2	2.43	0.51
24:X:123:ARG:NH2	24:X:337:LEU:O	2.44	0.50
1:A:812:A:O2'	1:A:814:A:N1	2.44	0.50
1:A:905:A:O2'	1:A:907:A:OP1	2.27	0.50
4:D:245:VAL:HG22	4:D:271:ALA:HB1	1.93	0.50
19:S:98:ARG:NH2	19:S:128:GLU:OE1	2.42	0.50
2:B:138:ARG:NH1	19:S:30:LEU:O	2.44	0.50
27:0:84:SER:N	27:0:138:ASP:OD1	2.39	0.50
32:7:357:GLY:O	32:7:431:ILE:N	2.41	0.50
1:A:1583:MA6:H93	1:A:1584:MA6:N6	2.27	0.49
7:G:320:VAL:HG23	7:G:322:ARG:HG2	1.93	0.49
9:I:151:VAL:HG11	9:I:158:ARG:HG3	1.94	0.49
22:V:266:VAL:HG21	22:V:275:LEU:HG	1.94	0.49
1:A:1451:U:OP1	7:G:382:PRO:O	2.30	0.49
25:Y:326:SER:O	28:1:217:GLN:NE2	2.42	0.49
32:7:411:TYR:HB2	32:7:412:PRO:HD2	1.92	0.49
7:G:381:LYS:N	7:G:381:LYS:HD2	2.27	0.49
24:X:127:TYR:OH	28:1:306:GLU:OE2	2.29	0.49
21:U:137:LEU:O	21:U:141:ARG:N	2.40	0.49
28:1:103:LEU:O	28:1:107:LYS:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1415:G:OP2	1:A:1415:G:N2	2.37	0.49
7:G:143:ASP:OD1	7:G:144:GLY:N	2.45	0.49
7:G:150:LEU:O	7:G:153:THR:OG1	2.31	0.49
1:A:745:A:H5'	13:M:11:ALA:HB2	1.95	0.49
1:A:1190:C:O2'	1:A:1467:C:N3	2.42	0.49
1:A:1115:U:OP1	19:S:55:LYS:NZ	2.43	0.48
1:A:1325:U:OP1	4:D:112:LYS:NZ	2.44	0.48
4:D:165:GLN:NE2	4:D:169:GLU:OE2	2.46	0.48
1:A:1227:G:OP1	8:H:128:LYS:NZ	2.30	0.48
22:V:134:GLN:NE2	27:0:108:ASN:OD1	2.46	0.48
2:B:243:PRO:O	2:B:247:HIS:ND1	2.43	0.48
22:V:123:ASP:OD1	22:V:123:ASP:N	2.46	0.48
1:A:1444:A:N7	43:A:1803:HOH:O	2.35	0.48
3:C:39:ALA:O	3:C:41:ARG:NH1	2.47	0.48
19:S:87:LEU:HD12	23:W:116:PHE:O	2.14	0.48
24:X:347:ASN:HB3	24:X:386:ALA:O	2.14	0.48
27:0:41:LEU:HD13	27:0:55:TRP:CG	2.48	0.48
4:D:173:ILE:HG23	4:D:176:ARG:NH2	2.28	0.48
32:7:538:TYR:OH	32:7:544:CYS:O	2.20	0.48
6:F:84:SER:OG	24:X:379:GLU:OE1	2.22	0.48
18:R:275:PHE:O	18:R:279:LYS:N	2.47	0.48
27:0:54:ALA:O	27:0:58:VAL:HG23	2.14	0.47
7:G:320:VAL:O	7:G:321:ASP:OD1	2.31	0.47
19:S:75:TYR:O	19:S:79:GLY:N	2.47	0.47
1:A:948:U:OP2	1:A:1045:G:N1	2.41	0.47
18:R:191:ARG:HG3	18:R:204:ILE:HG23	1.97	0.47
19:S:87:LEU:HD13	23:W:89:LEU:HD13	1.96	0.47
1:A:965:C:H3'	1:A:966:A:H5"	1.97	0.47
22:V:361:LYS:O	22:V:361:LYS:HG2	2.15	0.47
1:A:1136:C:H2'	1:A:1137:A:H5"	1.96	0.47
1:A:1557:A:HO2'	1:A:1558:A:P	2.37	0.46
27:0:68:LEU:HA	27:0:71:LEU:HD12	1.97	0.46
10:J:78:ARG:NH1	10:J:117:ASP:OD2	2.47	0.46
21:U:161:GLN:O	21:U:164:VAL:HG12	2.16	0.46
3:C:57:HIS:HB2	3:C:66:LYS:HD2	1.97	0.46
28:1:255:ASN:N	28:1:259:GLU:OE2	2.47	0.46
31:4:436:HIS:O	31:4:440:LYS:HG2	2.15	0.46
33:8:207:GLU:O	33:8:207:GLU:HG2	2.15	0.46
1:A:782:A:OP1	34:A:1701:NAD:O2D	2.18	0.46
1:A:1267:U:H2'	1:A:1268:C:C6	2.50	0.46
1:A:1450:C:O2'	8:H:131:ARG:NH2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:231:CYS:SG	18:R:242:TYR:HA	2.55	0.46
1:A:1343:A:O2'	1:A:1345:G:N7	2.42	0.46
6:F:176:ASP:OD2	6:F:180:ARG:NH1	2.49	0.46
33:8:231:GLN:O	33:8:234:LYS:HG2	2.16	0.46
1:A:958:C:C4'	1:A:959:C:H5'	2.46	0.46
7:G:270:SER:OG	7:G:351:ALA:O	2.28	0.46
1:A:1531:C:O3'	1:A:1532:C:H6	1.98	0.46
2:B:134:HIS:O	2:B:138:ARG:HG3	2.17	0.45
22:V:269:SER:HB2	22:V:270:PRO:HD2	1.98	0.45
1:A:1416:A:H5'	1:A:1416:A:H8	1.81	0.45
21:U:80:ARG:O	21:U:84:GLU:N	2.49	0.45
1:A:1259:U:OP2	1:A:1327:G:OP2	2.35	0.45
1:A:959:C:H2'	1:A:960:C:H5"	1.99	0.45
1:A:1143:C:N4	1:A:1576:G:OP1	2.49	0.45
2:B:239:ASN:ND2	2:B:242:SER:OG	2.50	0.45
25:Y:296:ASN:OD1	25:Y:298:PHE:N	2.49	0.45
31:4:58:VAL:HG23	31:4:58:VAL:O	2.17	0.45
3:C:58:ALA:HB1	3:C:59:PRO:CD	2.46	0.45
10:J:70:PRO:HB3	10:J:117:ASP:HB3	1.99	0.45
1:A:1046:A:O2'	1:A:1048:C:OP2	2.29	0.44
11:K:90:ARG:NH1	11:K:95:SER:O	2.50	0.44
22:V:46:GLU:OE2	22:V:74:ARG:NE	2.47	0.44
22:V:391:GLN:O	22:V:395:GLN:N	2.40	0.44
32:7:192:GLY:HA2	42:7:801:GNP:H8	2.00	0.44
22:V:252:LYS:O	22:V:258:ARG:NH1	2.50	0.44
24:X:80:PRO:HB2	24:X:190:ASN:OD1	2.17	0.44
24:X:265:ILE:HG12	24:X:265:ILE:O	2.17	0.44
1:A:974:U:O2'	1:A:975:A:N7	2.48	0.44
32:7:224:LEU:HB3	32:7:225:PRO:HD2	1.99	0.44
33:8:243:LEU:HD11	33:8:247:GLU:HB3	1.98	0.44
1:A:1033:U:H4'	5:E:94:VAL:HG12	2.00	0.44
3:C:103:CYS:O	3:C:123:VAL:HA	2.17	0.44
15:O:137:ALA:HB3	15:O:138:PRO:HD3	1.99	0.44
7:G:299:ASP:OD2	24:X:385:ASN:ND2	2.51	0.44
7:G:384:GLN:HB3	7:G:389:ARG:O	2.17	0.44
21:U:84:GLU:O	21:U:84:GLU:HG2	2.18	0.44
28:1:118:ALA:O	28:1:122:HIS:N	2.45	0.44
3:C:89:ASP:O	3:C:93:ARG:HG3	2.18	0.44
21:U:199:ARG:HG3	21:U:200:PRO:HD2	2.00	0.44
2:B:103:GLU:N	2:B:104:PRO:CD	2.80	0.43
4:D:368:LEU:HD22	18:R:107:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:120:VAL:HG13	15:O:163:LEU:HD13	2.00	0.43
24:X:48:ILE:O	24:X:48:ILE:HG12	2.18	0.43
24:X:233:VAL:HG12	24:X:233:VAL:O	2.18	0.43
1:A:727:U:H2'	1:A:728:C:O4'	2.17	0.43
32:7:401:ASP:OD1	32:7:405:LYS:N	2.44	0.43
12:L:221:LYS:HA	12:L:221:LYS:HE2	1.99	0.43
33:8:241:ARG:NH2	33:8:247:GLU:OE1	2.52	0.43
7:G:196:GLY:O	7:G:248:VAL:N	2.45	0.43
8:H:121:LEU:HD21	8:H:128:LYS:HD2	1.99	0.43
3:C:123:VAL:HG23	3:C:157:THR:HG22	2.00	0.43
1:A:940:A:H8	1:A:940:A:H5"	1.83	0.43
11:K:55:ASN:OD1	11:K:58:ARG:NH2	2.51	0.43
13:M:85:LYS:O	13:M:89:LYS:HG3	2.19	0.43
15:O:146:GLN:OE1	15:O:146:GLN:HA	2.18	0.43
33:8:130:LEU:HD12	33:8:130:LEU:O	2.19	0.43
1:A:1430:A:OP1	7:G:388:ARG:NH2	2.47	0.43
7:G:315:PHE:HB3	7:G:316:PRO:HD3	2.00	0.43
7:G:395:LYS:O	7:G:396:ARG:OXT	2.36	0.43
10:J:84:ARG:NH1	32:7:565:GLU:OE1	2.45	0.42
31:4:509:ILE:N	31:4:510:PRO:CD	2.82	0.42
1:A:928:A:OP2	10:J:47:ARG:NH2	2.53	0.42
1:A:1136:C:C2'	1:A:1137:A:H5"	2.49	0.42
1:A:1366:C:H3'	1:A:1367:A:H5'	2.01	0.42
6:F:161:ILE:HD12	6:F:170:VAL:HG21	2.01	0.42
32:7:311:CYS:SG	32:7:312:GLU:N	2.92	0.42
33:8:222:THR:HG21	33:8:243:LEU:HD13	2.00	0.42
1:A:1378:C:O2	24:X:389:SER:OG	2.26	0.42
12:L:212:ARG:NH1	12:L:216:GLU:OE2	2.49	0.42
32:7:654:GLU:HB2	32:7:657:LYS:HG2	2.01	0.42
18:R:315:GLN:HA	18:R:315:GLN:OE1	2.19	0.42
18:R:76:GLN:HA	18:R:76:GLN:OE1	2.19	0.42
29:2:7:ARG:O	29:2:9:ARG:NH1	2.53	0.42
2:B:110:ARG:NH2	23:W:90:THR:O	2.49	0.42
5:E:31:ASP:OD1	21:U:170:ARG:NH2	2.52	0.42
7:G:116:LEU:O	7:G:122:ARG:NH2	2.45	0.42
8:H:76:LEU:HB2	8:H:148:LEU:HD13	2.01	0.42
12:L:181:ILE:HG23	12:L:185:LEU:HD12	2.02	0.42
24:X:196:GLU:OE2	24:X:196:GLU:HA	2.20	0.42
1:A:1198:A:C2'	1:A:1199:G:H5'	2.49	0.42
18:R:262:LEU:O	18:R:265:THR:OG1	2.25	0.42
25:Y:393:GLN:O	25:Y:393:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:0:163:SER:HA	27:0:191:LEU:O	2.19	0.42
16:P:73:ASP:OD1	16:P:74:TYR:N	2.52	0.42
32:7:311:CYS:O	32:7:316:GLY:N	2.47	0.42
32:7:663:ARG:NH2	32:7:702:GLU:O	2.52	0.42
6:F:52:ARG:NH2	7:G:319:PHE:O	2.53	0.42
10:J:70:PRO:HD3	10:J:76:ALA:O	2.20	0.42
1:A:1079:G:C2'	1:A:1080:A:H5'	2.50	0.42
8:H:184:ILE:O	8:H:184:ILE:HG22	2.20	0.42
24:X:186:THR:O	24:X:190:ASN:ND2	2.51	0.42
32:7:614:LEU:O	32:7:718:GLN:NE2	2.52	0.42
31:4:318:GLU:OE1	31:4:318:GLU:HA	2.19	0.41
8:H:188:ILE:O	8:H:188:ILE:HG13	2.19	0.41
1:A:663:A:H2'	1:A:664:G:C8	2.55	0.41
1:A:1119:U:O4'	19:S:50:ARG:NH1	2.51	0.41
2:B:157:ASN:OD1	7:G:163:HIS:NE2	2.54	0.41
5:E:109:VAL:HG23	5:E:109:VAL:O	2.19	0.41
6:F:235:ALA:O	6:F:238:HIS:NE2	2.53	0.41
7:G:305:PRO:O	7:G:310:ARG:NH2	2.51	0.41
8:H:50:LEU:HD12	31:4:79:ASN:HB3	2.02	0.41
32:7:484:LEU:O	32:7:489:ARG:NH1	2.53	0.41
32:7:617:ALA:N	32:7:717:ILE:O	2.47	0.41
3:C:84:GLU:O	3:C:88:GLU:HG3	2.21	0.41
6:F:71:THR:O	7:G:253:LYS:NZ	2.50	0.41
12:L:123:ARG:O	12:L:123:ARG:HG2	2.21	0.41
20:T:103:ARG:O	20:T:103:ARG:HG2	2.20	0.41
31:4:650:MET:HA	31:4:654:ALA:HB3	2.03	0.41
3:C:62:ILE:O	3:C:66:LYS:O	2.38	0.41
4:D:380:LEU:HD12	4:D:381:PRO:HD2	2.02	0.41
12:L:76:TYR:O	12:L:79:VAL:HG22	2.19	0.41
15:O:217:ARG:NE	22:V:318:ASP:OD2	2.48	0.41
22:V:376:GLU:HA	22:V:376:GLU:OE1	2.20	0.41
24:X:285:GLU:OE2	24:X:285:GLU:N	2.48	0.41
31:4:56:GLU:HA	31:4:56:GLU:OE1	2.21	0.41
15:O:220:TYR:O	15:O:224:LEU:HG	2.21	0.41
16:P:54:MET:HG2	16:P:55:GLU:N	2.35	0.41
24:X:338:ASP:OD1	28:1:292:TYR:OH	2.36	0.41
31:4:508:VAL:O	31:4:508:VAL:HG12	2.20	0.41
32:7:268:GLN:OE1	32:7:268:GLN:HA	2.21	0.41
32:7:457:GLN:HA	32:7:457:GLN:OE1	2.19	0.41
3:C:58:ALA:HB3	3:C:60:HIS:CE1	2.56	0.41
10:J:99:GLY:O	10:J:127:ARG:NH2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:151:LEU:HD21	24:X:247:LEU:HD22	2.02	0.41
1:A:1184:U:H2'	1:A:1185:C:O4'	2.21	0.41
12:L:83:GLU:HA	12:L:83:GLU:OE1	2.21	0.41
19:S:67:GLU:OE2	19:S:67:GLU:N	2.52	0.41
27:0:194:GLN:HA	27:0:194:GLN:OE1	2.21	0.41
31:4:324:VAL:O	31:4:324:VAL:HG12	2.21	0.41
4:D:263:ASP:OD1	4:D:264:ARG:N	2.53	0.41
22:V:269:SER:HB2	22:V:273:ILE:HD12	2.03	0.41
31:4:558:ALA:O	31:4:561:SER:O	2.39	0.41
33:8:190:GLN:NE2	33:8:237:MET:SD	2.94	0.41
1:A:1078:A:N6	1:A:1563:U:OP1	2.50	0.40
20:T:9:ILE:O	20:T:12:THR:OG1	2.24	0.40
25:Y:319:ALA:O	28:1:164:ARG:NH1	2.55	0.40
5:E:26:ILE:HG23	5:E:36:VAL:HG21	2.02	0.40
10:J:95:ILE:HG12	10:J:102:LEU:HD12	2.03	0.40
11:K:52:LEU:HD11	26:Z:36:LEU:HB3	2.03	0.40
20:T:89:ASP:OD2	21:U:120:ARG:NH2	2.45	0.40
1:A:1591:C:OP1	17:Q:52:ARG:NH2	2.55	0.40
1:A:1591:C:OP1	17:Q:48:PRO:HB2	2.21	0.40
8:H:50:LEU:HD13	8:H:53:ASP:O	2.21	0.40
15:O:71:ARG:HB3	15:O:72:PRO:HD2	2.03	0.40
23:W:114:ILE:HB	23:W:122:CYS:SG	2.62	0.40
1:A:906:C:C2	7:G:50:ARG:HG2	2.57	0.40
4:D:316:CYS:HB3	4:D:334:ALA:HB3	2.03	0.40
18:R:253:ILE:O	18:R:257:GLY:N	2.54	0.40
24:X:103:LYS:N	24:X:104:PRO:CD	2.84	0.40
12:L:67:PRO:HA	12:L:68:PRO:HD3	1.99	0.40
15:O:208:PRO:HG2	15:O:213:LEU:HD21	2.04	0.40
24:X:53:GLU:HA	24:X:53:GLU:OE2	2.21	0.40
32:7:310:VAL:HG23	32:7:316:GLY:HA3	2.02	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%)	212 (95%)	11 (5%)	0	100	100
3	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
4	D	341/430 (79%)	329 (96%)	12 (4%)	0	100	100
5	E	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
6	F	206/242 (85%)	202 (98%)	4 (2%)	0	100	100
7	G	326/396 (82%)	314 (96%)	12 (4%)	0	100	100
8	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	22	56
9	I	135/194 (70%)	126 (93%)	8 (6%)	1 (1%)	22	56
10	J	106/138 (77%)	100 (94%)	6 (6%)	0	100	100
11	K	99/128 (77%)	99 (100%)	0	0	100	100
12	L	172/257 (67%)	168 (98%)	4 (2%)	0	100	100
13	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
14	N	108/130 (83%)	102 (94%)	6 (6%)	0	100	100
15	O	192/258 (74%)	184 (96%)	8 (4%)	0	100	100
16	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
17	Q	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
18	R	293/360 (81%)	287 (98%)	6 (2%)	0	100	100
19	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
20	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	U	174/205 (85%)	171 (98%)	3 (2%)	0	100	100
22	V	358/414 (86%)	350 (98%)	8 (2%)	0	100	100
23	W	98/187 (52%)	93 (95%)	5 (5%)	0	100	100
24	X	350/398 (88%)	344 (98%)	6 (2%)	0	100	100
25	Y	147/395 (37%)	145 (99%)	2 (1%)	0	100	100
26	Z	98/106 (92%)	94 (96%)	4 (4%)	0	100	100
27	0	213/218 (98%)	207 (97%)	6 (3%)	0	100	100
28	1	274/323 (85%)	260 (95%)	14 (5%)	0	100	100
29	2	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
30	3	68/199 (34%)	65 (96%)	3 (4%)	0	100	100
31	4	584/689 (85%)	563 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	7	569/699 (81%)	548 (96%)	21 (4%)	0	100	100
33	8	189/285 (66%)	184 (97%)	4 (2%)	1 (0%)	29	63
All	All	6421/8285 (78%)	6225 (97%)	193 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	184	ASN
8	H	126	ILE
33	8	218	PRO

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%)	197 (100%)	1 (0%)	88	95
3	C	115/143 (80%)	115 (100%)	0	100	100
4	D	286/357 (80%)	284 (99%)	2 (1%)	84	93
5	E	104/107 (97%)	103 (99%)	1 (1%)	76	89
6	F	185/209 (88%)	185 (100%)	0	100	100
7	G	288/342 (84%)	287 (100%)	1 (0%)	92	97
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	105/147 (71%)	105 (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	175/230 (76%)	175 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	324 (100%)	1 (0%)	92	97
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	310 (100%)	1 (0%)	92	97
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%)	186 (99%)	2 (1%)	73	88
28	1	254/291 (87%)	254 (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	526/609 (86%)	525 (100%)	1 (0%)	93	97
32	7	481/595 (81%)	481 (100%)	0	100	100
33	8	172/253 (68%)	171 (99%)	1 (1%)	86	94
All	All	5708/7192 (79%)	5697 (100%)	11 (0%)	93	97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	178	ASN
4	D	296	LEU
4	D	316	CYS
5	E	92	ASN
7	G	389	ARG
22	V	226	TYR
24	X	81	HIS
27	0	79	LEU
27	0	135	MET
31	4	486	TYR
33	8	238	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	90	HIS
2	B	167	HIS
2	B	178	ASN
5	E	58	HIS
15	O	223	HIS
20	T	51	ASN
22	V	380	GLN
22	V	391	GLN
24	X	159	HIS
24	X	302	HIS
24	X	326	GLN
25	Y	290	ASN
26	Z	55	HIS
31	4	257	HIS
31	4	453	HIS
31	4	504	ASN
31	4	577	ASN
32	7	377	GLN
32	7	621	HIS
33	8	198	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	951/955 (99%)	282 (29%)	10 (1%)

All (282) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	649	A
1	A	657	G
1	A	676	G
1	A	680	U
1	A	688	A
1	A	689	U
1	A	690	U
1	A	693	A
1	A	695	A
1	A	704	U
1	A	715	G
1	A	718	A
1	A	721	U

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Mol	Chain	Res	Type
1	A	722	C
1	A	723	A
1	A	724	C
1	A	730	A
1	A	737	C
1	A	738	A
1	A	749	G
1	A	753	A
1	A	757	A
1	A	760	A
1	A	761	A
1	A	763	C
1	A	764	A
1	A	770	C
1	A	776	A
1	A	777	G
1	A	791	G
1	A	792	C
1	A	793	C
1	A	794	U
1	A	796	G
1	A	801	A
1	A	803	C
1	A	804	C
1	A	806	C
1	A	807	A
1	A	808	C
1	A	814	A
1	A	815	C
1	A	826	A
1	A	828	C
1	A	829	C
1	A	830	U
1	A	832	U
1	A	835	C
1	A	836	A
1	A	844	A
1	A	859	U
1	A	860	A
1	A	861	U
1	A	868	C
1	A	869	C

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Mol	Chain	Res	Type
1	A	870	C
1	A	871	A
1	A	879	U
1	A	881	A
1	A	889	G
1	A	890	C
1	A	896	A
1	A	902	G
1	A	903	U
1	A	904	C
1	A	905	A
1	A	907	A
1	A	908	C
1	A	919	A
1	A	922	C
1	A	929	A
1	A	930	G
1	A	931	C
1	A	932	C
1	A	933	G
1	A	935	C
1	A	937	U
1	A	938	A
1	A	939	A
1	A	940	A
1	A	941	G
1	A	942	A
1	A	953	U
1	A	955	A
1	A	956	C
1	A	957	C
1	A	958	C
1	A	959	C
1	A	960	C
1	A	962	C
1	A	965	C
1	A	966	A
1	A	967	A
1	A	974	U
1	A	975	A
1	A	987	A
1	A	992	U

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Mol	Chain	Res	Type
1	A	999	C
1	A	1001	C
1	A	1002	C
1	A	1011	C
1	A	1015	A
1	A	1017	A
1	A	1018	G
1	A	1021	U
1	A	1031	G
1	A	1038	C
1	A	1039	A
1	A	1040	U
1	A	1042	U
1	A	1049	A
1	A	1050	C
1	A	1064	C
1	A	1065	C
1	A	1069	A
1	A	1074	G
1	A	1078	A
1	A	1080	A
1	A	1081	U
1	A	1082	A
1	A	1100	C
1	A	1103	A
1	A	1105	C
1	A	1106	C
1	A	1107	U
1	A	1108	C
1	A	1109	A
1	A	1110	A
1	A	1115	U
1	A	1116	A
1	A	1117	A
1	A	1118	A
1	A	1119	U
1	A	1120	C
1	A	1121	A
1	A	1122	A
1	A	1125	A
1	A	1126	A
1	A	1127	A

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Mol	Chain	Res	Type
1	A	1136	C
1	A	1138	G
1	A	1139	A
1	A	1144	U
1	A	1151	C
1	A	1153	C
1	A	1155	G
1	A	1160	A
1	A	1166	A
1	A	1178	G
1	A	1179	G
1	A	1181	G
1	A	1185	C
1	A	1187	U
1	A	1188	A
1	A	1189	U
1	A	1190	C
1	A	1194	C
1	A	1199	G
1	A	1200	G
1	A	1201	A
1	A	1213	A
1	A	1215	U
1	A	1219	U
1	A	1221	A
1	A	1222	A
1	A	1223	C
1	A	1225	C
1	A	1227	G
1	A	1231	A
1	A	1233	C
1	A	1237	A
1	A	1244	C
1	A	1245	U
1	A	1246	U
1	A	1247	G
1	A	1248	C
1	A	1249	U
1	A	1250	C
1	A	1251	A
1	A	1253	C
1	A	1256	A

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Mol	Chain	Res	Type
1	A	1266	A
1	A	1267	U
1	A	1269	U
1	A	1271	C
1	A	1272	A
1	A	1273	G
1	A	1282	G
1	A	1284	U
1	A	1286	A
1	A	1289	G
1	A	1290	C
1	A	1291	U
1	A	1292	A
1	A	1295	A
1	A	1298	U
1	A	1309	A
1	A	1310	C
1	A	1311	C
1	A	1312	C
1	A	1313	A
1	A	1320	G
1	A	1325	U
1	A	1326	A
1	A	1327	G
1	A	1329	U
1	A	1336	G
1	A	1341	C
1	A	1342	C
1	A	1343	A
1	A	1345	G
1	A	1352	C
1	A	1354	A
1	A	1355	G
1	A	1357	A
1	A	1358	A
1	A	1368	U
1	A	1377	C
1	A	1378	C
1	A	1379	A
1	A	1382	A
1	A	1383	A
1	A	1384	A

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Mol	Chain	Res	Type
1	A	1385	C
1	A	1387	A
1	A	1389	G
1	A	1390	A
1	A	1391	U
1	A	1392	A
1	A	1399	A
1	A	1402	A
1	A	1404	A
1	A	1405	C
1	A	1407	U
1	A	1415	G
1	A	1416	A
1	A	1419	G
1	A	1421	G
1	A	1430	A
1	A	1443	U
1	A	1444	A
1	A	1447	G
1	A	1448	U
1	A	1465	C
1	A	1466	C
1	A	1478	A
1	A	1480	A
1	A	1482	A
1	A	1483	C
1	A	1493	C
1	A	1501	A
1	A	1511	C
1	A	1512	A
1	A	1516	G
1	A	1519	A
1	A	1522	U
1	A	1523	A
1	A	1524	A
1	A	1525	C
1	A	1527	A
1	A	1529	A
1	A	1532	C
1	A	1533	C
1	A	1536	A
1	A	1537	C

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Mol	Chain	Res	Type
1	A	1539	C
1	A	1553	A
1	A	1558	A
1	A	1563	U
1	A	1564	A
1	A	1565	A
1	A	1568	U
1	A	1571	U
1	A	1572	A
1	A	1582	G
1	A	1593	U
1	A	1594	G
1	A	1595	G
1	A	1597	C
1	A	1598	G
1	A	1599	A
1	A	1602	C

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	723	A
1	A	930	G
1	A	965	C
1	A	1246	U
1	A	1342	C
1	A	1488	5MC
1	A	1512	A
1	A	1531	C
1	A	1532	C
1	A	1557	A

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	$\#\|Z\| > 2$
29	AYA	2	2	29	6,7,8	1.35	1 (16%)	5,8,10	1.35	1 (20%)
1	MA6	A	1583	1	18,26,27	1.06	2 (11%)	19,38,41	1.39	2 (10%)
1	5MU	A	1076	1	19,22,23	1.13	3 (15%)	28,32,35	2.15	8 (28%)
1	5MC	A	1488	1	18,22,23	1.22	2 (11%)	26,32,35	1.92	8 (30%)
17	AYA	Q	2	17	6,7,8	1.40	1 (16%)	5,8,10	1.15	0
1	B8T	A	1486	1	19,22,23	0.88	2 (10%)	26,31,34	0.98	1 (3%)
1	MA6	A	1584	1	18,26,27	1.07	2 (11%)	19,38,41	1.33	2 (10%)

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
29	AYA	2	2	29	-	0/4/6/8	-
1	MA6	A	1583	1	-	0/7/29/30	0/3/3/3
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
17	AYA	Q	2	17	-	1/4/6/8	-
1	B8T	A	1486	1	-	0/7/27/28	0/2/2/2
1	MA6	A	1584	1	-	1/7/29/30	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	2	AYA	CA-N	-2.97	1.43	1.46
1	A	1583	MA6	C8-N7	-2.86	1.29	1.34
1	A	1584	MA6	C8-N7	-2.80	1.29	1.34
29	2	2	AYA	CA-N	-2.76	1.43	1.46
1	A	1076	5MU	C2-N1	-2.68	1.34	1.38
1	A	1488	5MC	C2-N1	-2.66	1.34	1.40
1	A	1076	5MU	C4-C5	-2.62	1.40	1.44
1	A	1583	MA6	C4-N3	-2.39	1.32	1.35
1	A	1584	MA6	C4-N3	-2.32	1.32	1.35
1	A	1486	B8T	C6-N1	2.22	1.43	1.38
1	A	1486	B8T	C2-N1	-2.14	1.35	1.40
1	A	1076	5MU	C4-N3	-2.05	1.35	1.38
1	A	1488	5MC	C2'-C3'	-2.04	1.47	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1076	5MU	C4-N3-C2	-5.62	120.07	127.35
1	A	1583	MA6	N3-C2-N1	-4.77	121.22	128.68
1	A	1076	5MU	N3-C2-N1	4.66	121.07	114.89
1	A	1584	MA6	N3-C2-N1	-4.61	121.48	128.68
1	A	1076	5MU	C5-C4-N3	4.32	119.00	115.31
1	A	1488	5MC	O3'-C3'-C4'	4.19	123.15	111.05
1	A	1076	5MU	O4-C4-C5	-4.18	120.05	124.90
1	A	1488	5MC	O3'-C3'-C2'	3.75	123.96	111.82
1	A	1488	5MC	C5-C6-N1	-3.71	119.52	123.34
1	A	1076	5MU	C5-C6-N1	-3.34	119.90	123.34
1	A	1488	5MC	O2'-C2'-C3'	3.08	121.78	111.82
29	2	2	AYA	CB-CA-N	2.74	112.65	109.61
1	A	1584	MA6	C4-C5-N7	-2.70	106.59	109.40
1	A	1488	5MC	O2'-C2'-C1'	2.65	118.88	110.02
1	A	1076	5MU	C5M-C5-C6	-2.61	119.36	122.85
1	A	1488	5MC	CM5-C5-C6	-2.55	119.44	122.85
1	A	1076	5MU	O2-C2-N1	-2.50	119.46	122.79
1	A	1583	MA6	C4-C5-N7	-2.48	106.81	109.40
1	A	1486	B8T	C5-C4-N4	-2.36	117.81	122.61
1	A	1488	5MC	C1'-N1-C6	-2.17	117.51	121.12
1	A	1076	5MU	C6-C5-C4	2.09	119.78	118.03
1	A	1488	5MC	C5-C4-N3	-2.07	119.44	121.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	Q	2	AYA	C-CA-N-CT
1	A	1584	MA6	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1583	MA6	3	0
1	A	1584	MA6	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 87 ligands modelled in this entry, 79 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
34	NAD	A	1701	37	42,48,48	1.11	5 (11%)	50,73,73	1.23	5 (10%)
36	SRY	A	1703	-	40,42,42	0.78	2 (5%)	49,63,63	1.33	6 (12%)
42	GNP	X	503	-	29,34,34	1.60	7 (24%)	33,54,54	2.25	6 (18%)
42	GNP	7	801	37	29,34,34	1.59	7 (24%)	33,54,54	2.24	6 (18%)
40	FES	T	201	20,13	0,4,4	-	-	-		
35	SPM	A	1702	-	13,13,13	0.15	0	12,12,12	1.15	0
41	ATP	X	501	37	26,33,33	0.90	1 (3%)	31,52,52	1.37	5 (16%)
40	FES	P	201	16,5	0,4,4	-	-	-		

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
34	NAD	A	1701	37	-	0/26/62/62	0/5/5/5
36	SRY	A	1703	-	-	1/20/87/87	0/3/3/3
42	GNP	X	503	-	-	5/14/38/38	0/3/3/3
42	GNP	7	801	37	-	4/14/38/38	0/3/3/3
40	FES	T	201	20,13	-	-	0/1/1/1
35	SPM	A	1702	-	-	0/11/11/11	-
41	ATP	X	501	37	-	0/18/38/38	0/3/3/3
40	FES	P	201	16,5	-	-	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	X	503	GNP	PB-O3A	4.36	1.64	1.59
42	7	801	GNP	PB-O3A	4.27	1.64	1.59
42	7	801	GNP	C6-N1	3.08	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	X	503	GNP	C6-N1	3.06	1.38	1.33
42	X	503	GNP	PB-O1B	3.04	1.51	1.46
42	7	801	GNP	PB-O1B	3.02	1.50	1.46
36	A	1703	SRY	CD1-N31	2.93	1.38	1.33
42	X	503	GNP	PG-N3B	2.91	1.71	1.63
42	7	801	GNP	PG-N3B	2.86	1.70	1.63
34	A	1701	NAD	C8A-N7A	-2.73	1.29	1.34
34	A	1701	NAD	O4B-C1B	2.72	1.44	1.41
36	A	1703	SRY	CA1-N11	2.68	1.37	1.33
42	X	503	GNP	PG-O1G	2.67	1.50	1.46
42	7	801	GNP	PG-O1G	2.62	1.50	1.46
34	A	1701	NAD	C2N-N1N	-2.52	1.31	1.35
34	A	1701	NAD	O4D-C1D	2.49	1.44	1.41
42	7	801	GNP	PB-O2B	-2.29	1.50	1.56
42	X	503	GNP	PB-O2B	-2.23	1.50	1.56
41	X	501	ATP	C5-C4	2.16	1.46	1.40
34	A	1701	NAD	C4A-N3A	-2.15	1.32	1.35
42	7	801	GNP	C5-C6	2.09	1.45	1.41
42	X	503	GNP	C5-C6	2.05	1.44	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	X	503	GNP	C5-C6-N1	-8.45	111.88	123.43
42	7	801	GNP	C5-C6-N1	-8.44	111.88	123.43
42	X	503	GNP	C2-N1-C6	5.84	125.21	115.93
42	7	801	GNP	C2-N1-C6	5.84	125.21	115.93
36	A	1703	SRY	C12-O42-C42	-4.64	101.08	108.38
34	A	1701	NAD	N3A-C2A-N1A	-4.12	122.24	128.68
41	X	501	ATP	N3-C2-N1	-3.72	122.87	128.68
34	A	1701	NAD	PN-O3-PA	-3.54	120.68	132.83
36	A	1703	SRY	O42-C12-C22	-3.17	103.88	107.30
42	7	801	GNP	N3-C2-N1	-2.79	123.51	127.22
42	7	801	GNP	PB-O3A-PA	-2.75	122.93	132.62
42	X	503	GNP	N3-C2-N1	-2.75	123.56	127.22
36	A	1703	SRY	CH2-C42-C32	-2.71	111.85	116.65
42	X	503	GNP	PB-O3A-PA	-2.67	123.22	132.62
41	X	501	ATP	PA-O3A-PB	-2.59	123.93	132.83
42	7	801	GNP	C4-C5-C6	-2.56	118.35	120.80
36	A	1703	SRY	O42-C42-C32	-2.54	100.71	104.33
41	X	501	ATP	PB-O3B-PG	-2.53	124.15	132.83
42	X	503	GNP	C4-C5-C6	-2.53	118.39	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	1701	NAD	C4A-C5A-N7A	-2.51	106.78	109.40
41	X	501	ATP	C4-C5-N7	-2.46	106.84	109.40
34	A	1701	NAD	C5A-C6A-N6A	2.43	124.04	120.35
42	X	503	GNP	C2-N3-C4	-2.21	112.83	115.36
36	A	1703	SRY	C41-C31-N31	-2.18	107.30	110.91
42	7	801	GNP	C2-N3-C4	-2.17	112.87	115.36
41	X	501	ATP	C3'-C2'-C1'	2.16	104.23	100.98
34	A	1701	NAD	O7N-C7N-N7N	-2.06	119.65	122.58
36	A	1703	SRY	CI3-N23-C23	-2.05	111.40	114.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	X	503	GNP	PG-N3B-PB-O3A
42	X	503	GNP	PA-O3A-PB-O1B
42	X	503	GNP	PA-O3A-PB-O2B
42	7	801	GNP	PG-N3B-PB-O1B
42	7	801	GNP	O4'-C4'-C5'-O5'
42	7	801	GNP	C5'-O5'-PA-O3A
42	X	503	GNP	PG-N3B-PB-O1B
36	A	1703	SRY	C13-C23-N23-CI3
42	X	503	GNP	C5'-O5'-PA-O1A
42	7	801	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

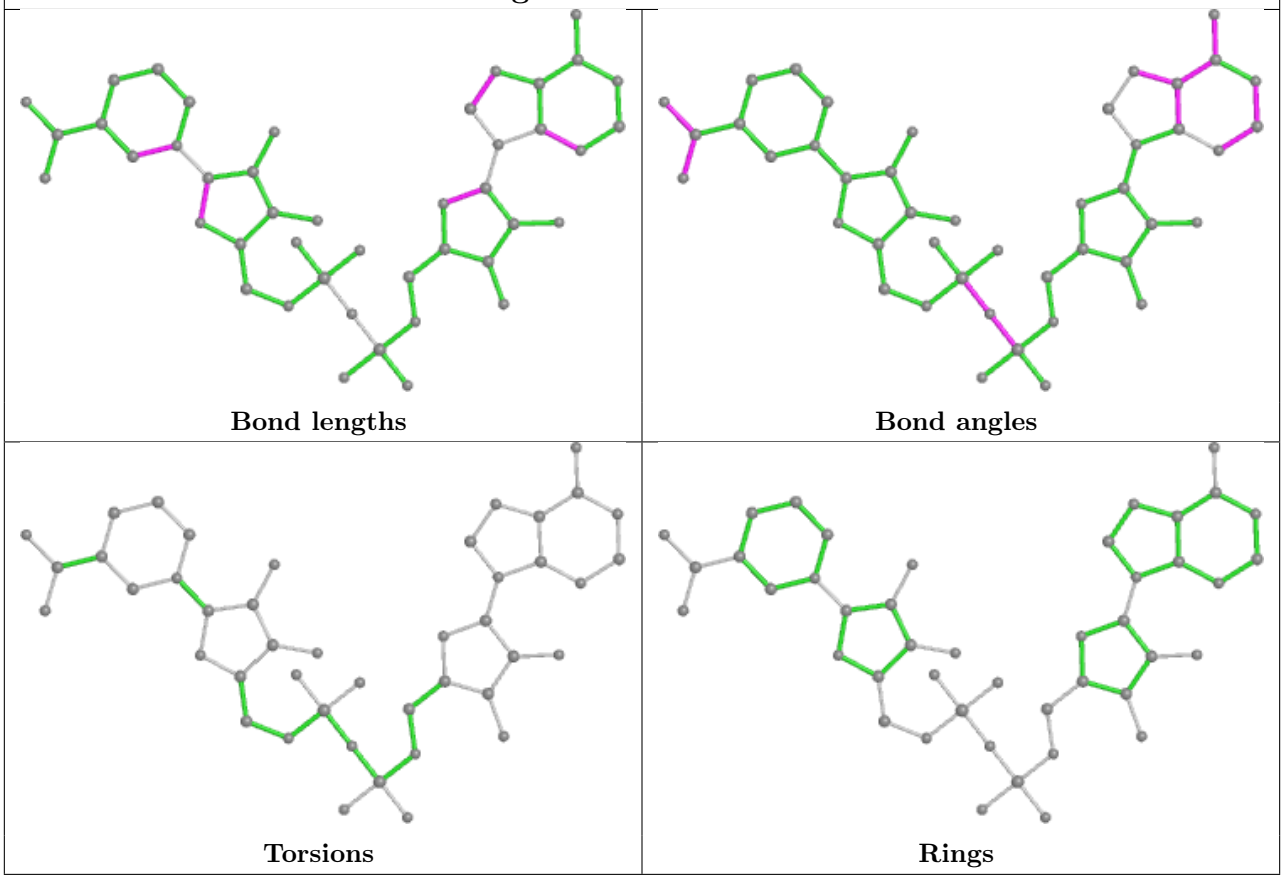
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	1701	NAD	1	0
42	7	801	GNP	1	0

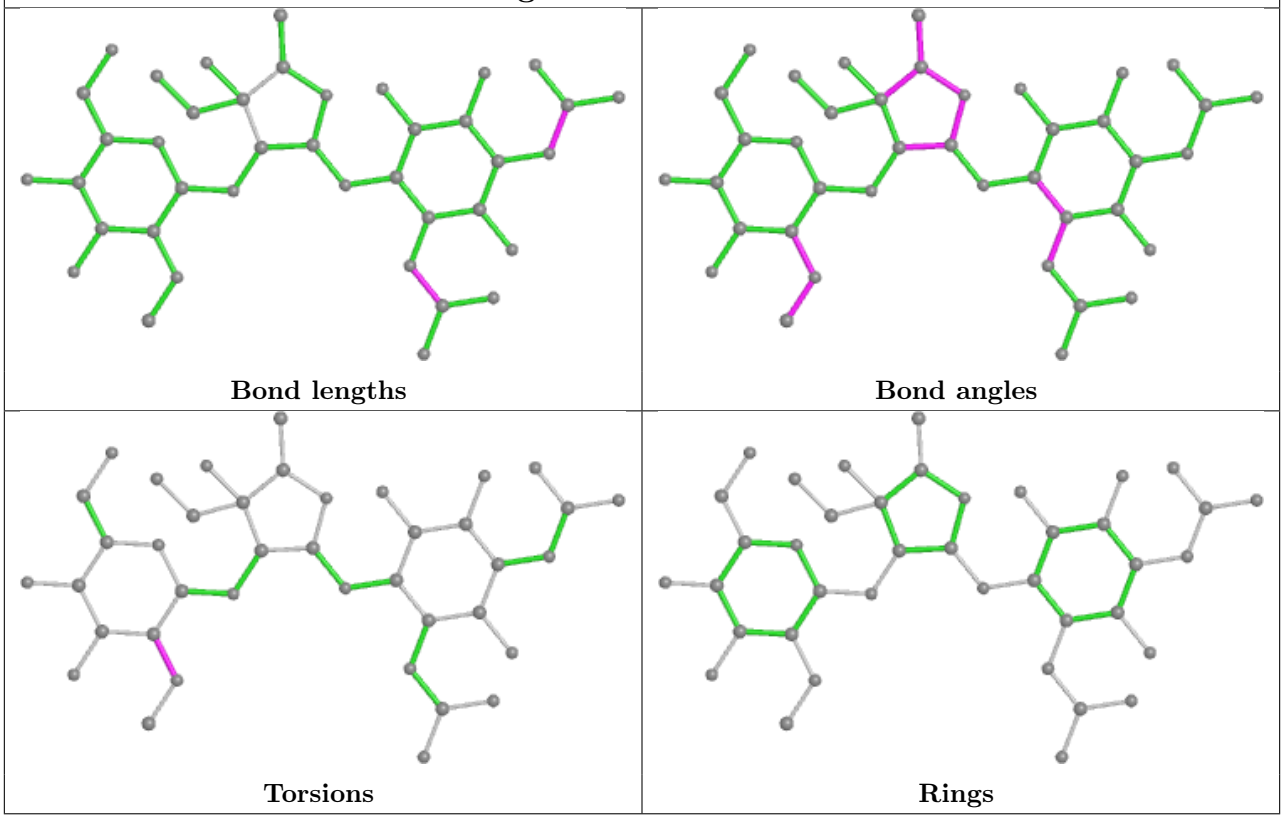
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

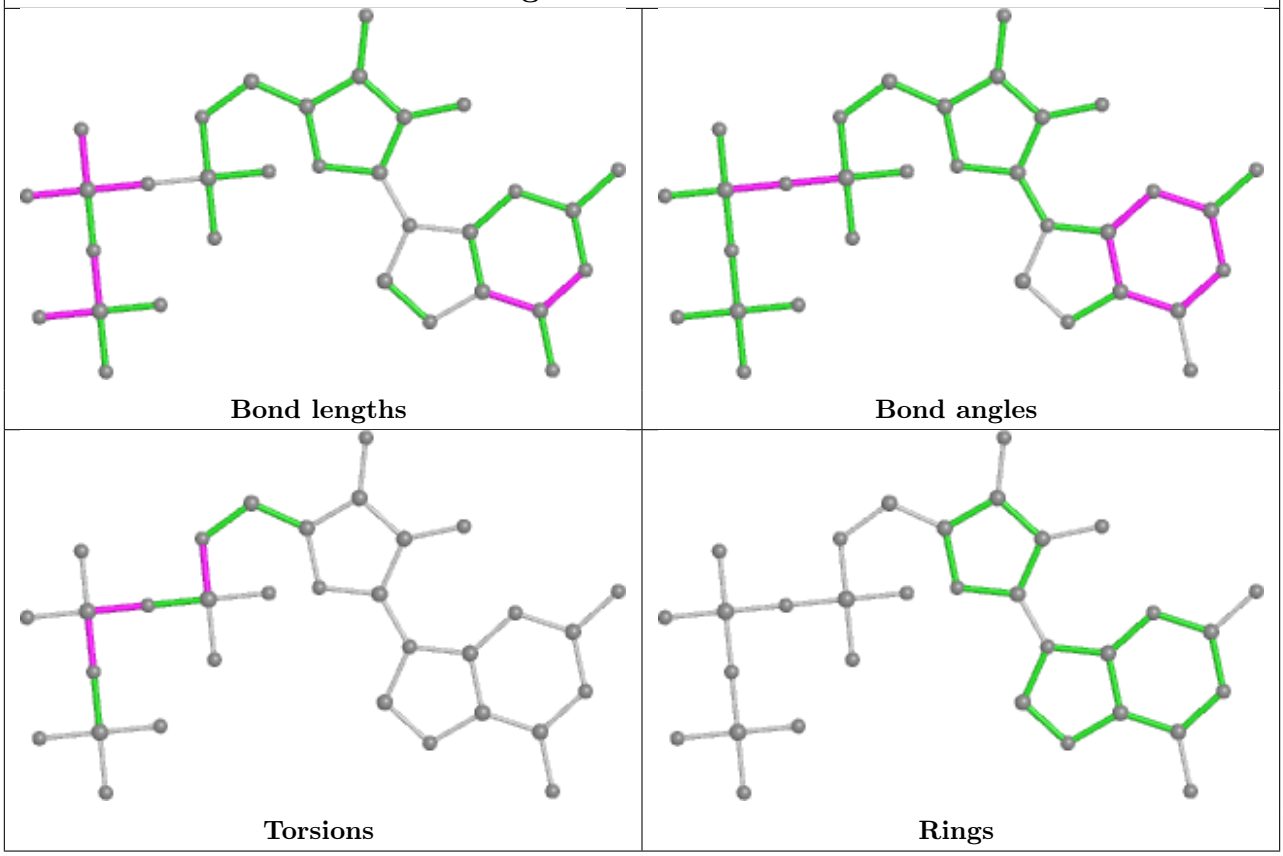
Ligand NAD A 1701



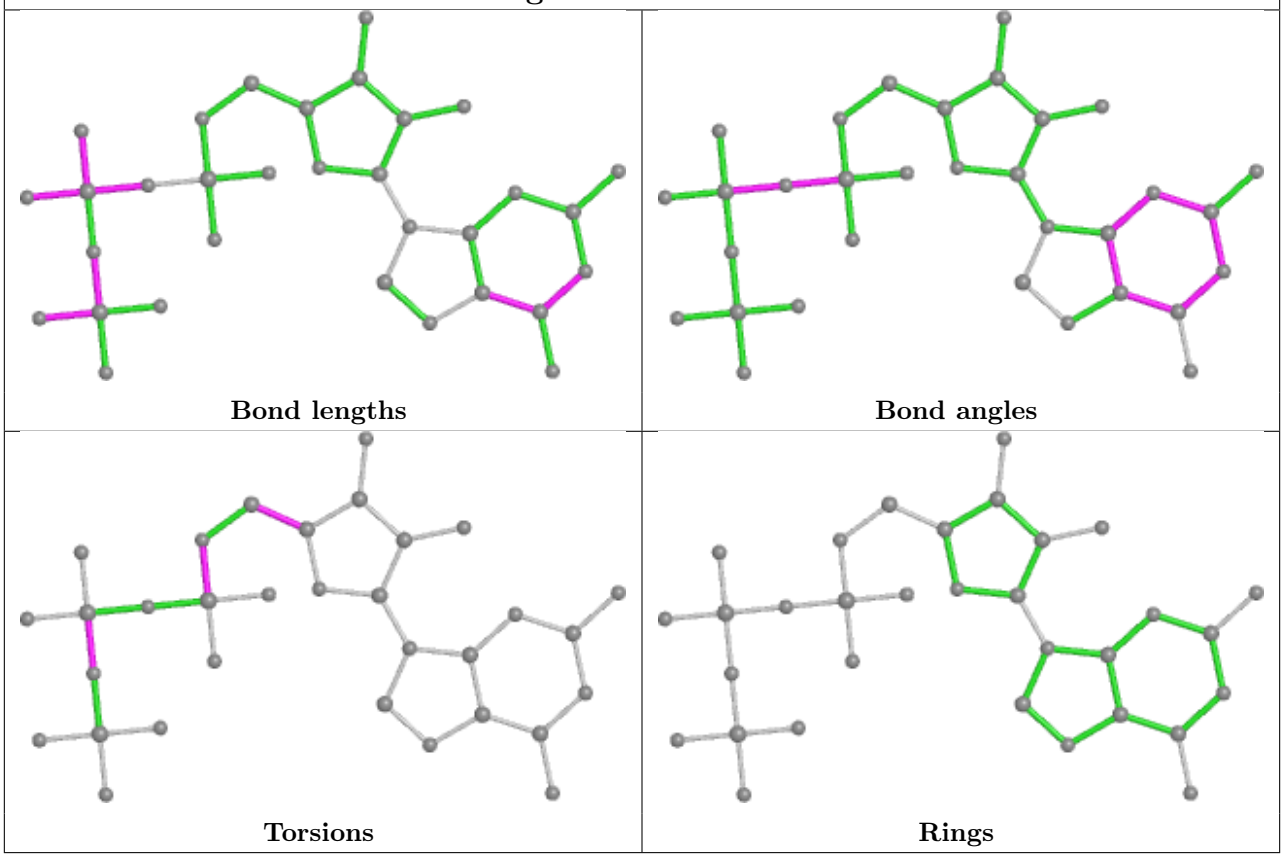
Ligand SRY A 1703

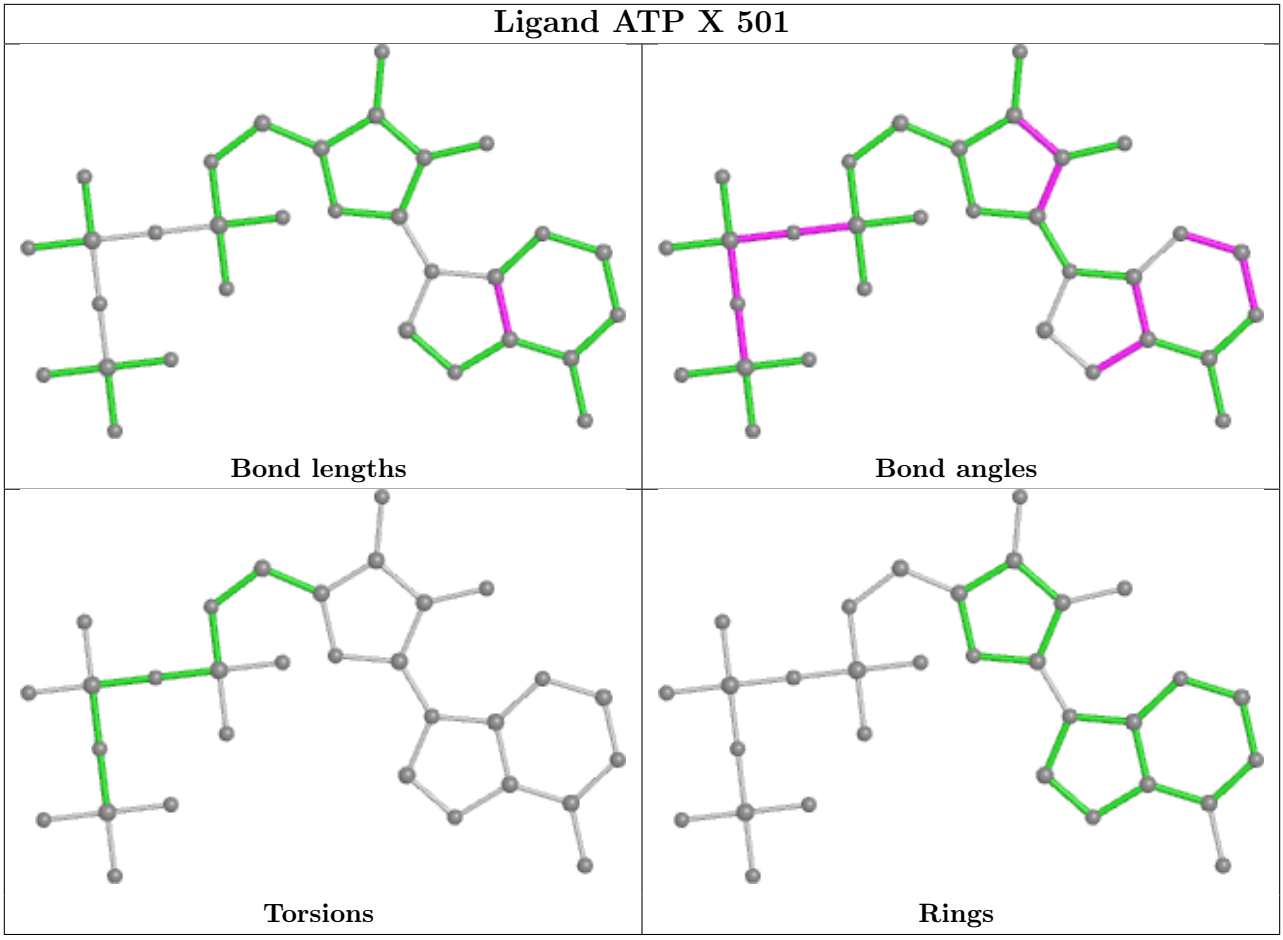


Ligand GNP X 503



Ligand GNP 7 801





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.

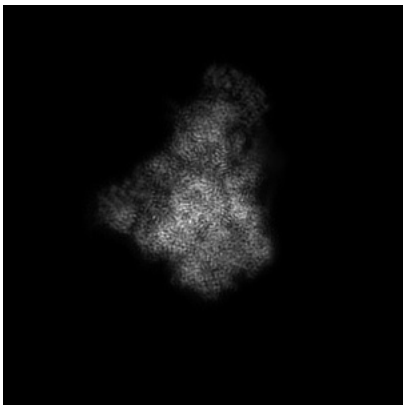
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10022. These allow visual inspection of the internal detail of the map and identification of artifacts.

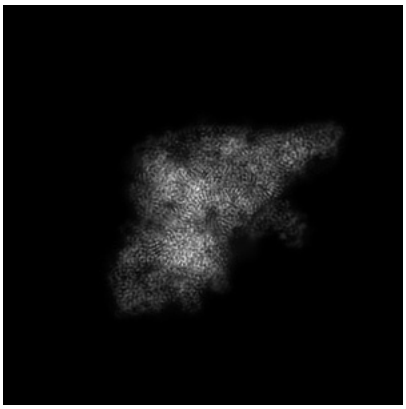
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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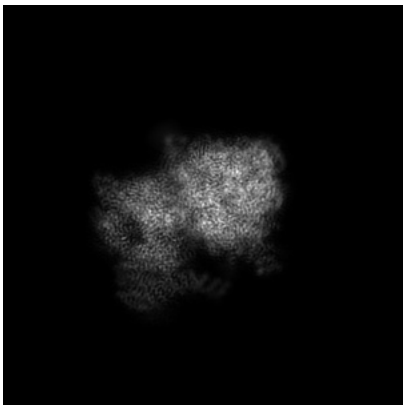
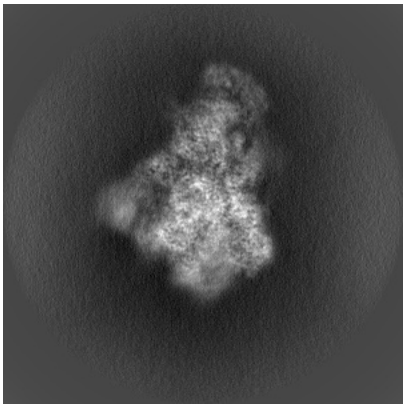
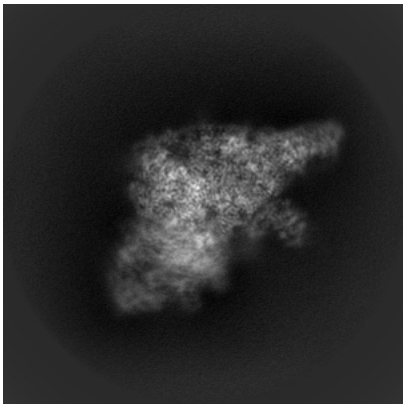


Z

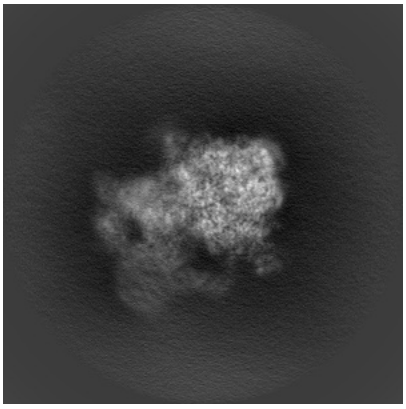
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

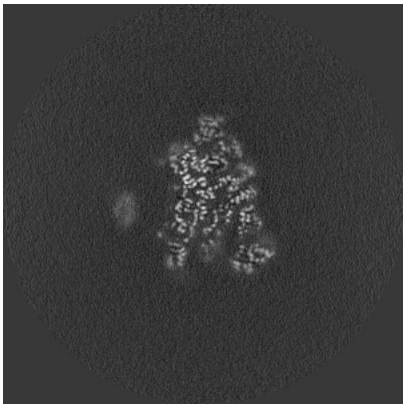
6.2.1 Primary map

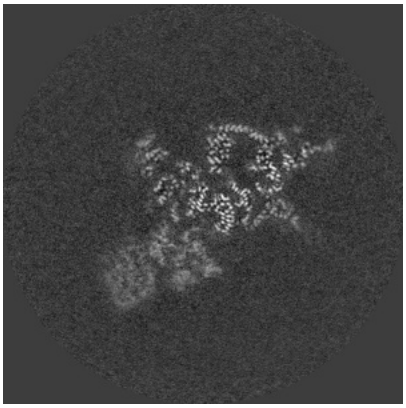
X Index: 240

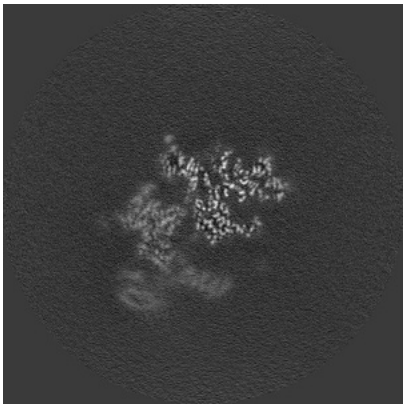
Y Index: 240

Z Index: 240

6.2.2 Raw map


X Index: 240


Y Index: 240


Z Index: 240

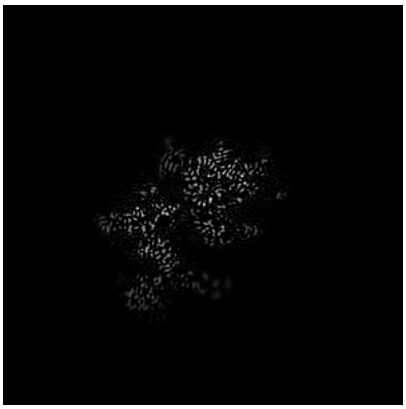
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

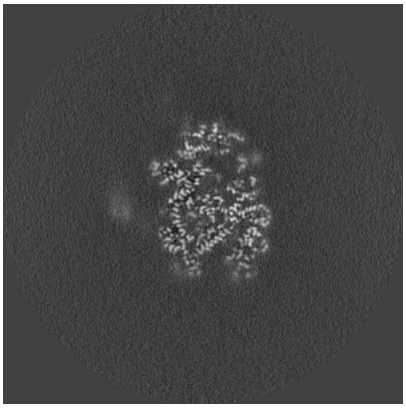
X Index: 259

Y Index: 239

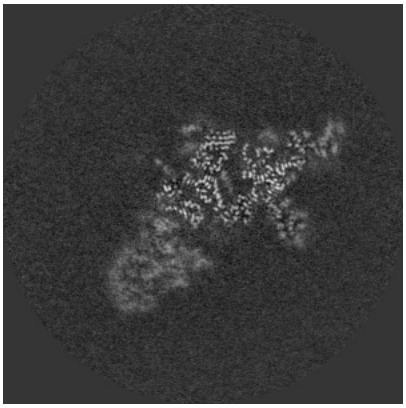


Z Index: 234

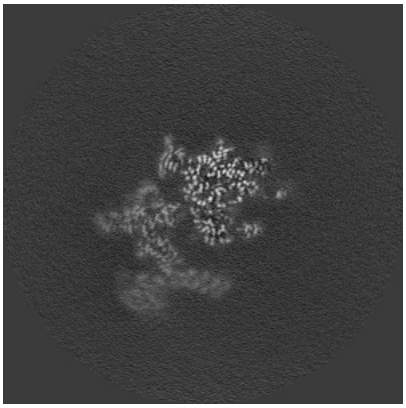
6.3.2 Raw map



X Index: 259



Y Index: 255

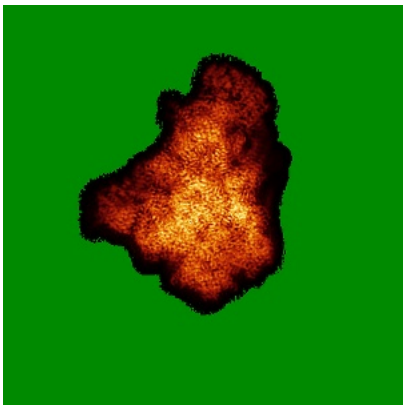


Z Index: 234

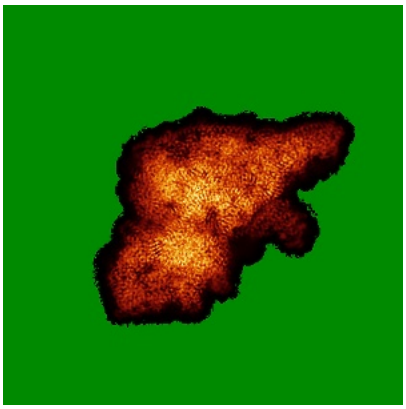
The images above show the largest variance slices of the map in three orthogonal directions.

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

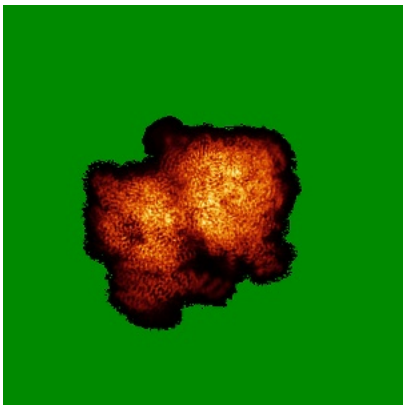
6.4.1 Primary map



X

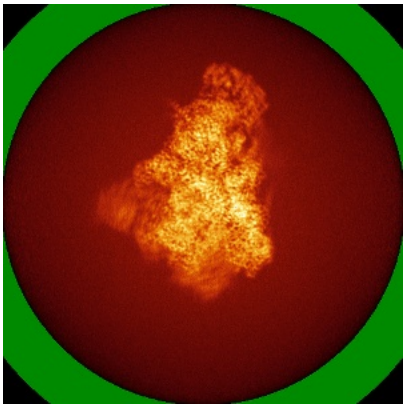


Y

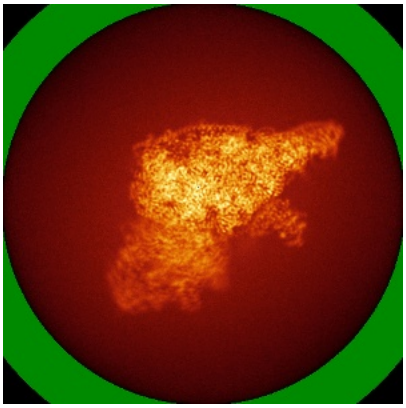


Z

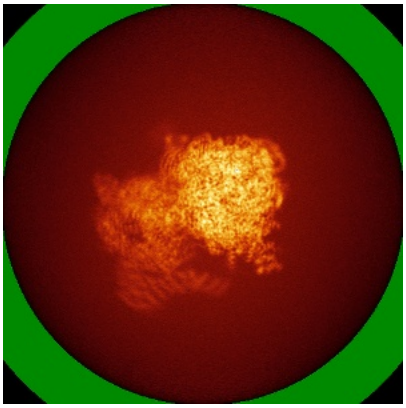
6.4.2 Raw map



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.

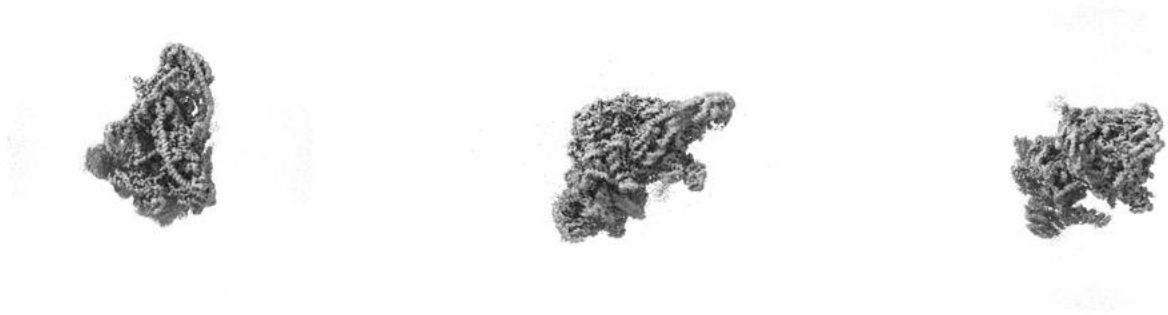
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

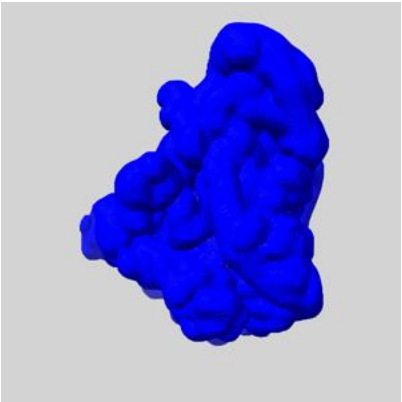
6.6 Mask visualisation (i)

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

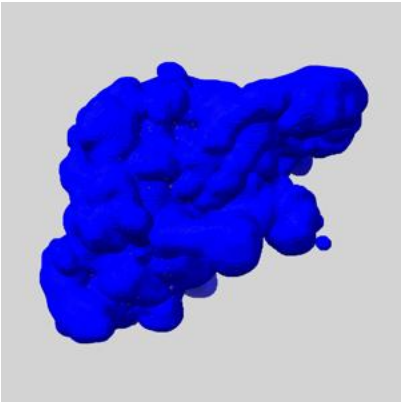
A mask typically either:

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

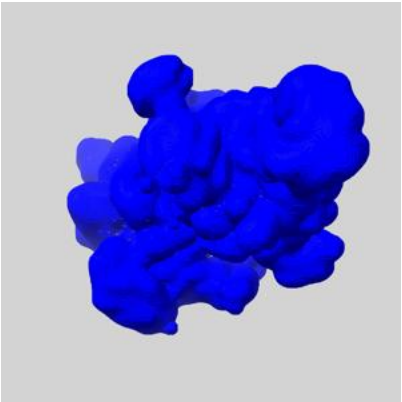
6.6.1 emd_10022_msk_1.map (i)



X



Y

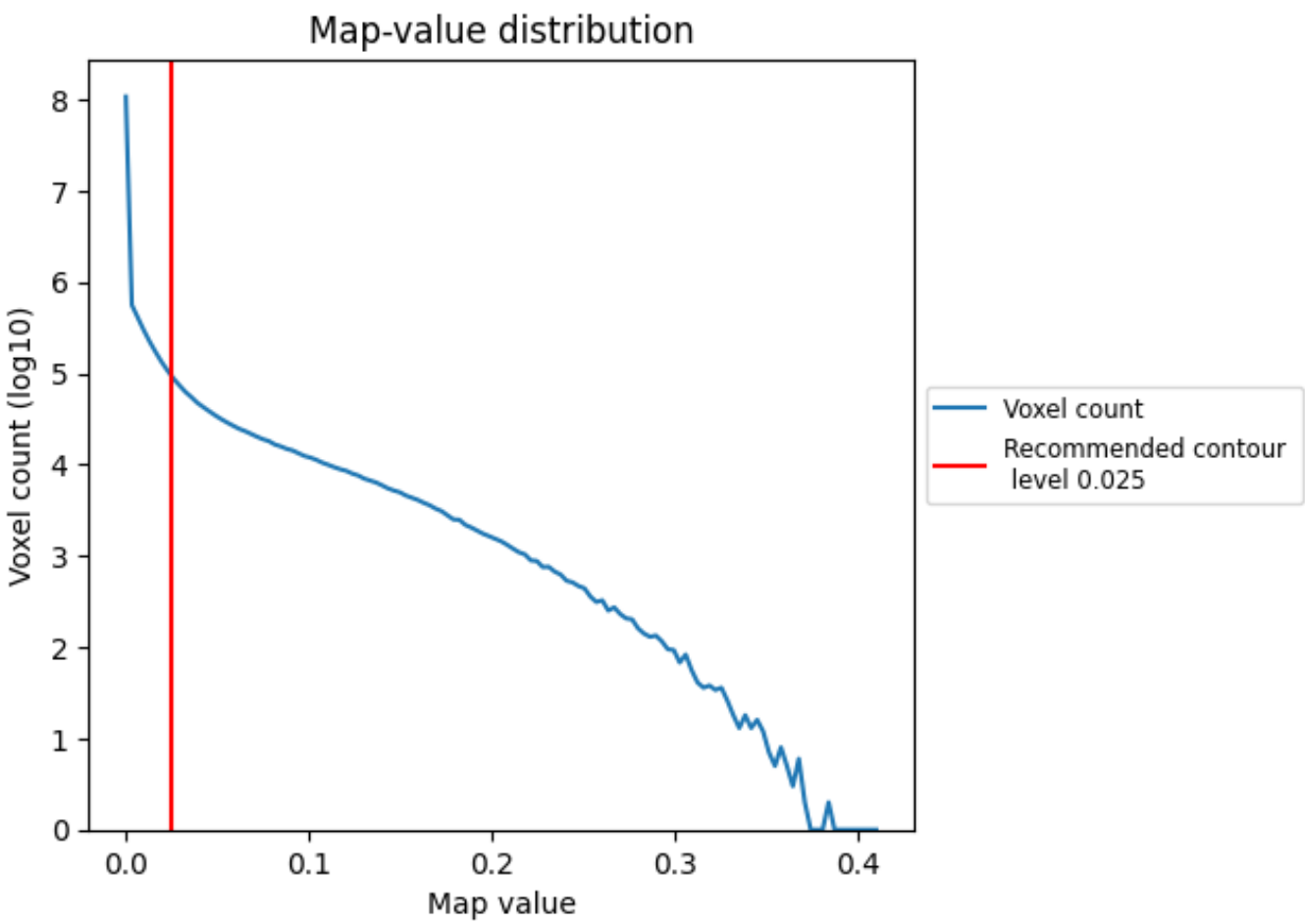


Z

7 Map analysis (i)

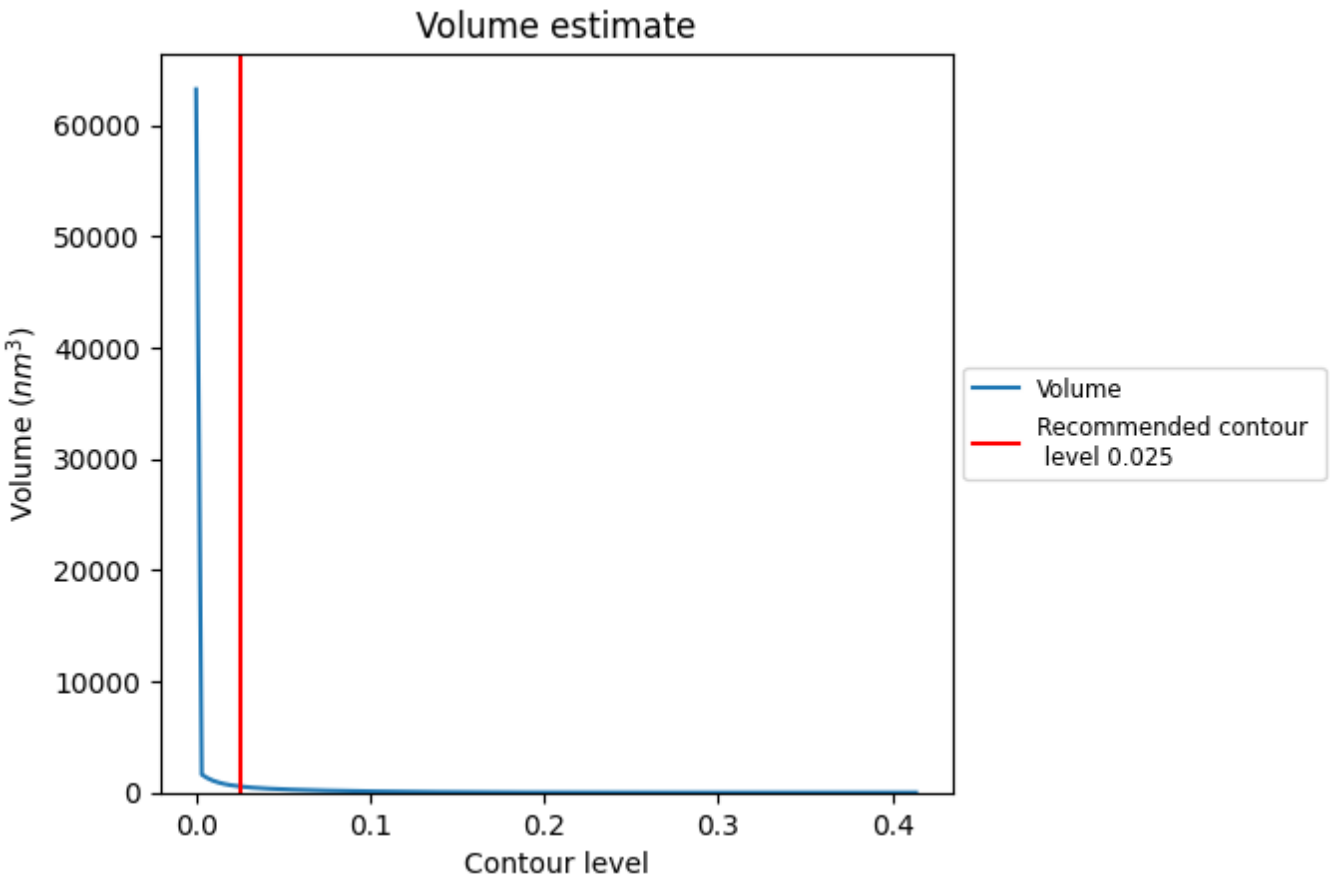
This section contains the results of statistical analysis of the map.

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.

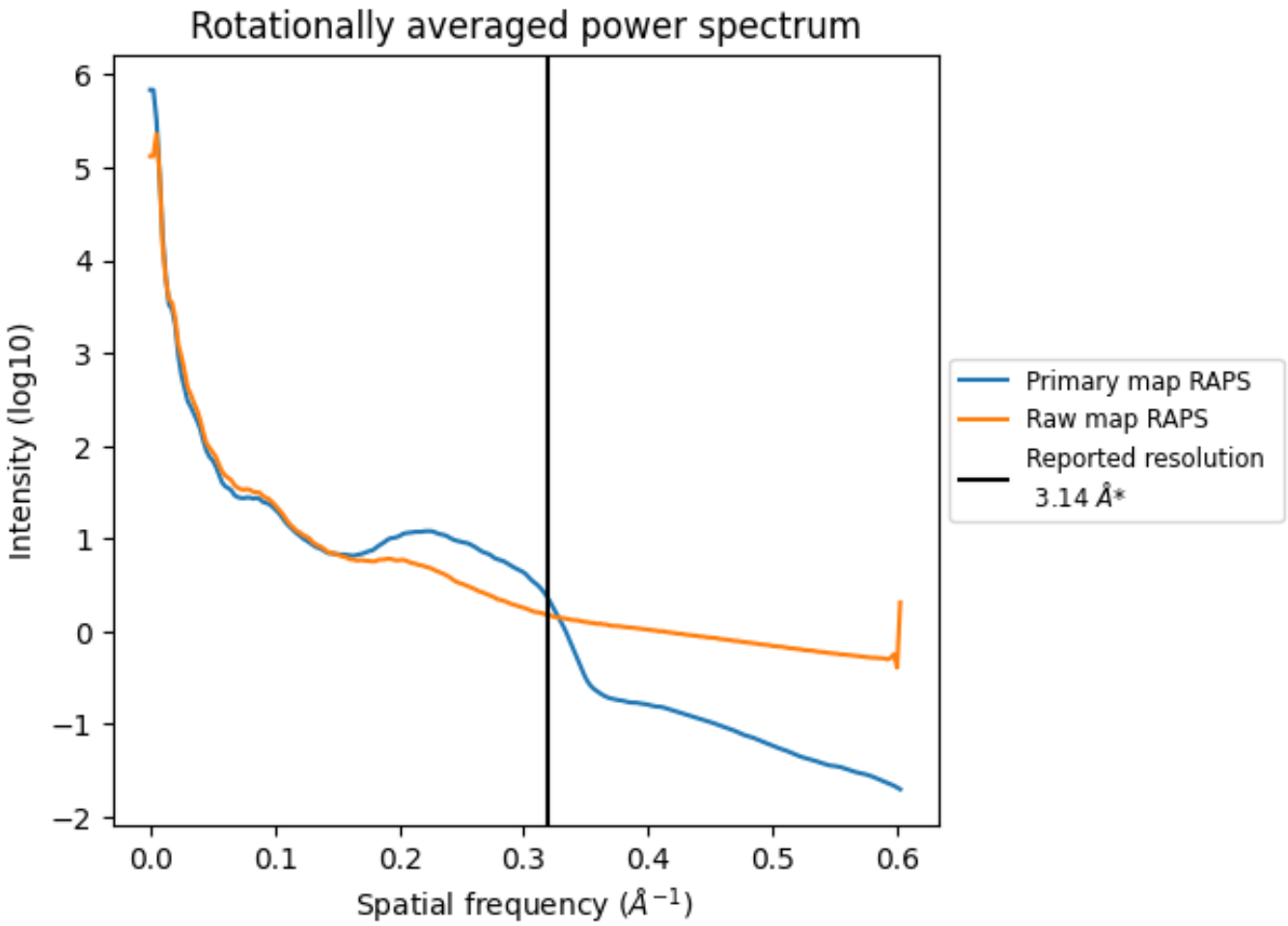
7.2 Volume estimate (i)



The volume at the recommended contour level is 554 nm^3; this corresponds to an approximate mass of 500 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)

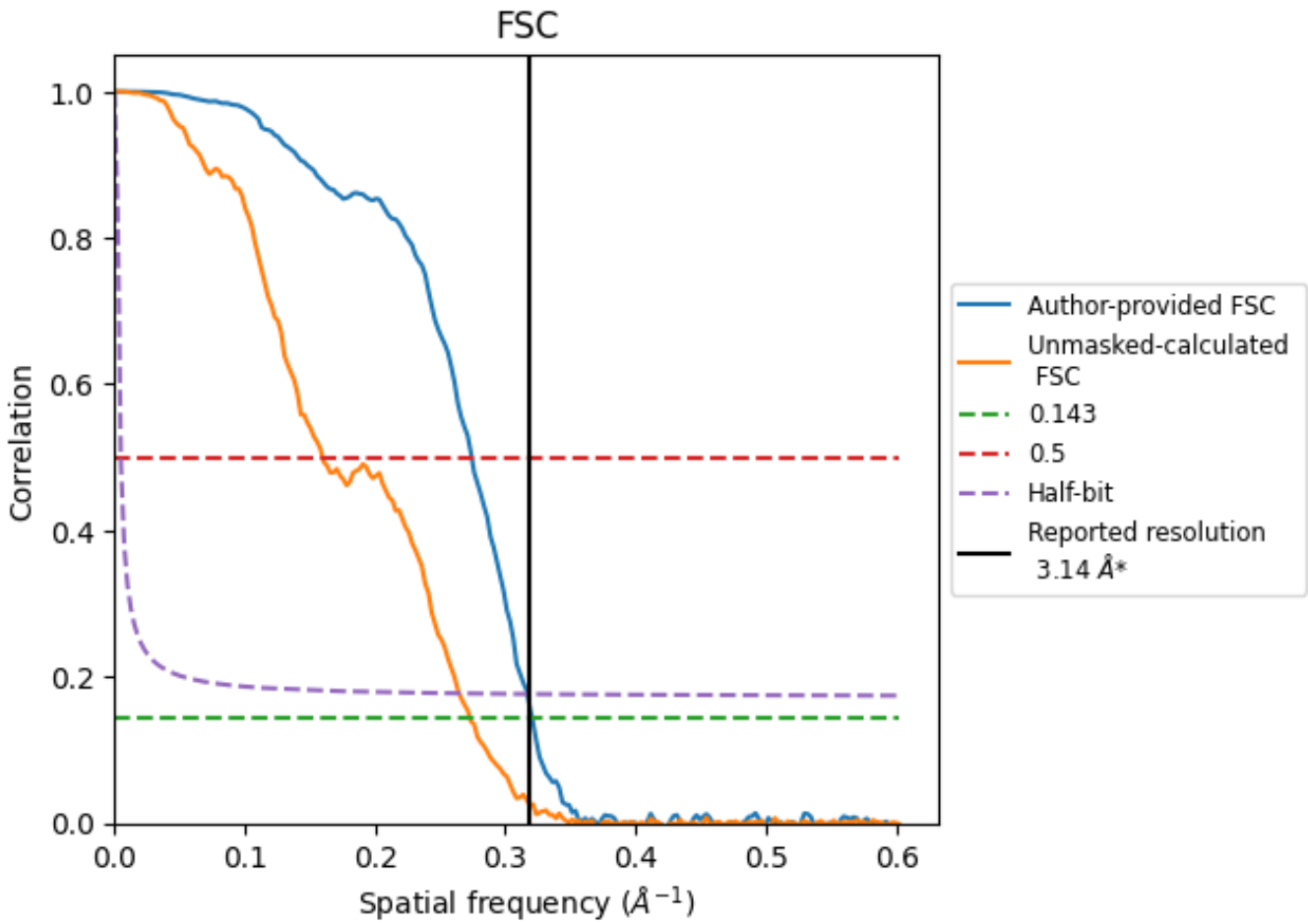


*Reported resolution corresponds to spatial frequency of 0.318 Å^{-1}

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 0.318 Å^{-1}

8.2 Resolution estimates (i)

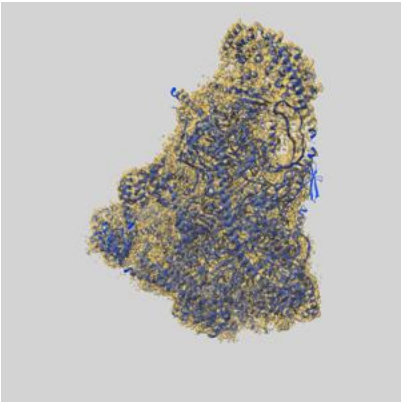
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.12	3.65	3.16
Unmasked-calculated*	3.66	6.26	3.78

*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 3.66 differs from the reported value 3.14 by more than 10 %

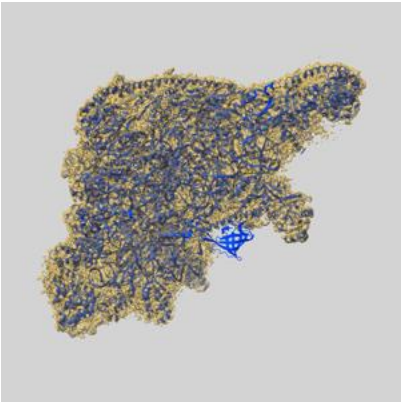
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10022 and PDB model 6RW5. Per-residue inclusion information can be found in section 3 on page 16.

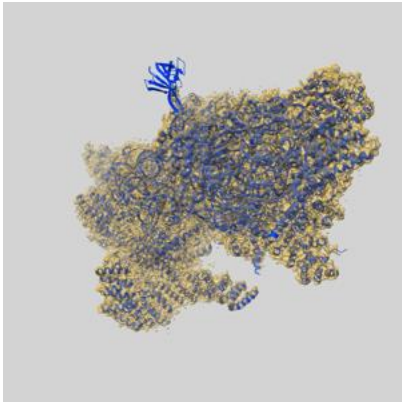
9.1 Map-model overlay (i)



X



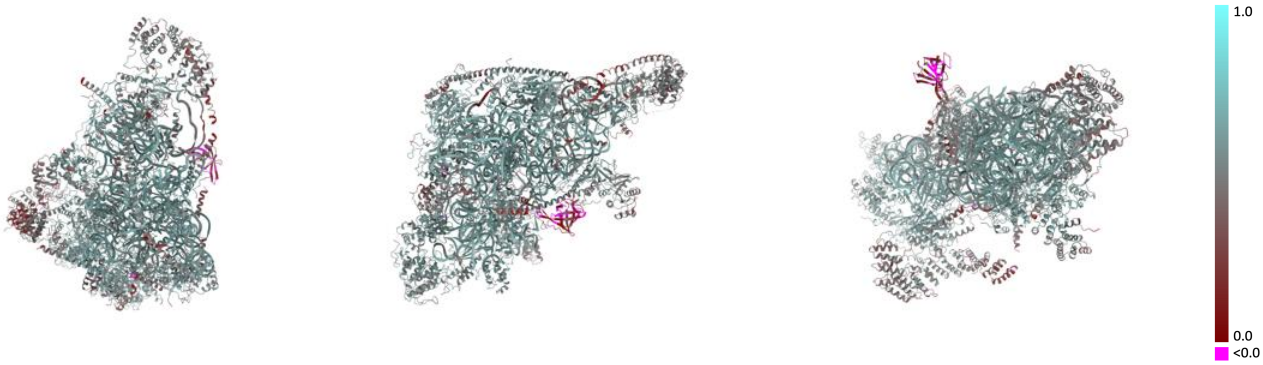
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

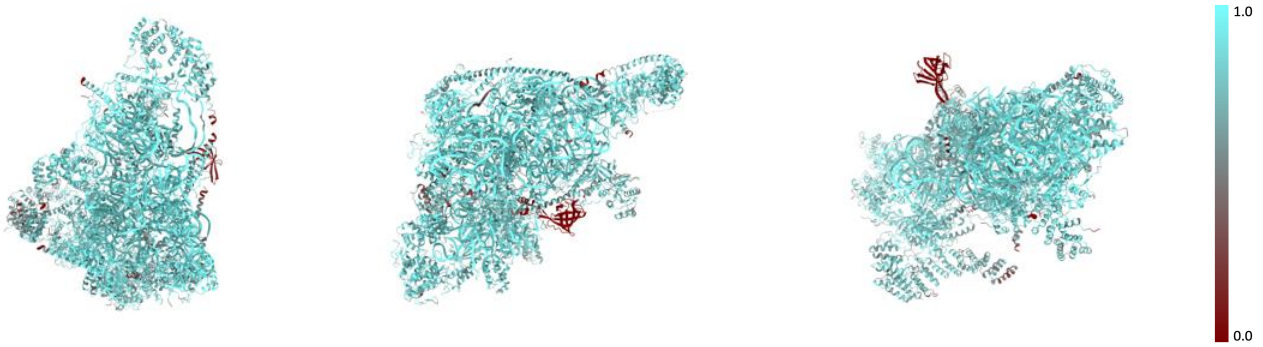
9.2 Q-score mapped to coordinate model (i)



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.

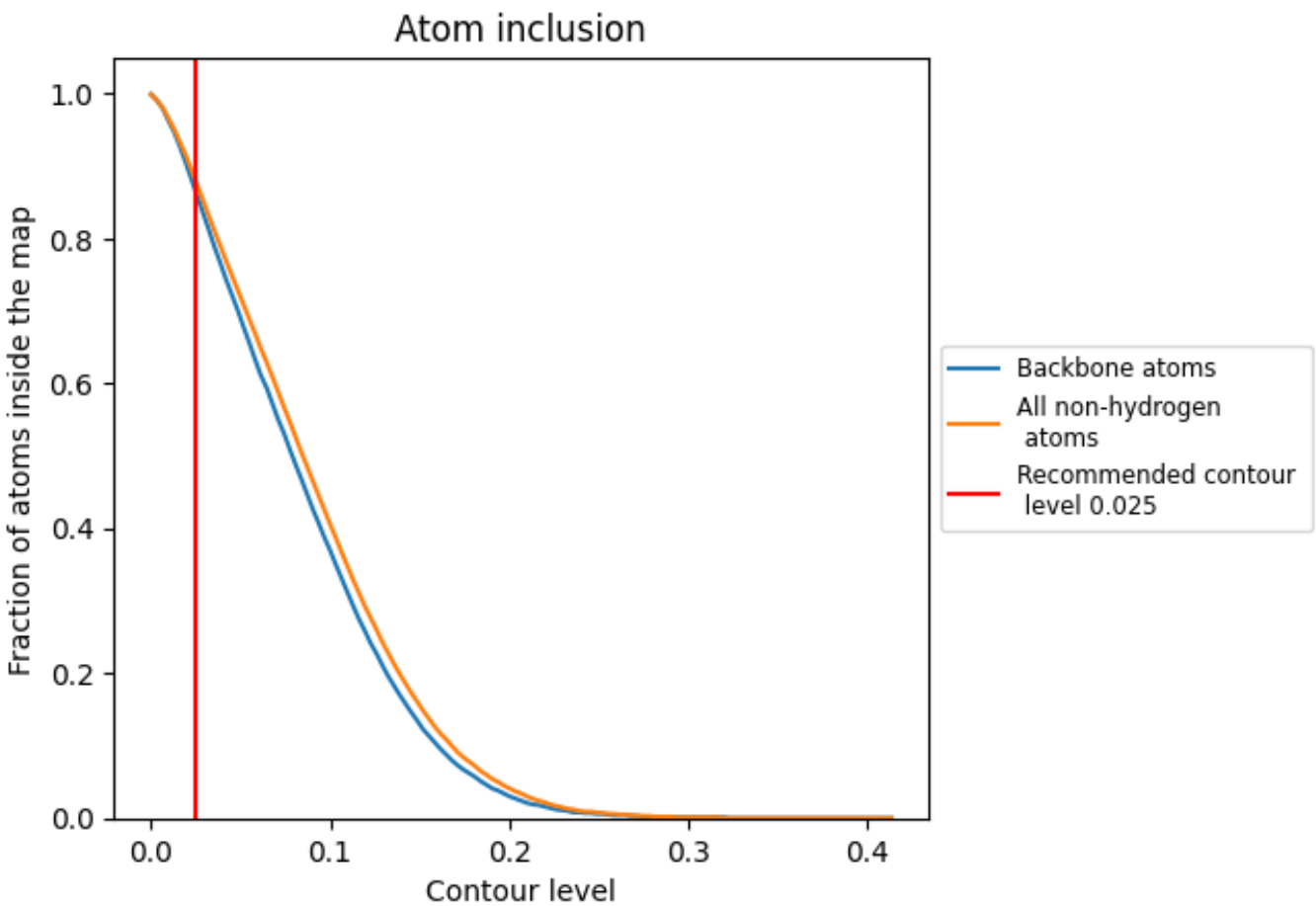
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 88% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8800	0.5510
0	0.8820	0.5300
1	0.8710	0.5550
2	0.7890	0.4890
3	0.9140	0.5940
4	0.7570	0.4400
7	0.5990	0.4150
8	0.6180	0.4170
A	0.9780	0.6120
B	0.9100	0.5900
C	0.9500	0.6290
D	0.8990	0.5660
E	0.8930	0.5670
F	0.8640	0.5430
G	0.8380	0.5310
H	0.9110	0.5880
I	0.9040	0.5680
J	0.9340	0.5970
K	0.9410	0.6320
L	0.8460	0.5400
M	0.9090	0.5940
N	0.9330	0.6090
O	0.9120	0.5840
P	0.9170	0.5870
Q	0.9270	0.5970
R	0.8480	0.5370
S	0.8450	0.5280
T	0.9060	0.5770
U	0.8290	0.5150
V	0.8070	0.4600
W	0.8960	0.5740
X	0.8840	0.5570
Y	0.7780	0.5030
Z	0.8960	0.5860