



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:17 AM UTC

PDB ID : 6RW4 / pdb_00006rw4
EMDB ID : EMD-10021
Title : Structure of human mitochondrial 28S ribosome in complex with mitochondrial IF3
Authors : Itoh, Y.; Khawaja, A.; Rorbach, J.; Amunts, A.
Deposited on : 2019-06-03
Resolution : 2.97 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

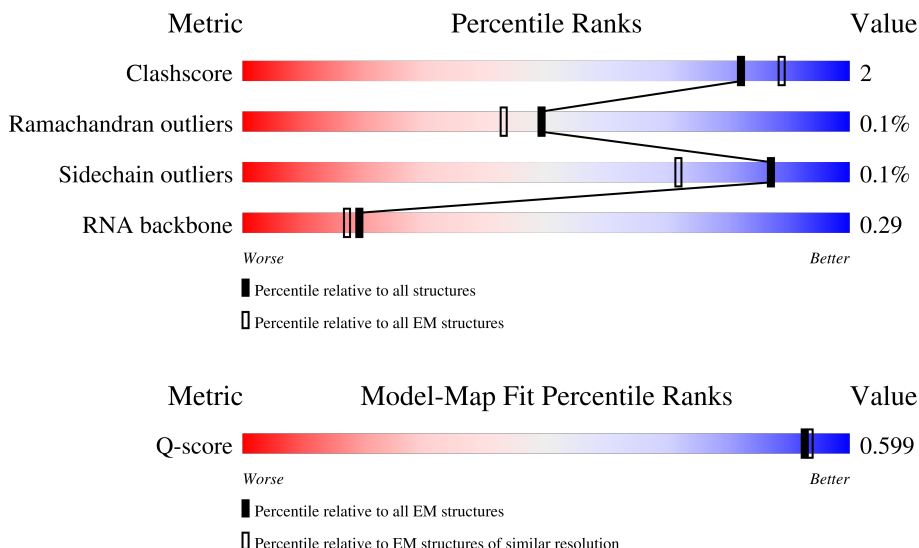
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.97 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.



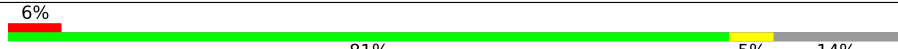
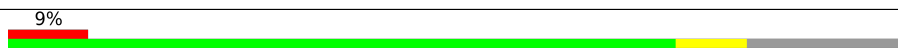
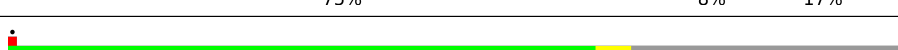
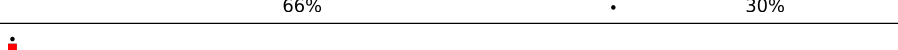
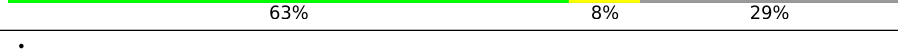
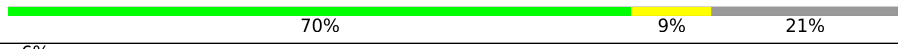
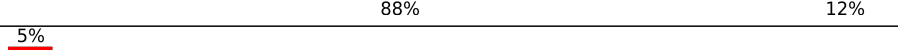
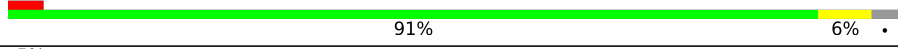
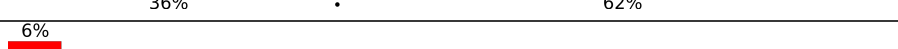
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13205 (2.47 - 3.47)

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 $\leq 5\%$. 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	
2	B	296	
3	C	167	

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Mol	Chain	Length	Quality of chain
4	D	430	
5	E	125	
6	F	242	
7	G	396	
8	H	201	
9	I	194	
10	J	138	
11	K	128	
12	L	257	
13	M	137	
14	N	130	
15	O	258	
16	P	142	
17	Q	86	
18	R	360	
19	S	190	
20	T	173	
21	U	205	
22	V	414	
23	W	187	
24	X	398	
25	Y	395	
26	Z	106	
27	0	218	
28	1	323	

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Mol	Chain	Length	Quality of chain
29	2	117	28% 93% 7%
30	3	199	32% 65%
31	4	689	13% 78% 7% 15%
32	8	285	16% 61% 6% 33%

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 128280 atoms, of which 59411 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
1	A	955	Total	C	H	N	O	P	0	0
			30595	9098	10313	3652	6577	955		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	122	Total	C	H	N	O	S	0	0
			1972	614	1000	177	177	4		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	330	Total	C	H	N	O	S	0	0
			5434	1726	2718	485	491	14		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	137	Total	C	H	N	O	S	0	0
			2079	641	1060	193	181	4		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	194	Total	C	H	N	O	S	0	0
			3165	1019	1566	295	278	7		

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

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

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

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

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
18	R	295	Total	C	H	N	O	S	0	0
			4838	1533	2429	413	455	8		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	168	Total	C	H	N	O	S	0	0
			2764	877	1393	239	244	11		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	276	Total	C	H	N	O	S	0	0
			4507	1419	2269	381	427	11		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	3	70	Total	C	H	N	O	S	0	0
			1325	401	700	134	89	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	588	Total	C	H	N	O	S	0	0
			9536	3053	4768	808	879	28		

- Molecule 32 is a protein called Translation initiation factor IF-3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	8	191	Total	C	H	N	O	S	0	0
			3131	953	1588	289	293	8		

There are 9 discrepancies between the modelled and reference sequences:

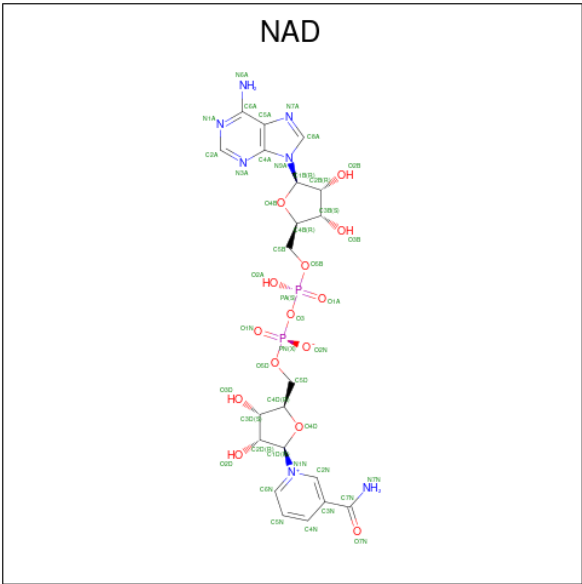
Chain	Residue	Modelled	Actual	Comment	Reference
8	68	ILE	THR	variant	UNP Q9H2K0
8	243	LEU	PHE	variant	UNP Q9H2K0
8	279	GLY	-	expression tag	UNP Q9H2K0
8	280	LEU	-	expression tag	UNP Q9H2K0
8	281	GLU	-	expression tag	UNP Q9H2K0

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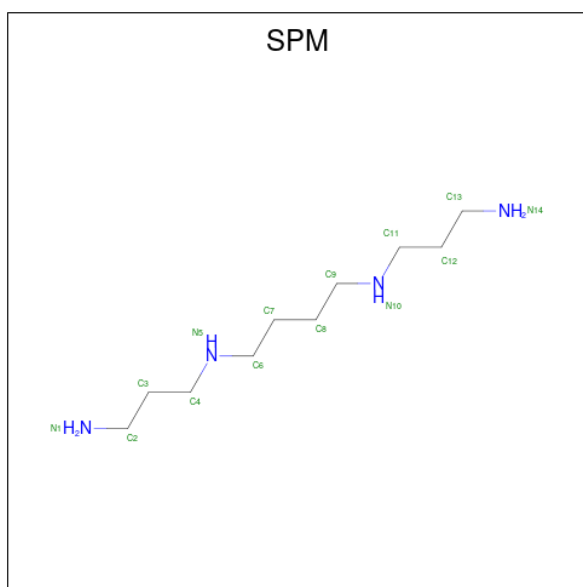
Chain	Residue	Modelled	Actual	Comment	Reference
8	282	VAL	-	expression tag	UNP Q9H2K0
8	283	LEU	-	expression tag	UNP Q9H2K0
8	284	PHE	-	expression tag	UNP Q9H2K0
8	285	GLN	-	expression tag	UNP Q9H2K0

- Molecule 33 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



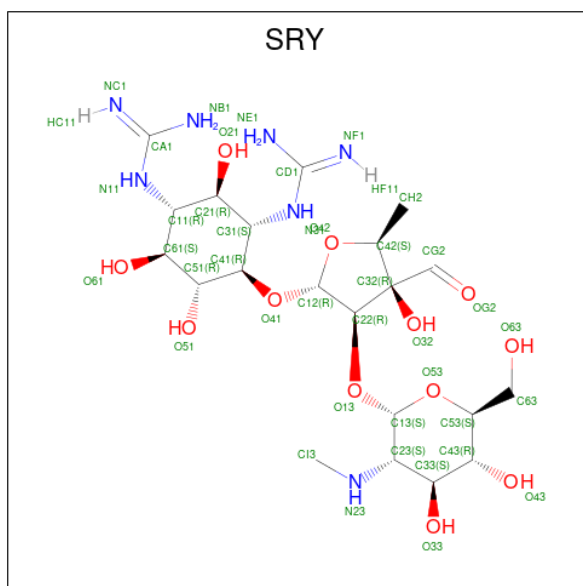
Mol	Chain	Residues	Atoms						AltConf
33	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 34 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	H	N	0
			40	10	26	4	

- Molecule 35 is STREPTOMYCIN (CCD ID: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



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

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

Mol	Chain	Residues	Atoms		AltConf
36	A	57	Total	Mg	0
			57	57	
36	B	1	Total	Mg	0
			1	1	
36	X	1	Total	Mg	0
			1	1	
36	3	1	Total	Mg	0
			1	1	

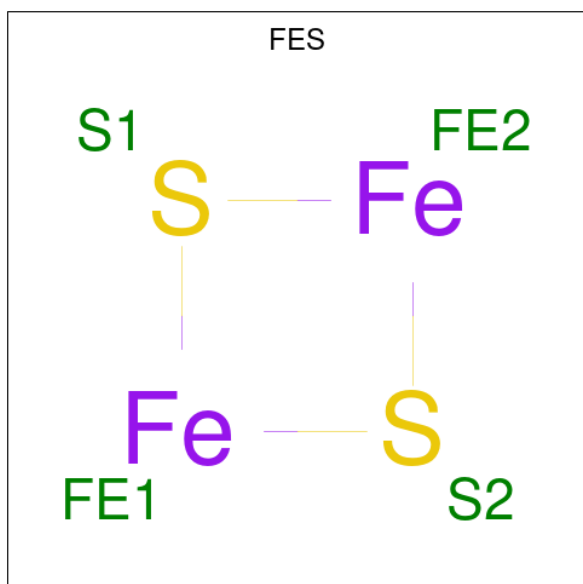
- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



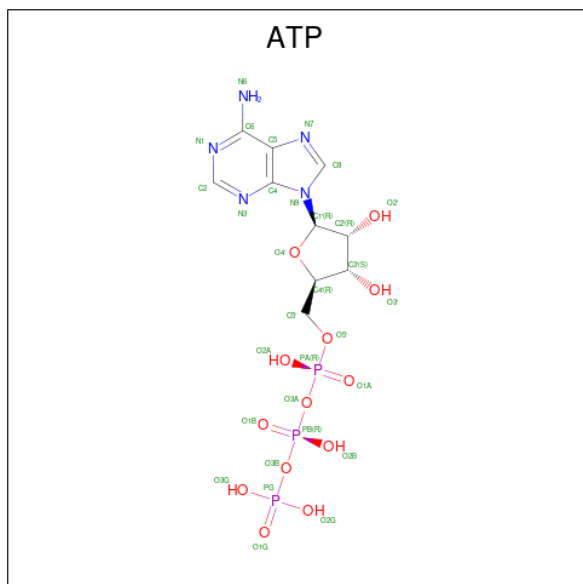
Mol	Chain	Residues	Atoms			AltConf
39	P	1	Total	Fe	S	0
			4	2	2	

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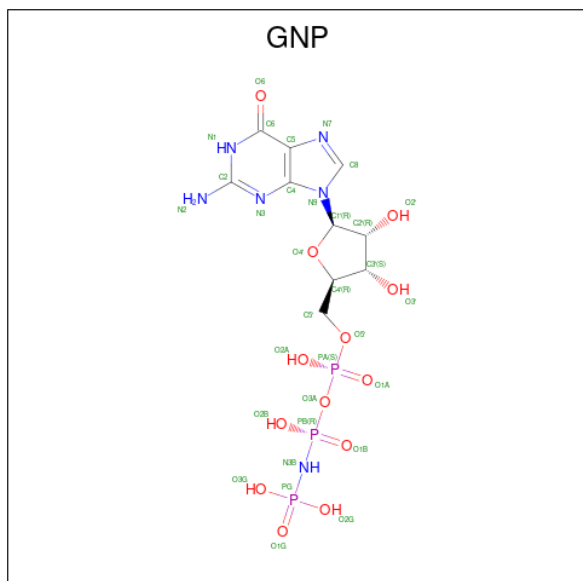
Mol	Chain	Residues	Atoms			AltConf
39	T	1	Total	Fe	S	0
			4	2	2	

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



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

- Molecule 41 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

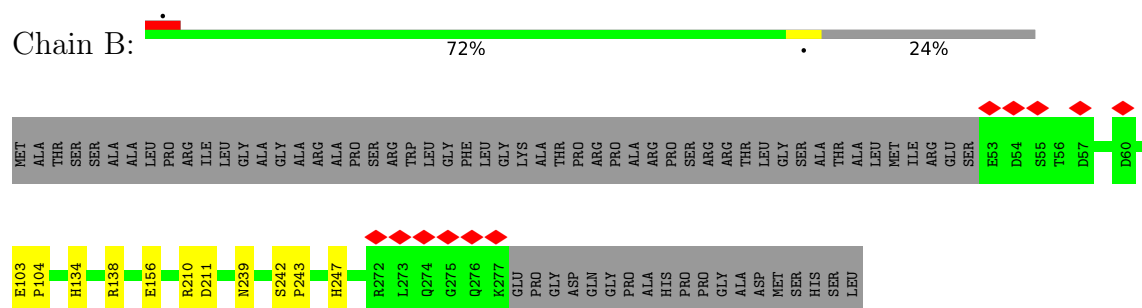


Mol	Chain	Residues	Atoms						AltConf
41	X	1	Total	C	H	N	O	P	0
			45	10	13	6	13	3	

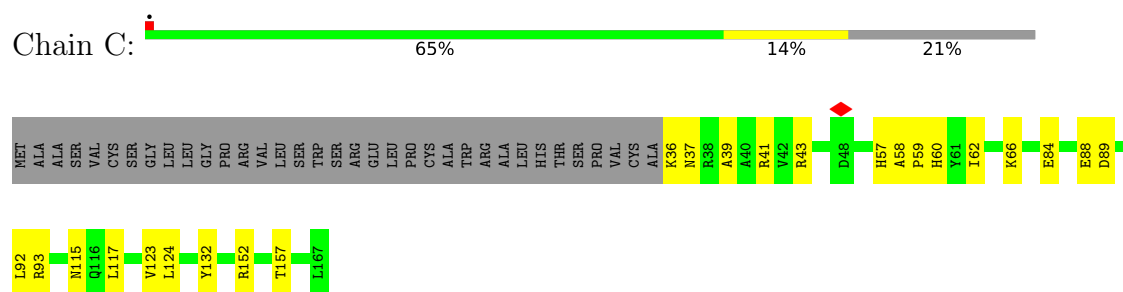
- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	49	Total	O	0
			49	49	
42	C	2	Total	O	0
			2	2	
42	G	1	Total	O	0
			1	1	
42	I	1	Total	O	0
			1	1	
42	T	1	Total	O	0
			1	1	
42	X	3	Total	O	0
			3	3	
42	0	1	Total	O	0
			1	1	
42	2	1	Total	O	0
			1	1	

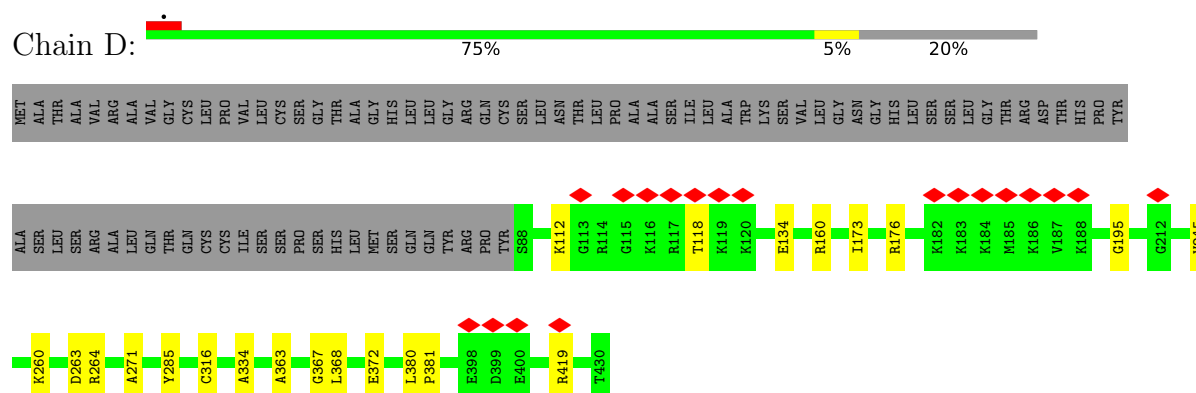
- Molecule 2: 28S ribosomal protein S2, mitochondrial



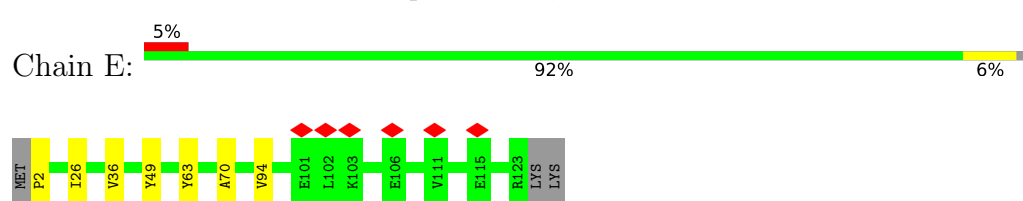
- Molecule 3: 28S ribosomal protein S24, mitochondrial



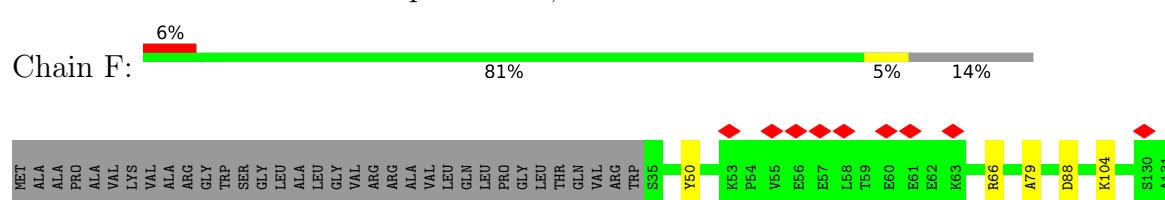
- Molecule 4: 28S ribosomal protein S5, mitochondrial

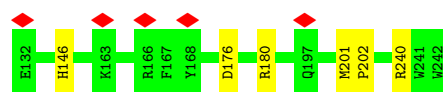


- Molecule 5: 28S ribosomal protein S6, mitochondrial

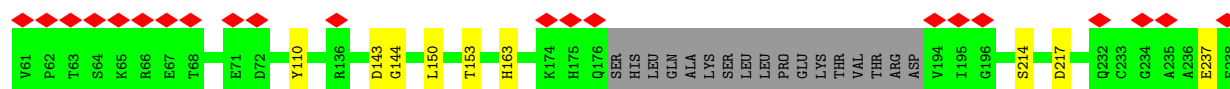
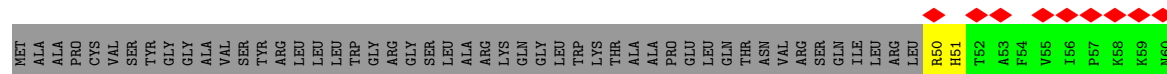
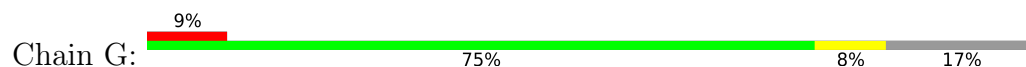


- Molecule 6: 28S ribosomal protein S7, mitochondrial

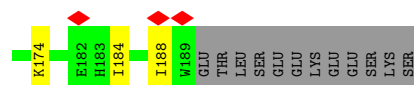
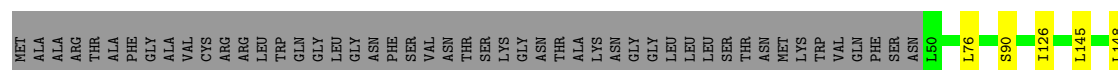




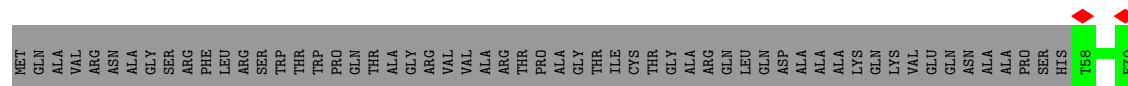
- Molecule 7: 28S ribosomal protein S9, mitochondrial



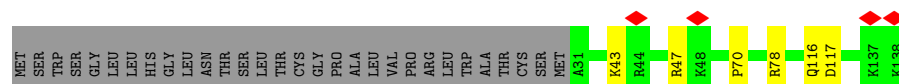
- Molecule 8: 28S ribosomal protein S10, mitochondrial



- Molecule 9: 28S ribosomal protein S11, mitochondrial

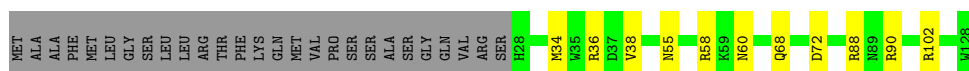


- Molecule 10: 28S ribosomal protein S12, mitochondrial

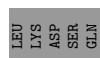
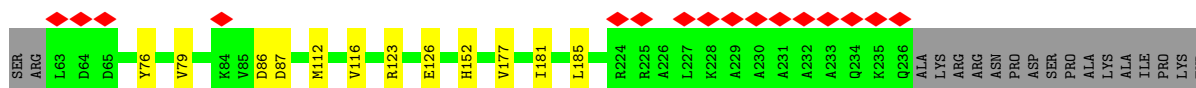


- Molecule 11: 28S ribosomal protein S14, mitochondrial

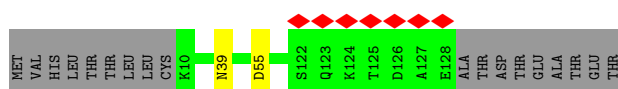
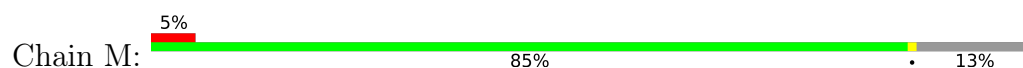




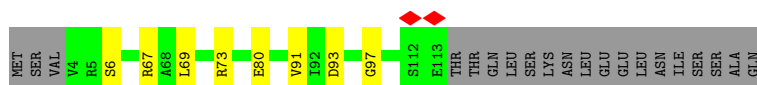
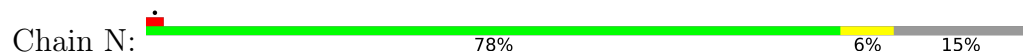
- Molecule 12: 28S ribosomal protein S15, mitochondrial



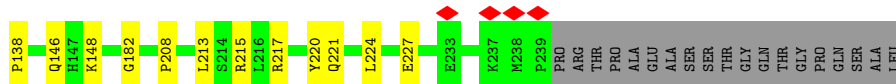
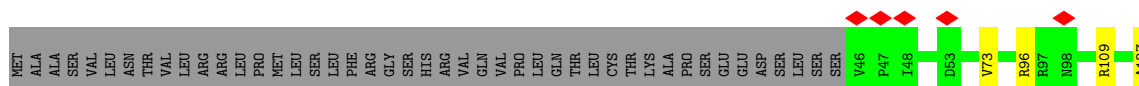
- Molecule 13: 28S ribosomal protein S16, mitochondrial



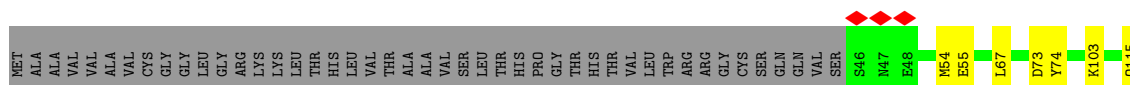
- Molecule 14: 28S ribosomal protein S17, mitochondrial

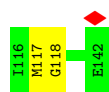


- Molecule 15: 28S ribosomal protein S18b, mitochondrial



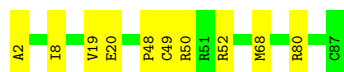
- Molecule 16: 28S ribosomal protein S18c, mitochondrial





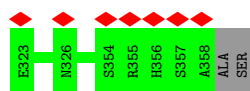
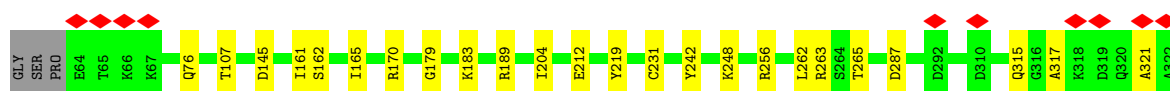
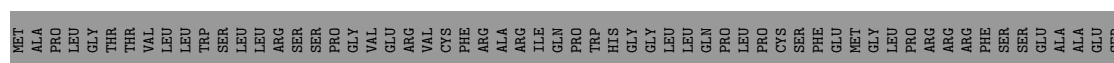
- Molecule 17: 28S ribosomal protein S21, mitochondrial

Chain Q: 88% 12%



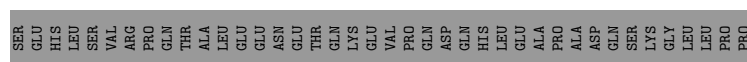
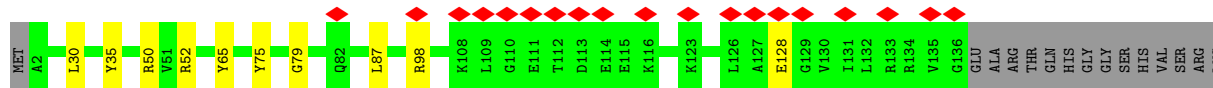
- Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R: 5% 75% 7% 18%



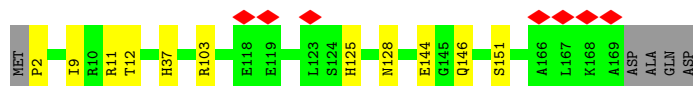
- Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S: 10% 66% 5% 29%



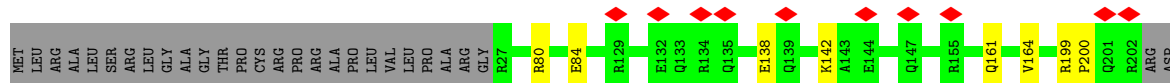
- Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T: 91% 6%



- Molecule 21: 28S ribosomal protein S26, mitochondrial

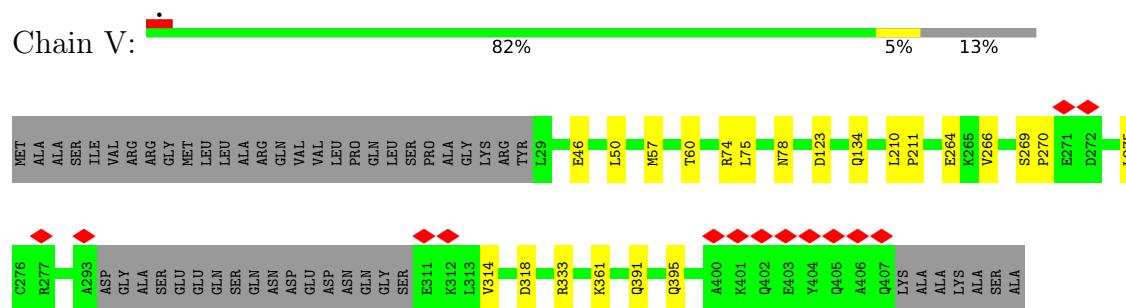
Chain U: 5% 82% 14%



SER

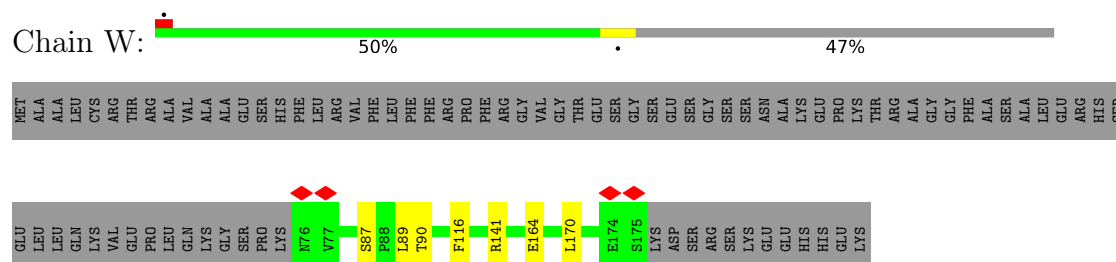
- Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V:



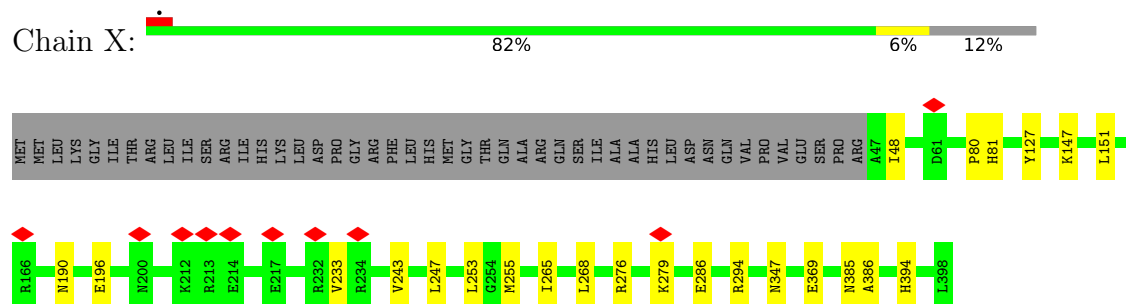
- Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain W:



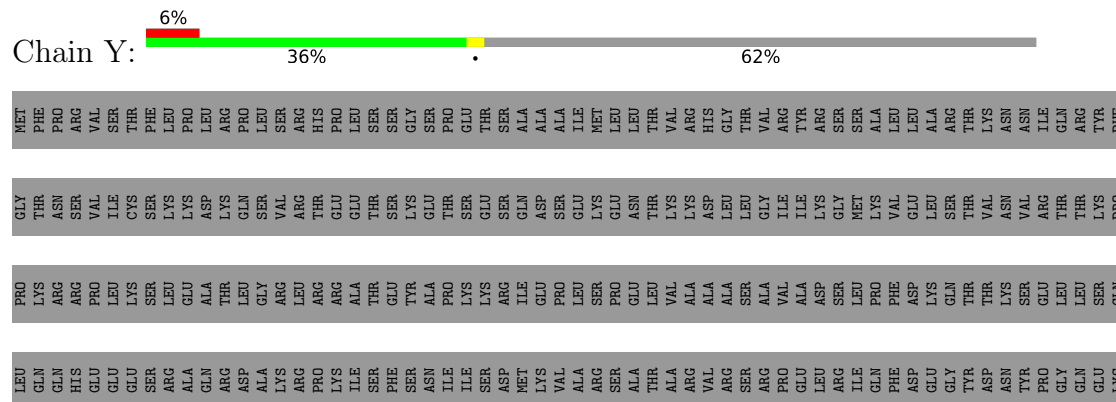
- Molecule 24: 28S ribosomal protein S29, mitochondrial

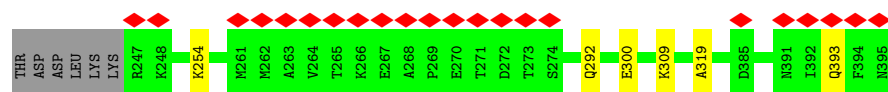
Chain X:



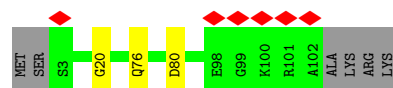
- Molecule 25: 28S ribosomal protein S31, mitochondrial

Chain Y:

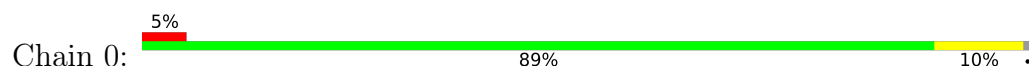




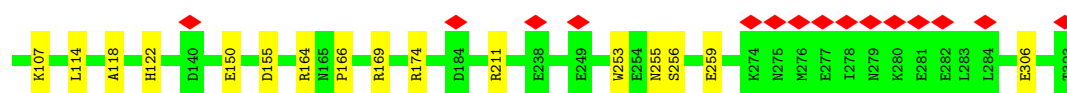
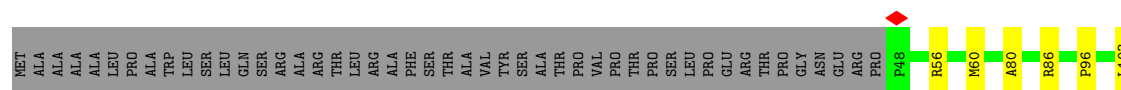
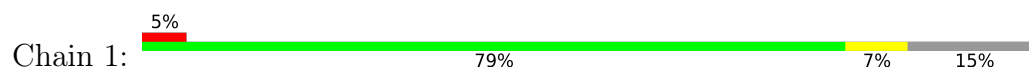
- Molecule 26: 28S ribosomal protein S33, mitochondrial



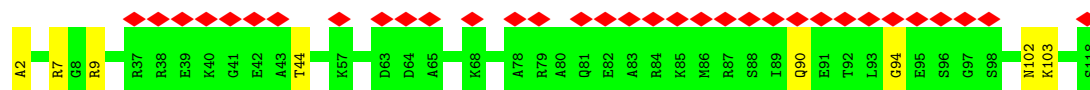
- Molecule 27: 28S ribosomal protein S34, mitochondrial



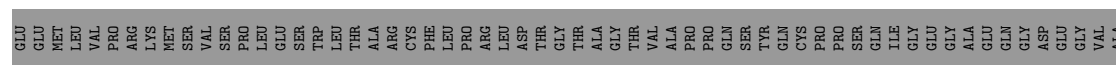
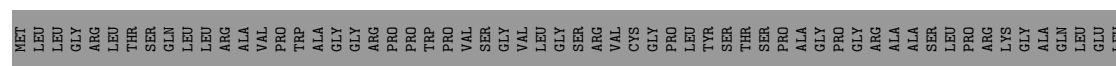
- Molecule 28: 28S ribosomal protein S35, mitochondrial



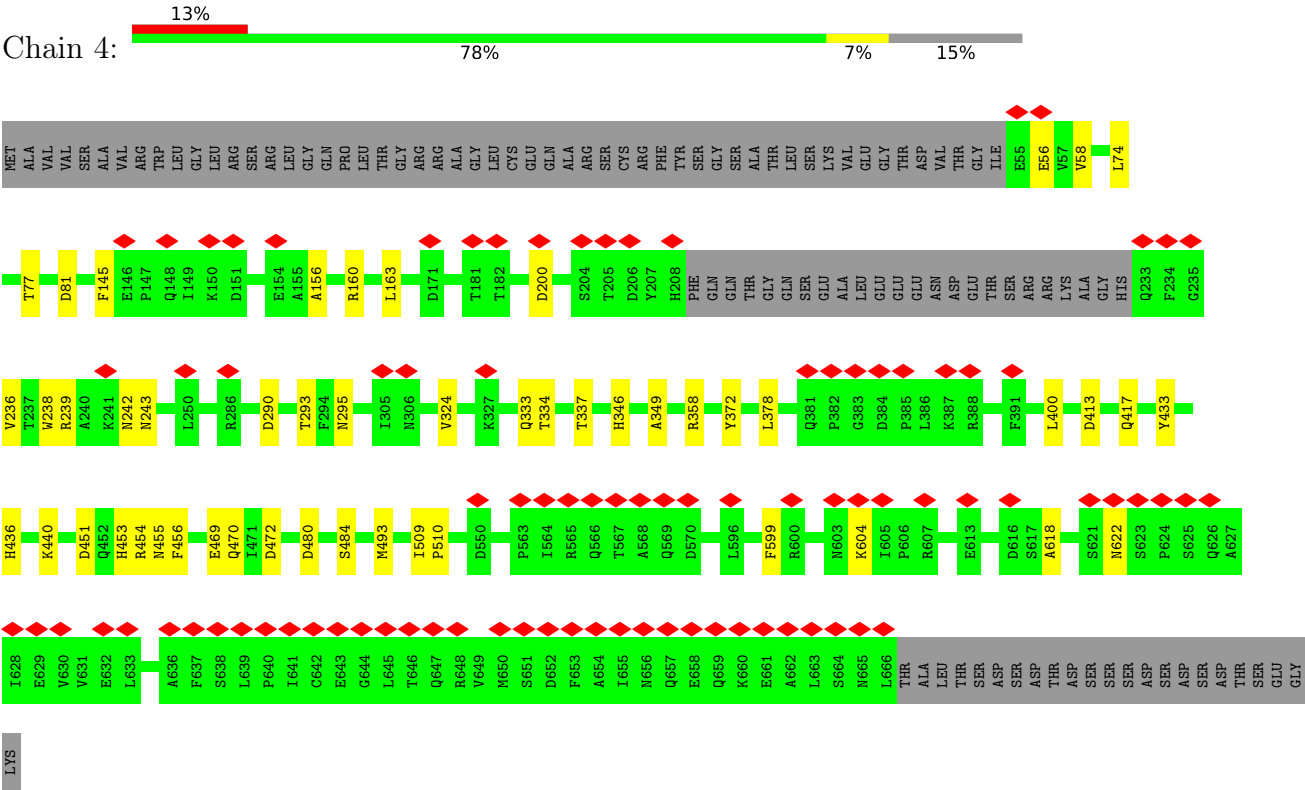
- Molecule 29: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1



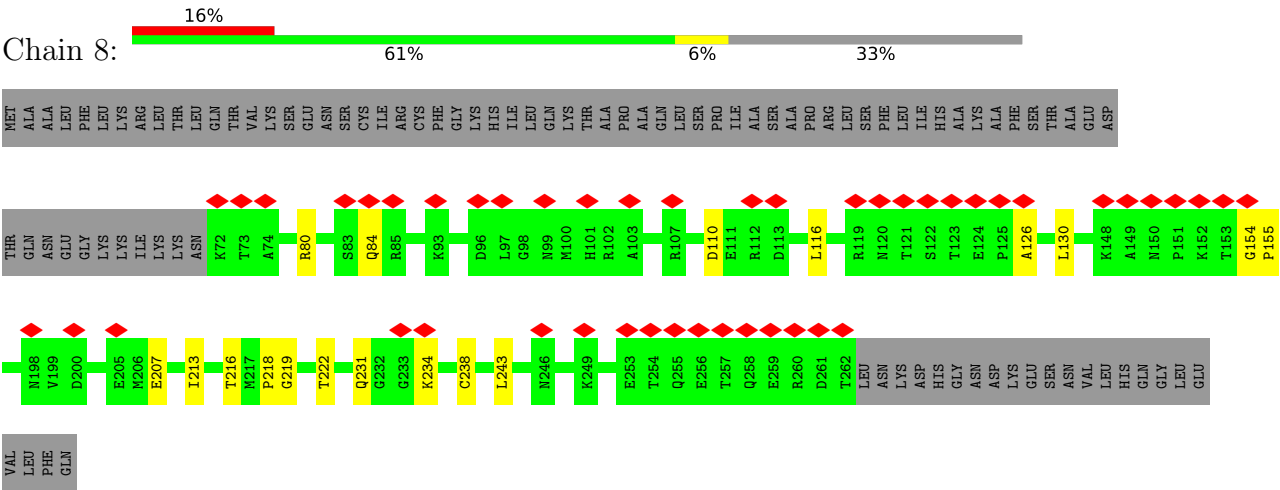
- Molecule 30: Aurora kinase A-interacting protein



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



• Molecule 32: Translation initiation factor IF-3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	379761	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 ($e^-/\text{\AA}^2$)	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	0.562	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, GNP, ZN, NAD, SRY, MA6, SPM, B8T, MG, 5MC, K, 5MU, ATP, FES

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	0.29	0/22562	0.33	0/35124
2	B	0.31	0/1871	0.37	0/2531
3	C	0.36	0/1113	0.40	0/1505
4	D	0.29	0/2783	0.36	0/3724
5	E	0.26	0/989	0.36	0/1335
6	F	0.25	0/1767	0.35	0/2373
7	G	0.27	0/2775	0.36	0/3720
8	H	0.33	0/1178	0.37	0/1598
9	I	0.35	0/1039	0.39	0/1400
10	J	0.32	0/855	0.37	0/1148
11	K	0.37	0/880	0.41	0/1182
12	L	0.29	0/1477	0.36	0/1974
13	M	0.34	0/963	0.42	0/1295
14	N	0.32	0/886	0.34	0/1199
15	O	0.31	0/1655	0.37	0/2254
16	P	0.32	0/798	0.35	0/1070
17	Q	0.34	0/748	0.46	1/994 (0.1%)
18	R	0.26	0/2456	0.33	0/3317
19	S	0.24	0/1138	0.33	0/1533
20	T	0.31	0/1402	0.39	0/1883
21	U	0.26	0/1510	0.38	0/2025
22	V	0.24	0/3030	0.34	0/4093
23	W	0.26	0/801	0.33	0/1079
24	X	0.25	0/2921	0.34	0/3954
25	Y	0.27	0/1280	0.33	0/1725
26	Z	0.29	0/857	0.34	0/1141
27	0	0.30	0/1834	0.40	0/2484
28	1	0.28	0/2285	0.35	0/3090
29	2	0.23	0/941	0.37	0/1257
30	3	0.32	0/636	0.46	0/839
31	4	0.25	0/4877	0.37	0/6598
32	8	0.21	0/1560	0.38	0/2089

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.29	0/71867	0.35	1/101533 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	8	ILE	N-CA-C	-5.04	107.64	111.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	183	HIS	Peptide

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	75	0
2	B	1828	1816	1815	8	0
3	C	1083	1089	1088	14	0
4	D	2731	2805	2804	14	0
5	E	972	1000	1000	5	0
6	F	1725	1770	1769	7	0
7	G	2716	2718	2714	26	0
8	H	1152	1184	1183	6	0
9	I	1019	1060	1059	9	0
10	J	839	888	887	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	862	886	885	8	0
12	L	1453	1541	1540	7	0
13	M	942	966	965	2	0
14	N	868	929	928	4	0
15	O	1599	1566	1565	12	0
16	P	781	807	806	7	0
17	Q	744	758	758	7	0
18	R	2409	2429	2428	16	0
19	S	1111	1116	1115	9	0
20	T	1371	1393	1393	10	0
21	U	1488	1500	1499	5	0
22	V	2969	2964	2961	14	0
23	W	789	803	802	5	0
24	X	2849	2845	2843	18	0
25	Y	1246	1198	1197	6	0
26	Z	839	860	858	2	0
27	0	1787	1797	1796	15	0
28	1	2238	2269	2269	14	0
29	2	935	969	969	5	0
30	3	625	700	699	5	0
31	4	4768	4768	4766	30	0
32	8	1543	1588	1587	10	0
33	A	44	26	26	0	0
34	A	14	26	26	1	0
35	A	40	39	39	0	0
36	3	1	0	0	0	0
36	A	57	0	0	0	0
36	B	1	0	0	0	0
36	X	1	0	0	0	0
37	A	17	0	0	0	0
38	O	1	0	0	0	0
39	P	4	0	0	0	0
39	T	4	0	0	0	0
40	X	31	12	12	0	0
41	X	32	13	13	0	0
42	0	1	0	0	0	0
42	2	1	0	0	0	0
42	A	49	0	0	3	0
42	C	2	0	0	0	0
42	G	1	0	0	2	0
42	I	1	0	0	0	0
42	T	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	X	3	0	0	0	0
All	All	68869	59411	59361	306	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 (306) 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)
4:D:285:TYR:OH	4:D:372:GLU:OE2	1.92	0.86
1:A:1037:A:O2'	12:L:152:HIS:NE2	2.08	0.86
1:A:1021:U:OP2	29:2:9:ARG:NH2	2.09	0.86
3:C:37:ASN:O	3:C:43:ARG:NH2	2.14	0.81
31:4:470:GLN:NE2	31:4:472:ASP:OD2	2.16	0.78
1:A:1107:U:O4	30:3:128:LYS:NZ	2.16	0.77
7:G:276:ARG:NH1	42:G:2001:HOH:O	2.16	0.77
7:G:375:ARG:O	42:G:2001:HOH:O	2.03	0.76
7:G:214:SER:N	7:G:217:ASP:OD2	2.21	0.74
31:4:451:ASP:OD1	31:4:455:ASN:ND2	2.22	0.73
15:O:182:GLY:O	18:R:183:LYS:NZ	2.22	0.72
1:A:1433:A:OP2	42:A:1801:HOH:O	2.07	0.71
31:4:480:ASP:O	31:4:484:SER:OG	2.08	0.71
22:V:74:ARG:O	22:V:78:ASN:ND2	2.24	0.70
31:4:295:ASN:OD1	31:4:334:THR:OG1	2.02	0.70
17:Q:80:ARG:NH1	23:W:164:GLU:OE1	2.25	0.70
24:X:276:ARG:NH2	24:X:286:GLU:OE1	2.27	0.68
1:A:1583:MA6:H93	1:A:1584:MA6:H92	1.75	0.67
18:R:262:LEU:O	18:R:265:THR:OG1	2.11	0.67
1:A:1530:A:OP1	27:0:29:ARG:NH2	2.27	0.66
1:A:1511:C:OP1	27:0:7:ARG:NH1	2.28	0.66
6:F:50:TYR:O	6:F:66:ARG:NH2	2.28	0.66
1:A:1583:MA6:H93	1:A:1584:MA6:C9	2.26	0.66
1:A:1199:G:N1	1:A:1422:G:OP2	2.28	0.64
3:C:115:ASN:ND2	25:Y:309:LYS:O	2.30	0.64
31:4:156:ALA:O	31:4:160:ARG:NH1	2.31	0.64
15:O:73:VAL:O	15:O:109:ARG:NH2	2.31	0.64
1:A:906:C:O2	7:G:50:ARG:N	2.30	0.64
31:4:200:ASP:OD2	31:4:243:ASN:N	2.31	0.64
31:4:349:ALA:HB3	31:4:378:LEU:HD11	1.80	0.64
1:A:904:C:O2	4:D:118:THR:OG1	2.14	0.63
1:A:1028:G:OP2	42:A:1802:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:C:OP1	27:0:19:ARG:NH1	2.33	0.62
18:R:317:ALA:O	18:R:321:ALA:N	2.33	0.61
1:A:932:C:N3	20:T:11:ARG:NH1	2.48	0.61
12:L:86:ASP:OD1	12:L:87:ASP:N	2.33	0.61
1:A:1231:A:OP1	11:K:88:ARG:NH2	2.26	0.61
7:G:388:ARG:O	7:G:390:LYS:NZ	2.34	0.61
28:1:56:ARG:NH2	31:4:81:ASP:OD2	2.34	0.61
1:A:1532:C:O2'	1:A:1533:C:OP1	2.16	0.60
31:4:372:TYR:CE2	31:4:400:LEU:HD21	2.37	0.60
1:A:1591:C:OP1	17:Q:52:ARG:NH2	2.34	0.60
1:A:1322:C:OP2	3:C:36:LYS:NZ	2.34	0.60
2:B:156:GLU:OE1	7:G:163:HIS:ND1	2.35	0.60
1:A:684:U:O2'	20:T:151:SER:OG	2.11	0.60
22:V:134:GLN:NE2	27:0:108:ASN:OD1	2.35	0.60
3:C:124:LEU:O	3:C:132:TYR:OH	2.17	0.60
4:D:363:ALA:O	4:D:367:GLY:N	2.34	0.59
29:2:7:ARG:O	29:2:9:ARG:NH1	2.36	0.59
1:A:946:U:OP2	34:A:1702:SPM:N10	2.36	0.59
15:O:208:PRO:HG2	15:O:213:LEU:HD21	1.84	0.59
1:A:992:U:O2'	1:A:994:A:OP2	2.19	0.58
20:T:128:ASN:O	42:T:301:HOH:O	2.17	0.58
1:A:905:A:O2'	1:A:907:A:OP1	2.20	0.58
18:R:219:TYR:O	18:R:256:ARG:NH1	2.36	0.58
1:A:1235:U:OP1	11:K:36:ARG:NH2	2.37	0.58
25:Y:254:LYS:O	31:4:358:ARG:NH1	2.37	0.57
28:1:150:GLU:OE1	28:1:174:ARG:NH2	2.38	0.57
1:A:1528:A:OP1	27:0:99:ARG:NH2	2.38	0.56
6:F:240:ARG:NH2	29:2:44:THR:O	2.39	0.56
7:G:320:VAL:HG23	7:G:322:ARG:HG2	1.87	0.56
31:4:239:ARG:O	31:4:242:ASN:ND2	2.38	0.56
17:Q:49:CYS:SG	17:Q:50:ARG:NH1	2.78	0.56
19:S:87:LEU:HD13	23:W:89:LEU:HD13	1.88	0.56
22:V:46:GLU:OE2	22:V:74:ARG:NE	2.36	0.56
32:8:213:ILE:O	32:8:216:THR:OG1	2.23	0.56
20:T:9:ILE:O	20:T:12:THR:OG1	2.20	0.55
18:R:161:ILE:O	20:T:125:HIS:NE2	2.40	0.55
31:4:413:ASP:N	31:4:413:ASP:OD1	2.40	0.55
14:N:6:SER:OG	14:N:69:LEU:O	2.24	0.55
24:X:147:LYS:HE2	24:X:147:LYS:HA	1.89	0.55
31:4:618:ALA:O	31:4:622:ASN:N	2.35	0.55
1:A:1451:U:OP1	7:G:382:PRO:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:299:ASP:OD2	24:X:385:ASN:ND2	2.40	0.54
1:A:812:A:O2'	1:A:814:A:N1	2.41	0.54
1:A:958:C:H4'	1:A:959:C:H5'	1.89	0.54
19:S:87:LEU:HD12	23:W:116:PHE:O	2.08	0.53
4:D:173:ILE:HG23	4:D:176:ARG:NH2	2.24	0.53
32:8:154:GLY:N	32:8:155:PRO:CD	2.70	0.53
3:C:152:ARG:NH1	25:Y:300:GLU:OE2	2.39	0.53
21:U:80:ARG:O	21:U:84:GLU:N	2.40	0.53
2:B:138:ARG:NH1	19:S:30:LEU:O	2.42	0.53
1:A:1376:C:H4'	1:A:1377:C:H5'	1.90	0.53
32:8:222:THR:CG2	32:8:243:LEU:HD13	2.38	0.53
1:A:1429:C:H4'	1:A:1430:A:H5''	1.90	0.53
23:W:87:SER:OG	23:W:90:THR:OG1	2.26	0.53
24:X:268:LEU:O	24:X:294:ARG:NH1	2.34	0.53
27:0:110:ASP:OD1	27:0:110:ASP:N	2.39	0.52
11:K:58:ARG:NE	11:K:72:ASP:OD1	2.39	0.52
28:1:166:PRO:O	28:1:169:ARG:NH2	2.42	0.52
29:2:102:ASN:OD1	29:2:103:LYS:N	2.41	0.52
31:4:346:HIS:HA	31:4:378:LEU:HD12	1.90	0.52
1:A:841:A:OP1	13:M:39:ASN:ND2	2.32	0.52
23:W:141:ARG:NH2	23:W:170:LEU:O	2.43	0.52
9:I:71:SER:O	9:I:74:ARG:NH1	2.43	0.52
13:M:55:ASP:OD2	20:T:146:GLN:NE2	2.42	0.52
7:G:263:ASP:OD1	7:G:267:MET:N	2.42	0.52
7:G:312:GLN:OE1	7:G:345:ARG:NH2	2.41	0.52
4:D:134:GLU:OE2	4:D:160:ARG:NH1	2.35	0.51
1:A:1190:C:O2'	1:A:1467:C:N3	2.36	0.51
1:A:1443:U:OP2	11:K:102:ARG:NH2	2.43	0.51
9:I:151:VAL:HG11	9:I:158:ARG:HG3	1.93	0.51
2:B:134:HIS:O	2:B:138:ARG:HG3	2.11	0.51
7:G:267:MET:HA	7:G:267:MET:HE2	1.93	0.51
6:F:88:ASP:OD2	6:F:146:HIS:NE2	2.42	0.50
3:C:92:LEU:HD11	3:C:117:LEU:HD21	1.93	0.50
24:X:347:ASN:HB3	24:X:386:ALA:O	2.11	0.50
22:V:57:MET:O	22:V:60:THR:OG1	2.28	0.50
7:G:270:SER:OG	7:G:351:ALA:O	2.28	0.50
8:H:174:LYS:NZ	28:1:155:ASP:OD2	2.30	0.50
1:A:1416:A:H5'	1:A:1416:A:H8	1.77	0.49
7:G:143:ASP:OD1	7:G:144:GLY:N	2.45	0.49
1:A:1488:5MC:O2	1:A:1584:MA6:O2'	2.20	0.49
7:G:150:LEU:O	7:G:153:THR:OG1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:320:VAL:O	7:G:321:ASP:OD1	2.29	0.49
11:K:60:ASN:OD1	11:K:68:GLN:NE2	2.44	0.49
1:A:1136:C:H2'	1:A:1137:A:H5''	1.94	0.49
7:G:237:GLU:OE2	7:G:237:GLU:N	2.45	0.49
31:4:436:HIS:O	31:4:440:LYS:HG2	2.13	0.49
1:A:769:G:OP2	14:N:73:ARG:NH2	2.46	0.49
1:A:1583:MA6:H93	1:A:1584:MA6:N6	2.27	0.49
28:1:86:ARG:NH1	28:1:96:PRO:O	2.45	0.49
1:A:1430:A:OP1	7:G:388:ARG:NH2	2.43	0.49
1:A:1325:U:OP1	4:D:112:LYS:NZ	2.37	0.49
22:V:391:GLN:O	22:V:395:GLN:N	2.41	0.49
27:0:43:ARG:O	27:0:47:GLY:N	2.42	0.49
32:8:116:LEU:HD12	32:8:116:LEU:O	2.12	0.49
3:C:57:HIS:HB2	3:C:66:LYS:HD2	1.94	0.48
9:I:83:ILE:O	9:I:148:ARG:NH1	2.46	0.48
28:1:253:TRP:O	28:1:256:SER:OG	2.29	0.48
11:K:34:MET:O	11:K:38:VAL:HG23	2.13	0.48
15:O:221:GLN:NE2	22:V:314:VAL:O	2.41	0.48
1:A:958:C:C4'	1:A:959:C:H5'	2.44	0.48
1:A:1287:A:OP2	4:D:260:LYS:NZ	2.40	0.48
2:B:243:PRO:O	2:B:247:HIS:ND1	2.42	0.48
7:G:381:LYS:N	7:G:381:LYS:HD2	2.29	0.48
7:G:315:PHE:HB3	7:G:316:PRO:HD3	1.95	0.48
12:L:126:GLU:HG2	12:L:177:VAL:HG11	1.95	0.47
22:V:123:ASP:OD1	22:V:123:ASP:N	2.48	0.47
15:O:217:ARG:NE	22:V:318:ASP:OD2	2.42	0.47
1:A:965:C:H3'	1:A:966:A:H5''	1.97	0.47
3:C:58:ALA:HB1	3:C:59:PRO:CD	2.45	0.47
16:P:73:ASP:OD1	16:P:74:TYR:N	2.48	0.47
28:1:118:ALA:O	28:1:122:HIS:N	2.43	0.47
22:V:269:SER:HB2	22:V:270:PRO:HD2	1.96	0.47
32:8:231:GLN:O	32:8:234:LYS:HG2	2.15	0.47
18:R:212:GLU:OE1	18:R:248:LYS:NZ	2.36	0.47
29:2:90:GLN:O	29:2:94:GLY:N	2.40	0.47
6:F:176:ASP:OD2	6:F:180:ARG:NH1	2.47	0.47
8:H:76:LEU:HB2	8:H:148:LEU:HD13	1.97	0.47
31:4:74:LEU:O	31:4:77:THR:OG1	2.33	0.47
26:Z:76:GLN:O	26:Z:80:ASP:N	2.44	0.46
32:8:207:GLU:O	32:8:207:GLU:HG2	2.14	0.46
27:0:41:LEU:HD13	27:0:55:TRP:CG	2.50	0.46
1:A:1569:G:OP2	1:A:1572:A:O2'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:217:ARG:NH2	15:O:227:GLU:OE2	2.48	0.46
1:A:928:A:OP2	10:J:47:ARG:NH2	2.48	0.46
9:I:129:GLN:NE2	9:I:167:MET:SD	2.86	0.46
30:3:148:LYS:O	30:3:151:ARG:NH2	2.45	0.46
1:A:756:C:P	10:J:43:LYS:HD3	2.56	0.46
31:4:236:VAL:HG12	31:4:238:TRP:H	1.79	0.46
24:X:369:GLU:CD	24:X:369:GLU:H	2.22	0.46
31:4:493:MET:HA	31:4:493:MET:HE2	1.96	0.46
21:U:138:GLU:O	21:U:142:LYS:N	2.44	0.46
10:J:70:PRO:HB3	10:J:117:ASP:HB3	1.99	0.45
7:G:395:LYS:O	7:G:396:ARG:OXT	2.34	0.45
18:R:263:ARG:NH1	18:R:287:ASP:OD1	2.49	0.45
1:A:959:C:H2'	1:A:960:C:H5''	1.98	0.45
31:4:433:TYR:OH	31:4:469:GLU:OE2	2.35	0.45
1:A:1149:G:OP2	30:3:165:LYS:NZ	2.44	0.45
1:A:1154:A:OP2	30:3:155:ARG:NH1	2.44	0.45
7:G:110:TYR:OH	28:1:114:LEU:O	2.29	0.45
9:I:81:GLU:OE1	9:I:81:GLU:N	2.41	0.45
21:U:84:GLU:O	21:U:84:GLU:HG2	2.17	0.45
28:1:103:LEU:O	28:1:107:LYS:HG3	2.16	0.45
4:D:380:LEU:HD12	4:D:381:PRO:HD2	1.99	0.45
21:U:161:GLN:O	21:U:164:VAL:HG12	2.16	0.45
1:A:1458:A:OP1	6:F:104:LYS:NZ	2.45	0.45
24:X:48:ILE:O	24:X:48:ILE:HG12	2.17	0.45
12:L:76:TYR:O	12:L:79:VAL:HG22	2.17	0.45
15:O:215:ARG:NH1	27:0:90:ASP:OD1	2.46	0.45
11:K:55:ASN:OD1	11:K:58:ARG:NH2	2.47	0.44
24:X:253:LEU:HD12	24:X:255:MET:HE3	1.99	0.44
1:A:843:G:N2	1:A:846:A:OP2	2.44	0.44
1:A:1412:G:OP1	24:X:279:LYS:NZ	2.49	0.44
24:X:233:VAL:HG12	24:X:233:VAL:O	2.18	0.44
7:G:110:TYR:CD1	8:H:90:SER:OG	2.71	0.44
1:A:1119:U:O4'	19:S:50:ARG:NH1	2.47	0.44
6:F:79:ALA:O	7:G:312:GLN:NE2	2.51	0.44
14:N:93:ASP:O	14:N:97:GLY:N	2.46	0.44
19:S:75:TYR:O	19:S:79:GLY:N	2.51	0.44
21:U:199:ARG:HG3	21:U:200:PRO:HD2	2.00	0.44
24:X:265:ILE:HG12	24:X:265:ILE:O	2.17	0.44
31:4:145:PHE:O	31:4:163:LEU:HD13	2.18	0.44
1:A:704:U:OP1	27:0:53:ARG:NH1	2.51	0.44
1:A:1184:U:H2'	1:A:1185:C:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:384:GLN:HB3	7:G:389:ARG:O	2.18	0.44
22:V:361:LYS:O	22:V:361:LYS:HG2	2.18	0.44
3:C:62:ILE:O	3:C:66:LYS:O	2.36	0.44
27:0:78:ARG:NH1	27:0:142:VAL:O	2.49	0.44
5:E:49:TYR:OH	16:P:115:GLN:O	2.22	0.43
18:R:231:CYS:SG	18:R:242:TYR:HA	2.58	0.43
1:A:1445:G:O6	42:A:1803:HOH:O	2.20	0.43
19:S:98:ARG:NH2	19:S:128:GLU:OE1	2.44	0.43
31:4:417:GLN:HG3	31:4:456:PHE:CD1	2.53	0.43
32:8:130:LEU:HD12	32:8:130:LEU:O	2.18	0.43
1:A:1136:C:C2'	1:A:1137:A:H5''	2.47	0.43
3:C:39:ALA:O	3:C:41:ARG:NH1	2.51	0.43
8:H:188:ILE:O	8:H:188:ILE:HG13	2.18	0.43
16:P:54:MET:HE1	19:S:65:TYR:O	2.18	0.43
27:0:30:ASP:OD1	27:0:212:ARG:NH1	2.44	0.43
31:4:509:ILE:N	31:4:510:PRO:CD	2.82	0.43
15:O:220:TYR:O	15:O:224:LEU:HG	2.19	0.43
16:P:54:MET:HG2	16:P:55:GLU:N	2.33	0.43
19:S:35:TYR:C	19:S:35:TYR:CD1	2.97	0.43
1:A:1481:C:O2	1:A:1481:C:O2'	2.34	0.43
15:O:146:GLN:OE1	15:O:146:GLN:HA	2.19	0.43
1:A:743:C:H2'	1:A:744:A:O4'	2.19	0.43
27:0:83:LYS:N	27:0:138:ASP:OD1	2.52	0.43
1:A:940:A:H8	1:A:940:A:H5''	1.84	0.43
2:B:239:ASN:ND2	2:B:242:SER:OG	2.52	0.43
9:I:163:HIS:NE2	17:Q:20:GLU:OE1	2.47	0.43
24:X:80:PRO:HB2	24:X:190:ASN:OD1	2.19	0.43
3:C:89:ASP:O	3:C:93:ARG:HG3	2.19	0.42
10:J:116:GLN:OE1	10:J:116:GLN:N	2.39	0.42
25:Y:292:GLN:OE1	31:4:454:ARG:NH2	2.52	0.42
1:A:932:C:O2'	20:T:2:PRO:O	2.33	0.42
15:O:148:LYS:HE3	15:O:148:LYS:HB2	1.93	0.42
1:A:1267:U:H2'	1:A:1268:C:C6	2.54	0.42
3:C:84:GLU:O	3:C:88:GLU:HG3	2.19	0.42
5:E:94:VAL:HG11	16:P:117:MET:HE1	2.02	0.42
12:L:123:ARG:O	12:L:123:ARG:HG2	2.20	0.42
24:X:151:LEU:CD2	24:X:247:LEU:HD22	2.49	0.42
25:Y:319:ALA:O	28:1:164:ARG:NH1	2.50	0.42
31:4:290:ASP:OD1	31:4:293:THR:OG1	2.37	0.42
1:A:1235:U:O3'	11:K:90:ARG:NH2	2.53	0.42
6:F:201:MET:HB3	6:F:202:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:67:ARG:NH1	14:N:80:GLU:OE1	2.53	0.42
18:R:76:GLN:HA	18:R:76:GLN:OE1	2.19	0.42
1:A:919:A:OP2	15:O:96:ARG:NH2	2.44	0.42
3:C:58:ALA:HB3	3:C:60:HIS:CE1	2.55	0.42
4:D:245:VAL:HG22	4:D:271:ALA:HB1	2.00	0.42
18:R:204:ILE:HB	20:T:144:GLU:HG3	2.02	0.42
22:V:266:VAL:HG21	22:V:275:LEU:HG	2.01	0.42
1:A:1198:A:C2'	1:A:1199:G:H5'	2.50	0.42
15:O:137:ALA:HB3	15:O:138:PRO:HD3	2.02	0.42
22:V:264:GLU:OE1	22:V:333:ARG:NH1	2.43	0.42
4:D:195:GLY:HA3	7:G:51:HIS:CE1	2.55	0.42
8:H:184:ILE:O	8:H:184:ILE:HG22	2.20	0.42
24:X:151:LEU:HD21	24:X:247:LEU:HD22	2.02	0.42
24:X:243:VAL:O	24:X:247:LEU:HG	2.19	0.42
31:4:58:VAL:O	31:4:58:VAL:HG23	2.19	0.41
4:D:263:ASP:OD1	4:D:264:ARG:N	2.53	0.41
18:R:162:SER:HB2	18:R:165:ILE:HD12	2.02	0.41
18:R:170:ARG:O	18:R:189:ARG:NH2	2.49	0.41
24:X:196:GLU:HA	24:X:196:GLU:OE2	2.20	0.41
31:4:56:GLU:HA	31:4:56:GLU:OE1	2.20	0.41
32:8:84:GLN:OE1	32:8:126:ALA:HB2	2.21	0.41
1:A:663:A:H2'	1:A:664:G:C8	2.55	0.41
1:A:860:A:N7	1:A:919:A:O2'	2.44	0.41
2:B:103:GLU:N	2:B:104:PRO:CD	2.83	0.41
1:A:929:A:O2'	4:D:419:ARG:O	2.23	0.41
1:A:955:A:C8	20:T:37:HIS:HE1	2.39	0.41
2:B:210:ARG:NH2	2:B:211:ASP:OD1	2.41	0.41
5:E:26:ILE:HG23	5:E:36:VAL:HG21	2.02	0.41
5:E:63:TYR:OH	16:P:118:GLY:O	2.15	0.41
16:P:67:LEU:O	16:P:103:LYS:HE2	2.21	0.41
1:A:1068:A:H5''	9:I:190:LYS:HD3	2.02	0.41
22:V:210:LEU:HB2	22:V:211:PRO:HD3	2.03	0.41
27:0:54:ALA:O	27:0:58:VAL:HG23	2.20	0.41
31:4:333:GLN:O	31:4:337:THR:HG23	2.20	0.41
2:B:103:GLU:OE2	19:S:52:ARG:NH2	2.53	0.41
3:C:123:VAL:HG23	3:C:157:THR:HG22	2.03	0.41
9:I:175:ILE:HD11	17:Q:19:VAL:HG13	2.02	0.41
18:R:315:GLN:HA	18:R:315:GLN:OE1	2.20	0.41
20:T:103:ARG:O	20:T:103:ARG:HG2	2.21	0.41
32:8:219:GLY:O	32:8:243:LEU:HD22	2.21	0.41
1:A:866:A:H2'	1:A:867:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:C:H3'	1:A:1367:A:H5'	2.02	0.41
8:H:76:LEU:HD23	8:H:145:LEU:HD12	2.02	0.41
10:J:78:ARG:NH1	10:J:117:ASP:OD2	2.53	0.41
18:R:242:TYR:CD1	18:R:242:TYR:C	2.98	0.41
26:Z:20:GLY:O	28:1:211:ARG:NH2	2.37	0.41
28:1:255:ASN:N	28:1:259:GLU:OE2	2.51	0.41
31:4:599:PHE:O	31:4:604:LYS:N	2.47	0.41
1:A:1571:U:O2	9:I:193:LYS:HD3	2.21	0.41
4:D:368:LEU:HD22	18:R:107:THR:HG22	2.02	0.41
17:Q:68:MET:HE3	17:Q:68:MET:HA	2.02	0.41
25:Y:393:GLN:O	25:Y:393:GLN:HG3	2.20	0.41
1:A:648:A:N3	1:A:929:A:H2'	2.36	0.41
22:V:50:LEU:CD1	22:V:75:LEU:HG	2.51	0.41
30:3:177:TRP:CD1	30:3:177:TRP:C	2.98	0.41
5:E:2:PRO:N	5:E:70:ALA:O	2.54	0.40
1:A:872:G:H2'	1:A:873:G:C8	2.56	0.40
1:A:1591:C:OP1	17:Q:48:PRO:HB2	2.22	0.40
32:8:80:ARG:NH2	32:8:110:ASP:OD1	2.53	0.40
4:D:316:CYS:HB3	4:D:334:ALA:HB3	2.03	0.40
12:L:112:MET:O	12:L:116:VAL:HG22	2.21	0.40
12:L:181:ILE:HG23	12:L:185:LEU:HD12	2.03	0.40
24:X:127:TYR:OH	28:1:306:GLU:OE2	2.37	0.40
28:1:60:MET:HE1	28:1:80:ALA:O	2.20	0.40
31:4:324:VAL:O	31:4:324:VAL:HG12	2.21	0.40
18:R:145:ASP:O	18:R:179:GLY:HA3	2.21	0.40
24:X:394:HIS:ND1	24:X:394:HIS:O	2.53	0.40
27:0:68:LEU:HA	27:0:71:LEU:HD12	2.03	0.40
31:4:417:GLN:OE1	31:4:453:HIS:CD2	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	126 (97%)	4 (3%)	0	100	100
4	D	341/430 (79%)	326 (96%)	15 (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%)	316 (97%)	10 (3%)	0	100	100
8	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18	50
9	I	135/194 (70%)	128 (95%)	6 (4%)	1 (1%)	18	50
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%)	84 (100%)	0	0	100	100
18	R	293/360 (81%)	287 (98%)	6 (2%)	0	100	100
19	S	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
20	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
22	V	358/414 (86%)	351 (98%)	7 (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%)	206 (97%)	7 (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%)	561 (96%)	23 (4%)	0	100	100
32	8	189/285 (66%)	183 (97%)	5 (3%)	1 (0%)	24	58
All	All	5852/7586 (77%)	5675 (97%)	174 (3%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	184	ASN
8	H	126	ILE
32	8	218	PRO

5.3.2 Protein sidechains ⓘ

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%)	286 (100%)	0	100	100
5	E	104/107 (97%)	104 (100%)	0	100	100
6	F	185/209 (88%)	185 (100%)	0	100	100
7	G	288/342 (84%)	288 (100%)	0	100	100
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%)	95 (99%)	1 (1%)	68	83
15	O	175/230 (76%)	175 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	310 (100%)	1 (0%)	86	91
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	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%)	526 (100%)	0	100	100
32	8	172/253 (68%)	171 (99%)	1 (1%)	78	88
All	All	5227/6597 (79%)	5224 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	91	VAL
24	X	81	HIS
32	8	238	CYS

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

Mol	Chain	Res	Type
2	B	74	ASN
2	B	90	HIS
2	B	167	HIS
2	B	178	ASN
4	D	359	HIS
4	D	369	HIS
6	F	169	GLN
6	F	224	HIS
7	G	308	GLN
8	H	109	HIS
8	H	176	GLN
10	J	134	HIS
12	L	162	GLN
13	M	16	HIS

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Mol	Chain	Res	Type
13	M	61	HIS
13	M	75	HIS
15	O	130	HIS
17	Q	4	HIS
18	R	194	GLN
18	R	214	ASN
19	S	66	HIS
22	V	38	HIS
22	V	87	HIS
22	V	380	GLN
22	V	391	GLN
24	X	140	HIS
24	X	159	HIS
24	X	302	HIS
24	X	326	GLN
24	X	363	ASN
25	Y	290	ASN
26	Z	55	HIS
27	0	137	HIS
31	4	243	ASN
31	4	257	HIS
31	4	285	ASN
31	4	453	HIS
31	4	577	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	954/955 (99%)	285 (29%)	8 (0%)

All (285) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	649	A
1	A	657	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

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Mol	Chain	Res	Type
1	A	704	U
1	A	715	G
1	A	718	A
1	A	721	U
1	A	722	C
1	A	723	A
1	A	724	C
1	A	730	A
1	A	736	C
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	859	U

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Mol	Chain	Res	Type
1	A	860	A
1	A	861	U
1	A	868	C
1	A	869	C
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	891	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

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Mol	Chain	Res	Type
1	A	967	A
1	A	974	U
1	A	975	A
1	A	987	A
1	A	992	U
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	1021	U
1	A	1030	G
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	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

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Mol	Chain	Res	Type
1	A	1125	A
1	A	1126	A
1	A	1127	A
1	A	1136	C
1	A	1138	G
1	A	1142	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	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

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Mol	Chain	Res	Type
1	A	1253	C
1	A	1256	A
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	1296	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	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	1388	C
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	1429	C
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	1488	5MC
1	A	1489	G
1	A	1492	A
1	A	1494	C
1	A	1495	C
1	A	1501	A
1	A	1511	C
1	A	1512	A
1	A	1515	G
1	A	1516	G
1	A	1519	A
1	A	1522	U
1	A	1523	A
1	A	1524	A

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Mol	Chain	Res	Type
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
1	A	1539	C
1	A	1553	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	1583	MA6
1	A	1584	MA6
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 (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
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

5.4 Non-standard residues in protein, DNA, RNA chains

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	5MC	A	1488	1	19,22,23	1.72	3 (15%)	26,32,35	1.89	8 (30%)
1	B8T	A	1486	1	19,22,23	0.86	2 (10%)	25,31,34	1.01	2 (8%)
1	MA6	A	1583	1	23,26,27	0.96	2 (8%)	33,38,41	2.05	8 (24%)
17	AYA	Q	2	17	6,7,8	1.41	1 (16%)	6,8,10	1.21	1 (16%)
1	5MU	A	1076	1	19,22,23	1.19	3 (15%)	27,32,35	2.14	9 (33%)
29	AYA	2	2	29	6,7,8	1.28	1 (16%)	6,8,10	1.31	1 (16%)
1	MA6	A	1584	1	23,26,27	0.90	1 (4%)	33,38,41	2.07	8 (24%)

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	5MC	A	1488	1	-	0/7/25/26	0/2/2/2
1	B8T	A	1486	1	-	0/7/27/28	0/2/2/2
1	MA6	A	1583	1	-	0/11/29/30	0/3/3/3
17	AYA	Q	2	17	-	1/5/6/8	-
1	5MU	A	1076	1	-	0/7/25/26	0/2/2/2
29	AYA	2	2	29	-	1/5/6/8	-
1	MA6	A	1584	1	-	1/11/29/30	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1488	5MC	C5-C4	-5.37	1.40	1.44
17	Q	2	AYA	CA-N	-3.02	1.43	1.46
1	A	1076	5MU	C2-N1	-2.80	1.34	1.38
1	A	1488	5MC	C2-N1	-2.75	1.34	1.40
1	A	1076	5MU	C4-C5	-2.72	1.40	1.44
29	2	2	AYA	CA-N	-2.49	1.43	1.46
1	A	1076	5MU	C4-N3	-2.31	1.34	1.38
1	A	1584	MA6	C5-N7	-2.29	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1486	B8T	C6-N1	2.26	1.43	1.38
1	A	1486	B8T	C2-N1	-2.22	1.35	1.40
1	A	1583	MA6	C5-N7	-2.19	1.35	1.39
1	A	1488	5MC	C2'-C3'	-2.09	1.47	1.53
1	A	1583	MA6	C2-N3	-2.05	1.30	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1076	5MU	C4-N3-C2	-5.25	120.46	127.34
1	A	1584	MA6	C5-C4-N3	-4.82	120.09	126.72
1	A	1584	MA6	N1-C2-N3	-4.77	121.36	128.58
1	A	1583	MA6	N1-C2-N3	-4.73	121.42	128.58
1	A	1583	MA6	C2-N1-C6	4.66	123.22	111.83
1	A	1076	5MU	N3-C2-N1	4.62	120.91	114.89
1	A	1584	MA6	C2-N1-C6	4.34	122.42	111.83
1	A	1488	5MC	O3'-C3'-C4'	4.24	123.26	111.08
1	A	1583	MA6	C5-C4-N3	-4.13	121.03	126.72
1	A	1076	5MU	C5-C4-N3	4.03	118.83	115.32
1	A	1488	5MC	O3'-C3'-C2'	3.94	124.45	111.82
1	A	1076	5MU	O4-C4-C5	-3.94	120.41	124.92
1	A	1584	MA6	C5-N7-C8	3.92	109.61	103.45
1	A	1583	MA6	C5-N7-C8	3.92	109.61	103.45
1	A	1584	MA6	N3-C4-N9	3.71	133.48	127.17
1	A	1584	MA6	C2-N3-C4	3.65	120.74	111.83
1	A	1583	MA6	C4-C5-N7	-3.51	106.57	110.58
1	A	1583	MA6	C2-N3-C4	3.36	120.04	111.83
1	A	1584	MA6	C4-C5-N7	-3.25	106.86	110.58
1	A	1583	MA6	N9-C8-N7	-3.23	109.35	113.94
1	A	1488	5MC	C5-C6-N1	-3.16	119.88	123.31
1	A	1076	5MU	C5M-C5-C6	-3.05	118.72	122.85
1	A	1584	MA6	N9-C8-N7	-3.05	109.61	113.94
29	2	2	AYA	CB-CA-N	3.03	113.10	109.68
1	A	1583	MA6	N3-C4-N9	3.01	132.29	127.17
1	A	1488	5MC	O2'-C2'-C3'	2.94	121.25	111.82
1	A	1076	5MU	C5-C6-N1	-2.94	120.12	123.31
1	A	1076	5MU	C5M-C5-C4	2.62	121.58	118.78
1	A	1488	5MC	CM5-C5-C6	-2.59	119.34	122.85
17	Q	2	AYA	CA-N-CT	2.28	124.44	121.50
1	A	1488	5MC	O2'-C2'-C1'	2.27	117.93	110.10
1	A	1486	B8T	C5-C4-N4	-2.24	117.47	122.40
1	A	1076	5MU	O2-C2-N1	-2.14	120.00	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1488	5MC	C1'-N1-C6	-2.08	117.73	121.15
1	A	1076	5MU	C6-C5-C4	2.04	119.70	118.02
1	A	1486	B8T	C5-C6-N1	-2.03	118.54	121.84
1	A	1488	5MC	O2-C2-N3	-2.00	119.17	122.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	2	2	AYA	O-C-CA-CB
17	Q	2	AYA	C-CA-N-CT
1	A	1584	MA6	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1488	5MC	1	0
1	A	1583	MA6	3	0
1	A	1584	MA6	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 78 are monoatomic - leaving 7 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	$\# Z > 2$
41	GNP	X	503	-	34,34,34	1.29	5 (14%)	47,54,54	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	SRY	A	1703	-	40,42,42	0.79	2 (5%)	49,63,63	1.27	4 (8%)
39	FES	T	201	20,13	0,4,4	-	-	-	-	-
40	ATP	X	501	36	32,33,33	1.34	5 (15%)	48,52,52	1.73	9 (18%)
33	NAD	A	1701	36	46,48,48	1.01	2 (4%)	64,73,73	1.57	9 (14%)
39	FES	P	201	16,5	0,4,4	-	-	-	-	-
34	SPM	A	1702	-	13,13,13	0.14	0	12,12,12	1.15	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
41	GNP	X	503	-	-	3/18/38/38	0/3/3/3
35	SRY	A	1703	-	-	1/20/87/87	0/3/3/3
39	FES	T	201	20,13	-	-	0/1/1/1
40	ATP	X	501	36	-	0/22/38/38	0/3/3/3
33	NAD	A	1701	36	-	1/30/62/62	0/5/5/5
39	FES	P	201	16,5	-	-	0/1/1/1
34	SPM	A	1702	-	-	0/11/11/11	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	503	GNP	PB-O3A	4.38	1.64	1.59
40	X	501	ATP	C5-C4	4.27	1.46	1.39
41	X	503	GNP	PB-O1B	3.19	1.51	1.46
35	A	1703	SRY	CD1-N31	3.03	1.38	1.33
41	X	503	GNP	PG-N3B	2.91	1.71	1.63
33	A	1701	NAD	O4D-C1D	2.78	1.44	1.40
41	X	503	GNP	PG-O1G	2.73	1.50	1.46
35	A	1703	SRY	CA1-N11	2.69	1.37	1.33
40	X	501	ATP	C5-N7	-2.60	1.34	1.39
33	A	1701	NAD	C2N-N1N	-2.58	1.32	1.35
40	X	501	ATP	C5-C6	2.44	1.47	1.41
41	X	503	GNP	PB-O2B	-2.25	1.50	1.56
40	X	501	ATP	C8-N7	2.07	1.35	1.31
40	X	501	ATP	C4-N9	-2.01	1.33	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	X	501	ATP	C5-C4-N3	-5.77	118.77	126.72
33	A	1701	NAD	C5A-C4A-N3A	-5.60	119.00	126.72
40	X	501	ATP	N3-C4-N9	4.67	135.11	127.17
35	A	1703	SRY	C12-O42-C42	-4.51	101.19	108.48
33	A	1701	NAD	N3A-C4A-N9A	4.21	134.33	127.17
33	A	1701	NAD	N3A-C2A-N1A	-4.20	122.23	128.58
40	X	501	ATP	C2-N3-C4	3.79	121.09	111.83
33	A	1701	NAD	C5A-N7A-C8A	3.77	109.38	103.45
33	A	1701	NAD	C2A-N3A-C4A	3.67	120.80	111.83
35	A	1703	SRY	O42-C12-C22	-3.61	103.44	107.31
40	X	501	ATP	N3-C2-N1	-3.53	123.23	128.58
33	A	1701	NAD	C4A-C5A-N7A	-3.49	106.59	110.58
40	X	501	ATP	C4-C5-N7	-3.24	106.88	110.58
40	X	501	ATP	C4-N9-C8	2.74	108.61	105.74
33	A	1701	NAD	N9A-C8A-N7A	-2.60	110.25	113.94
40	X	501	ATP	C5-N7-C8	2.55	107.46	103.45
35	A	1703	SRY	CH2-C42-C32	-2.47	111.16	116.27
33	A	1701	NAD	C3N-C7N-N7N	2.43	120.73	117.74
33	A	1701	NAD	O7N-C7N-N7N	-2.34	119.24	122.62
35	A	1703	SRY	CI3-N23-C23	-2.24	111.34	114.23
40	X	501	ATP	N9-C8-N7	-2.12	110.92	113.94
40	X	501	ATP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	X	503	GNP	PG-N3B-PB-O3A
41	X	503	GNP	PA-O3A-PB-O2B
35	A	1703	SRY	C13-C23-N23-CI3
41	X	503	GNP	PG-N3B-PB-O1B
33	A	1701	NAD	C2B-C1B-N9A-C8A

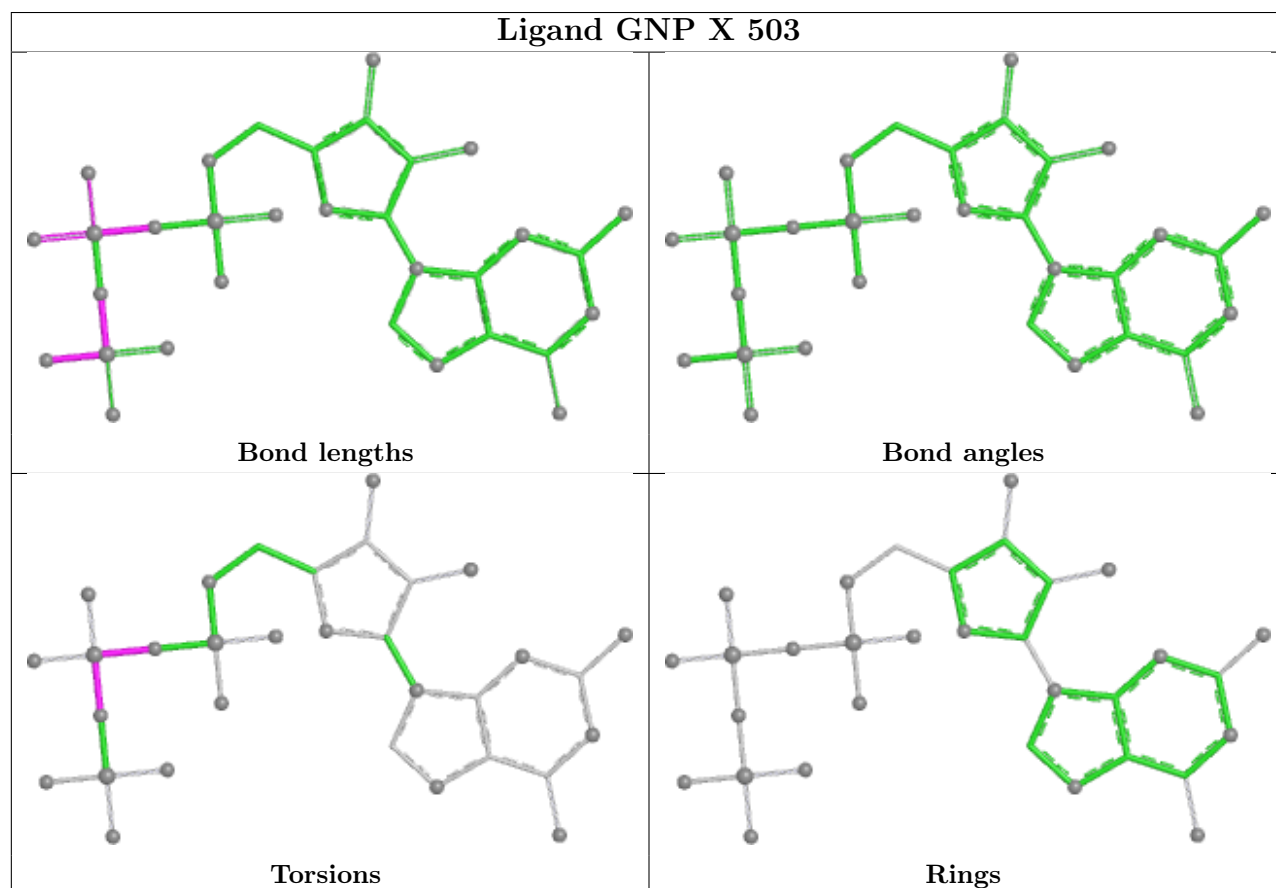
There are no ring outliers.

1 monomer is involved in 1 short contact:

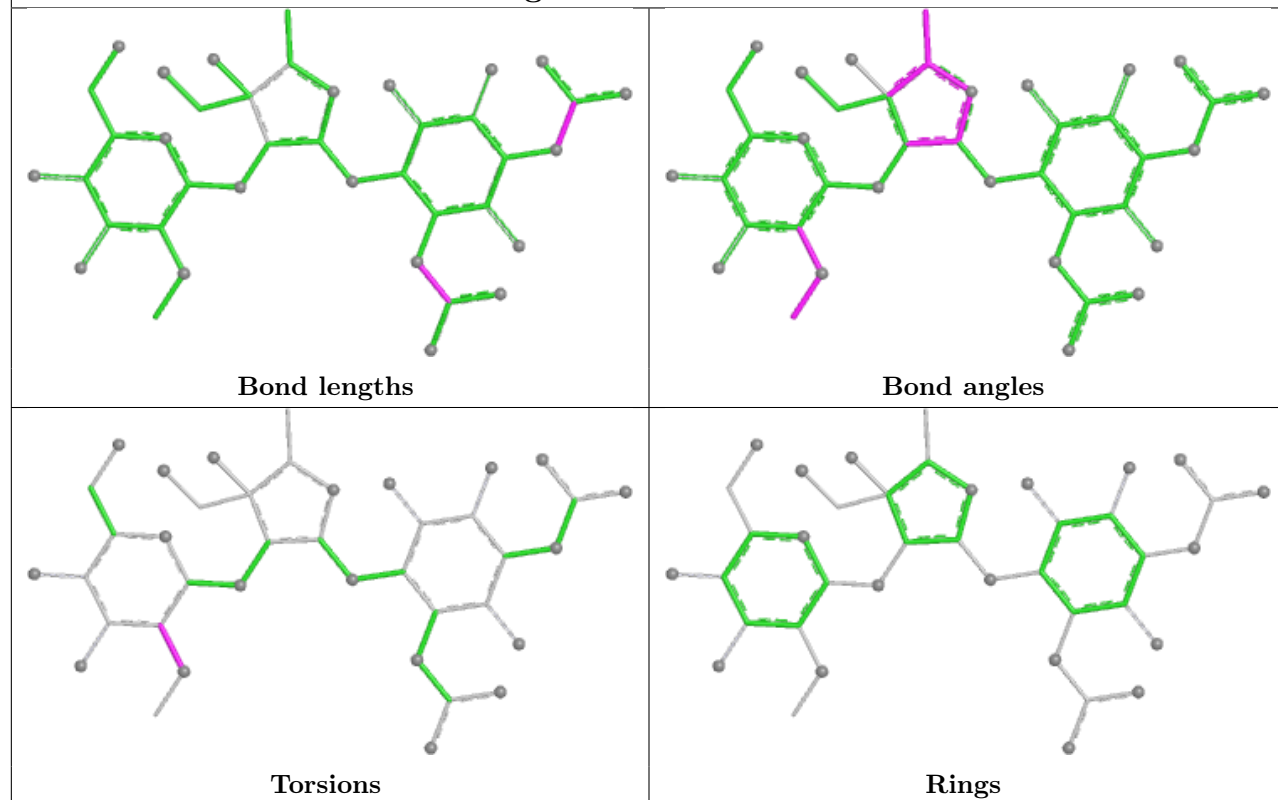
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	1702	SPM	1	0

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

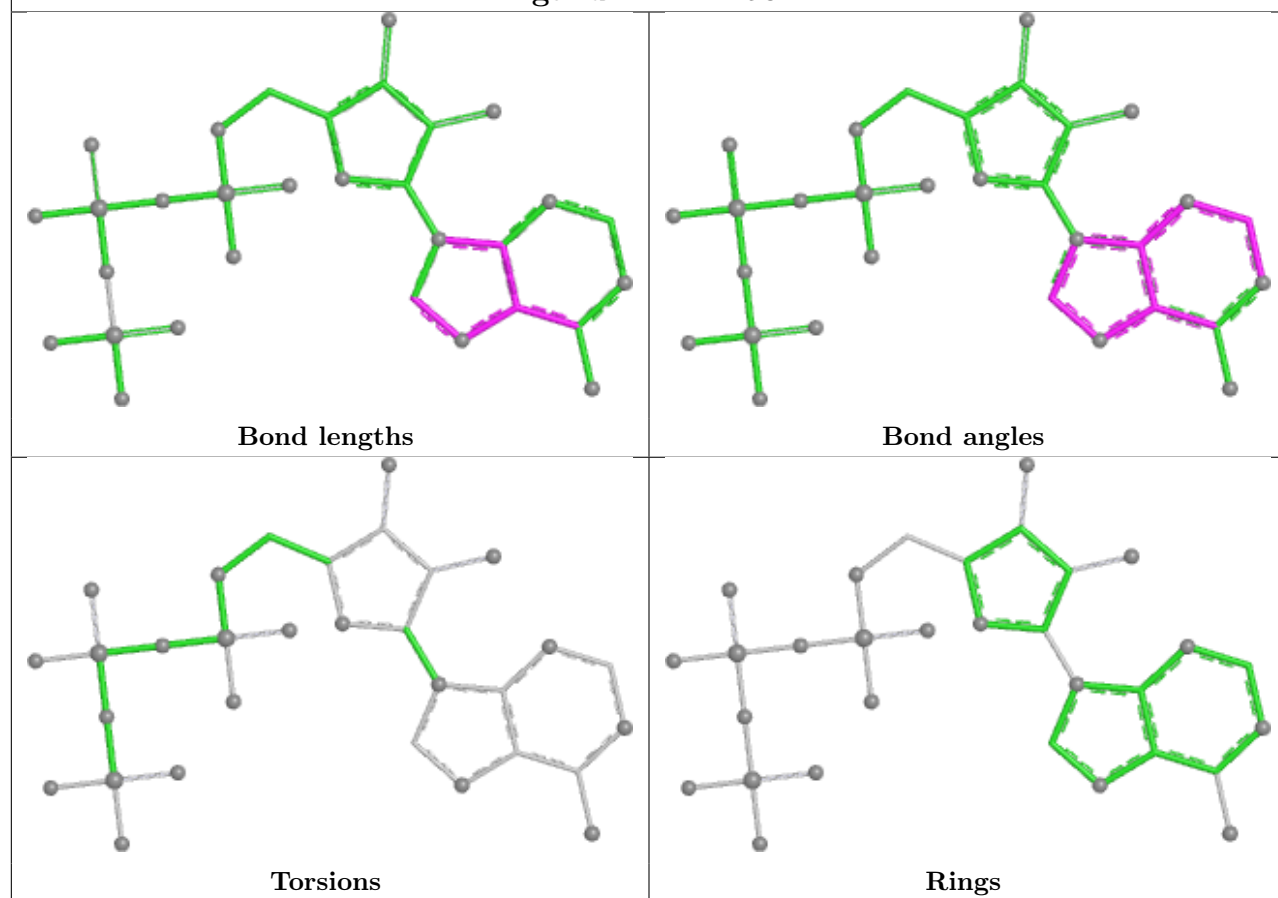
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

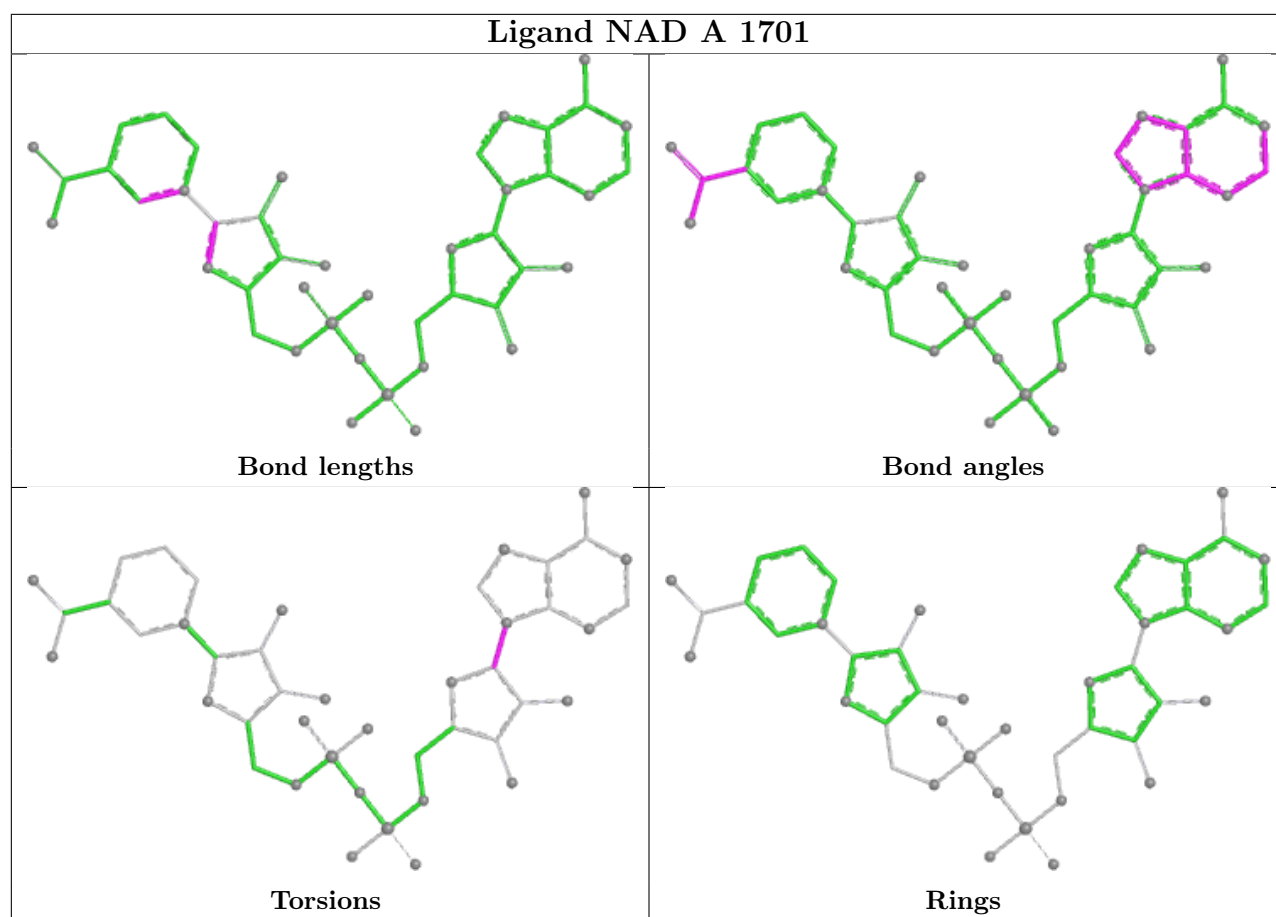


Ligand SRY A 1703



Ligand ATP X 501





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.

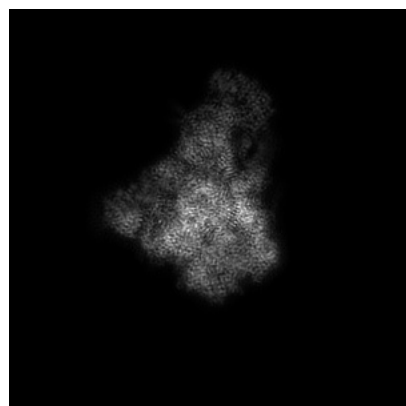
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10021. These allow visual inspection of the internal detail of the map and identification of artifacts.

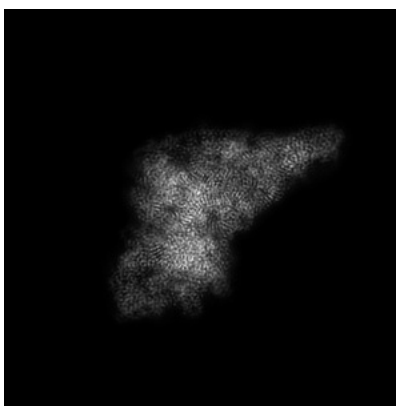
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

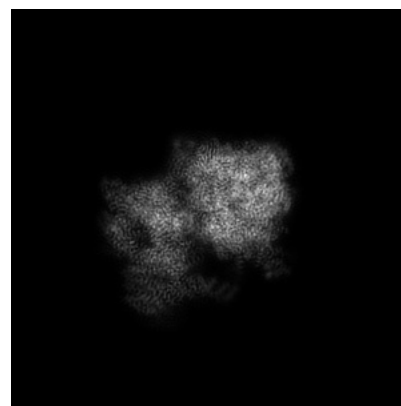
6.1.1 Primary map



X

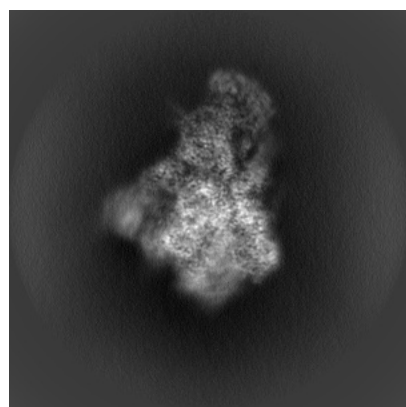


Y

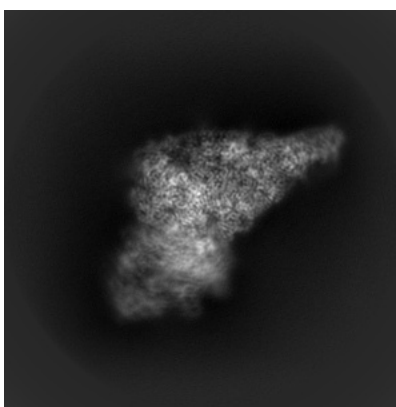


Z

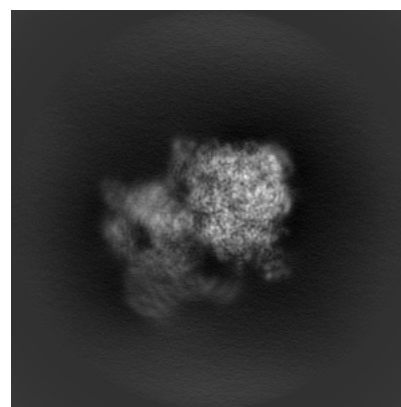
6.1.2 Raw map



X



Y

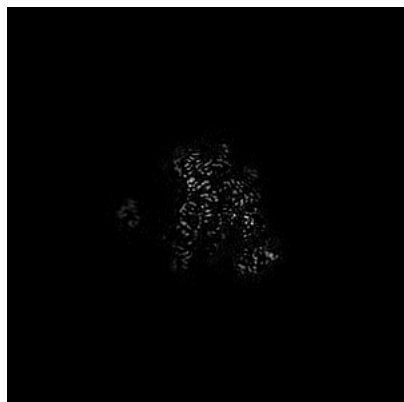


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

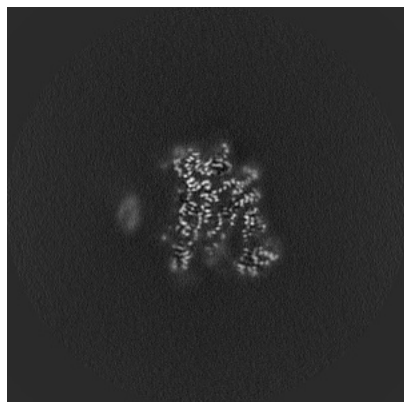


Y Index: 240

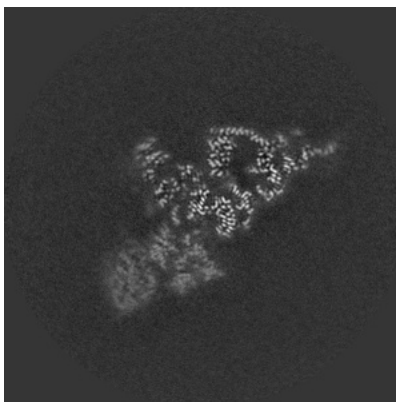


Z Index: 240

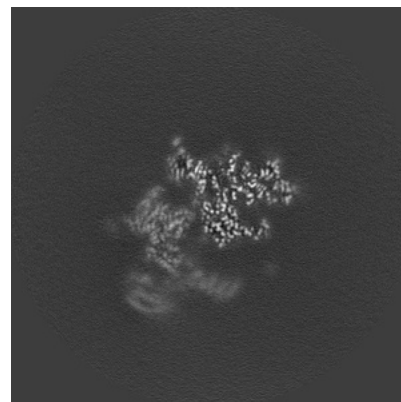
6.2.2 Raw map



X Index: 240



Y Index: 240

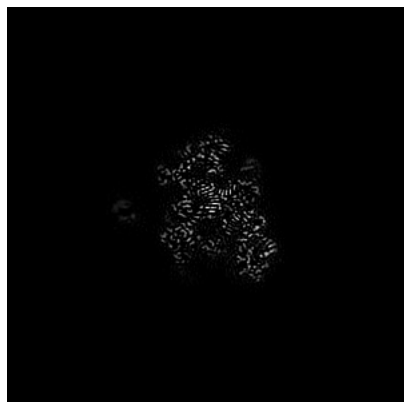


Z Index: 240

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

6.3 Largest variance slices [i](#)

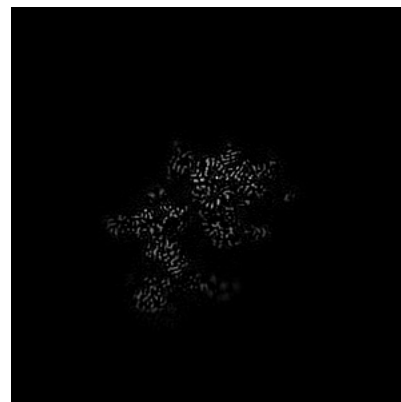
6.3.1 Primary map



X Index: 248

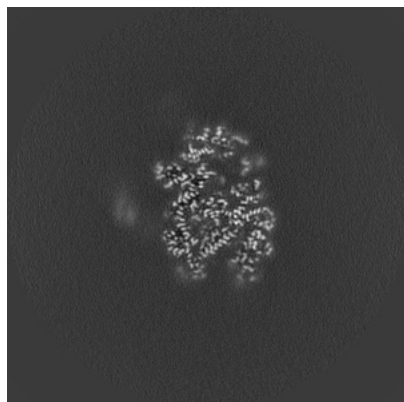


Y Index: 232

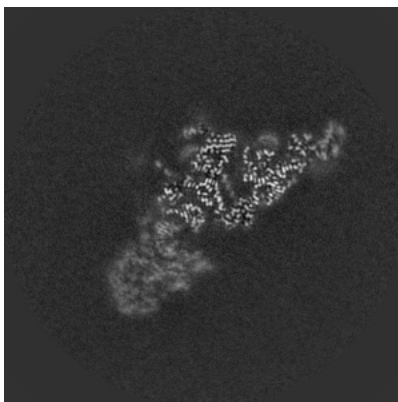


Z Index: 234

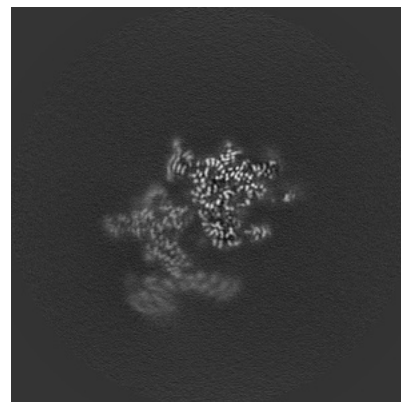
6.3.2 Raw map



X Index: 259



Y Index: 255

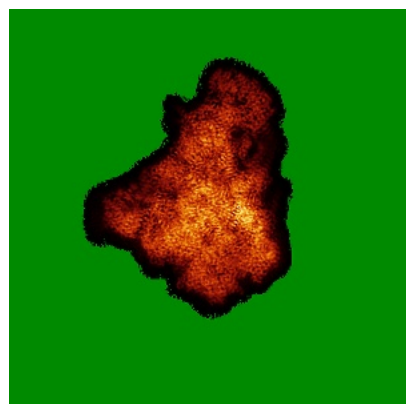


Z Index: 234

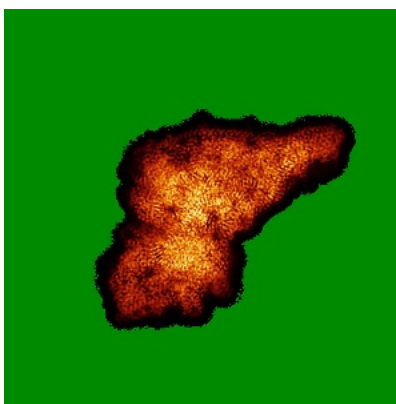
The images above show the largest variance slices of the map in three orthogonal directions.

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

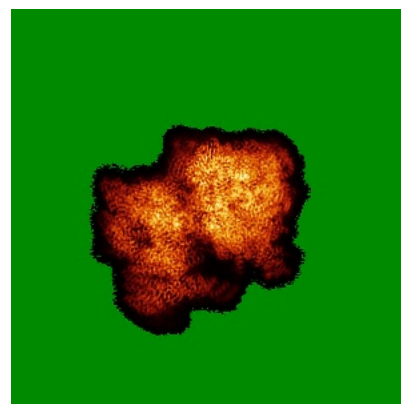
6.4.1 Primary map



X

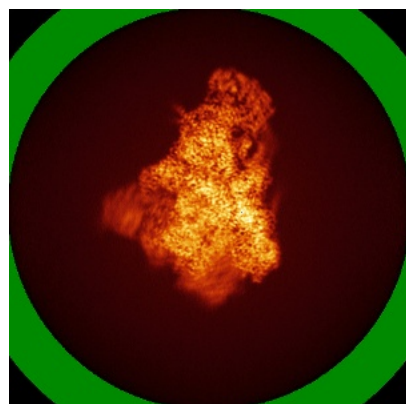


Y



Z

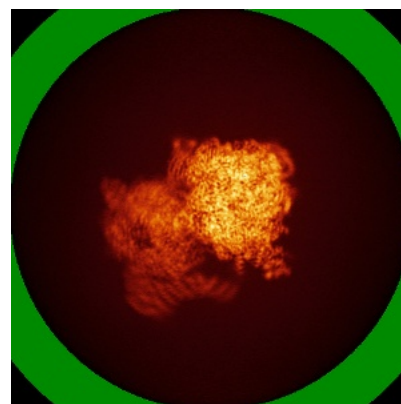
6.4.2 Raw map



X



Y

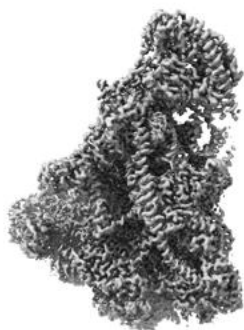


Z

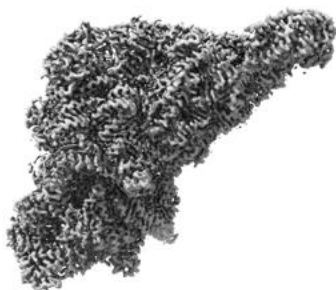
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

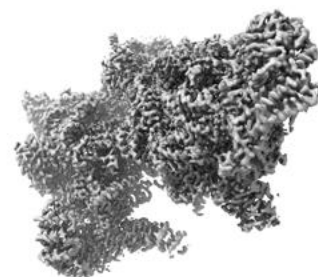
6.5.1 Primary map



X



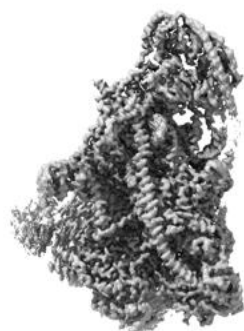
Y



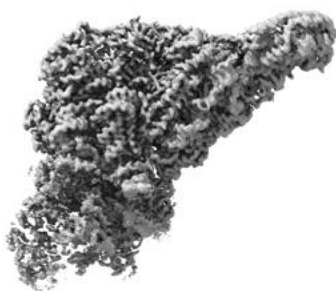
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

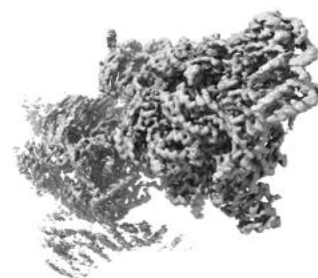
6.5.2 Raw map



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.

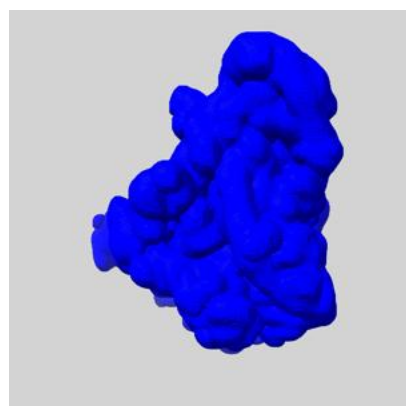
6.6 Mask visualisation [i](#)

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

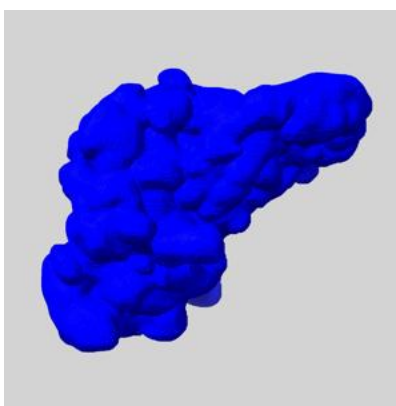
A mask typically either:

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

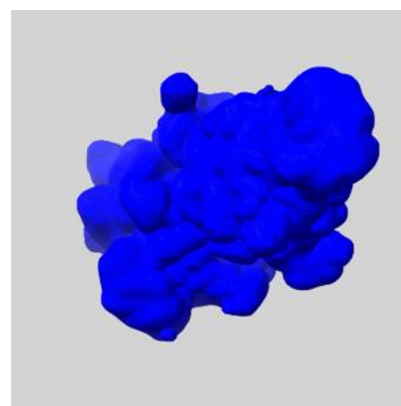
6.6.1 emd_10021_msk_1.map [i](#)



X



Y

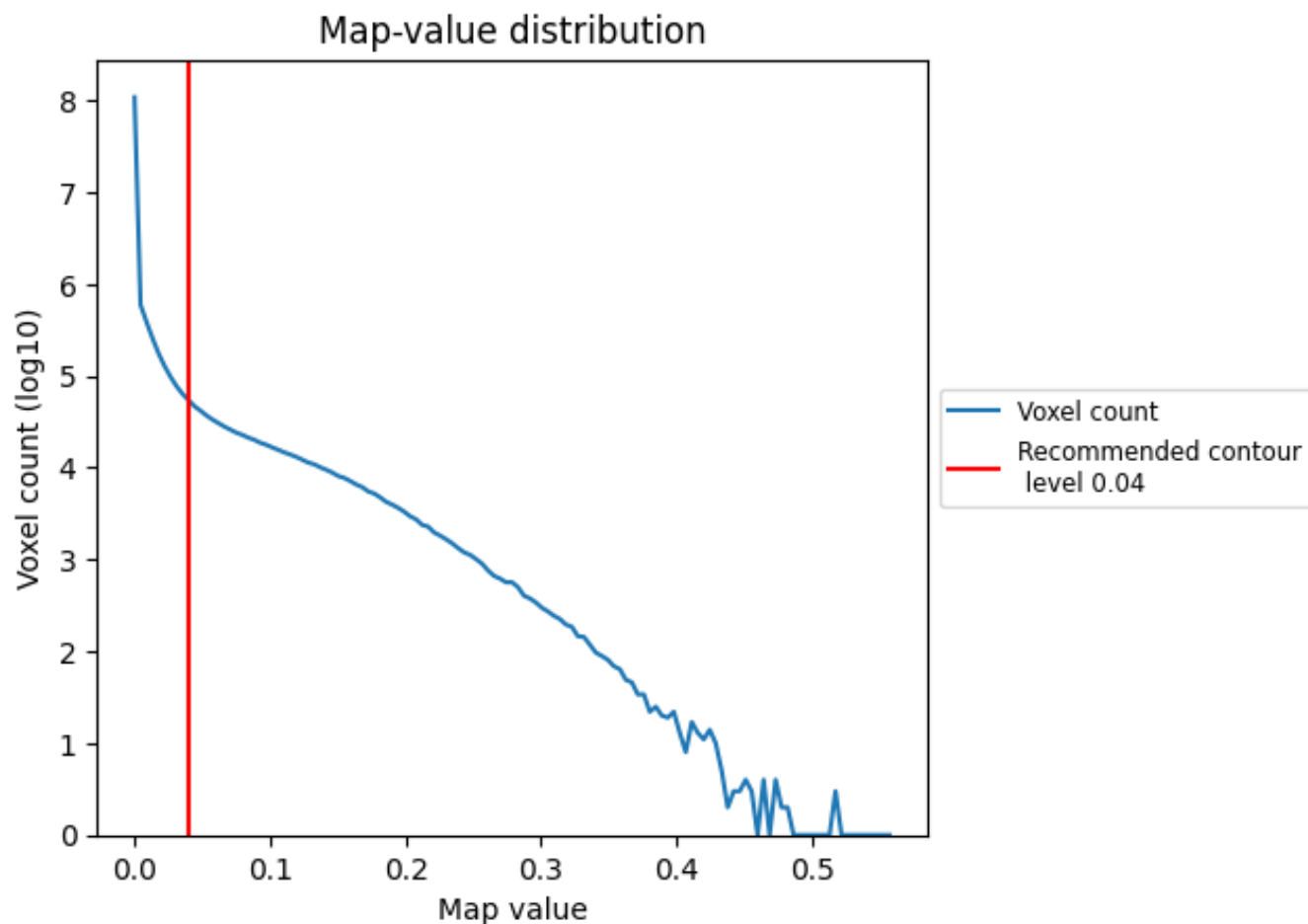


Z

7 Map analysis [i](#)

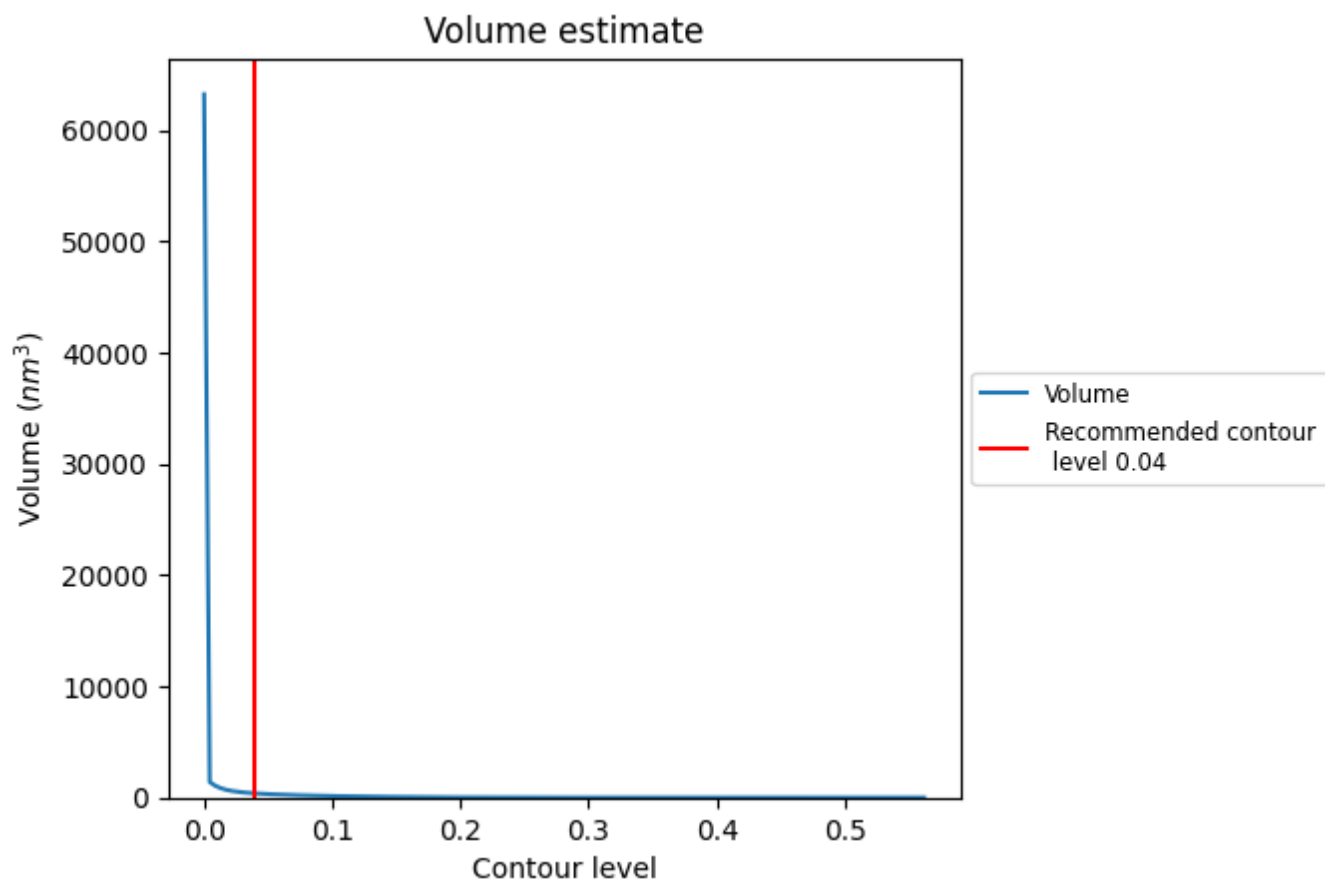
This section contains the results of statistical analysis of the map.

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.

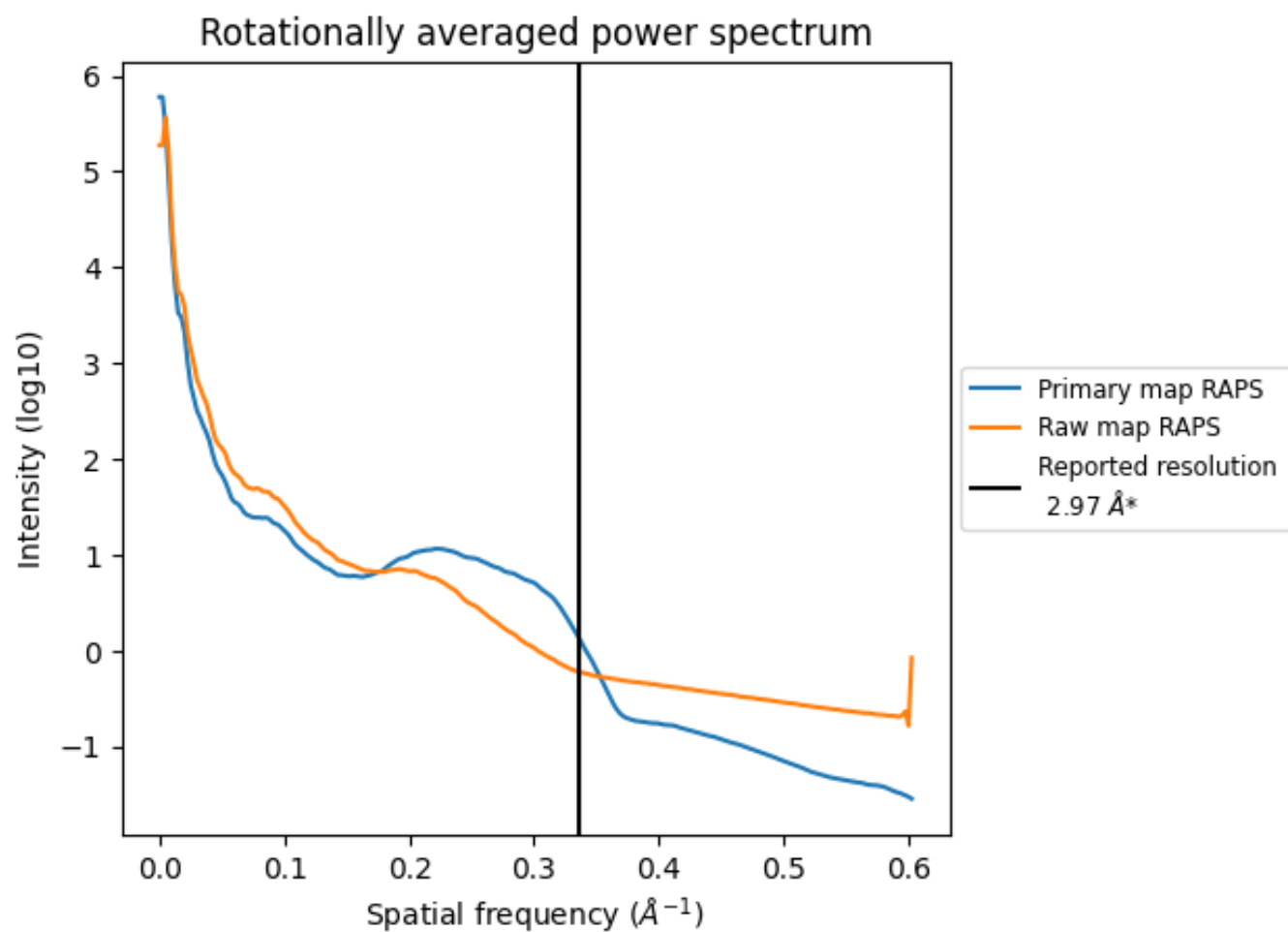
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 374 nm^3 ; this corresponds to an approximate mass of 338 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 ⓘ

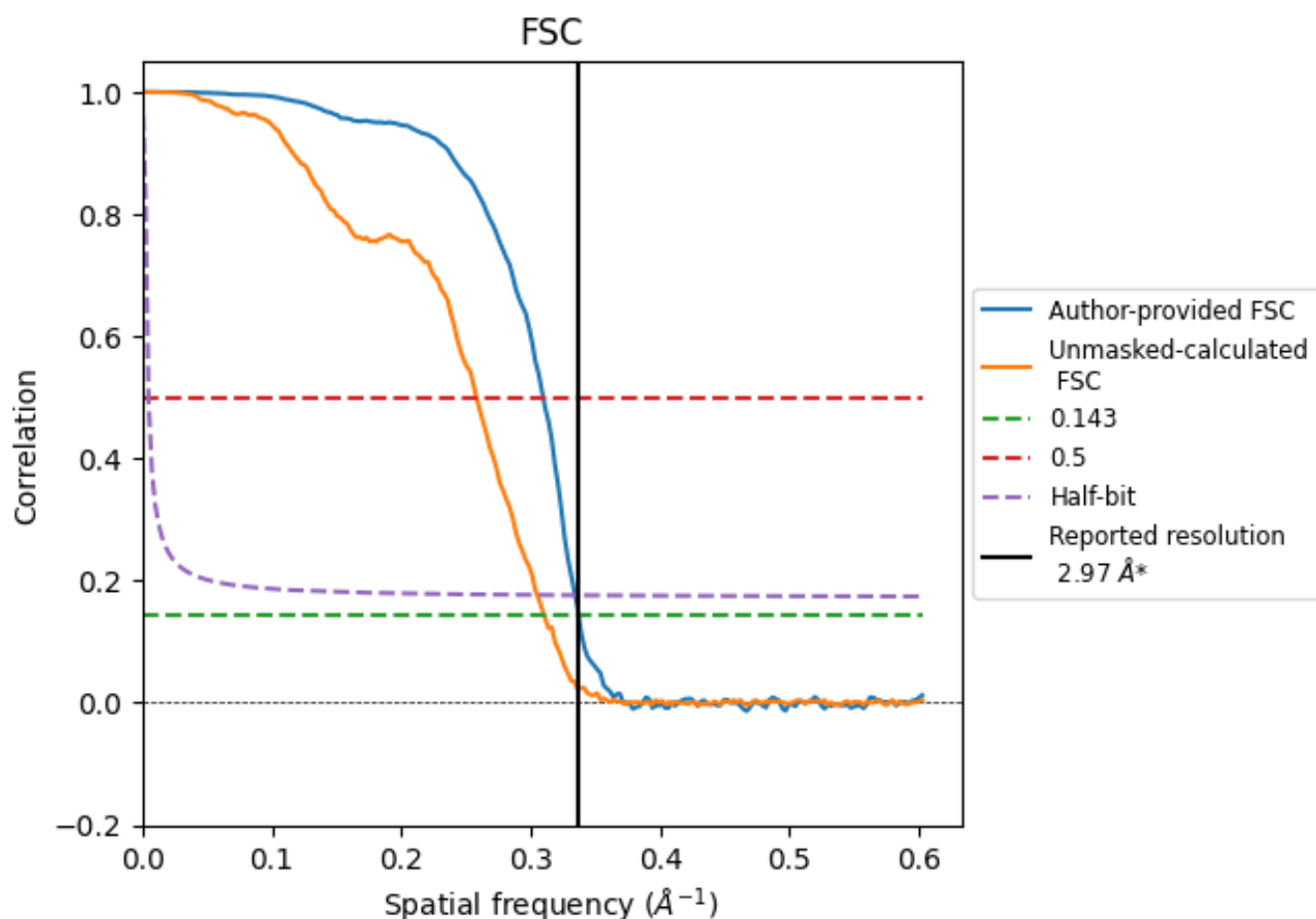


*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

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 0.337 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.23	2.99
Unmasked-calculated*	3.22	3.87	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

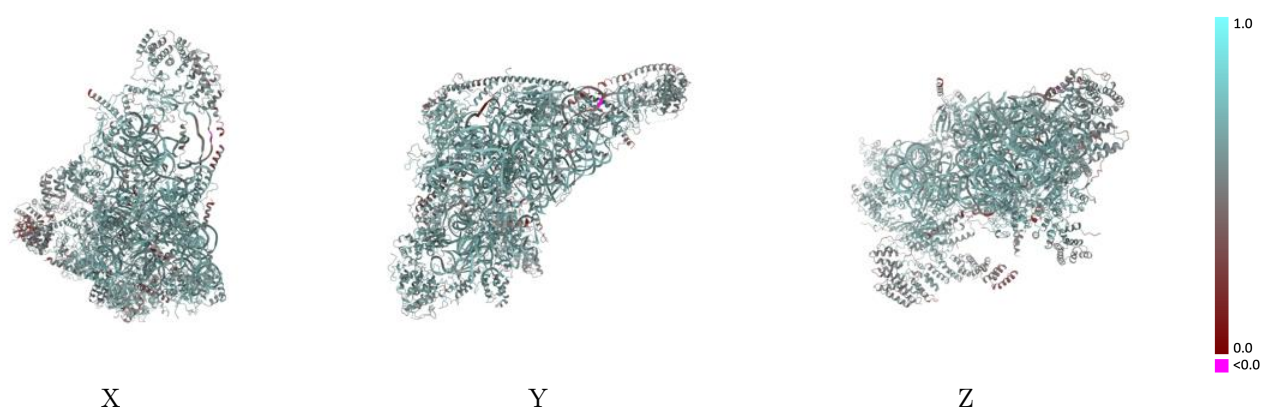
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10021 and PDB model 6RW4. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)

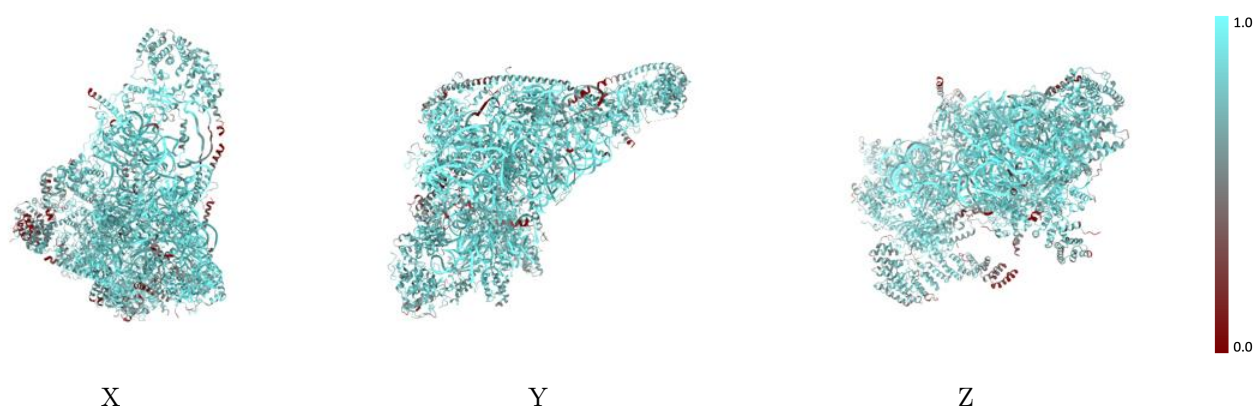
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



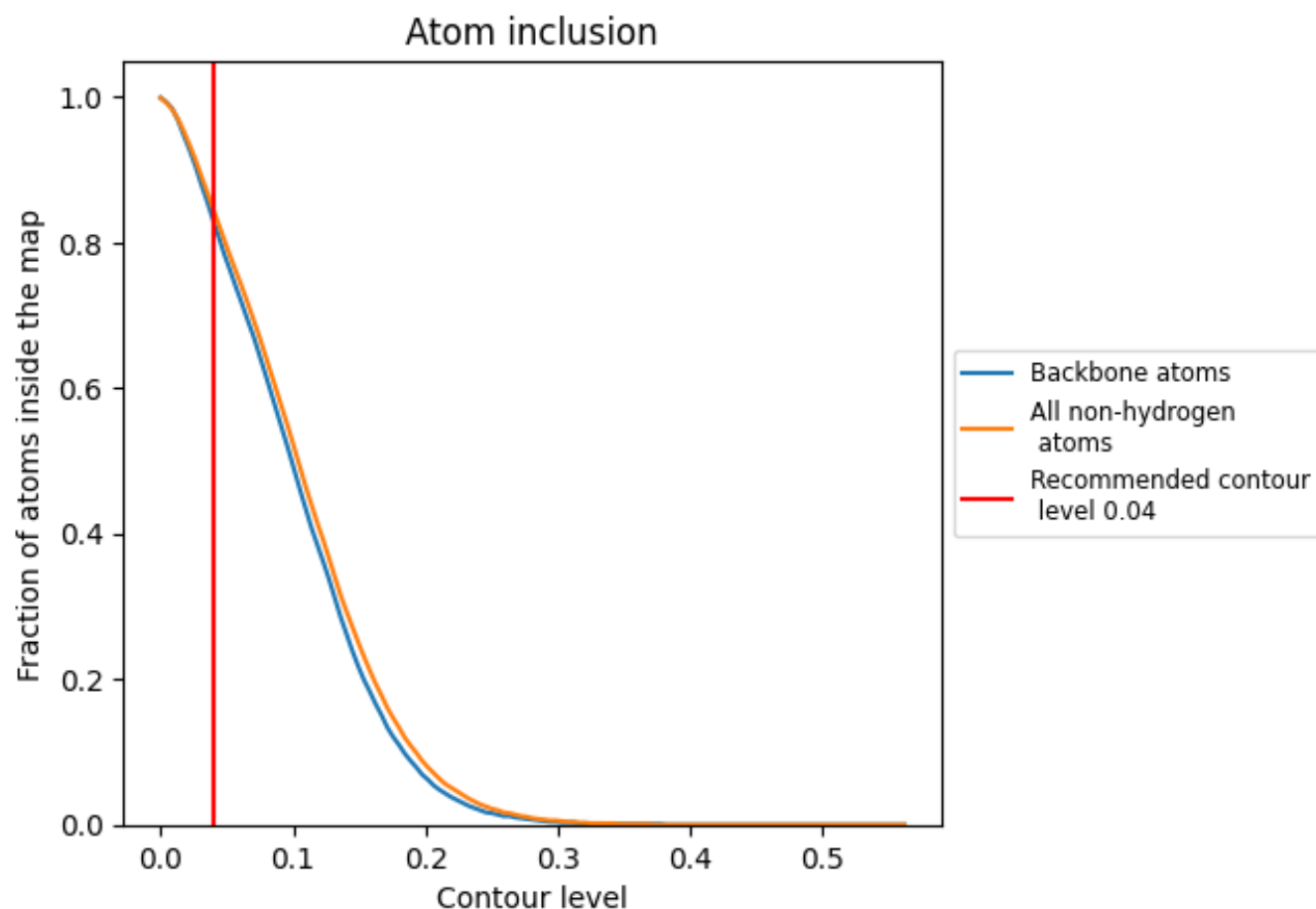
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.5990
0	 0.8300	 0.5730
1	 0.8000	 0.5940
2	 0.6320	 0.5330
3	 0.8570	 0.6390
4	 0.6910	 0.5090
8	 0.6120	 0.5220
A	 0.9490	 0.6360
B	 0.8750	 0.6210
C	 0.9420	 0.6650
D	 0.8380	 0.6000
E	 0.8370	 0.6130
F	 0.7720	 0.5840
G	 0.7600	 0.5730
H	 0.8750	 0.6170
I	 0.9110	 0.6240
J	 0.8820	 0.6180
K	 0.9230	 0.6600
L	 0.7720	 0.5770
M	 0.8820	 0.6190
N	 0.9070	 0.6400
O	 0.8640	 0.6210
P	 0.8720	 0.6150
Q	 0.9010	 0.6390
R	 0.7780	 0.5840
S	 0.7400	 0.5680
T	 0.8650	 0.6220
U	 0.7270	 0.5490
V	 0.7440	 0.5270
W	 0.8480	 0.6110
X	 0.8190	 0.5990
Y	 0.7170	 0.5570
Z	 0.8330	 0.6100

