



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 11:50 PM UTC

PDB ID : 6RW5 / pdb_00006rw5
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 ⓘ 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:

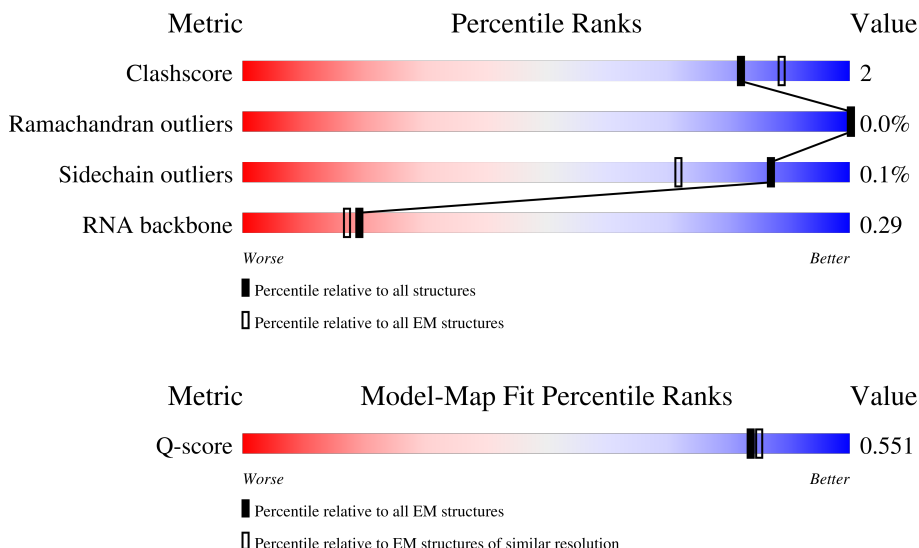
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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



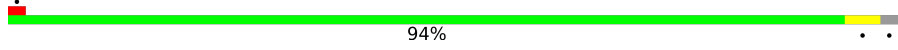
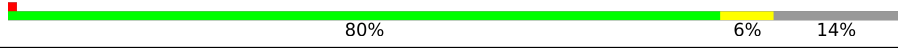
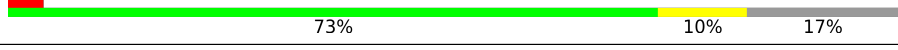
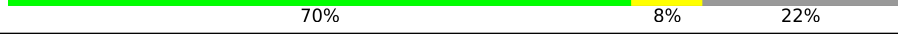
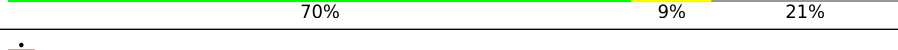
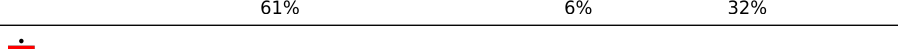
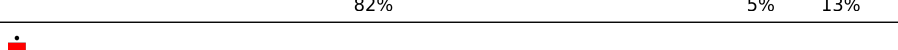
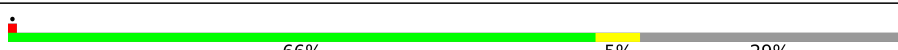
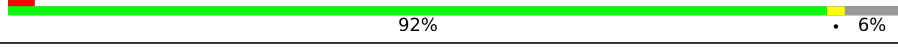
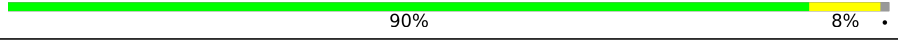
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14483 (2.64 - 3.64)

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	
30	3	199	
31	4	689	
32	7	699	
33	8	285	

2 Entry composition

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
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-2, mitochondrial.

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

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

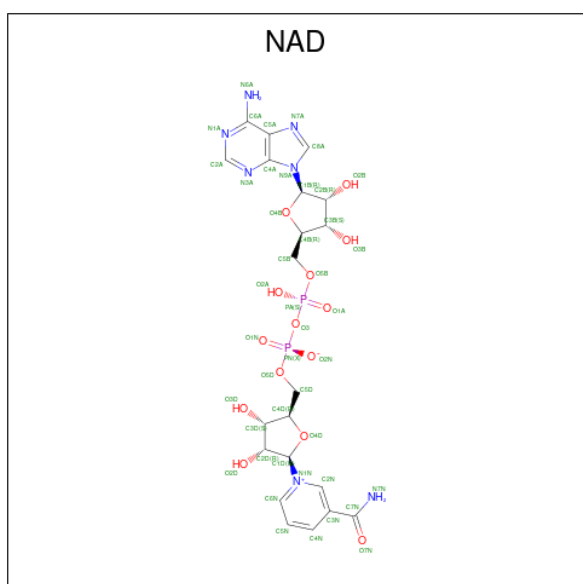
- Molecule 33 is a protein called Translation initiation factor IF-3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	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:

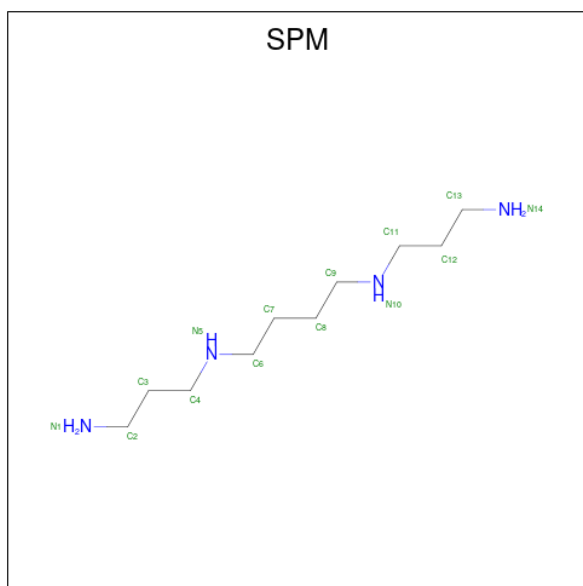
Chain	Residue	Modelled	Actual	Comment	Reference
8	68	ILE	THR	variant	UNP Q9H2K0
8	243	LEU	PHE	variant	UNP Q9H2K0
8	279	GLY	-	expression tag	UNP Q9H2K0
8	280	LEU	-	expression tag	UNP Q9H2K0
8	281	GLU	-	expression tag	UNP Q9H2K0
8	282	VAL	-	expression tag	UNP Q9H2K0
8	283	LEU	-	expression tag	UNP Q9H2K0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

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



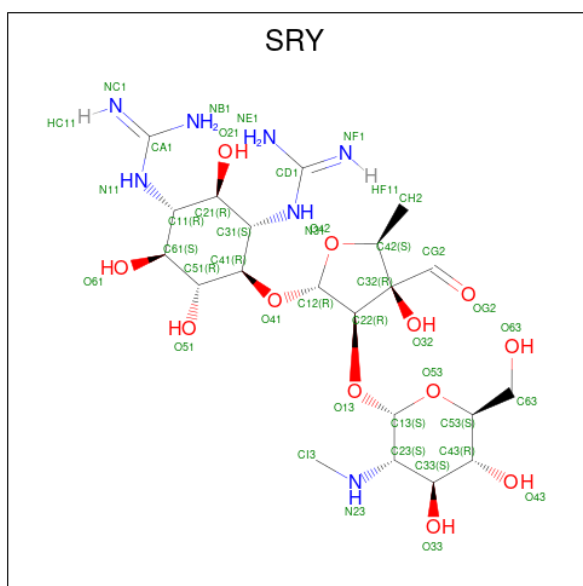
Mol	Chain	Residues	Atoms						AltConf
34	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 35 is SPERMINE (CCD ID: SPM) (formula: $\text{C}_{10}\text{H}_{26}\text{N}_4$).



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

- Molecule 36 is STREPTOMYCIN (CCD ID: SRY) (formula: $\text{C}_{21}\text{H}_{39}\text{N}_7\text{O}_{12}$).



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

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

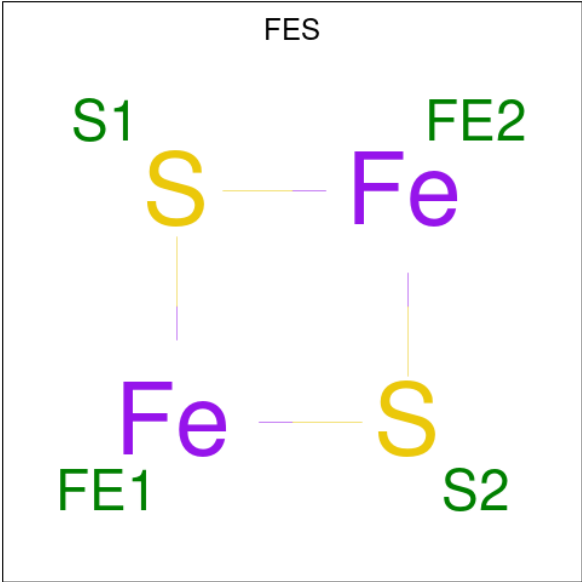
- Molecule 38 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

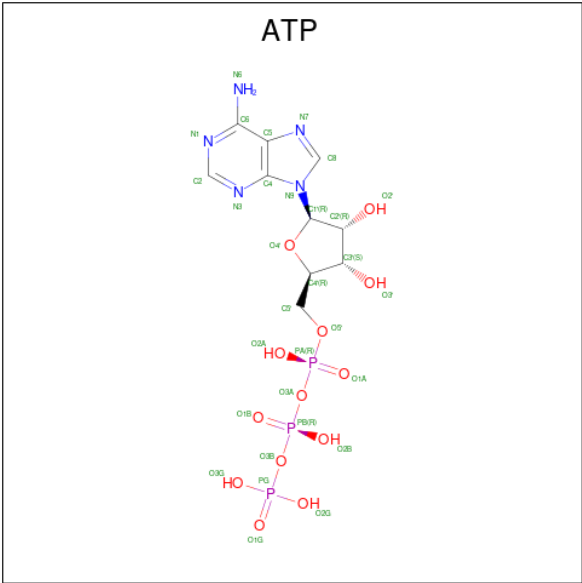
Mol	Chain	Residues	Atoms		AltConf
39	O	1	Total	Zn	0
			1	1	

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

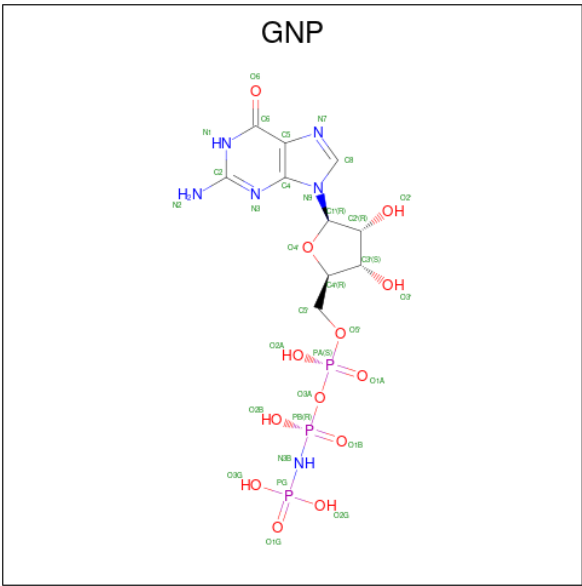
- Molecule 41 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 42 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID:

GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 43 is water.

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

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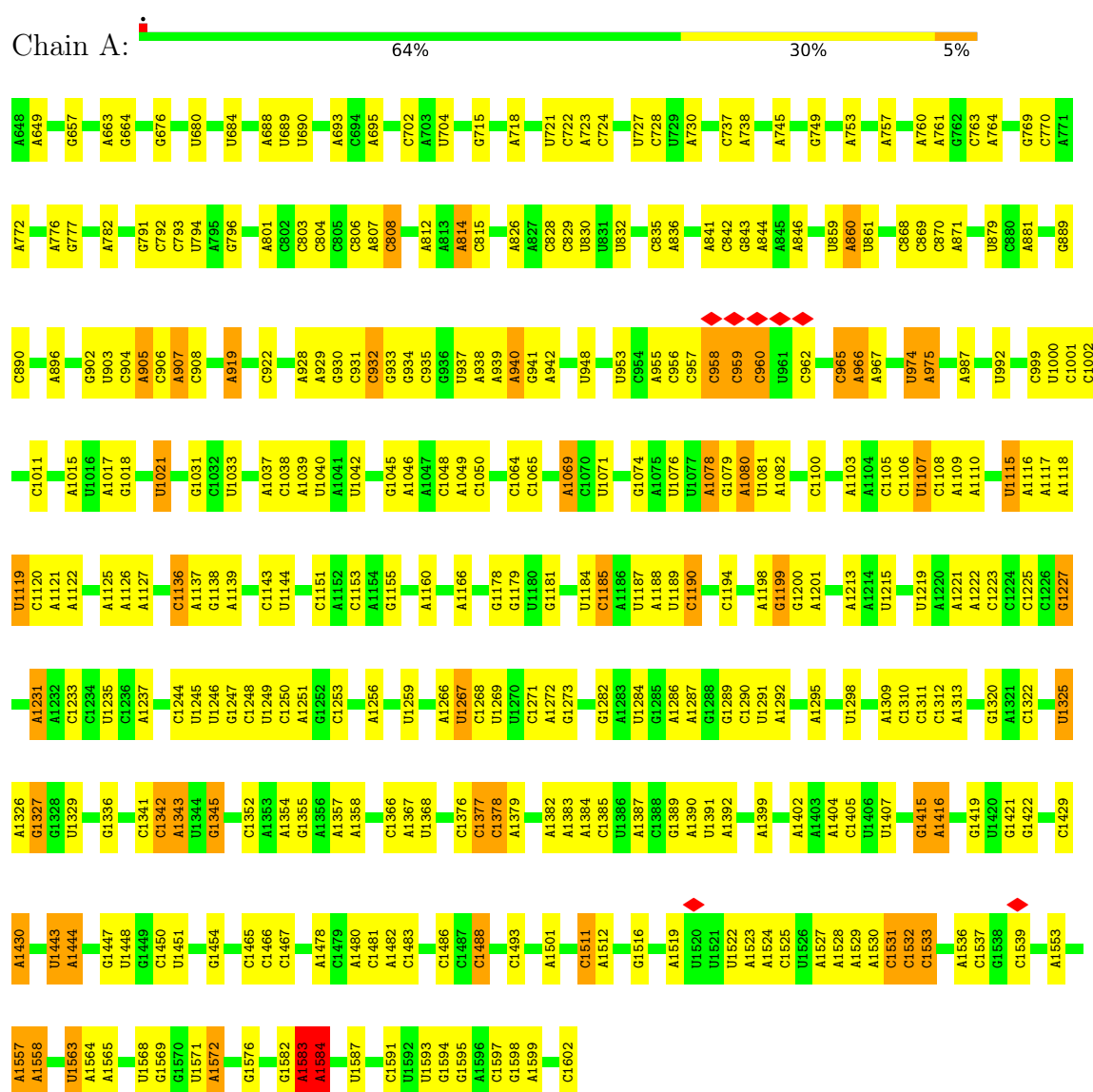
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Mol	Chain	Residues	Atoms		AltConf
43	7	2	Total	O	0
			2	2	

3 Residue-property plots

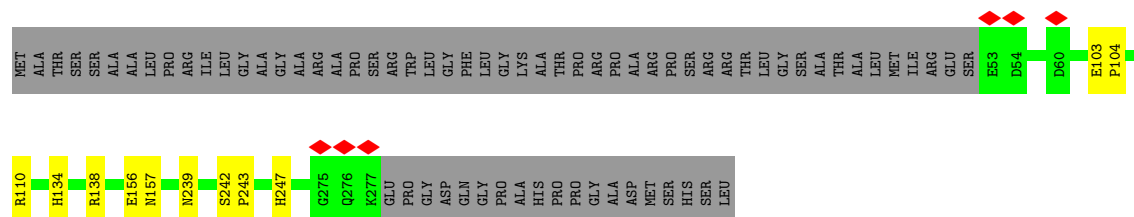
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

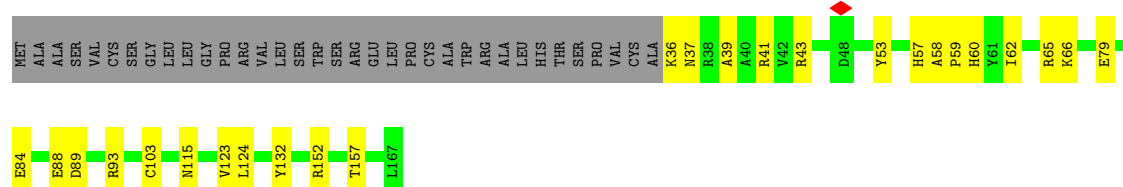


• Molecule 2: 28S ribosomal protein S2, mitochondrial

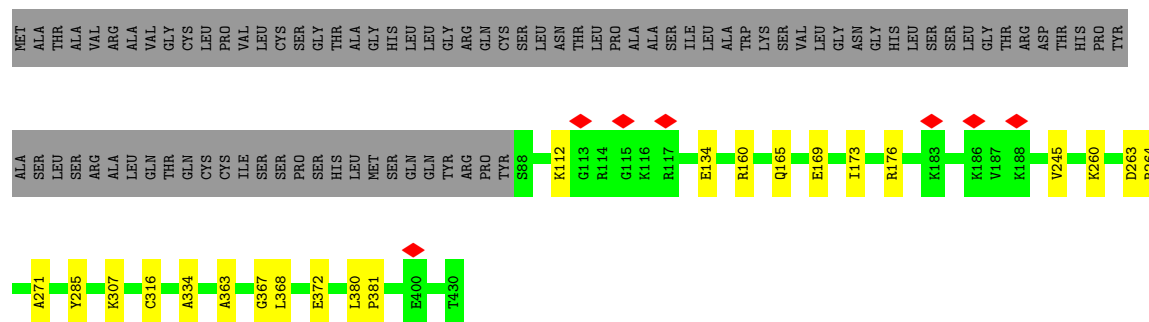
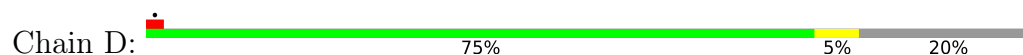




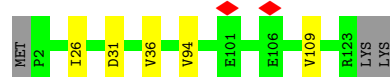
- Molecule 3: 28S ribosomal protein S24, mitochondrial



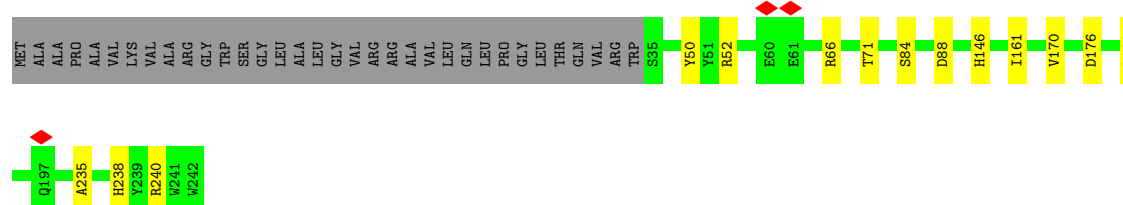
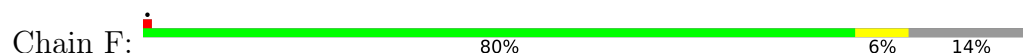
- Molecule 4: 28S ribosomal protein S5, mitochondrial



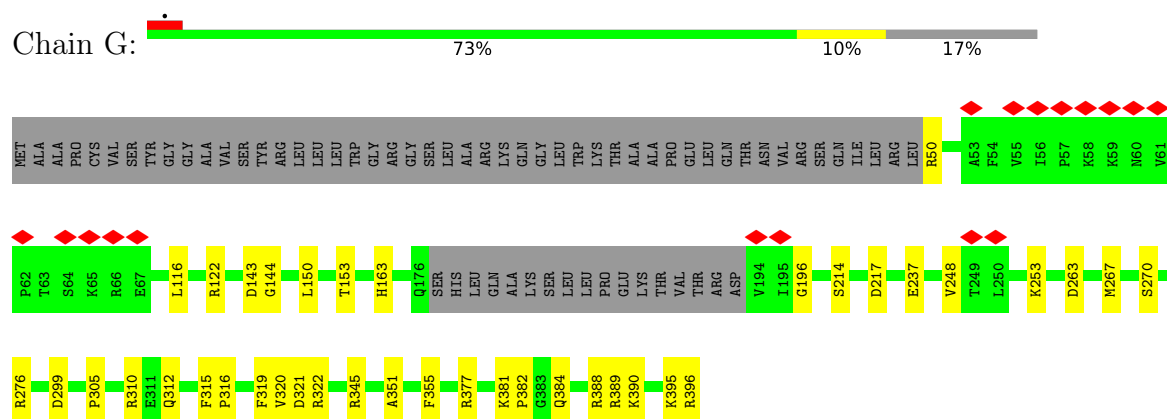
- Molecule 5: 28S ribosomal protein S6, mitochondrial



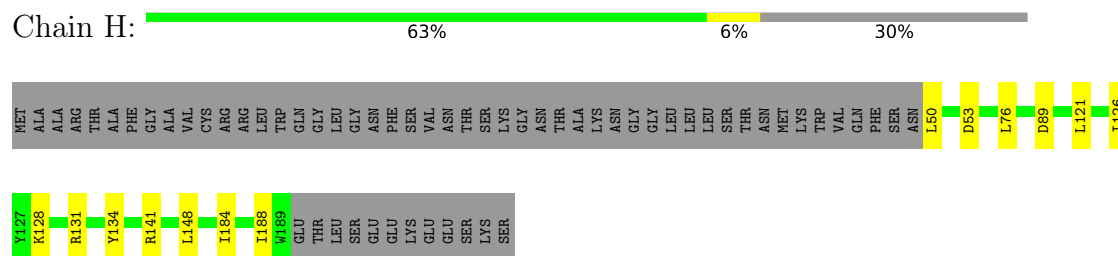
- Molecule 6: 28S ribosomal protein S7, mitochondrial



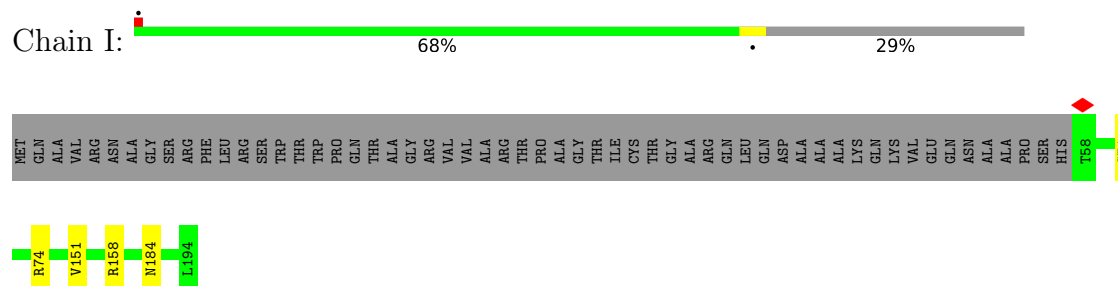
- Molecule 7: 28S ribosomal protein S9, mitochondrial



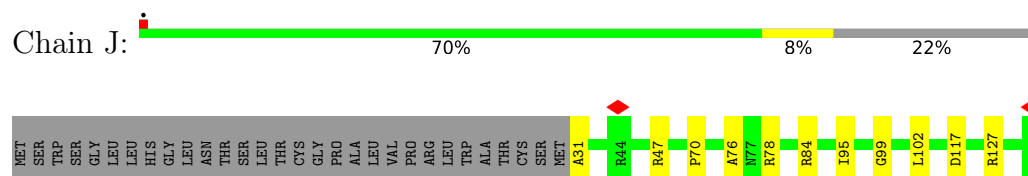
- Molecule 8: 28S ribosomal protein S10, mitochondrial



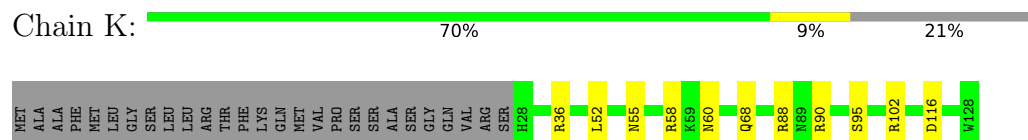
- Molecule 9: 28S ribosomal protein S11, mitochondrial



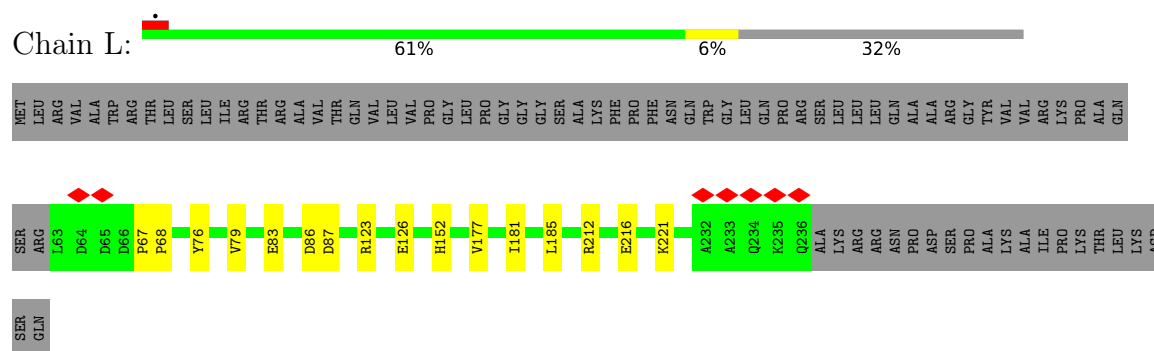
- Molecule 10: 28S ribosomal protein S12, mitochondrial



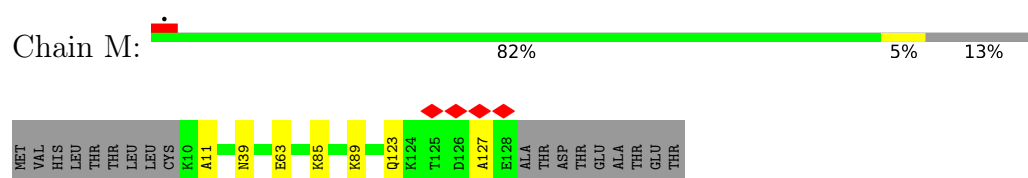
- Molecule 11: 28S ribosomal protein S14, mitochondrial



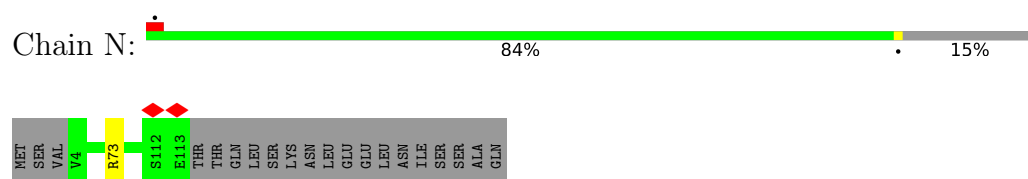
- Molecule 12: 28S ribosomal protein S15, mitochondrial



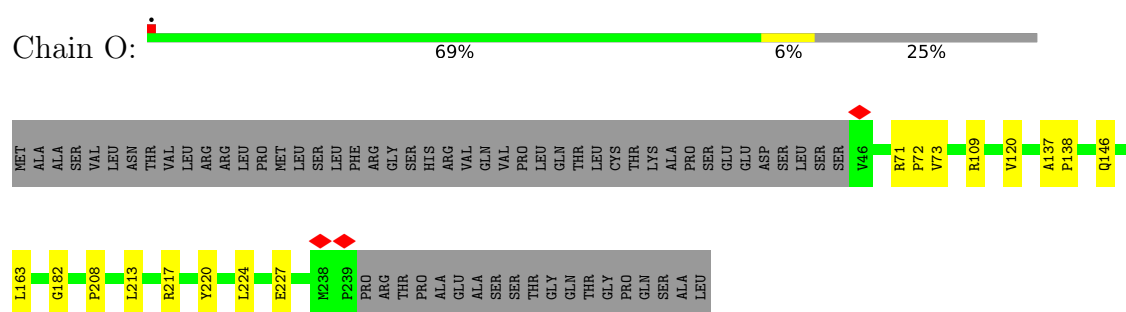
- Molecule 13: 28S ribosomal protein S16, mitochondrial



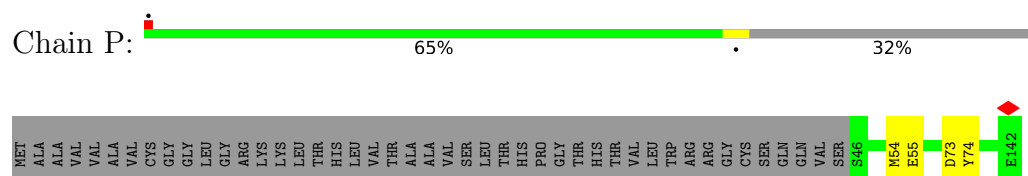
- Molecule 14: 28S ribosomal protein S17, mitochondrial



- Molecule 15: 28S ribosomal protein S18b, mitochondrial

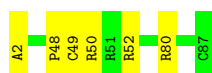


- Molecule 16: 28S ribosomal protein S18c, mitochondrial



- Molecule 17: 28S ribosomal protein S21, mitochondrial





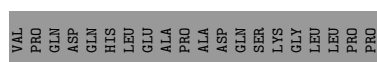
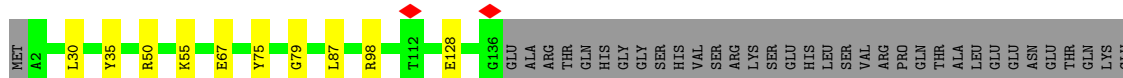
- Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R: 76% 6% 18%



- Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S: 66% 5% 29%



- Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T: 91% 6% 3%



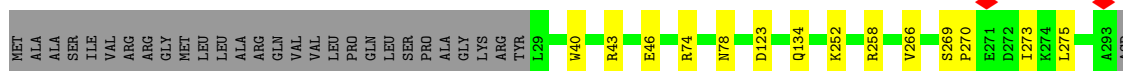
- Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U: 81% 5% 14%



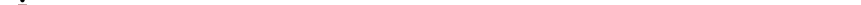
- Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V: 83% 5% 13%

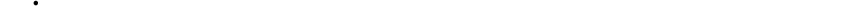


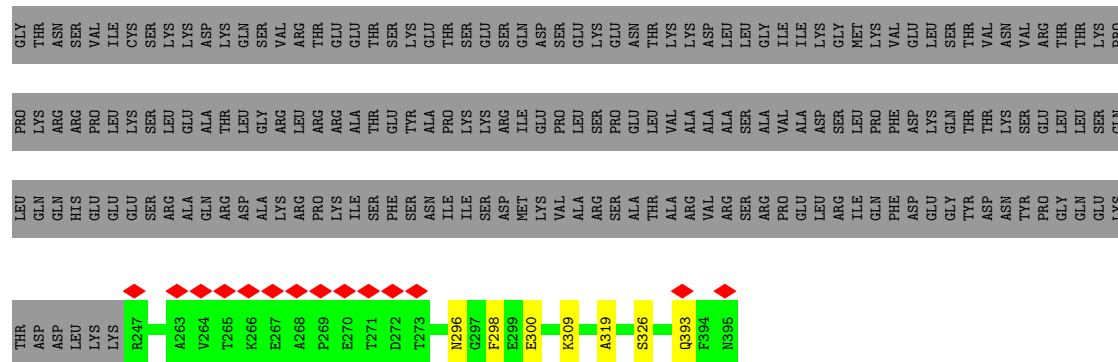
- Molecule 23: 28S ribosomal protein S28, mitochondrial

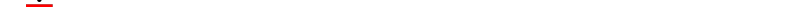


- Chain X: 
- | Residue | Category |
|---------|----------|
| MET | Green |
| LEU | Green |
| LEU | Green |
| LYS | Green |
| GLY | Green |
| ILE | Green |
| THR | Green |
| ARG | Green |
| LEU | Green |
| ILE | Green |
| SER | Green |
| ARG | Green |
| HIS | Green |
| LYS | Green |
| LEU | Green |
| ASP | Green |
| PRO | Green |
| GLY | Green |
| PHE | Green |
| LEU | Green |
| HIS | Green |
| MET | Green |
| GLY | Green |
| THR | Green |
| GLN | Green |
| ALA | Green |
| ARG | Green |
| GLN | Green |
| SER | Green |
| ILE | Green |
| ALA | Green |
| ALA | Green |
| HIS | Green |
| LEU | Green |
| ASP | Green |
| ASN | Green |
| GLN | Green |
| VAL | Green |
| PRO | Green |
| VAL | Green |
| GLU | Green |
| SER | Green |
| PRO | Green |
| ARG | Green |
| A47 | Yellow |
| I48 | Yellow |
| E53 | Yellow |
| P80 | Yellow |
| H81 | Yellow |
| K103 | Grey |
| P104 | Grey |
| R123 | Grey |
| V127 | Grey |

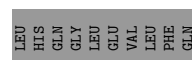


- Chain Y: 



- Chain Z:  92% 6%
- 
- MET SER S3 L36 K96 G97 E98 A102 ALA LYS ARG LYS

- Chain 0: 90% 8%



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.414	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: GNP, ATP, AYA, 5MC, 5MU, MA6, B8T, ZN, SRY, SPM, MG, FES, K, NAD

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	0.28	0/22562	0.33	0/35124
2	B	0.32	0/1871	0.38	0/2531
3	C	0.39	0/1113	0.41	0/1505
4	D	0.30	0/2783	0.37	0/3724
5	E	0.26	0/989	0.36	0/1335
6	F	0.26	0/1767	0.35	0/2373
7	G	0.28	0/2775	0.36	0/3720
8	H	0.35	0/1178	0.37	0/1598
9	I	0.26	0/1039	0.35	0/1400
10	J	0.34	0/855	0.38	0/1148
11	K	0.39	0/880	0.41	0/1182
12	L	0.29	0/1477	0.36	0/1974
13	M	0.34	0/963	0.41	0/1295
14	N	0.32	0/886	0.33	0/1199
15	O	0.30	0/1655	0.35	0/2254
16	P	0.31	0/798	0.36	0/1070
17	Q	0.32	0/748	0.44	0/994
18	R	0.26	0/2456	0.33	0/3317
19	S	0.25	0/1138	0.33	0/1533
20	T	0.31	0/1402	0.38	0/1883
21	U	0.23	0/1510	0.36	0/2025
22	V	0.18	0/3030	0.31	0/4093
23	W	0.27	0/801	0.33	0/1079
24	X	0.26	0/2921	0.35	0/3954
25	Y	0.26	0/1280	0.32	0/1725
26	Z	0.30	0/857	0.36	0/1141
27	0	0.26	0/1834	0.38	0/2484
28	1	0.29	0/2285	0.35	0/3090
29	2	0.24	0/941	0.38	0/1257
30	3	0.30	0/636	0.45	0/839
31	4	0.21	0/4877	0.34	0/6598
32	7	0.14	0/4501	0.29	0/6073

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	8	0.15	0/1560	0.35	0/2089
All	All	0.27	0/76368	0.35	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	80	0
2	B	1828	1816	1815	8	0
3	C	1083	1089	1088	16	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	16	0
19	S	1111	1116	1115	9	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	22	0

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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	13	0
29	2	935	969	969	4	0
30	3	625	700	699	1	0
31	4	4768	4768	4766	27	0
32	7	4431	4505	4502	21	0
33	8	1543	1588	1587	13	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	331	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 (331) 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
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
28:1:253:TRP:O	28:1:256:SER:OG	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
3:C:79:GLU:OE1	28:1:158:SER:OG	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:236:VAL:HG12	31:4:238:TRP:H	1.73	0.53
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
18:R:262:LEU:O	18:R:265:THR:OG1	2.25	0.52
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
20:T:9:ILE:O	20:T:12:THR:OG1	2.24	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
7:G:270:SER:OG	7:G:351:ALA:O	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1325:U:OP1	4:D:112:LYS:NZ	2.44	0.49
1:A:1115:U:OP1	19:S:55:LYS:NZ	2.43	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
31:4:255:ASN:O	31:4:258:SER:OG	2.30	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
28:1:60:MET:HE1	28:1:80:ALA:O	2.15	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1481:C:O2	1:A:1481:C:O2'	2.32	0.46
1:A:1531:C:O3'	1:A:1532:C:H6	1.98	0.46
31:4:493:MET:HA	31:4:493:MET:HE2	1.97	0.45
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:702:C:O2'	1:A:842:C:O2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:299:ASP:OD2	24:X:385:ASN:ND2	2.51	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
3:C:53:TYR:OH	3:C:65:ARG:O	2.23	0.43
4:D:368:LEU:HD22	18:R:107:THR:HG22	2.00	0.43
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
24:X:369:GLU:CD	24:X:369:GLU:H	2.26	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
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
33:8:235:ALA:C	33:8:236:LEU:HD12	2.44	0.43
10:J:84:ARG:NH1	32:7:565:GLU:OE1	2.45	0.42
15:O:146:GLN:OE1	15:O:146:GLN:HA	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1378:C:O2	24:X:389:SER:OG	2.26	0.42
25:Y:393:GLN:O	25:Y:393:GLN:HG3	2.19	0.42
27:O:163:SER:HA	27:O: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
28:1:173:LEU:HD23	28:1:173:LEU:C	2.45	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
31:4:290:ASP:OD1	31:4:293:THR:OG1	2.37	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
12:L:123:ARG:O	12:L:123:ARG:HG2	2.21	0.41
19:S:35:TYR:C	19:S:35:TYR:CD1	2.98	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
6:F:71:THR:O	7:G:253:LYS:NZ	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
18:R:242:TYR:CD1	18:R:242:TYR:C	2.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	18	47
9	I	135/194 (70%)	126 (93%)	8 (6%)	1 (1%)	18	47
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
32	7	569/699 (81%)	548 (96%)	21 (4%)	0	100	100
33	8	189/285 (66%)	184 (97%)	4 (2%)	1 (0%)	24	54
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 ⓘ

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	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
17	Q	78/78 (100%)	78 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100
19	S	116/164 (71%)	116 (100%)	0	100	100
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	V	325/364 (89%)	325 (100%)	0	100	100
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	310 (100%)	1 (0%)	86	85
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%)	187 (100%)	1 (0%)	81	82
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	7	481/595 (81%)	481 (100%)	0	100	100
33	8	172/253 (68%)	171 (99%)	1 (1%)	78	80
All	All	5708/7192 (79%)	5705 (100%)	3 (0%)	87	89

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

Mol	Chain	Res	Type
24	X	81	HIS
27	0	79	LEU
33	8	238	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	90	HIS
2	B	167	HIS
2	B	178	ASN
4	D	347	GLN
4	D	359	HIS
4	D	369	HIS
4	D	415	GLN
5	E	54	HIS
5	E	58	HIS
5	E	81	HIS
6	F	169	GLN
6	F	207	HIS
7	G	308	GLN
8	H	109	HIS
8	H	147	HIS
10	J	105	HIS
11	K	28	HIS
12	L	162	GLN
15	O	147	HIS
18	R	214	ASN
19	S	66	HIS
22	V	38	HIS
22	V	87	HIS
22	V	188	HIS
22	V	215	GLN
22	V	380	GLN
22	V	391	GLN
23	W	106	HIS
24	X	159	HIS
24	X	302	HIS
24	X	326	GLN
25	Y	290	ASN
26	Z	55	HIS
27	0	137	HIS
27	0	145	HIS
31	4	243	ASN

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Mol	Chain	Res	Type
31	4	257	HIS
31	4	453	HIS
31	4	489	HIS
31	4	504	ASN
31	4	577	ASN
32	7	330	ASN
32	7	377	GLN
33	8	198	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	954/955 (99%)	284 (29%)	10 (1%)

All (284) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	1583	MA6

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Mol	Chain	Res	Type
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 (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	$\# Z > 2$
1	5MC	A	1488	1	19,22,23	1.69	3 (15%)	26,32,35	1.91	8 (30%)
29	AYA	2	2	29	6,7,8	1.35	1 (16%)	6,8,10	1.22	1 (16%)
1	MA6	A	1583	1	23,26,27	0.82	1 (4%)	33,38,41	2.09	9 (27%)
17	AYA	Q	2	17	6,7,8	1.39	1 (16%)	6,8,10	1.10	0
1	B8T	A	1486	1	19,22,23	0.88	2 (10%)	25,31,34	0.98	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	A	1584	1	23,26,27	0.83	1 (4%)	33,38,41	2.12	9 (27%)
1	5MU	A	1076	1	19,22,23	1.13	3 (15%)	27,32,35	2.18	8 (29%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1488	5MC	C5-C4	-5.22	1.40	1.44
17	Q	2	AYA	CA-N	-2.89	1.43	1.46
1	A	1488	5MC	C2-N1	-2.80	1.34	1.40
1	A	1076	5MU	C2-N1	-2.76	1.34	1.38
1	A	1076	5MU	C4-C5	-2.70	1.40	1.44
29	2	2	AYA	CA-N	-2.69	1.43	1.46
1	A	1584	MA6	C5-N7	-2.26	1.35	1.39
1	A	1486	B8T	C2-N1	-2.26	1.35	1.40
1	A	1486	B8T	C6-N1	2.20	1.43	1.38
1	A	1488	5MC	C2'-C3'	-2.07	1.47	1.53
1	A	1583	MA6	C5-N7	-2.05	1.35	1.39
1	A	1076	5MU	C4-N3	-2.04	1.35	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1076	5MU	C4-N3-C2	-5.54	120.07	127.34
1	A	1584	MA6	C5-C4-N3	-5.17	119.60	126.72
1	A	1583	MA6	N1-C2-N3	-4.86	121.22	128.58
1	A	1076	5MU	N3-C2-N1	4.75	121.07	114.89
1	A	1584	MA6	N1-C2-N3	-4.69	121.48	128.58
1	A	1583	MA6	C5-C4-N3	-4.60	120.38	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1583	MA6	C2-N1-C6	4.50	122.81	111.83
1	A	1584	MA6	C2-N1-C6	4.31	122.35	111.83
1	A	1076	5MU	O4-C4-C5	-4.25	120.05	124.92
1	A	1076	5MU	C5-C4-N3	4.22	119.00	115.32
1	A	1488	5MC	O3'-C3'-C4'	4.20	123.15	111.08
1	A	1584	MA6	C5-N7-C8	4.07	109.85	103.45
1	A	1583	MA6	C5-N7-C8	3.95	109.66	103.45
1	A	1584	MA6	N3-C4-N9	3.89	133.79	127.17
1	A	1488	5MC	O3'-C3'-C2'	3.79	123.96	111.82
1	A	1584	MA6	C2-N3-C4	3.72	120.92	111.83
1	A	1583	MA6	N3-C4-N9	3.66	133.40	127.17
1	A	1583	MA6	C2-N3-C4	3.53	120.45	111.83
1	A	1488	5MC	C5-C6-N1	-3.50	119.52	123.31
1	A	1584	MA6	C4-C5-N7	-3.49	106.59	110.58
1	A	1583	MA6	N9-C8-N7	-3.31	109.23	113.94
1	A	1583	MA6	C4-C5-N7	-3.30	106.81	110.58
1	A	1076	5MU	C5-C6-N1	-3.14	119.90	123.31
1	A	1488	5MC	O2'-C2'-C3'	3.11	121.78	111.82
1	A	1584	MA6	N9-C8-N7	-3.00	109.68	113.94
29	2	2	AYA	CB-CA-N	2.63	112.65	109.68
1	A	1076	5MU	C5M-C5-C6	-2.58	119.36	122.85
1	A	1076	5MU	O2-C2-N1	-2.56	119.46	122.80
1	A	1488	5MC	O2'-C2'-C1'	2.55	118.88	110.10
1	A	1488	5MC	CM5-C5-C6	-2.52	119.44	122.85
1	A	1488	5MC	C5-C4-N3	-2.26	119.44	121.75
1	A	1584	MA6	C4-C5-C6	2.23	118.22	115.91
1	A	1583	MA6	C4-N9-C8	2.23	108.08	105.74
1	A	1488	5MC	C1'-N1-C6	-2.21	117.51	121.15
1	A	1076	5MU	C6-C5-C4	2.13	119.78	118.02
1	A	1486	B8T	C5-C4-N4	-2.09	117.81	122.40

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.

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 oligosaccharides 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	$\# Z > 2$
42	GNP	7	801	37	34,34,34	1.28	5 (14%)	47,54,54	0.89	0
36	SRY	A	1703	-	40,42,42	0.81	2 (5%)	49,63,63	1.26	5 (10%)
34	NAD	A	1701	37	46,48,48	1.02	2 (4%)	64,73,73	1.54	8 (12%)
42	GNP	X	503	-	34,34,34	1.29	5 (14%)	47,54,54	0.91	0
40	FES	P	201	5,16	0,4,4	-	-	-	-	-
40	FES	T	201	13,20	0,4,4	-	-	-	-	-
35	SPM	A	1702	-	13,13,13	0.15	0	12,12,12	1.15	0
41	ATP	X	501	37	32,33,33	1.32	5 (15%)	48,52,52	1.73	10 (20%)

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
42	GNP	7	801	37	-	3/18/38/38	0/3/3/3
36	SRY	A	1703	-	-	1/20/87/87	0/3/3/3
34	NAD	A	1701	37	-	1/30/62/62	0/5/5/5
42	GNP	X	503	-	-	4/18/38/38	0/3/3/3
40	FES	P	201	5,16	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	FES	T	201	13,20	-	-	0/1/1/1
35	SPM	A	1702	-	-	0/11/11/11	-
41	ATP	X	501	37	-	0/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	X	503	GNP	PB-O3A	4.41	1.64	1.59
42	7	801	GNP	PB-O3A	4.32	1.64	1.59
41	X	501	ATP	C5-C4	4.24	1.46	1.39
42	X	503	GNP	PB-O1B	3.16	1.51	1.46
42	7	801	GNP	PB-O1B	3.14	1.50	1.46
36	A	1703	SRY	CD1-N31	2.97	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	C2N-N1N	-2.82	1.31	1.35
34	A	1701	NAD	O4D-C1D	2.80	1.44	1.40
42	X	503	GNP	PG-O1G	2.78	1.50	1.46
42	7	801	GNP	PG-O1G	2.73	1.50	1.46
36	A	1703	SRY	CA1-N11	2.71	1.37	1.33
41	X	501	ATP	C5-N7	-2.49	1.34	1.39
41	X	501	ATP	C5-C6	2.40	1.47	1.41
42	7	801	GNP	PB-O2B	-2.34	1.50	1.56
42	X	503	GNP	PB-O2B	-2.27	1.50	1.56
41	X	501	ATP	C8-N7	2.24	1.36	1.31
41	X	501	ATP	C4-N9	-2.09	1.33	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	X	501	ATP	C5-C4-N3	-5.64	118.95	126.72
34	A	1701	NAD	C5A-C4A-N3A	-5.54	119.09	126.72
36	A	1703	SRY	C12-O42-C42	-4.58	101.08	108.48
41	X	501	ATP	N3-C4-N9	4.50	134.83	127.17
34	A	1701	NAD	N3A-C2A-N1A	-4.19	122.24	128.58
34	A	1701	NAD	N3A-C4A-N9A	4.16	134.24	127.17
41	X	501	ATP	C2-N3-C4	3.86	121.25	111.83
41	X	501	ATP	N3-C2-N1	-3.77	122.87	128.58
34	A	1701	NAD	C5A-N7A-C8A	3.63	109.15	103.45
34	A	1701	NAD	C2A-N3A-C4A	3.57	120.55	111.83
34	A	1701	NAD	C4A-C5A-N7A	-3.32	106.78	110.58
41	X	501	ATP	C4-C5-N7	-3.27	106.84	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	1703	SRY	O42-C12-C22	-3.20	103.88	107.31
41	X	501	ATP	C4-N9-C8	2.85	108.73	105.74
41	X	501	ATP	C5-N7-C8	2.50	107.39	103.45
34	A	1701	NAD	N9A-C8A-N7A	-2.36	110.58	113.94
36	A	1703	SRY	C41-C31-N31	-2.26	107.30	110.91
41	X	501	ATP	N9-C8-N7	-2.20	110.82	113.94
36	A	1703	SRY	CI3-N23-C23	-2.19	111.40	114.23
41	X	501	ATP	C6-C5-N7	2.17	136.26	132.09
36	A	1703	SRY	CH2-C42-C32	-2.13	111.85	116.27
34	A	1701	NAD	O7N-C7N-N7N	-2.06	119.65	122.62
41	X	501	ATP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (9) 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-O2B
42	7	801	GNP	PG-N3B-PB-O1B
42	7	801	GNP	O4'-C4'-C5'-O5'
42	X	503	GNP	C5'-O5'-PA-O1A
42	7	801	GNP	C5'-O5'-PA-O1A
36	A	1703	SRY	C13-C23-N23-CI3
42	X	503	GNP	PG-N3B-PB-O1B
34	A	1701	NAD	C2B-C1B-N9A-C8A

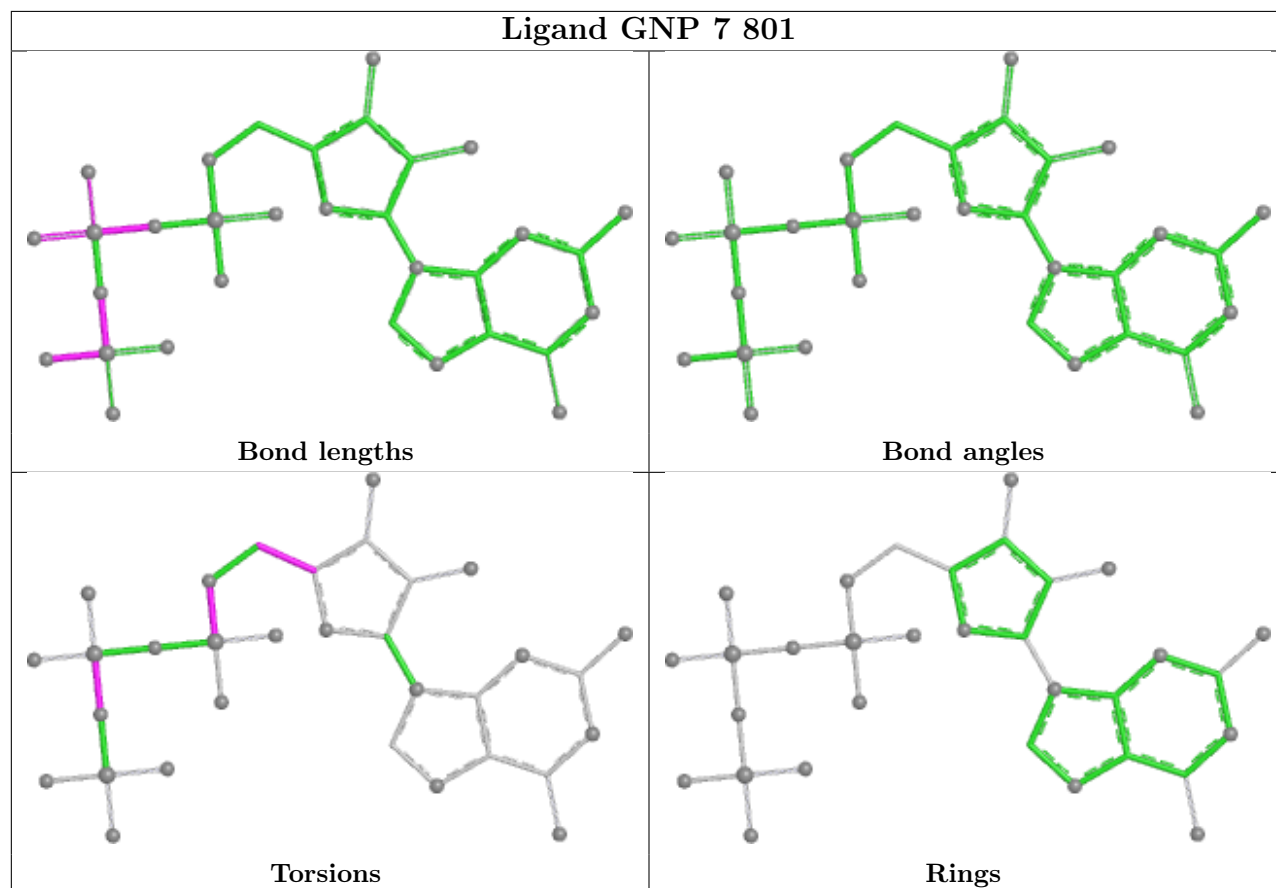
There are no ring outliers.

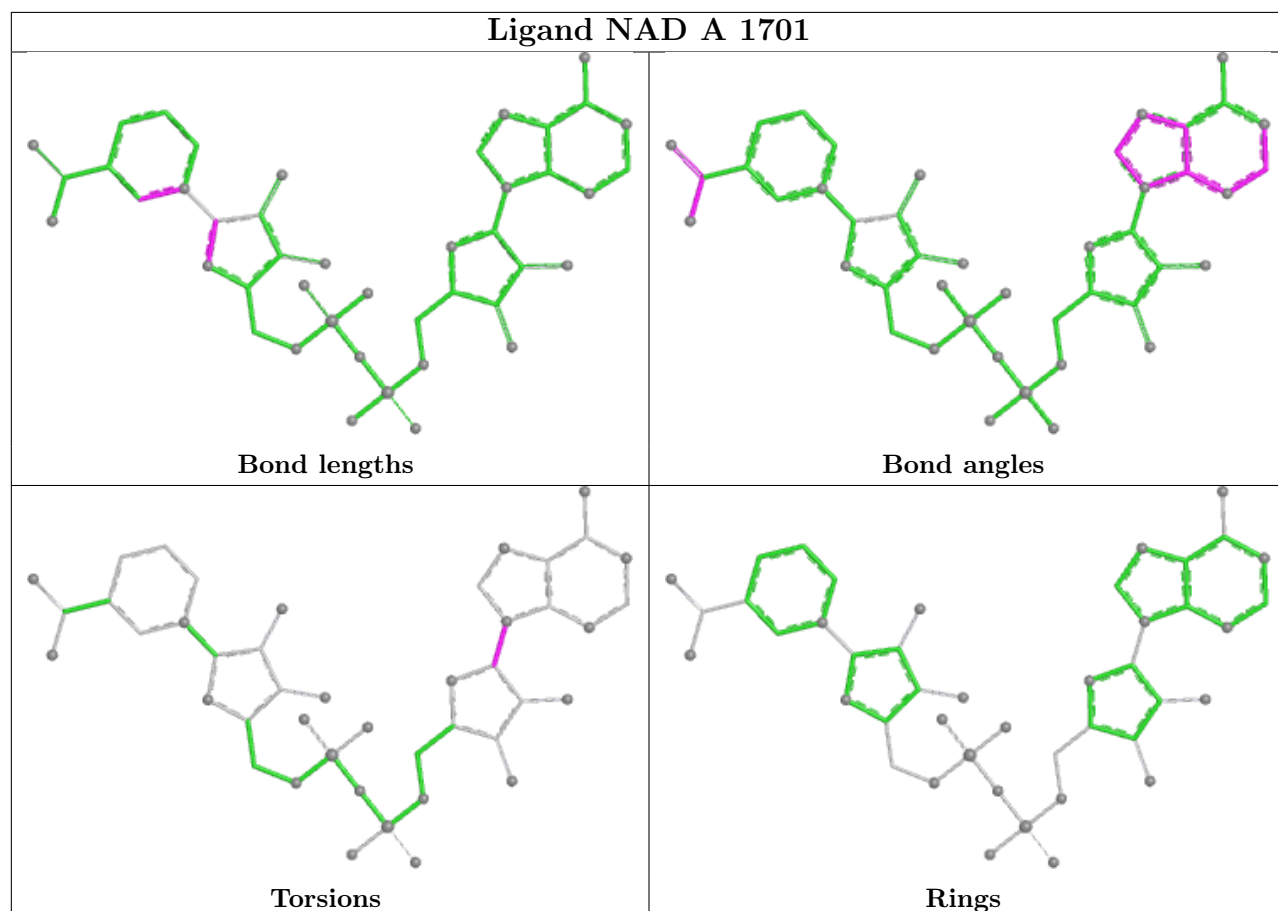
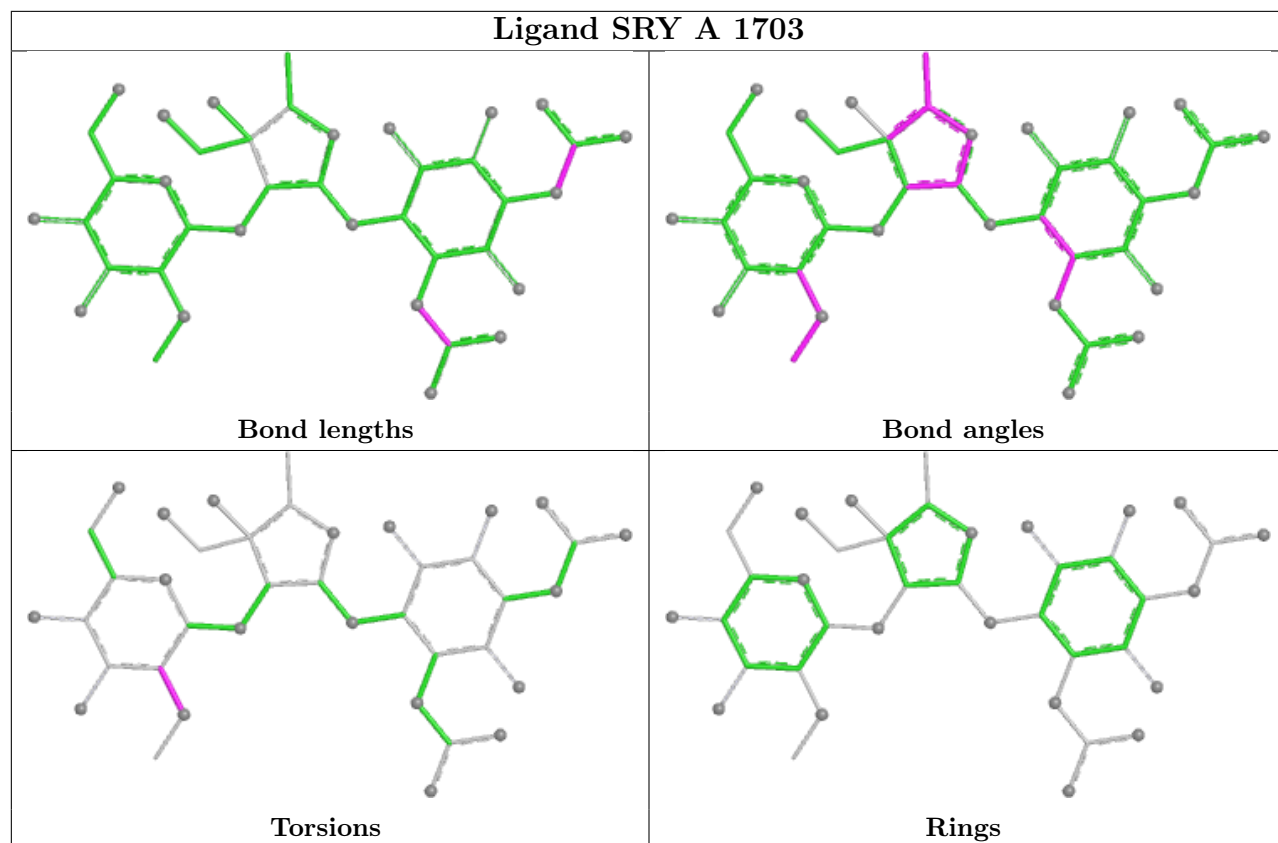
2 monomers are involved in 2 short contacts:

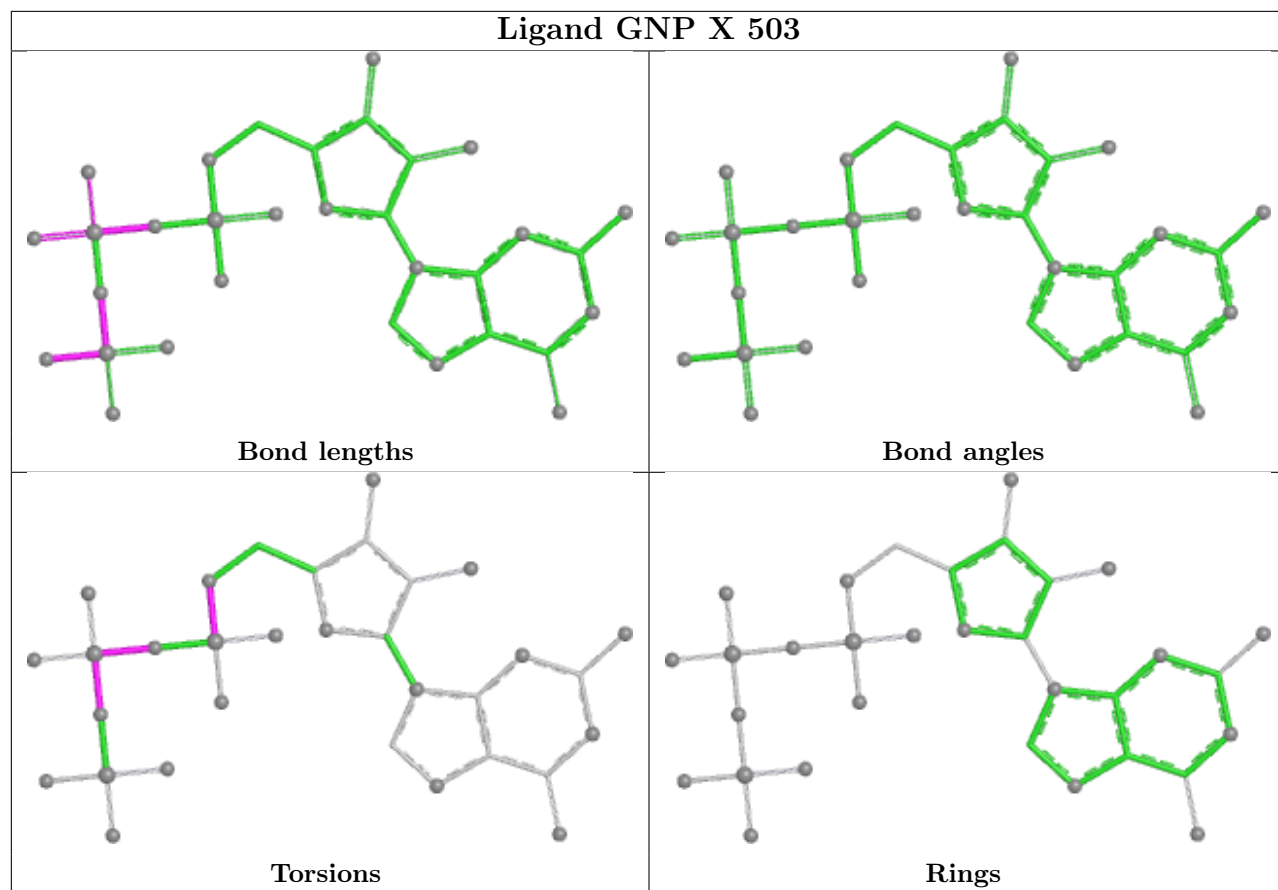
Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	7	801	GNP	1	0
34	A	1701	NAD	1	0

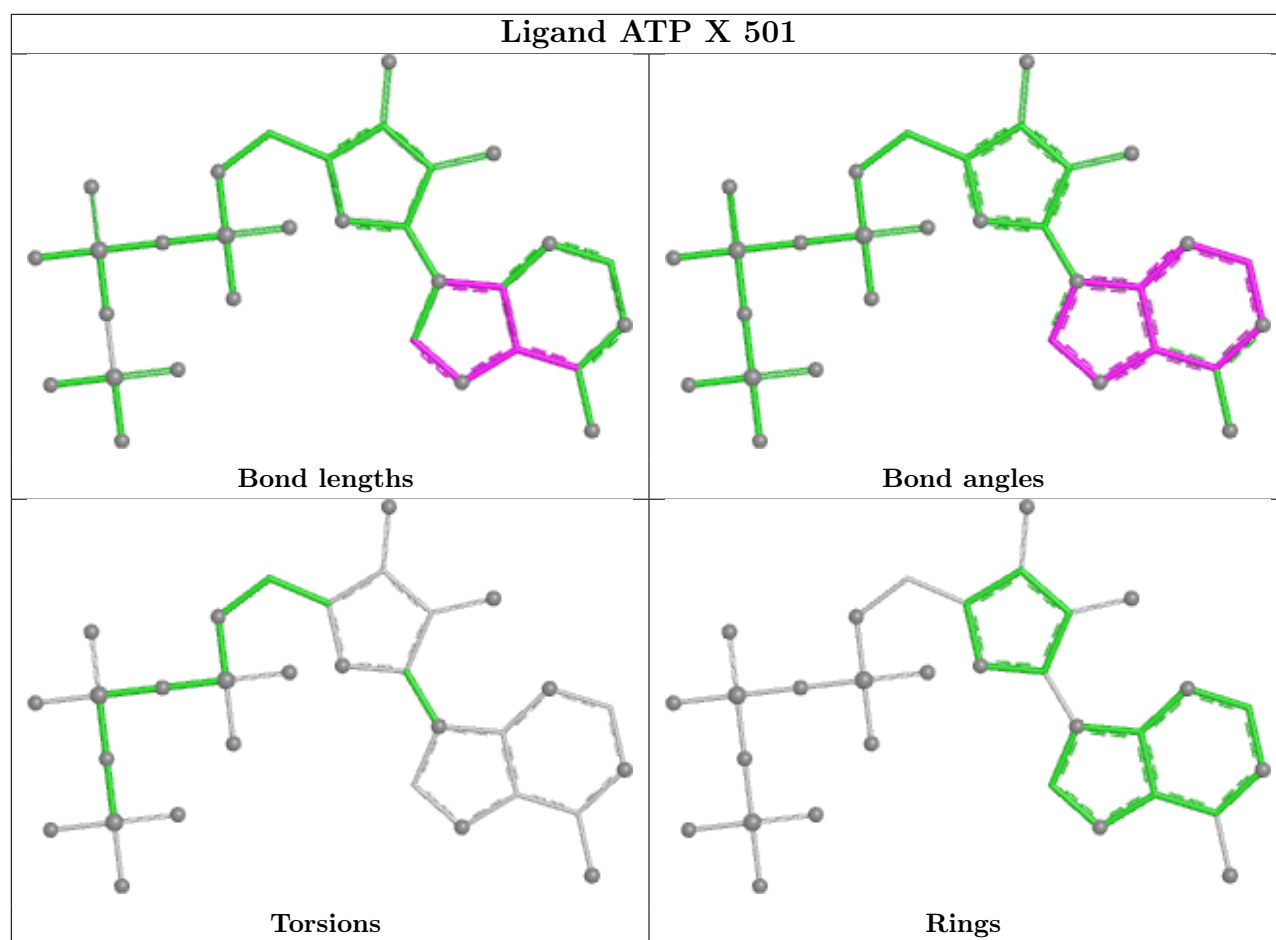
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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.

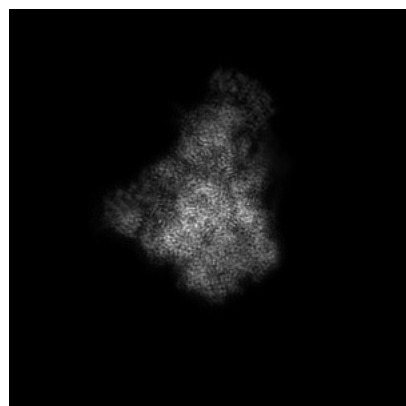
6 Map visualisation [i](#)

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.

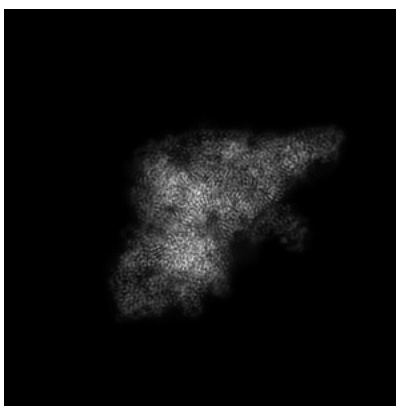
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

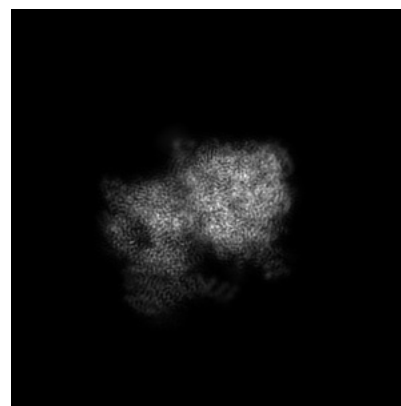
6.1.1 Primary map



X

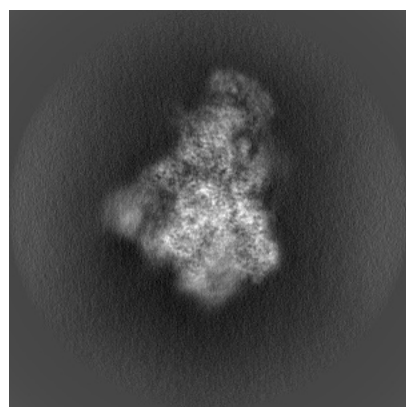


Y

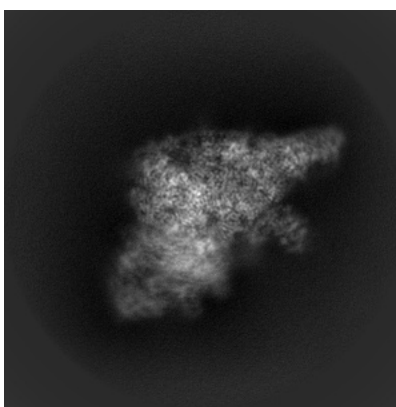


Z

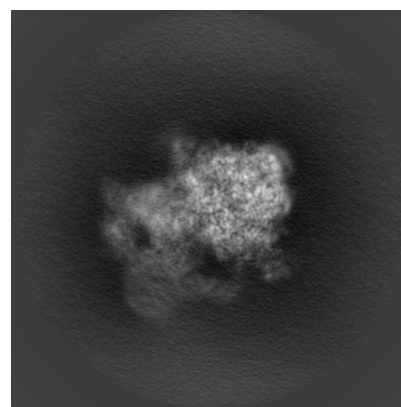
6.1.2 Raw map



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

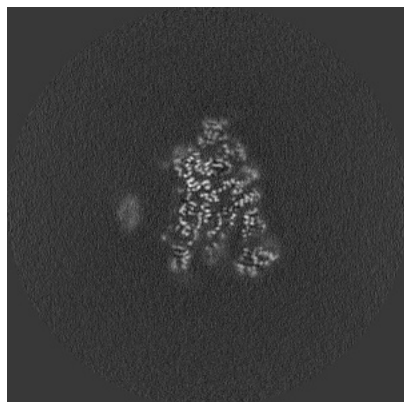


Y Index: 240

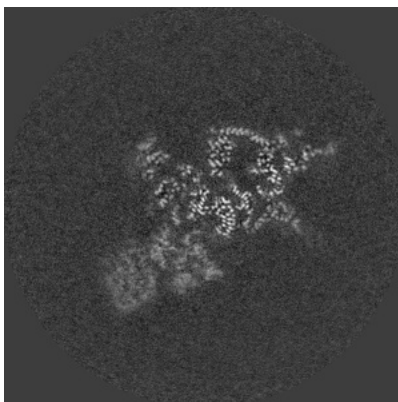


Z Index: 240

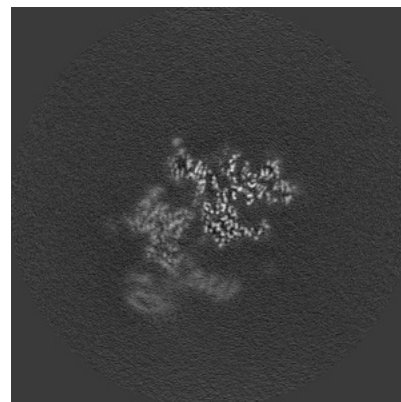
6.2.2 Raw map



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](#)

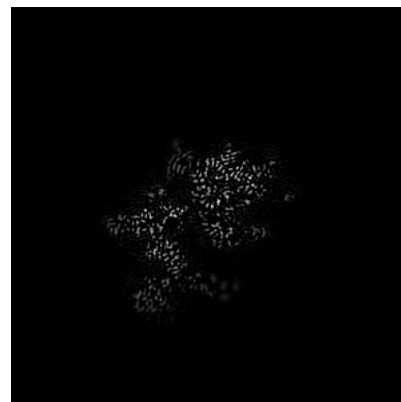
6.3.1 Primary map



X Index: 259

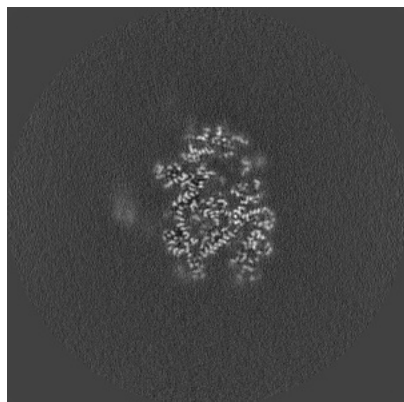


Y Index: 239

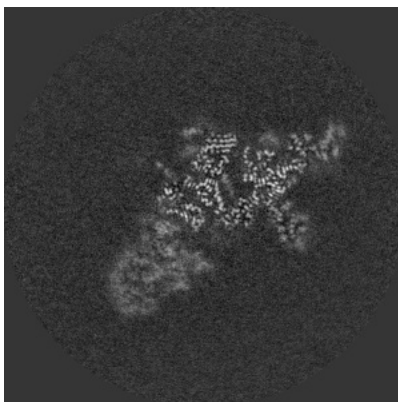


Z Index: 234

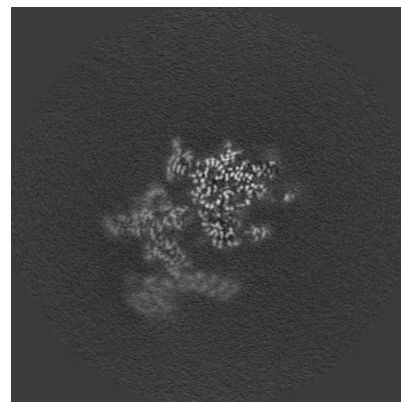
6.3.2 Raw map



X Index: 259



Y Index: 255

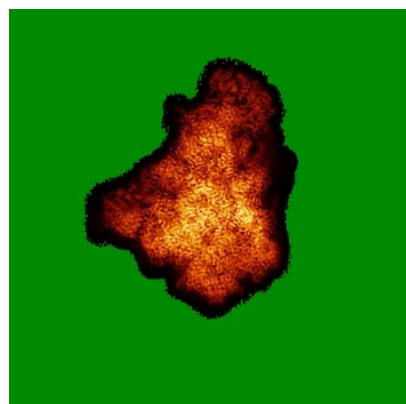


Z Index: 234

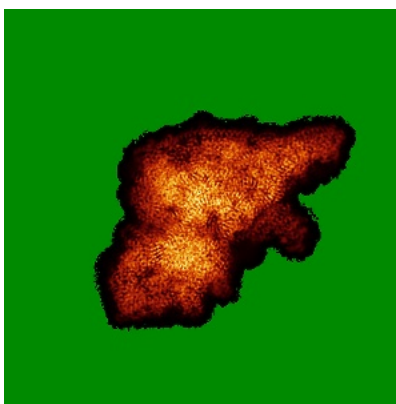
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

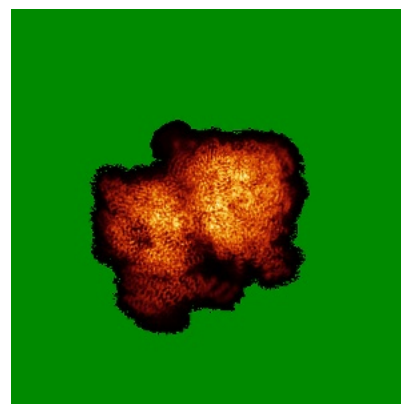
6.4.1 Primary map



X

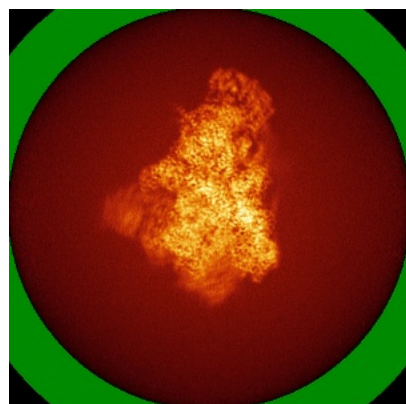


Y

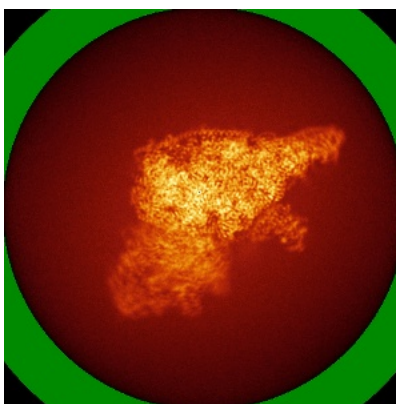


Z

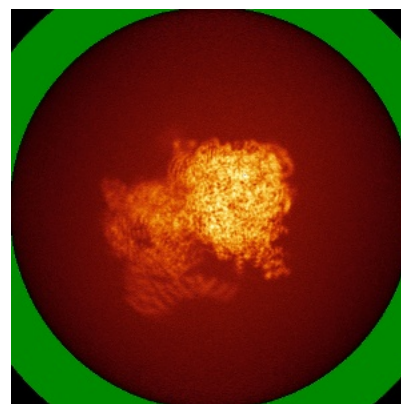
6.4.2 Raw map



X



Y

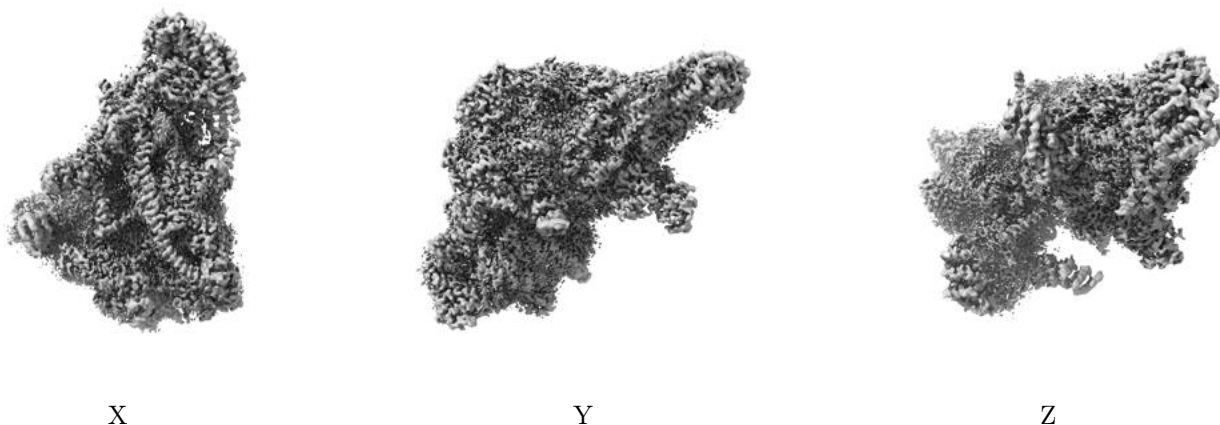


Z

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.

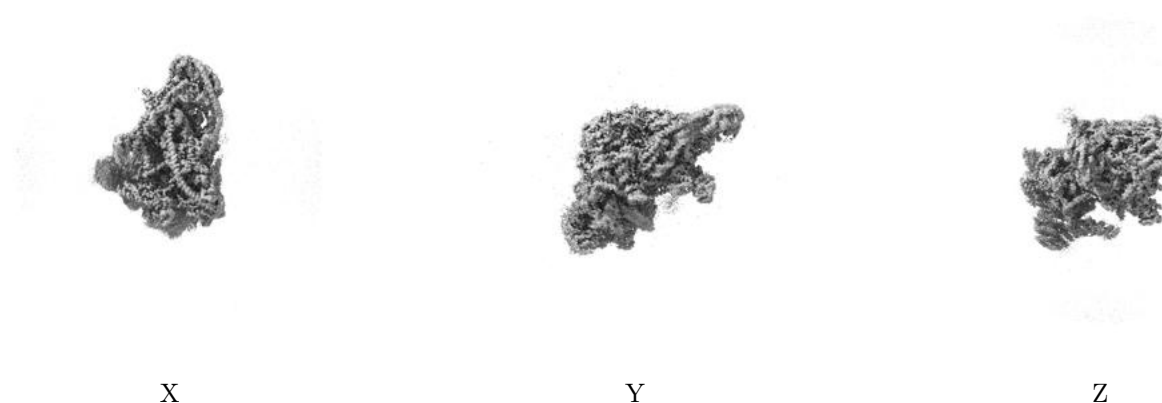
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

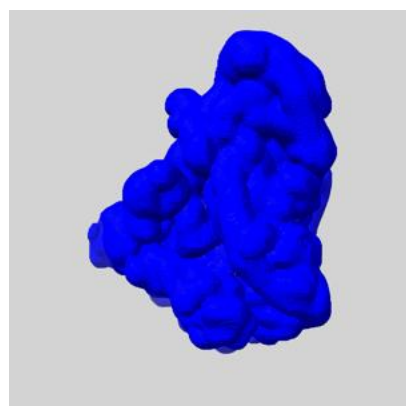
6.6 Mask visualisation [i](#)

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

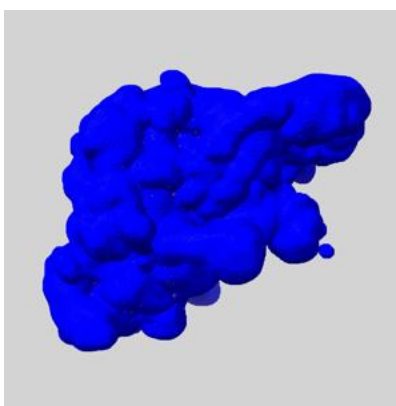
A mask typically either:

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

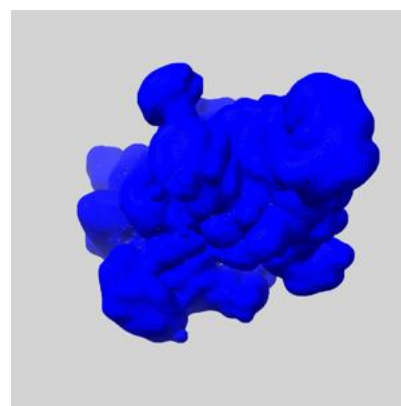
6.6.1 emd_10022_msk_1.map [i](#)



X



Y

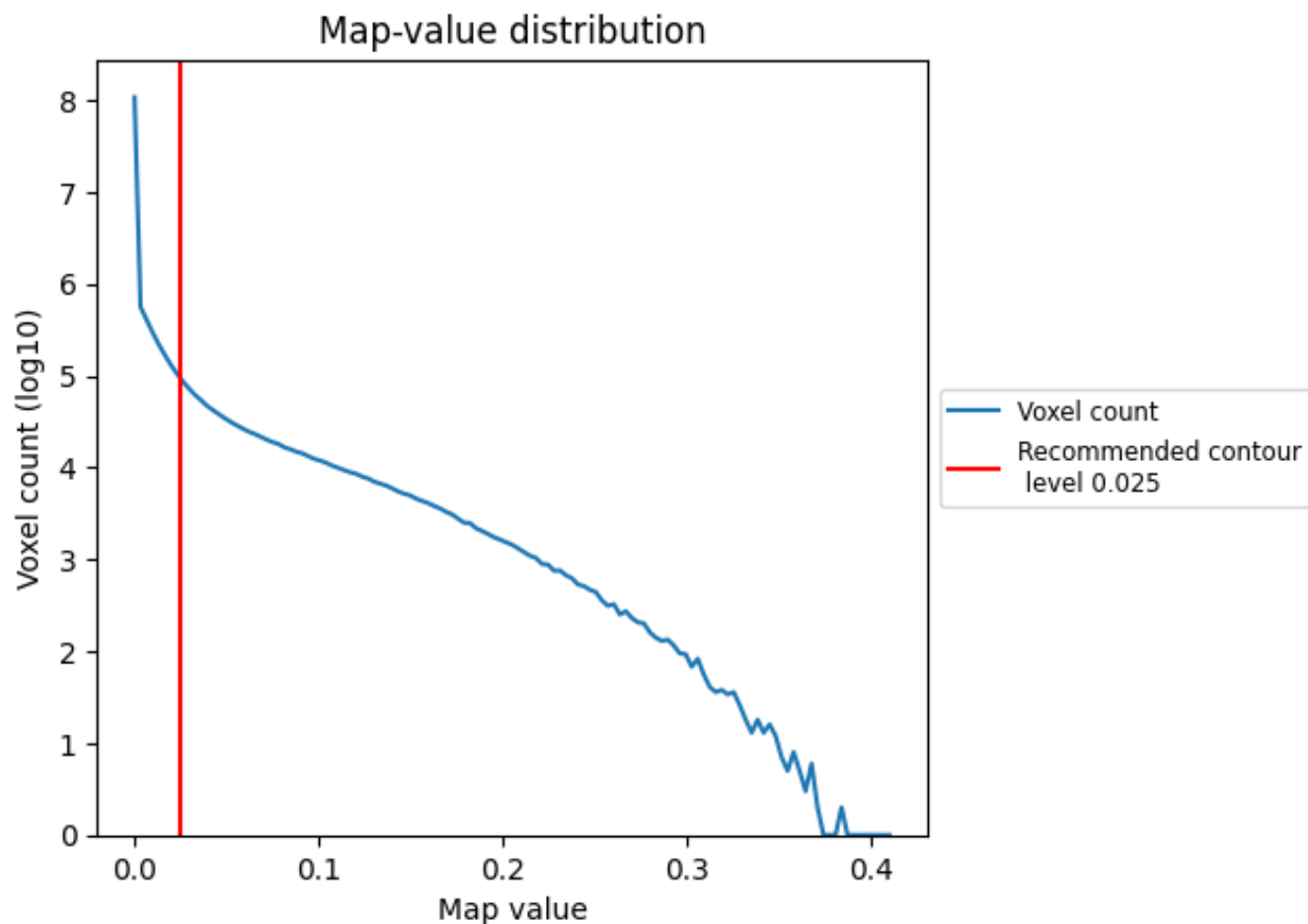


Z

7 Map analysis [i](#)

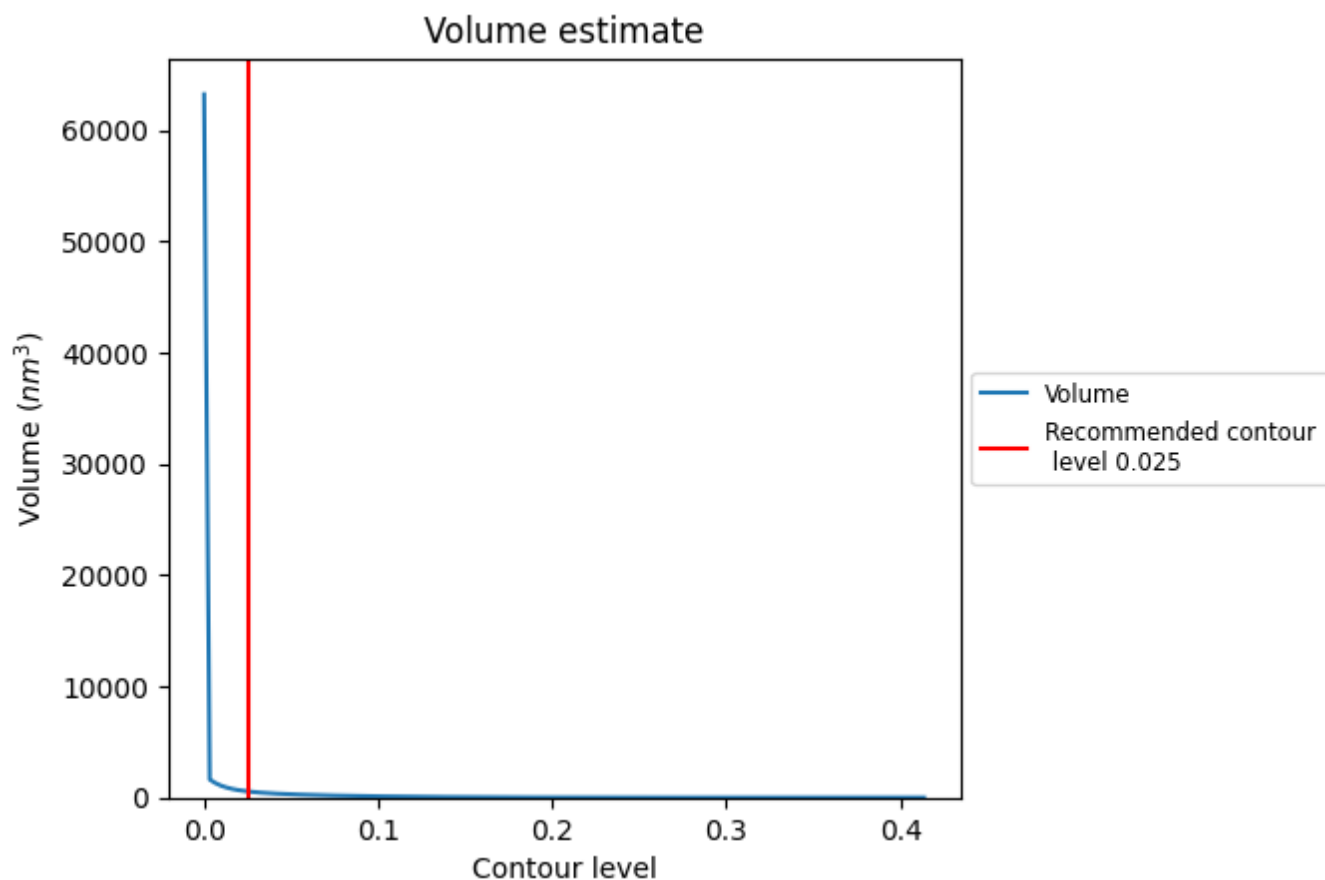
This section contains the results of statistical analysis of the map.

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.

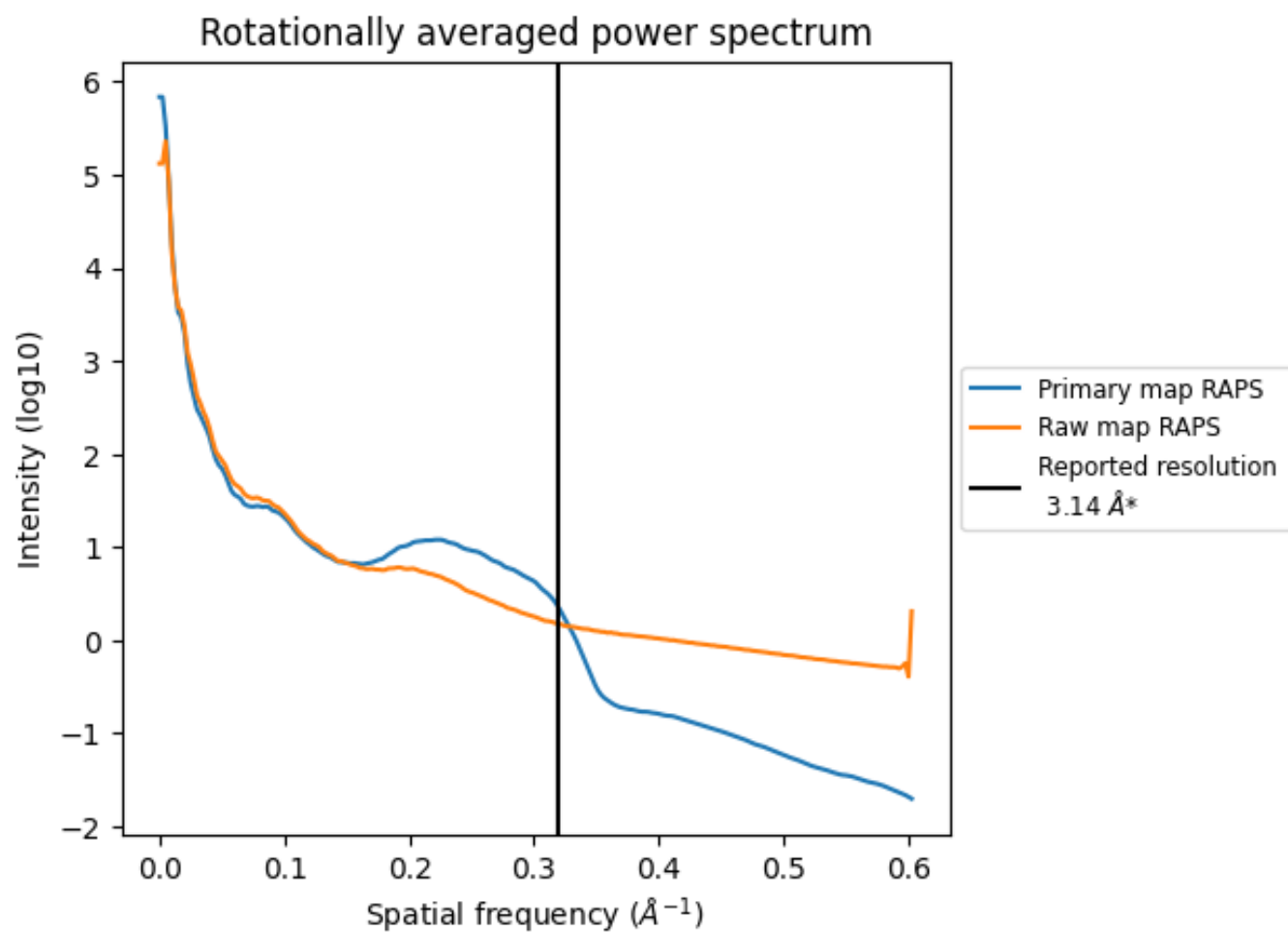
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 554 nm³; 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 ⓘ

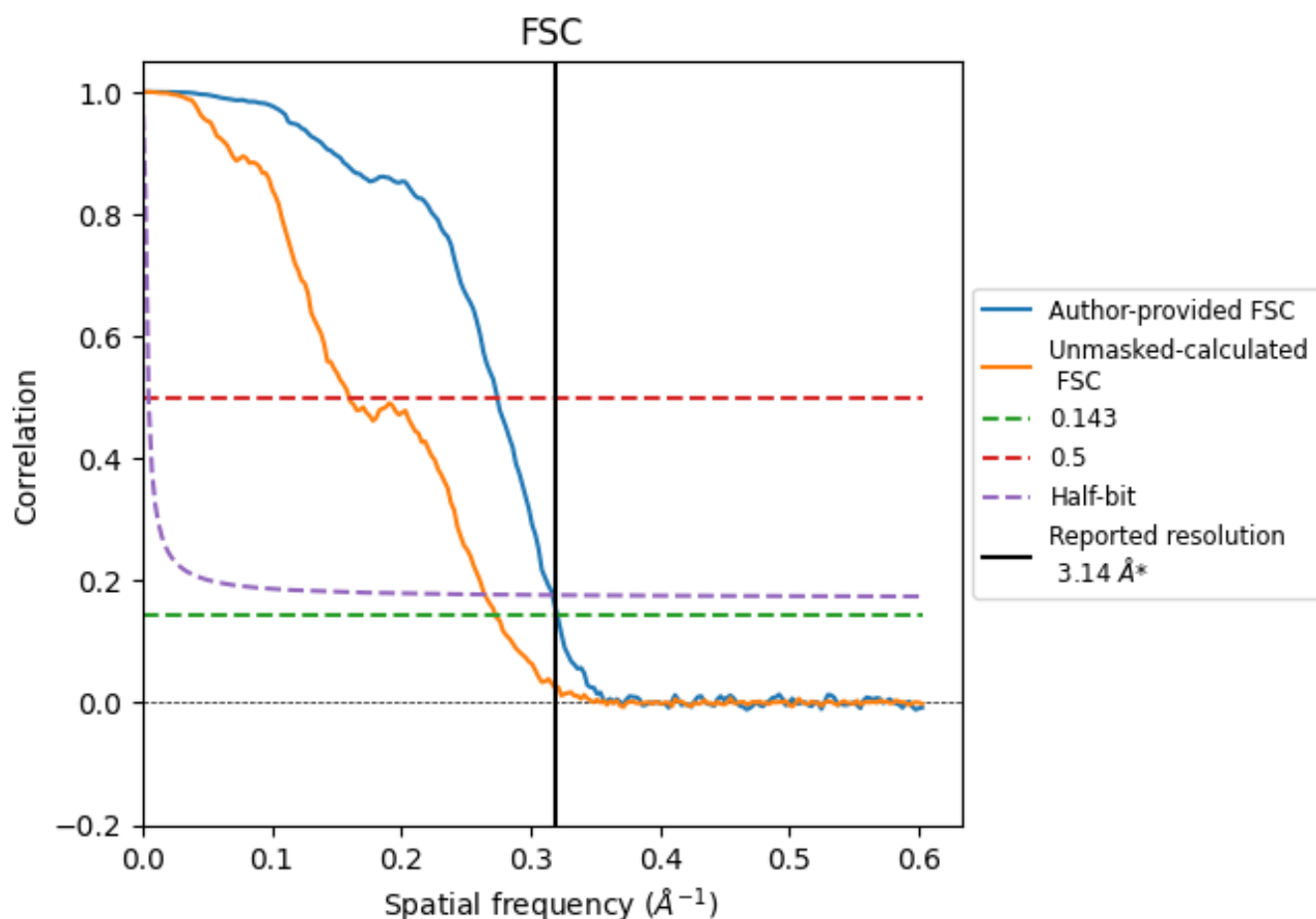


*Reported resolution corresponds to spatial frequency of $0.318 \text{ \AA}^{-1}$

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

8.2 Resolution estimates [i](#)

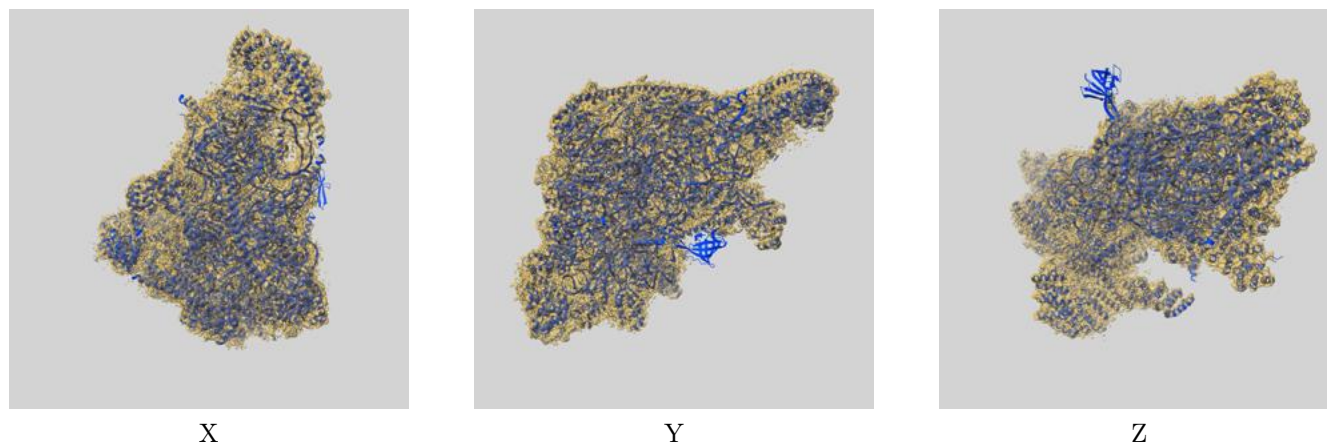
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.12	3.65	3.16
Unmasked-calculated*	3.66	6.26	3.78

*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](#)



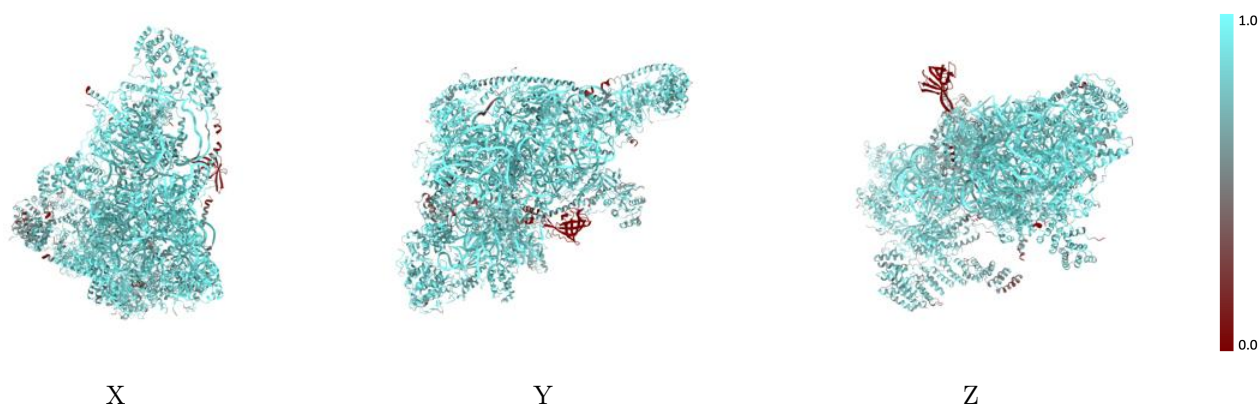
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



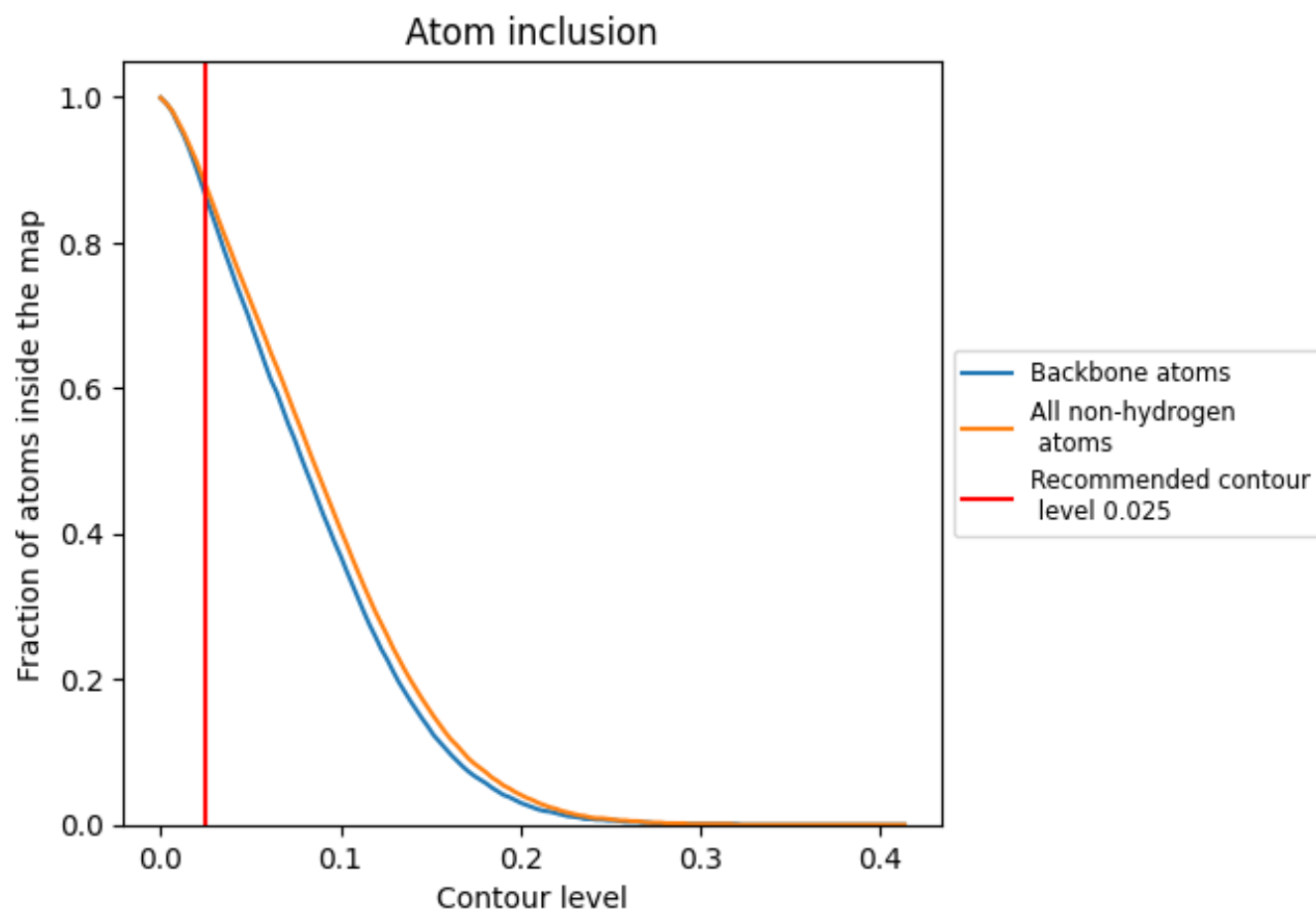
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion ⓘ



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 ⓘ

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

