



Full wwPDB EM Validation Report ⓘ

Dec 22, 2022 – 04:52 AM EST

PDB ID : 8CST
EMDB ID : EMD-26970
Title : Human mitochondrial small subunit assembly intermediate (State E)
Authors : Harper, N.J.; Burnside, C.; Klinge, S.
Deposited on : 2022-05-13
Resolution : 2.85 Å (reported)
Based on initial models : 6AAX, 6RW4, 2C2N

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

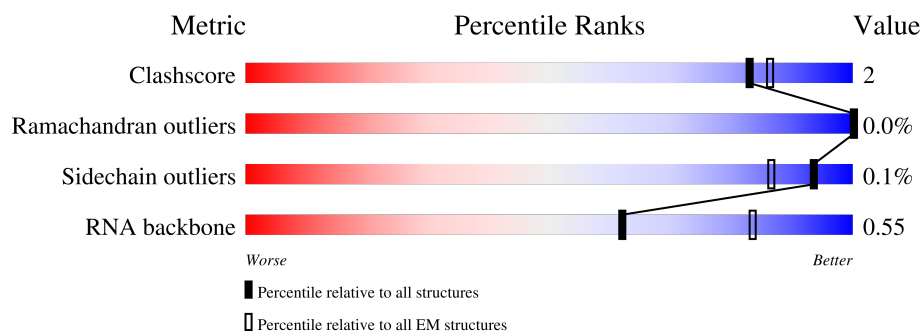
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0	218	<div> <div>19%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
2	1	323	<div> <div>5%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
3	3	199	<div> <div>19%</div> <div>34%</div> <div>65%</div> <div>.</div> </div>
4	4	689	<div> <div>35%</div> <div>72%</div> <div>10%</div> <div>18%</div> </div>
5	6	343	<div> <div>7%</div> <div>35%</div> <div>63%</div> <div>.</div> </div>
6	7	456	<div> <div>11%</div> <div>75%</div> <div>13%</div> <div>12%</div> </div>
7	A	955	<div> <div>16%</div> <div>65%</div> <div>23%</div> <div>5%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
8	B	296	
9	C	167	
10	D	430	
11	E	125	
12	F	242	
13	G	396	
14	H	201	
15	I	194	
16	J	138	
17	K	128	
18	L	257	
19	M	137	
20	N	130	
21	O	258	
22	P	142	
23	Q	87	
24	R	360	
25	S	190	
26	T	173	
27	U	205	
28	V	414	
29	W	187	
30	X	398	
31	Y	395	
32	Z	106	

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 66351 atoms, of which 0 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 protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	211	Total	C	N	O	S	0	0
			1754	1108	333	308	5		

- Molecule 2 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	259	Total	C	N	O	S	0	0
			2098	1333	353	402	10		

- Molecule 3 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 4 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	566	Total	C	N	O	S	0	0
			4585	2940	774	843	28		

- Molecule 5 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	126	Total	C	N	O	S	0	0
			994	630	177	182	5		

- Molecule 6 is a protein called Methyltransferase-like protein 17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	400	Total	C	N	O	S	0	0
			3160	2017	581	546	16		

- Molecule 7 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	888	Total	C	N	O	P	0	0
			18866	8461	3397	6120	888		

- Molecule 8 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	220	Total	C	N	O	S	0	0
			1789	1142	324	313	10		

- Molecule 9 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	126	Total	C	N	O	S	0	0
			1042	679	181	177	5		

- Molecule 10 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	232	Total	C	N	O	S	0	0
			1838	1155	345	329	9		

- Molecule 11 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	108	Total	C	N	O	S	0	0
			858	539	157	158	4		

- Molecule 12 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	206	Total	C	N	O	S	0	0
			1696	1082	308	295	11		

- Molecule 13 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	292	Total	C	N	O	S	0	0
			2395	1522	418	441	14		

- Molecule 14 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	130	Total	C	N	O	S	0	0
			1064	687	177	197	3		

- Molecule 15 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	137	Total	C	N	O	S	0	0
			1019	641	193	181	4		

- Molecule 16 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	107	Total	C	N	O	S	0	0
			829	515	167	141	6		

- Molecule 17 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	100	Total	C	N	O	S	0	0
			847	526	177	139	5		

- Molecule 18 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	161	Total	C	N	O	S	0	0
			1363	869	253	234	7		

- Molecule 19 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	115	Total	C	N	O	S	0	0
			913	578	181	148	6		

- Molecule 20 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	109	Total	C	N	O	S	0	0
			859	557	155	144	3		

- Molecule 21 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	190	Total	C	N	O	S	0	0
			1570	999	291	274	6		

- Molecule 22 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	96	Total	C	N	O	S	0	0
			774	498	133	135	8		

- Molecule 23 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	86	Total	C	N	O	S	0	0
			744	460	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 24 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	291	Total	C	N	O	S	0	0
			2382	1518	409	447	8		

- Molecule 25 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	133	Total	C	N	O	S	0	0
			1100	709	196	194	1		

- Molecule 26 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	164	Total	C	N	O	S	0	0
			1344	859	234	240	11		

- Molecule 27 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	174	Total	C	N	O	S	0	0
			1468	905	295	264	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	359	Total	C	N	O	S	0	0
			2946	1891	491	552	12		

- Molecule 29 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	98	Total	C	N	O	S	0	0
			775	491	138	142	4		

- Molecule 30 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

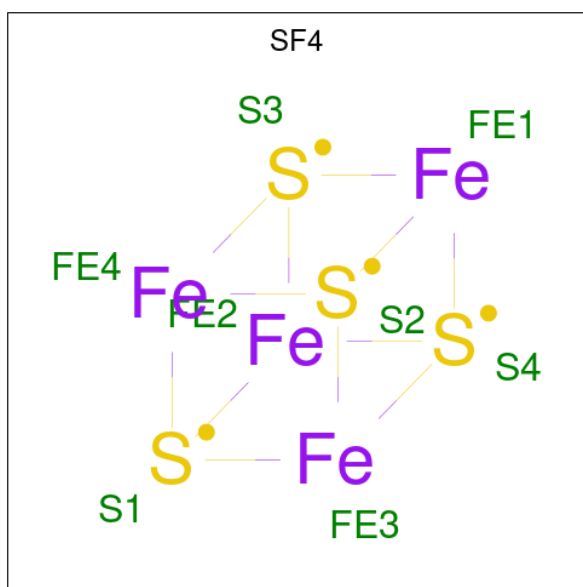
- Molecule 31 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	123	Total	C	N	O	S	0	0
			1043	676	175	189	3		

- Molecule 32 is a protein called 28S ribosomal protein S33, mitochondrial.

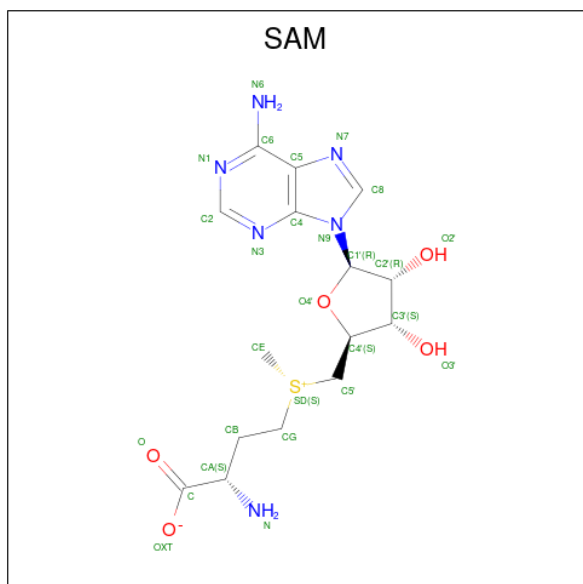
Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	69	Total	C	N	O	S	0	0
			581	377	101	100	3		

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
33	7	1	Total	Fe	S	0
			8	4	4	

- Molecule 34 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	7	1	Total	C	N	O	S	0
			27	15	6	5	1	

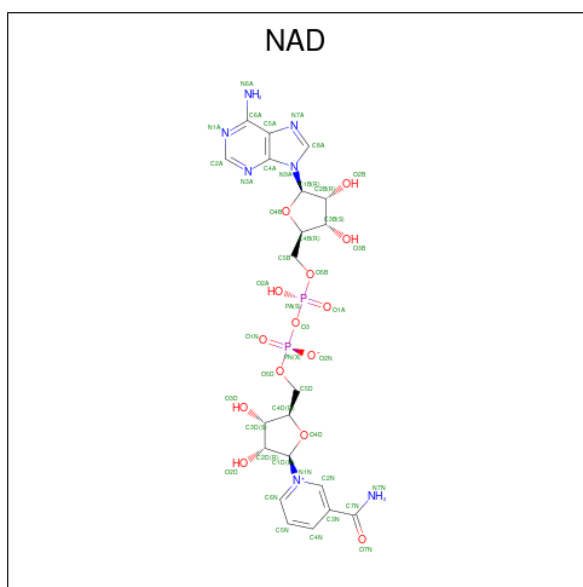
- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
35	A	4	Total	K	0
			4	4	

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

Mol	Chain	Residues	Atoms		AltConf
36	A	28	Total	Mg	0
			28	28	
36	B	1	Total	Mg	0
			1	1	
36	X	1	Total	Mg	0
			1	1	

- Molecule 37 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

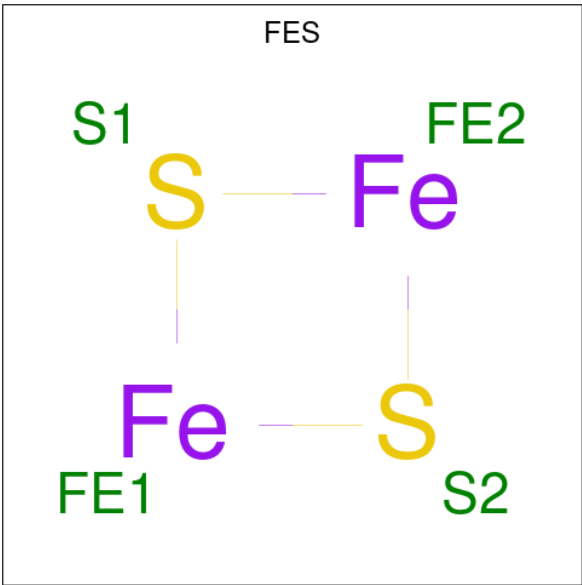


Mol	Chain	Residues	Atoms					AltConf
37	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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

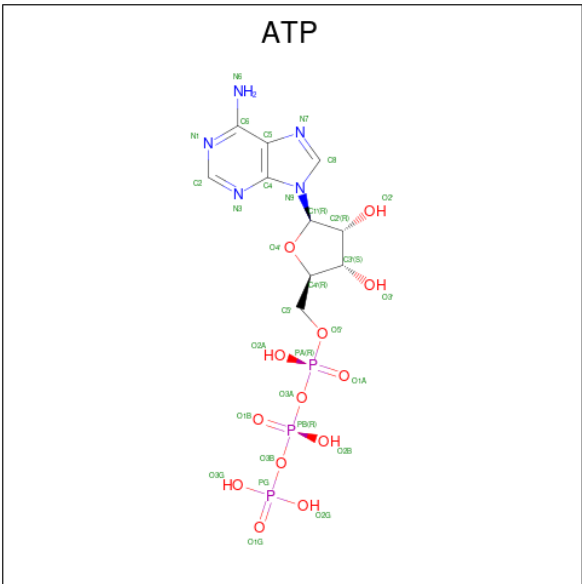
Mol	Chain	Residues	Atoms		AltConf
38	O	1	Total	Zn	0
			1	1	

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
40	X	1	Total	C	N	O	P	0
			31	10	5	13	3	

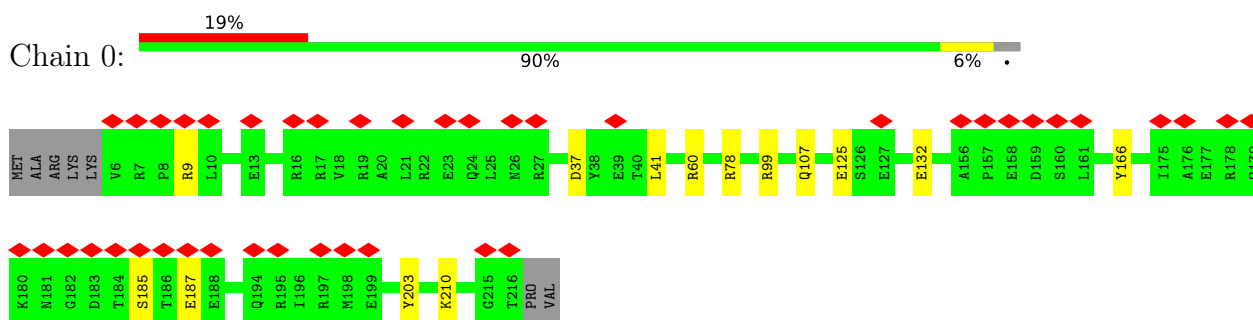
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- The image displays the chemical structure of Guanosine Diphosphate (GDP). It consists of a guanine base (a purine ring system with an amino group at C2 and a carbonyl group at C6) linked to a ribose sugar via a glycosidic bond. The ribose sugar is further linked to two phosphate groups (diphosphate) via a pyrophosphate bridge. The structure is labeled with atom names (N1, N2, N3, N7, N9, C2, C4, C5, C6, C8, C1', C2', C3', C4', C5') and includes stereochemical indicators (R, S, R, S) for the chiral centers in the ribose and phosphate groups. The phosphate groups are labeled with their respective atoms (O1A, O1B, O2A, O2B, O3A, O3B, O4A, O4B, O5A, O5B, O6A, O6B, O7A, O7B, O8A, O8B, O9A, O9B, O10A, O10B, O11A, O11B, O12A, O12B, O13A, O13B, O14A, O14B, O15A, O15B, O16A, O16B, O17A, O17B, O18A, O18B, O19A, O19B, O20A, O20B, O21A, O21B, O22A, O22B, O23A, O23B, O24A, O24B, O25A, O25B, O26A, O26B, O27A, O27B, O28A, O28B, O29A, O29B, O30A, O30B, O31A, O31B, O32A, O32B, O33A, O33B, O34A, O34B, O35A, O35B, O36A, O36B, O37A, O37B, O38A, O38B, O39A, O39B, O40A, O40B, O41A, O41B, O42A, O42B, O43A, O43B, O44A, O44B, O45A, O45B, O46A, O46B, O47A, O47B, O48A, O48B, O49A, O49B, O50A, O50B, O51A, O51B, O52A, O52B, O53A, O53B, O54A, O54B, O55A, O55B, O56A, O56B, O57A, O57B, O58A, O58B, O59A, O59B, O60A, O60B, O61A, O61B, O62A, O62B, O63A, O63B, O64A, O64B, O65A, O65B, O66A, O66B, O67A, O67B, O68A, O68B, O69A, O69B, O70A, O70B, O71A, O71B, O72A, O72B, O73A, O73B, O74A, O74B, O75A, O75B, O76A, O76B, O77A, O77B, O78A, O78B, O79A, O79B, O80A, O80B, O81A, O81B, O82A, O82B, O83A, O83B, O84A, O84B, O85A, O85B, O86A, O86B, O87A, O87B, O88A, O88B, O89A, O89B, O90A, O90B, O91A, O91B, O92A, O92B, O93A, O93B, O94A, O94B, O95A, O95B, O96A, O96B, O97A, O97B, O98A, O98B, O99A, O99B, O100A, O100B, O101A, O101B, O102A, O102B, O103A, O103B, O104A, O104B, O105A, O105B, O106A, O106B, O107A, O107B, O108A, O108B, O109A, O109B, O110A, O110B, O111A, O111B, O112A, O112B, O113A, O113B, O114A, O114B, O115A, O115B, O116A, O116B, O117A, O117B, O118A, O118B, O119A, O119B, O120A, O120B, O121A, O121B, O122A, O122B, O123A, O123B, O124A, O124B, O125A, O125B, O126A, O126B, O127A, O127B, O128A, O128B, O129A, O129B, O130A, O130B, O131A, O131B, O132A, O132B, O133A, O133B, O134A, O134B, O135A, O135B, O136A, O136B, O137A, O137B, O138A, O138B, O139A, O139B, O140A, O140B, O141A, O141B, O142A, O142B, O143A, O143B, O144A, O144B, O145A, O145B, O146A, O146B, O147A, O147B, O148A, O148B, O149A, O149B, O150A, O150B, O151A, O151B, O152A, O152B, O153A, O153B, O154A, O154B, O155A, O155B, O156A, O156B, O157A, O157B, O158A, O158B, O159A, O159B, O160A, O160B, O161A, O161B, O162A, O162B, O163A, O163B, O164A, O164B, O165A, O165B, O166A, O166B, O167A, O167B, O168A, O168B, O169A, O169B, O170A, O170B, O171A, O171B, O172A, O172B, O173A, O173B, O174A, O174B, O175A, O175B, O176A, O176B, O177A, O177B, O178A, O178B, O179A, O179B, O180A, O180B, O181A, O181B, O182A, O182B, O183A, O183B, O184A, O184B, O185A, O185B, O186A, O186B, O187A, O187B, O188A, O188B, O189A, O189B, O190A, O190B, O191A, O191B, O192A, O192B, O193A, O193B, O194A, O194B, O195A, O195B, O196A, O196B, O197A, O197B, O198A, O198B, O199A, O199B, O200A, O200B, O201A, O201B, O202A, O202B, O203A, O203B, O204A, O204B, O205A, O205B, O206A, O206B, O207A, O207B, O208A, O208B, O209A, O209B, O210A, O210B, O211A, O211B, O212A, O212B, O213A, O213B, O214A, O214B, O215A, O215B, O216A, O216B, O217A, O217B, O218A, O218B, O219A, O219B, O220A, O220B, O221A, O221B, O222A, O222B, O223A, O223B, O224A, O224B, O225A, O225B, O226A, O226B, O227A, O227B, O228A, O228B, O229A, O229B, O230A, O230B, O231A, O231B, O232A, O232B, O233A, O233B, O234A, O234B, O235A, O235B, O236A, O236B, O237A, O237B, O238A, O238B, O239A, O239B, O240A, O240B, O241A, O241B, O242A, O242B, O243A, O243B, O244A, O244B, O245A, O245B, O246A, O246B, O247A, O247B, O248A, O248B, O249A, O249B, O250A, O250B, O251A, O251B, O252A, O252B, O253A, O253B, O254A, O254B, O255A, O255B, O256A, O256B, O257A, O257B, O258A, O258B, O259A, O259B, O260A, O260B, O261A, O261B, O262A, O262B, O263A, O263B, O264A, O264B, O265A, O265B, O266A, O266B, O267A, O267B, O268A, O268B, O269A, O269B, O270A, O270B, O271A, O271B, O272A, O272B, O273A, O273B, O274A, O274B, O275A, O275B, O276A, O276B, O277A, O277B, O278A, O278B, O279A, O279B, O280A, O280B, O281A, O281B, O282A, O282B, O283A, O283B, O284A, O284B, O285A, O285B, O286A, O286B, O287A, O287B, O288A, O288B, O289A, O289B, O290A, O290B, O291A, O291B, O292A, O292B, O293A, O293B, O294A, O294B, O295A, O295B, O296A, O296B, O297A, O297B, O298A, O298B, O299A, O299B, O300A, O300B, O301A, O301B, O302A, O302B, O303A, O303B, O304A, O304B, O305A, O305B, O306A, O306B, O307A, O307B, O308A, O308B, O309A, O309B, O310A, O310B, O311A, O311B, O312A, O312B, O313A, O313B, O314A, O314B, O315A, O315B, O316A, O316B, O317A, O317B, O318A, O318B, O319A, O319B, O320A, O320B, O321A, O321B, O322A, O322B, O323A, O323B, O324A, O324B, O325A, O325B, O326A, O326B, O327A, O327B, O328A, O328B, O329A, O329B, O330A, O330B, O331A, O331B, O332A, O332B, O333A, O333B, O334A, O334B, O335A, O335B, O336A, O336B, O337A, O337B, O338A, O338B, O339A, O339B, O340A, O340B, O341A, O341B, O342A, O342B



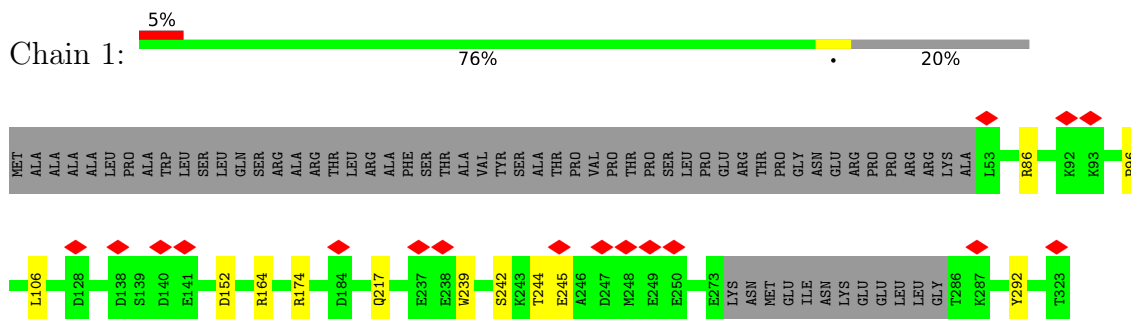
3 Residue-property plots

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.

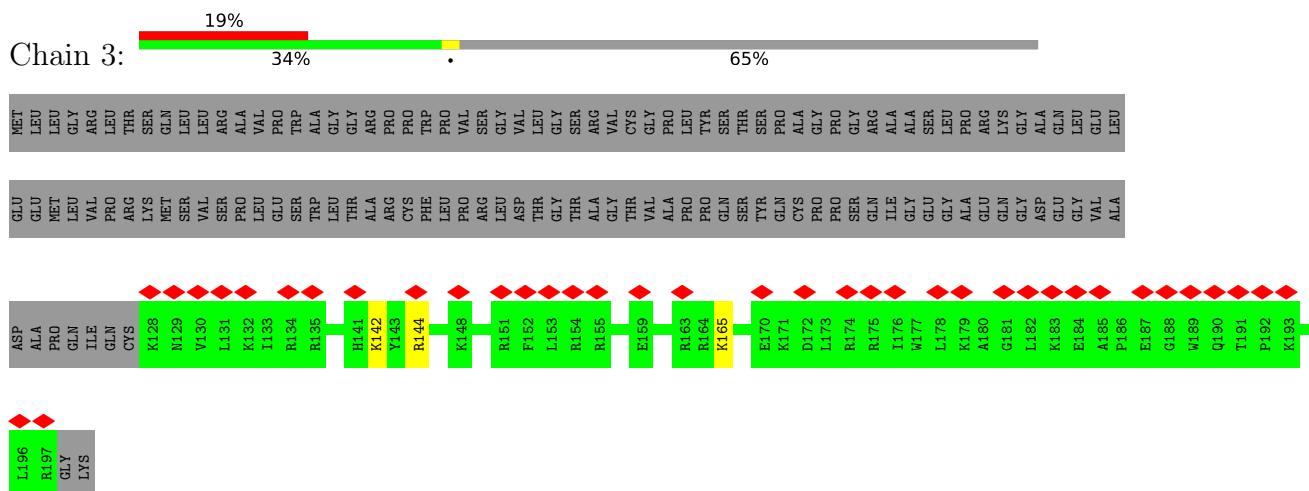
- Molecule 1: 28S ribosomal protein S34, mitochondrial



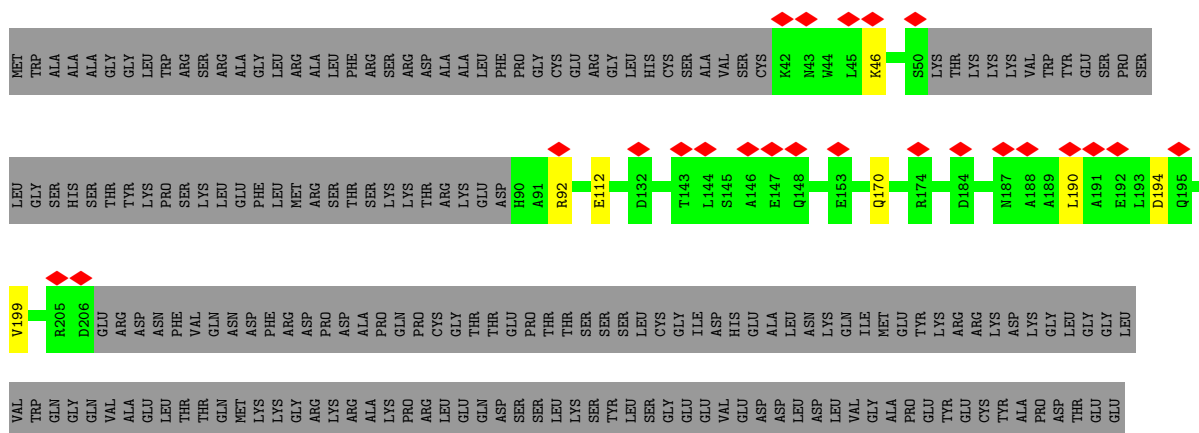
- Molecule 2: 28S ribosomal protein S35, mitochondrial



- Molecule 3: Aurora kinase A-interacting protein




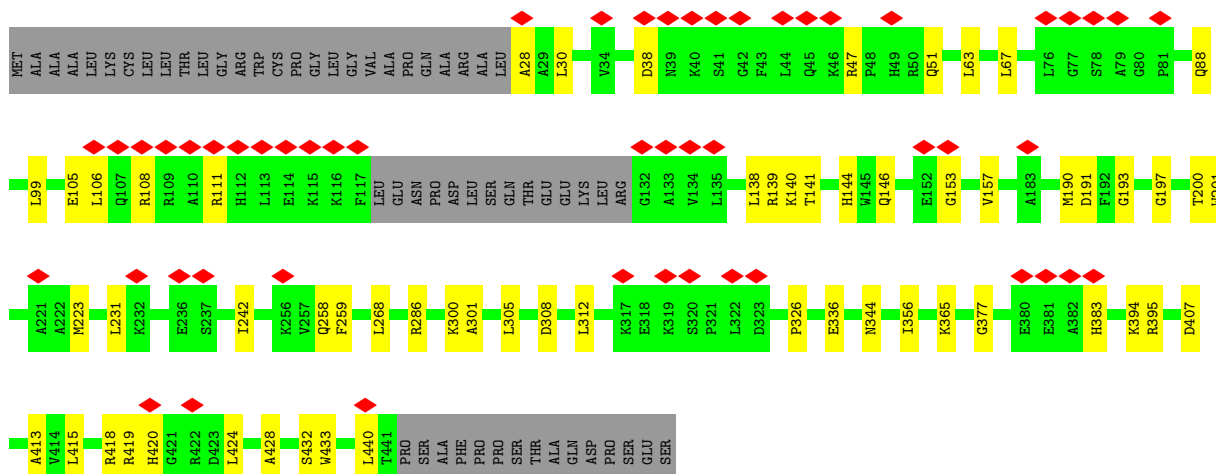
- Chain 4: 



LEU
GLU
ALA
GLU
ALA
GLY
ARG
LYS
CYS
GLY
GLY
ARG
THR
GLU
GLY
ASP
GLY
HIS
SER
CYS
GLY
ALA
SER
ARG
GLU

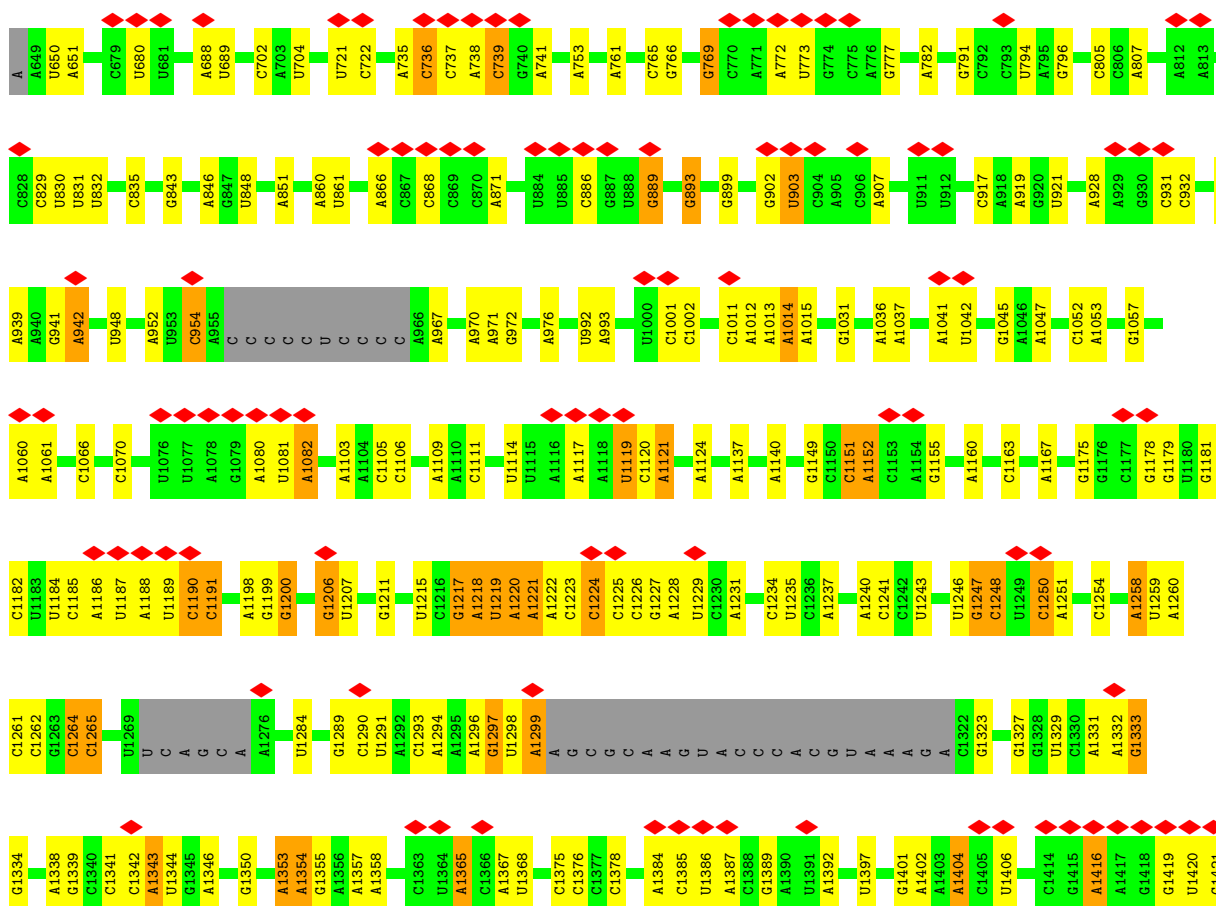
• Molecule 6: Methyltransferase-like protein 17, mitochondrial

Chain 7: 

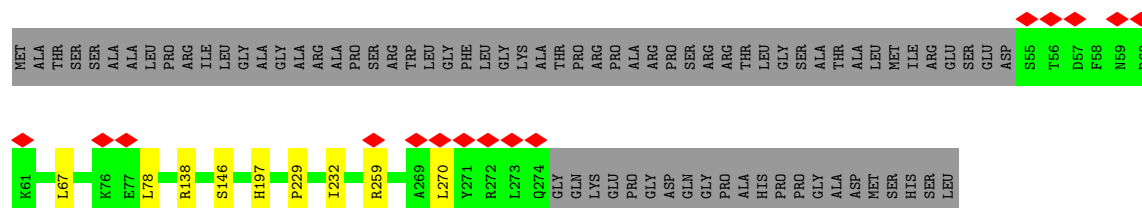


• Molecule 7: 12S mitochondrial rRNA

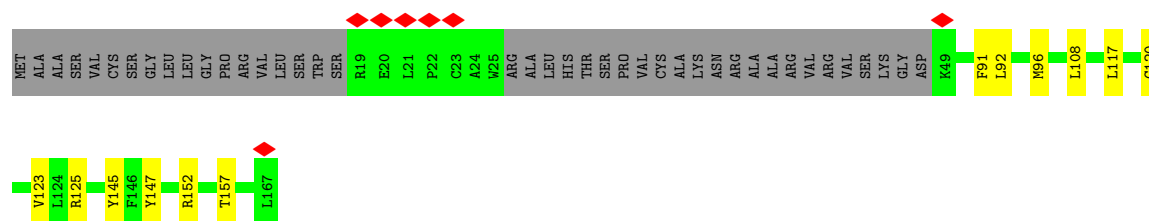
Chain A: 



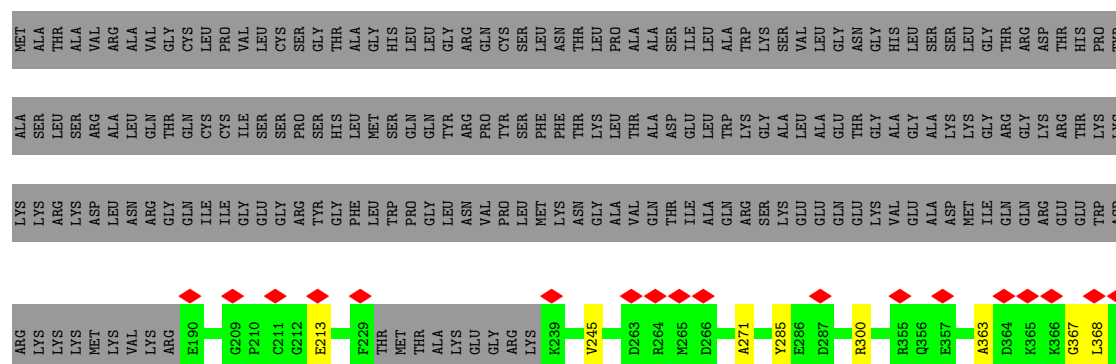
- Molecule 8: 28S ribosomal protein S2, mitochondrial

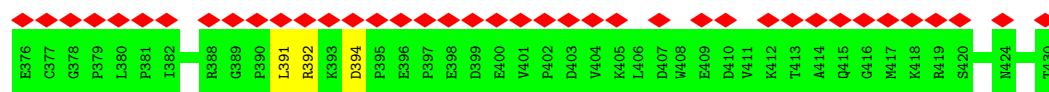


- Molecule 9: 28S ribosomal protein S24, mitochondrial

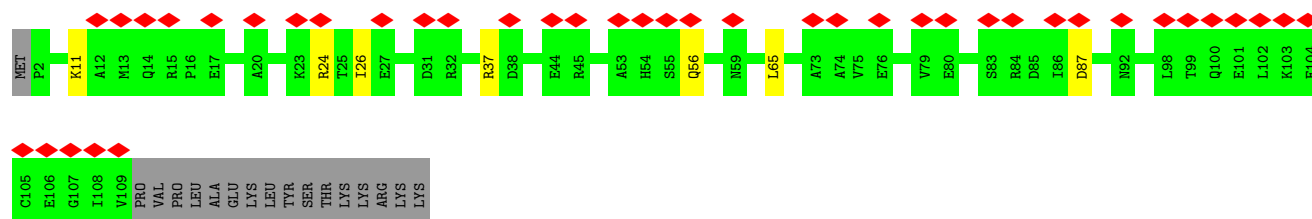
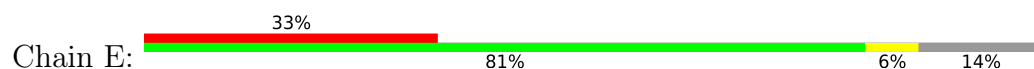


- Molecule 10: 28S ribosomal protein S5, mitochondrial

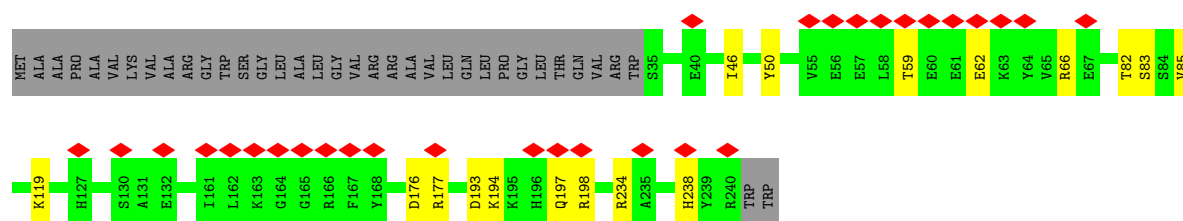
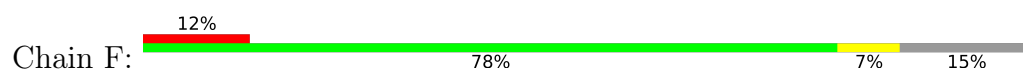




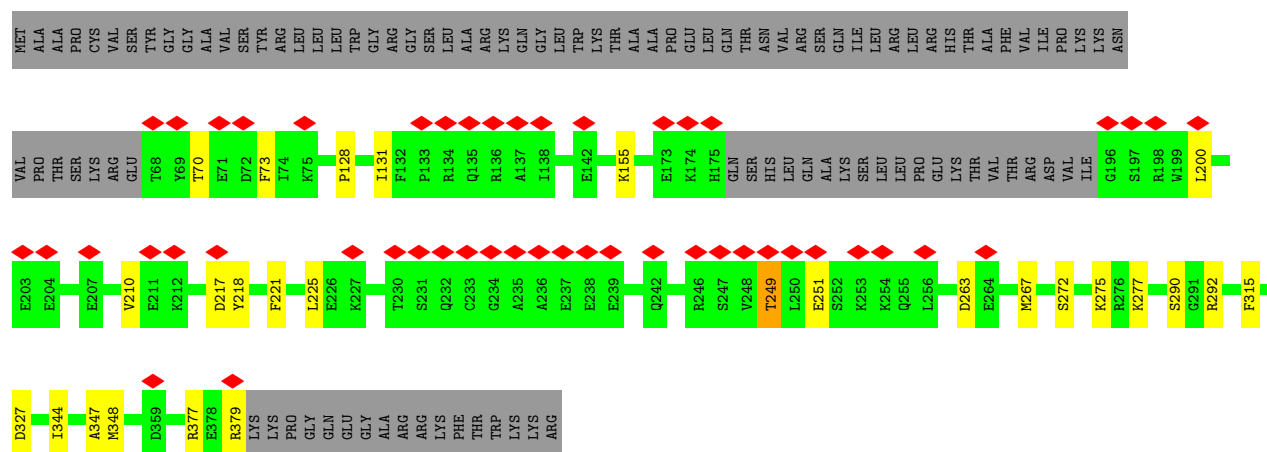
- Molecule 11: 28S ribosomal protein S6, mitochondrial



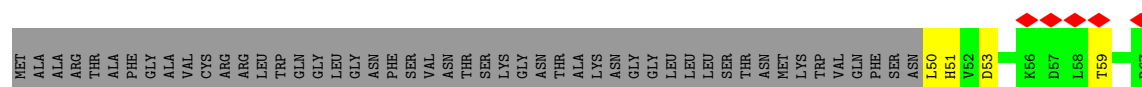
- Molecule 12: 28S ribosomal protein S7, mitochondrial



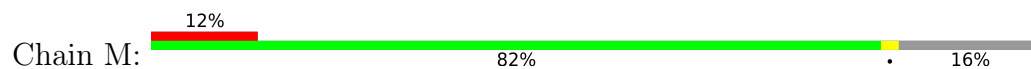
- Molecule 13: 28S ribosomal protein S9, mitochondrial



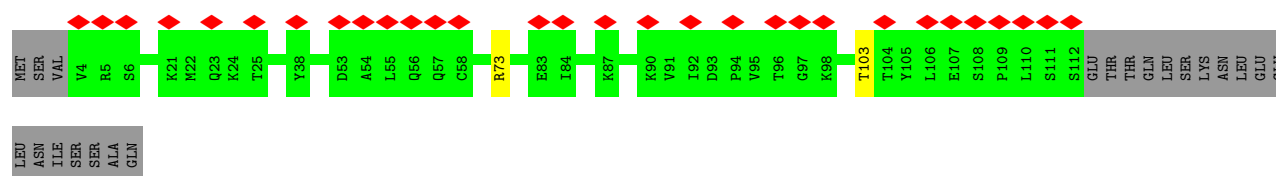
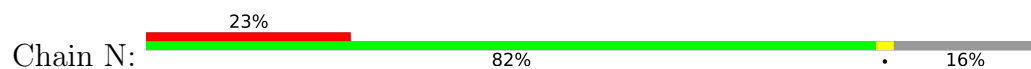
- Molecule 14: 28S ribosomal protein S10, mitochondrial



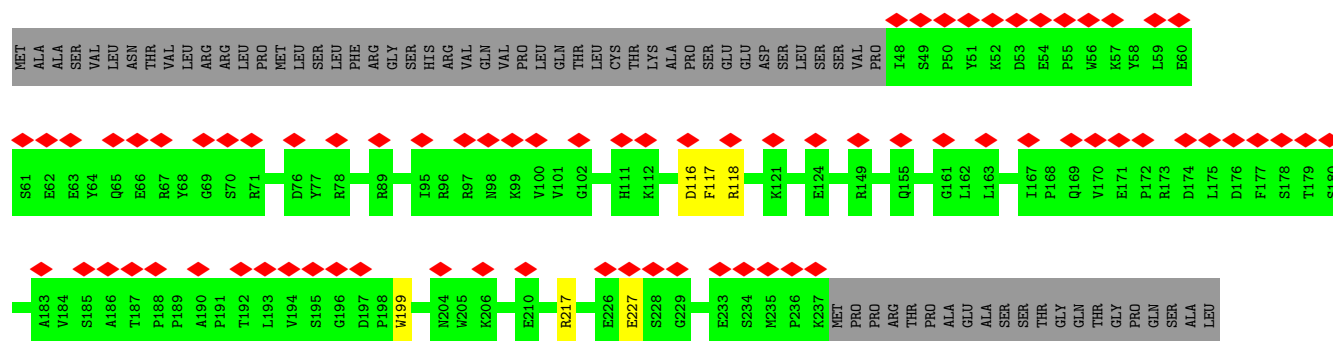
- Molecule 19: 28S ribosomal protein S16, mitochondrial



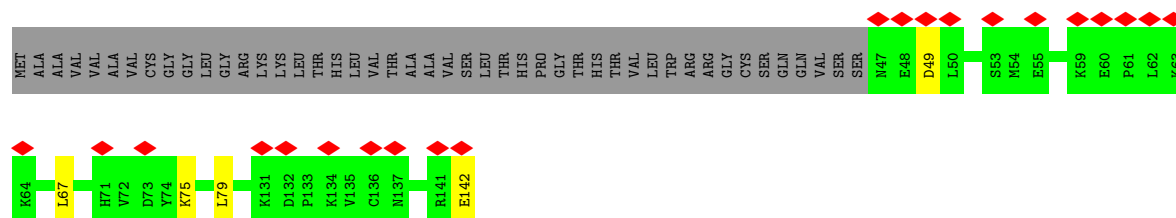
- Molecule 20: 28S ribosomal protein S17, mitochondrial



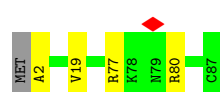
- Molecule 21: 28S ribosomal protein S18b, mitochondrial



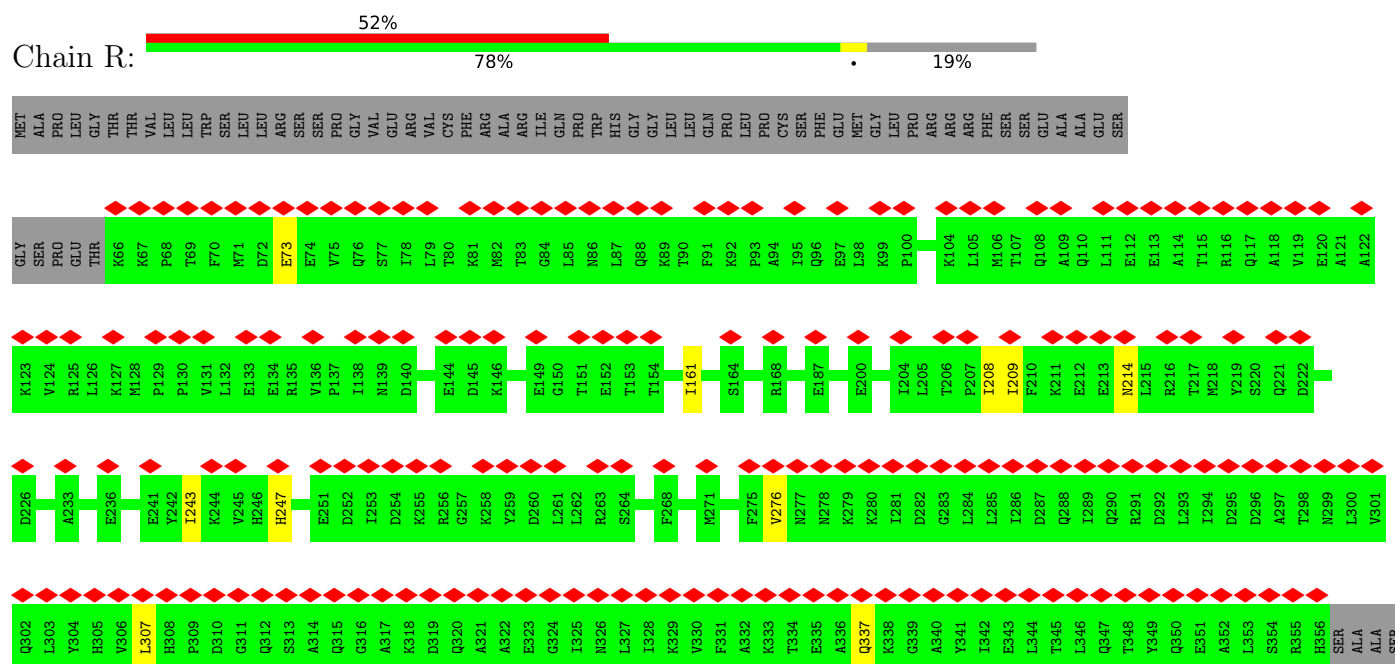
- Molecule 22: 28S ribosomal protein S18c, mitochondrial



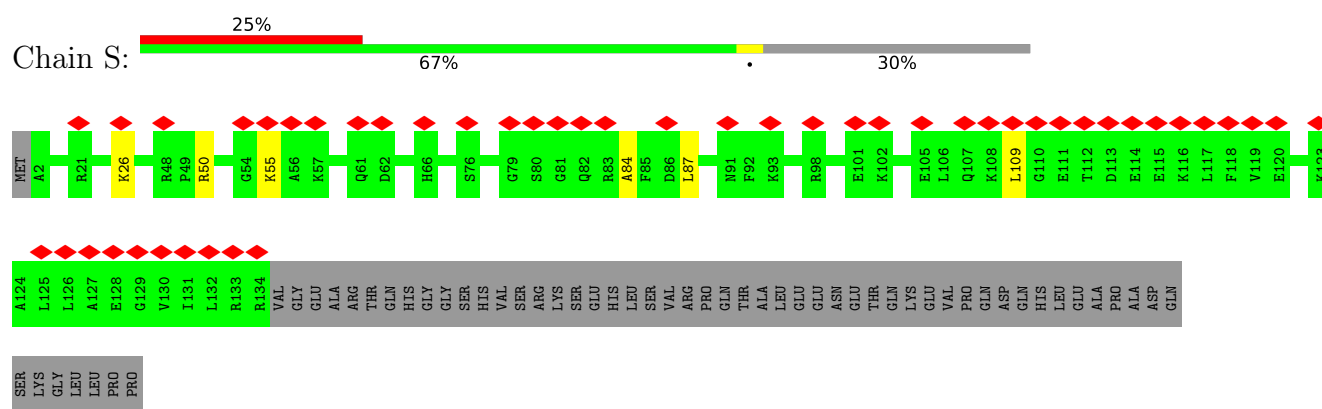
- Molecule 23: 28S ribosomal protein S21, mitochondrial



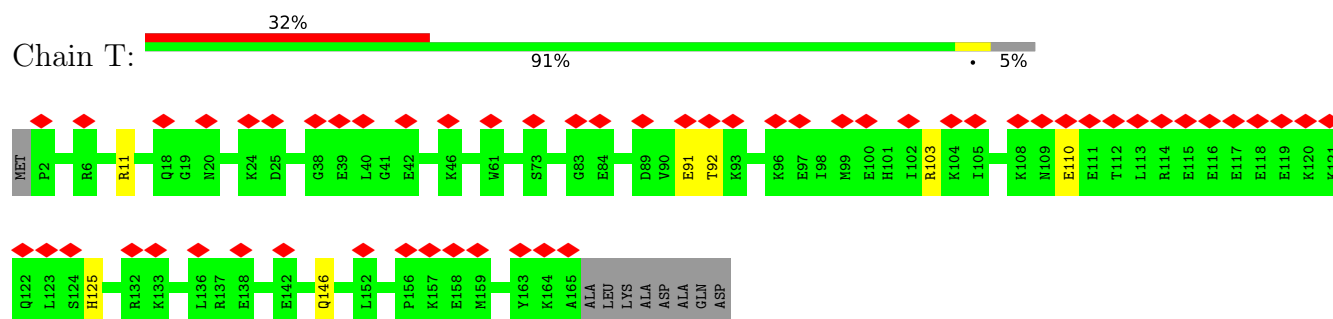
- Molecule 24: 28S ribosomal protein S22, mitochondrial



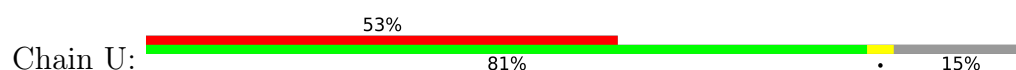
- Molecule 25: 28S ribosomal protein S23, mitochondrial

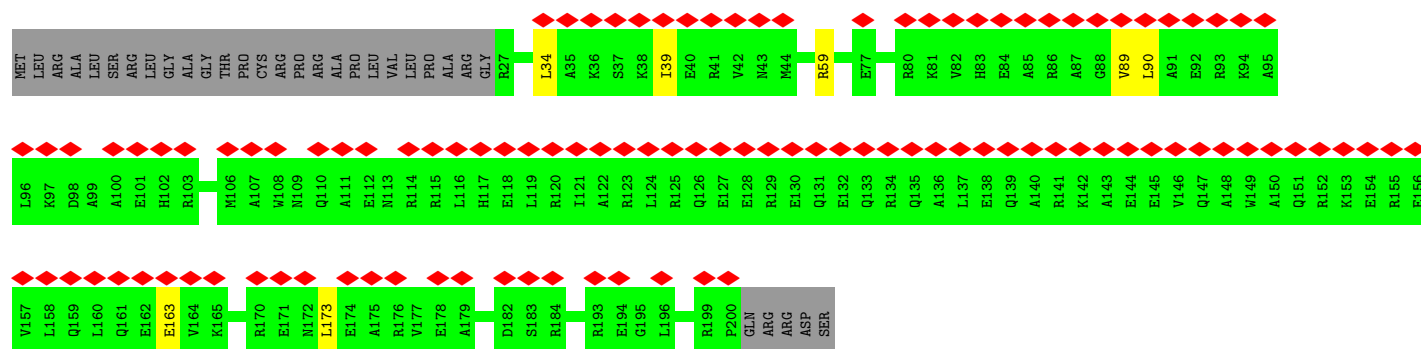


- Molecule 26: 28S ribosomal protein S25, mitochondrial



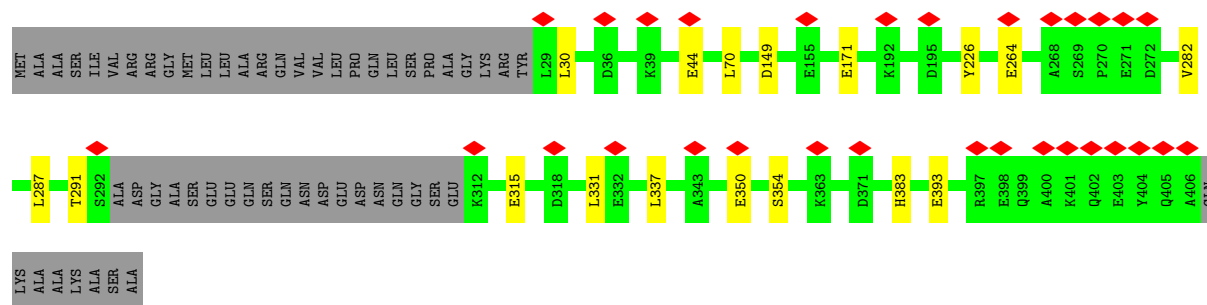
- Molecule 27: 28S ribosomal protein S26, mitochondrial





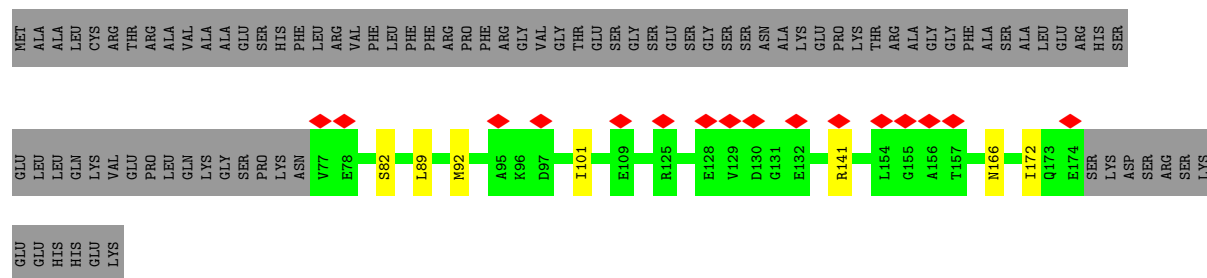
- Molecule 28: 28S ribosomal protein S27, mitochondrial

Chain V: 7% 83% 13%



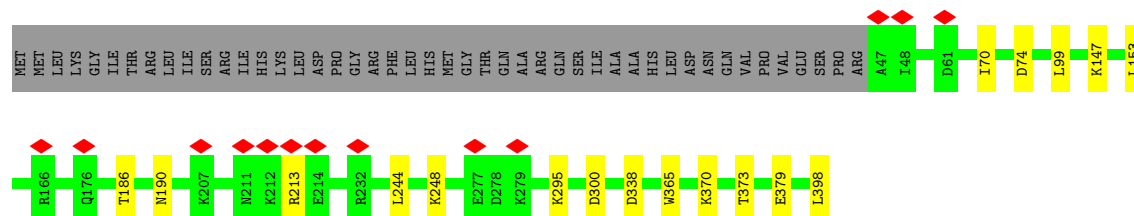
- Molecule 29: 28S ribosomal protein S28, mitochondrial

Chain W: 9% 49% 48%

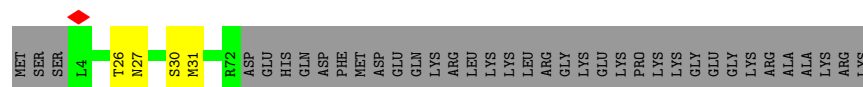


- Molecule 30: 28S ribosomal protein S29, mitochondrial

Chain X: 84% 5% 12%



- Molecule 31: 28S ribosomal protein S31, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39864	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.140	Depositor
Minimum map value	-17.779	Depositor
Average map value	0.035	Depositor
Map value standard deviation	1.235	Depositor
Recommended contour level	7.66	Depositor
Map size (Å)	424.80002, 424.80002, 424.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.062, 1.062, 1.062	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: FES, AYA, MA6, NAD, GDP, K, SAM, SF4, ATP, ZN, MG

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	0	0.28	0/1800	0.61	0/2440
2	1	0.30	0/2143	0.50	0/2902
3	3	0.26	0/636	0.66	0/839
4	4	0.30	1/4686 (0.0%)	0.52	2/6335 (0.0%)
5	6	0.26	0/1012	0.50	0/1371
6	7	0.29	0/3250	0.56	0/4411
7	A	0.31	0/21046	0.79	3/32755 (0.0%)
8	B	0.28	0/1832	0.57	0/2480
9	C	0.32	0/1074	0.54	0/1456
10	D	0.27	0/1877	0.58	0/2523
11	E	0.26	0/872	0.59	0/1177
12	F	0.27	0/1734	0.52	0/2327
13	G	0.29	0/2446	0.55	0/3283
14	H	0.31	0/1086	0.53	0/1473
15	I	0.27	0/1039	0.54	0/1400
16	J	0.26	0/845	0.59	0/1137
17	K	0.25	0/863	0.65	0/1159
18	L	0.26	0/1387	0.54	0/1853
19	M	0.27	0/934	0.60	0/1255
20	N	0.26	0/877	0.56	0/1187
21	O	0.27	0/1624	0.54	0/2210
22	P	0.28	0/791	0.49	0/1062
23	Q	0.28	0/748	0.61	0/994
24	R	0.26	0/2429	0.50	0/3280
25	S	0.29	0/1127	0.57	0/1518
26	T	0.26	0/1375	0.52	0/1847
27	U	0.27	0/1490	0.61	0/1999
28	V	0.29	0/3007	0.48	0/4062
29	W	0.28	0/787	0.55	0/1060
30	X	0.29	0/2921	0.49	0/3954
31	Y	0.29	0/1073	0.47	0/1444
32	Z	0.29	0/596	0.56	0/801

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.29	1/69407 (0.0%)	0.64	5/97994 (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
4	4	0	1
16	J	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	606	PRO	CG-CD	-5.39	1.32	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	606	PRO	N-CD-CG	-7.14	92.49	103.20
4	4	606	PRO	CA-N-CD	-6.13	102.92	111.50
7	A	765	C	C2-N1-C1'	5.31	124.64	118.80
7	A	1217	G	C4-N9-C1'	5.13	133.17	126.50
7	A	1217	G	C6-C5-N7	-5.01	127.39	130.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	264	ARG	Sidechain
16	J	72	LYS	Peptide

5.2 Too-close contacts ⓘ

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	0	1754	0	1754	10	0
2	1	2098	0	2115	8	0
3	3	625	0	699	3	0
4	4	4585	0	4595	46	0
5	6	994	0	1004	7	0
6	7	3160	0	3171	38	0
7	A	18866	0	9583	82	0
8	B	1789	0	1781	5	0
9	C	1042	0	1033	9	0
10	D	1838	0	1858	8	0
11	E	858	0	871	5	0
12	F	1696	0	1749	14	0
13	G	2395	0	2364	16	0
14	H	1064	0	1089	11	0
15	I	1019	0	1059	3	0
16	J	829	0	874	3	0
17	K	847	0	875	12	0
18	L	1363	0	1442	4	0
19	M	913	0	943	2	0
20	N	859	0	922	2	0
21	O	1570	0	1533	4	0
22	P	774	0	801	4	0
23	Q	744	0	758	3	0
24	R	2382	0	2405	8	0
25	S	1100	0	1103	7	0
26	T	1344	0	1359	5	0
27	U	1468	0	1478	5	0
28	V	2946	0	2942	10	0
29	W	775	0	791	7	0
30	X	2849	0	2843	11	0
31	Y	1043	0	996	11	0
32	Z	581	0	590	4	0
33	7	8	0	0	0	0
34	7	27	0	22	2	0
35	A	4	0	0	0	0
36	A	28	0	0	0	0
36	B	1	0	0	0	0
36	X	1	0	0	0	0
37	A	44	0	26	1	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	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	X	28	0	12	1	0
All	All	66351	0	57452	292	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 (292) 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)
7:A:1199:G:H21	7:A:1423:A:N6	1.62	0.97
7:A:1199:G:N2	7:A:1423:A:H62	1.64	0.96
6:7:30:LEU:HD21	6:7:415:LEU:HD21	1.53	0.91
7:A:1013:A:O2'	7:A:1014:A:O5'	1.94	0.84
7:A:1247:G:N2	7:A:1250:C:O2	2.14	0.80
7:A:1199:G:H21	7:A:1423:A:H62	0.85	0.80
7:A:1219:U:O2'	7:A:1220:A:OP2	1.98	0.80
3:3:142:LYS:NZ	7:A:1553:A:OP1	2.16	0.78
12:F:59:THR:OG1	12:F:62:GLU:OE1	2.02	0.78
7:A:738:A:O2'	7:A:739:C:O2	2.02	0.77
32:Z:26:THR:OG1	32:Z:30:SER:OG	2.02	0.77
4:4:118:LYS:NZ	9:C:145:TYR:OH	2.17	0.76
4:4:74:LEU:O	4:4:77:THR:OG1	2.03	0.76
1:0:185:SER:OG	1:0:187:GLU:OE1	2.05	0.75
4:4:358:ARG:NH1	31:Y:250:ILE:O	2.19	0.74
13:G:275:LYS:NZ	13:G:277:LYS:O	2.21	0.73
1:0:60:ARG:NH2	28:V:315:GLU:OE2	2.21	0.73
7:A:1262:C:O2	7:A:1333:G:N2	2.17	0.73
4:4:359:GLU:OE2	31:Y:256:LEU:N	2.22	0.72
7:A:941:G:O2'	7:A:1109:A:OP2	2.08	0.72
7:A:1114:U:OP1	25:S:55:LYS:NZ	2.24	0.70
5:6:194:ASP:OD1	12:F:234:ARG:NH2	2.25	0.70
7:A:702:C:OP1	7:A:848:U:O2'	2.10	0.69
6:7:193:GLY:O	34:7:502:SAM:N	2.25	0.69
17:K:81:ASP:OD1	17:K:86:ARG:NH1	2.26	0.69
6:7:197:GLY:O	6:7:200:THR:OG1	2.10	0.68
21:O:217:ARG:NH1	21:O:227:GLU:OE2	2.27	0.67
2:1:239:TRP:O	2:1:242:SER:OG	2.13	0.66
7:A:1455:U:O4	13:G:377:ARG:NH2	2.28	0.66
6:7:47:ARG:NH1	6:7:51:GLN:O	2.28	0.66
1:0:9:ARG:NE	7:A:805:C:O2	2.29	0.66
32:Z:26:THR:HG1	32:Z:30:SER:HG	1.38	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:112:GLU:OE2	5:6:170:GLN:NE2	2.30	0.65
4:4:448:ILE:HD12	4:4:454:ARG:HG2	1.79	0.65
7:A:1231:A:OP1	17:K:88:ARG:NH2	2.30	0.65
4:4:92:ASP:OD2	9:C:157:THR:OG1	2.08	0.64
6:7:420:HIS:HB3	6:7:424:LEU:HD23	1.79	0.64
7:A:1191:C:H42	7:A:1463:G:H1	1.45	0.64
7:A:1121:A:OP1	10:D:300:ARG:NH2	2.30	0.64
7:A:1434:A:O2'	7:A:1435:A:OP1	2.12	0.64
7:A:1248:C:O2	17:K:28:HIS:N	2.31	0.64
12:F:50:TYR:O	12:F:66:ARG:NH2	2.31	0.63
26:T:91:GLU:O	26:T:92:THR:OG1	2.14	0.63
24:R:276:VAL:HG11	24:R:307:LEU:HD12	1.80	0.63
30:X:153:LEU:HD11	30:X:244:LEU:CD2	2.28	0.63
6:7:144:HIS:CD2	6:7:146:GLN:HE21	2.16	0.63
4:4:577:ASN:OD1	4:4:607:ARG:NH2	2.33	0.62
2:1:164:ARG:NH2	31:Y:319:ALA:O	2.33	0.62
13:G:155:LYS:NZ	13:G:217:ASP:OD2	2.30	0.62
17:K:60:ASN:O	17:K:68:GLN:NE2	2.33	0.61
6:7:153:GLY:O	6:7:157:VAL:HG23	2.00	0.61
6:7:30:LEU:HD21	6:7:415:LEU:CD2	2.28	0.61
6:7:38:ASP:HA	6:7:440:LEU:HD23	1.83	0.61
6:7:140:LYS:O	6:7:141:THR:OG1	2.12	0.61
6:7:111:ARG:NH1	7:A:903:U:O2'	2.34	0.60
14:H:145:LEU:HD11	14:H:156:TYR:CE2	2.36	0.60
14:H:50:LEU:HD13	14:H:53:ASP:O	2.01	0.59
7:A:932:C:N3	26:T:11:ARG:NH2	2.51	0.59
17:K:53:ARG:NH2	31:Y:371:GLU:OE1	2.36	0.59
7:A:1389:G:N2	7:A:1416:A:N7	2.51	0.59
4:4:266:MET:HB3	4:4:271:ALA:HB3	1.85	0.59
10:D:285:TYR:OH	10:D:372:GLU:OE2	2.16	0.59
13:G:249:THR:HG22	13:G:251:GLU:H	1.68	0.59
7:A:736:C:O2'	7:A:738:A:OP2	2.20	0.58
4:4:355:GLN:HG2	31:Y:256:LEU:HD23	1.85	0.58
9:C:91:PHE:HD2	9:C:147:TYR:HH	1.50	0.58
18:L:115:ILE:HG21	18:L:181:ILE:HD13	1.84	0.58
7:A:1200:G:O6	7:A:1365:A:N1	2.37	0.57
7:A:1429:C:OP1	7:A:1459:A:N6	2.37	0.57
13:G:272:SER:OG	13:G:347:ALA:O	2.22	0.57
28:V:44:GLU:OE1	28:V:383:HIS:NE2	2.33	0.57
7:A:942:A:N6	7:A:1047:A:OP2	2.37	0.57
7:A:1218:A:OP1	7:A:1219:U:N3	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:46:LYS:NZ	7:A:1124:A:OP1	2.33	0.56
10:D:392:ARG:NH2	10:D:394:ASP:OD2	2.39	0.56
5:6:92:ARG:NH1	7:A:1570:G:O4'	2.39	0.56
6:7:88:GLN:OE1	7:A:1221:A:O2'	2.16	0.56
6:7:418:ARG:NH1	7:A:1343:A:OP2	2.39	0.56
13:G:292:ARG:NH2	13:G:327:ASP:OD2	2.37	0.56
11:E:11:LYS:NZ	11:E:56:GLN:OE1	2.31	0.56
11:E:37:ARG:NH2	27:U:163:GLU:OE2	2.37	0.56
13:G:290:SER:OG	13:G:292:ARG:NE	2.39	0.55
4:4:540:HIS:O	4:4:545:GLN:NE2	2.40	0.55
7:A:769:G:OP2	20:N:73:ARG:NH2	2.40	0.55
4:4:439:LEU:HD11	4:4:448:ILE:HG23	1.89	0.55
2:1:292:TYR:OH	30:X:338:ASP:OD2	2.24	0.55
13:G:217:ASP:OD1	13:G:218:TYR:N	2.39	0.55
6:7:99:LEU:CD2	6:7:301:ALA:HB1	2.36	0.55
7:A:1235:U:OP1	17:K:36:ARG:NH1	2.40	0.55
7:A:1293:C:N4	23:Q:80:ARG:O	2.39	0.54
4:4:238:TRP:HB3	4:4:271:ALA:HB2	1.88	0.54
4:4:479:GLU:OE1	14:H:51:HIS:ND1	2.39	0.54
6:7:88:GLN:NE2	7:A:1222:A:O4'	2.41	0.54
9:C:96:MET:HB3	9:C:108:LEU:HD11	1.88	0.54
12:F:119:LYS:NZ	30:X:365:TRP:O	2.30	0.54
22:P:49:ASP:OD2	29:W:82:SER:OG	2.25	0.54
4:4:439:LEU:HD11	4:4:448:ILE:CG2	2.37	0.54
6:7:300:LYS:NZ	6:7:344:ASN:O	2.39	0.53
6:7:308:ASP:O	6:7:312:LEU:HD13	2.08	0.53
10:D:213:GLU:OE1	25:S:26:LYS:NZ	2.20	0.53
4:4:302:VAL:HG21	4:4:341:CYS:HB3	1.90	0.53
7:A:1119:U:C4'	25:S:50:ARG:HH12	2.21	0.53
3:3:144:ARG:NH1	7:A:1155:G:OP1	2.42	0.52
7:A:1207:U:O2'	7:A:1224:C:N4	2.42	0.52
10:D:368:LEU:HD11	10:D:392:ARG:NH1	2.25	0.52
2:1:152:ASP:OD2	2:1:174:ARG:NH1	2.37	0.52
30:X:70:ILE:HD11	30:X:99:LEU:HD12	1.91	0.52
4:4:161:ILE:HD12	4:4:191:LEU:HA	1.91	0.52
7:A:1384:A:OP2	12:F:198:ARG:NH1	2.43	0.52
13:G:263:ASP:OD1	13:G:267:MET:N	2.39	0.52
12:F:119:LYS:NZ	30:X:398:LEU:OXT	2.32	0.51
28:V:350:GLU:OE2	28:V:354:SER:OG	2.26	0.51
21:O:116:ASP:OD2	21:O:118:ARG:NH2	2.42	0.51
30:X:295:LYS:NZ	41:X:503:GDP:O3A	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Z:26:THR:HG1	32:Z:27:ASN:H	1.59	0.51
7:A:1384:A:H61	12:F:197:GLN:HB2	1.75	0.50
6:7:106:LEU:HD22	6:7:138:LEU:HD21	1.94	0.50
6:7:419:ARG:NH2	7:A:1341:C:OP1	2.43	0.50
6:7:394:LYS:O	6:7:395:ARG:NH1	2.41	0.50
7:A:928:A:OP2	16:J:47:ARG:NH2	2.45	0.50
7:A:1228:A:OP2	17:K:108:ARG:NH1	2.45	0.50
6:7:63:LEU:HD22	6:7:356:ILE:HD11	1.94	0.50
7:A:952:A:N3	7:A:954:C:N4	2.60	0.50
7:A:1037:A:OP1	18:L:138:SER:OG	2.30	0.50
7:A:1206:G:OP2	7:A:1231:A:N6	2.45	0.50
8:B:78:LEU:HD11	8:B:259:ARG:NH2	2.27	0.50
4:4:87:TYR:OH	9:C:152:ARG:NH1	2.45	0.50
4:4:404:ARG:NH1	14:H:59:THR:OG1	2.45	0.50
1:0:125:GLU:OE2	1:0:203:TYR:OH	2.28	0.49
13:G:344:ILE:O	13:G:348:MET:HG3	2.12	0.49
6:7:144:HIS:CD2	6:7:146:GLN:NE2	2.80	0.49
4:4:339:LEU:CD1	4:4:371:THR:HG23	2.42	0.49
7:A:1227:G:OP2	7:A:1228:A:O2'	2.14	0.49
7:A:843:G:N2	7:A:846:A:OP2	2.40	0.49
2:1:86:ARG:NH1	2:1:96:PRO:O	2.44	0.49
19:M:108:GLU:OE2	27:U:59:ARG:NH2	2.44	0.49
7:A:1066:C:O2'	15:I:187:ARG:O	2.30	0.48
29:W:89:LEU:HD12	29:W:92:MET:HE2	1.95	0.48
7:A:1463:G:H2'	7:A:1464:G:H5'	1.95	0.48
10:D:245:VAL:HG22	10:D:271:ALA:HB1	1.94	0.48
27:U:34:LEU:HD23	27:U:39:ILE:HD13	1.95	0.48
12:F:176:ASP:OD1	12:F:177:ARG:N	2.46	0.48
4:4:59:ILE:HD11	14:H:70:ASP:O	2.14	0.48
4:4:360:MET:CE	4:4:371:THR:HG21	2.43	0.48
4:4:656:ASN:OD1	4:4:657:GLN:N	2.45	0.48
6:7:326:PRO:O	6:7:377:GLY:N	2.43	0.48
7:A:1496:U:OP1	16:J:82:ARG:NH2	2.46	0.48
24:R:161:ILE:O	26:T:125:HIS:NE2	2.44	0.48
4:4:57:VAL:HG23	4:4:57:VAL:O	2.14	0.48
4:4:293:THR:O	4:4:297:LEU:HG	2.13	0.48
10:D:363:ALA:O	10:D:367:GLY:N	2.45	0.48
4:4:526:ASP:N	4:4:526:ASP:OD1	2.44	0.48
7:A:1199:G:OP1	7:A:1365:A:N6	2.46	0.48
28:V:291:THR:HG21	28:V:331:LEU:HD22	1.96	0.48
30:X:248:LYS:NZ	30:X:300:ASP:OD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:342:LEU:HG	4:4:349:ALA:HB1	1.97	0.47
23:Q:77:ARG:NH2	29:W:166:ASN:OD1	2.48	0.47
8:B:67:LEU:HD11	8:B:138:ARG:NH2	2.28	0.47
13:G:200:LEU:O	13:G:218:TYR:OH	2.21	0.47
24:R:208:ILE:O	24:R:214:ASN:ND2	2.46	0.47
29:W:89:LEU:HD12	29:W:92:MET:CE	2.44	0.47
4:4:643:GLU:O	4:4:646:THR:OG1	2.28	0.47
14:H:108:VAL:HG22	14:H:143:LEU:CD2	2.44	0.47
4:4:289:ALA:HB3	4:4:294:PHE:CE2	2.50	0.47
18:L:212:ARG:NH1	18:L:215:GLN:OE1	2.48	0.47
2:1:217:GLN:NE2	31:Y:326:SER:O	2.47	0.47
11:E:24:ARG:NH2	11:E:87:ASP:OD2	2.47	0.47
4:4:94:TYR:HB2	9:C:125:ARG:HE	1.79	0.47
7:A:1070:C:OP1	7:A:1586:G:N2	2.40	0.47
28:V:70:LEU:HD23	28:V:393:GLU:OE1	2.14	0.47
29:W:141:ARG:NH1	29:W:172:ILE:O	2.48	0.47
4:4:349:ALA:HB3	4:4:378:LEU:HD11	1.96	0.47
13:G:221:PHE:CZ	13:G:225:LEU:HD11	2.50	0.47
12:F:193:ASP:OD1	12:F:194:LYS:N	2.49	0.46
13:G:128:PRO:HA	13:G:131:ILE:HG22	1.97	0.46
6:7:28:ALA:N	6:7:407:ASP:OD2	2.48	0.46
6:7:223:MET:SD	34:7:502:SAM:O3'	2.73	0.46
7:A:1119:U:H5'	25:S:50:ARG:HH12	1.79	0.46
4:4:509:ILE:HD12	4:4:509:ILE:H	1.80	0.46
12:F:46:ILE:HG23	13:G:315:PHE:CZ	2.51	0.46
22:P:67:LEU:HD21	22:P:79:LEU:HD11	1.96	0.46
7:A:899:G:O2'	7:A:907:A:N1	2.35	0.46
31:Y:249:ASN:OD1	31:Y:252:THR:HG23	2.16	0.46
6:7:258:GLN:NE2	6:7:286:ARG:O	2.46	0.46
7:A:1151:C:O2'	7:A:1152:A:OP1	2.27	0.46
13:G:70:THR:HG23	13:G:73:PHE:H	1.81	0.46
6:7:190:MET:HB2	6:7:259:PHE:HD2	1.81	0.46
15:I:62:ILE:HD13	22:P:142:GLU:HB2	1.98	0.46
4:4:161:ILE:HD11	4:4:191:LEU:HD13	1.97	0.46
6:7:268:LEU:HB2	6:7:305:LEU:HD21	1.97	0.46
7:A:893:G:N7	16:J:78:ARG:NH1	2.63	0.46
28:V:30:LEU:HD12	28:V:149:ASP:HB2	1.97	0.46
7:A:1190:C:H42	7:A:1464:G:H22	1.62	0.45
7:A:1401:G:N2	7:A:1404:A:OP2	2.47	0.45
14:H:108:VAL:HG13	14:H:143:LEU:HD23	1.98	0.45
6:7:336:GLU:N	6:7:336:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:383:HIS:O	6:7:383:HIS:ND1	2.50	0.45
7:A:917:C:O2'	7:A:921:U:OP1	2.33	0.45
7:A:1234:C:O2'	17:K:40:ARG:NH1	2.49	0.45
6:7:190:MET:SD	6:7:191:ASP:N	2.89	0.45
6:7:365:LYS:HZ3	7:A:1221:A:H5'	1.81	0.45
12:F:46:ILE:O	12:F:46:ILE:HG22	2.16	0.45
11:E:26:ILE:HG21	27:U:173:LEU:HD13	1.98	0.45
6:7:415:LEU:HD13	6:7:428:ALA:HB2	1.99	0.45
7:A:1237:A:O4'	17:K:33:ARG:NH2	2.49	0.45
10:D:391:LEU:HD23	10:D:392:ARG:O	2.17	0.45
28:V:226:TYR:CE2	28:V:282:VAL:HG21	2.52	0.45
4:4:540:HIS:HB3	4:4:541:PRO:HD2	1.97	0.45
5:6:190:LEU:HD11	12:F:238:HIS:HA	1.98	0.45
7:A:1057:G:H4'	7:A:1578:A:H4'	1.98	0.45
32:Z:26:THR:HG21	32:Z:31:MET:SD	2.57	0.45
20:N:103:THR:O	20:N:103:THR:HG22	2.18	0.44
4:4:262:MET:O	4:4:266:MET:HE2	2.17	0.44
24:R:73:GLU:N	24:R:73:GLU:OE2	2.49	0.44
2:1:244:THR:HG22	2:1:245:GLU:N	2.32	0.44
4:4:79:ASN:OD1	4:4:80:ARG:N	2.43	0.44
1:0:37:ASP:O	1:0:41:LEU:N	2.44	0.44
11:E:65:LEU:HD11	22:P:75:LYS:CD	2.46	0.44
17:K:67:LEU:HD11	31:Y:383:LYS:HD2	1.98	0.44
18:L:112:MET:O	18:L:116:VAL:HG12	2.18	0.44
2:1:106:LEU:HD11	9:C:120:CYS:SG	2.58	0.44
7:A:1258:A:H61	7:A:1329:U:H3'	1.83	0.44
4:4:166:VAL:HG23	4:4:167:LYS:N	2.33	0.44
13:G:210:VAL:HG12	13:G:210:VAL:O	2.17	0.44
28:V:287:LEU:O	28:V:291:THR:HG22	2.18	0.44
4:4:322:HIS:O	4:4:325:ALA:N	2.50	0.43
4:4:445:TRP:O	4:4:448:ILE:HG12	2.18	0.43
37:A:1733:NAD:O4B	37:A:1733:NAD:N7N	2.51	0.43
25:S:84:ALA:HB3	29:W:101:ILE:HD11	1.99	0.43
8:B:229:PRO:HA	8:B:232:ILE:HD13	2.00	0.43
24:R:209:ILE:HD12	24:R:214:ASN:HB3	1.99	0.43
31:Y:260:ASP:OD1	31:Y:260:ASP:N	2.50	0.43
1:0:132:GLU:OE1	1:0:210:LYS:NZ	2.46	0.43
25:S:87:LEU:HD13	29:W:89:LEU:HD13	2.01	0.43
7:A:1401:G:H22	7:A:1404:A:H5'	1.84	0.43
3:3:165:LYS:NZ	7:A:1149:G:OP2	2.39	0.43
17:K:70:VAL:HG11	31:Y:383:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:549:ALA:HB2	4:4:586:ALA:CB	2.49	0.43
4:4:649:VAL:HG12	4:4:655:ILE:HD11	1.99	0.43
7:A:889:G:HO2'	7:A:903:U:H5	1.65	0.43
24:R:243:ILE:HG23	24:R:247:HIS:CE1	2.54	0.43
4:4:302:VAL:HG11	4:4:341:CYS:HB3	2.01	0.42
7:A:1264:C:H5''	7:A:1265:C:OP2	2.19	0.42
14:H:120:LEU:HD11	17:K:111:PHE:HD2	1.84	0.42
21:O:116:ASP:OD1	21:O:117:PHE:N	2.52	0.42
12:F:82:THR:HG22	12:F:83:SER:N	2.34	0.42
28:V:264:GLU:HG2	28:V:337:LEU:HD21	2.00	0.42
1:O:166:TYR:O	21:O:199:TRP:NE1	2.42	0.42
4:4:359:GLU:HG2	31:Y:256:LEU:HD12	2.01	0.42
6:7:231:LEU:HD11	6:7:242:ILE:H	1.84	0.42
7:A:1140:A:H2	7:A:1163:C:H42	1.67	0.42
12:F:85:VAL:HG22	30:X:379:GLU:OE2	2.20	0.42
15:I:166:ILE:HD11	23:Q:19:VAL:HG11	2.01	0.42
4:4:305:ILE:HG22	4:4:306:ASN:N	2.35	0.42
14:H:106:ILE:HD12	14:H:145:LEU:HD21	2.01	0.42
30:X:186:THR:O	30:X:190:ASN:ND2	2.53	0.42
8:B:270:LEU:O	8:B:270:LEU:HD23	2.19	0.42
9:C:123:VAL:HG23	9:C:157:THR:HG22	2.02	0.42
30:X:370:LYS:O	30:X:373:THR:OG1	2.33	0.42
24:R:276:VAL:CG1	24:R:307:LEU:HD12	2.48	0.42
24:R:337:GLN:OE1	24:R:337:GLN:N	2.52	0.42
4:4:158:LYS:HD3	4:4:187:THR:HG23	2.00	0.42
7:A:1080:A:H1'	7:A:1082:A:N7	2.35	0.42
27:U:89:VAL:HG13	27:U:90:LEU:N	2.34	0.41
5:6:199:VAL:O	5:6:199:VAL:HG22	2.20	0.41
6:7:30:LEU:HD23	6:7:413:ALA:CB	2.51	0.41
9:C:92:LEU:HD11	9:C:117:LEU:HD21	2.02	0.41
7:A:948:U:OP2	7:A:1045:G:N1	2.46	0.41
7:A:1289:G:O2'	7:A:1297:G:OP2	2.31	0.41
5:6:92:ARG:NH1	7:A:1570:G:N3	2.68	0.41
14:H:181:PRO:O	14:H:184:ILE:HG22	2.21	0.41
1:O:78:ARG:NH2	28:V:171:GLU:OE1	2.53	0.41
14:H:108:VAL:HG22	14:H:143:LEU:HD23	2.02	0.41
19:M:55:ASP:OD2	26:T:146:GLN:NE2	2.52	0.41
30:X:74:ASP:OD2	30:X:147:LYS:NZ	2.31	0.41
4:4:420:MET:HE1	4:4:461:PHE:HD1	1.85	0.41
6:7:67:LEU:HD13	6:7:201:TRP:CE2	2.55	0.41
7:A:1298:U:H2'	7:A:1299:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1353:A:HO2'	7:A:1354:A:P	2.44	0.41
25:S:109:LEU:O	25:S:109:LEU:HD12	2.20	0.41
1:O:187:GLU:OE1	1:O:187:GLU:N	2.54	0.41
26:T:103:ARG:NH2	26:T:110:GLU:OE2	2.54	0.41
7:A:1013:A:HO2'	7:A:1014:A:P	2.37	0.40
7:A:1466:C:O2'	7:A:1467:C:OP1	2.29	0.40
8:B:146:SER:OG	8:B:197:HIS:ND1	2.45	0.40
1:O:99:ARG:HG3	7:A:1526:U:H2'	2.03	0.40
7:A:1375:C:H2'	7:A:1376:C:O4'	2.21	0.40
6:7:105:GLU:OE2	6:7:108:ARG:NH1	2.48	0.40
7:A:1211:G:H21	7:A:1353:A:H4'	1.87	0.40
4:4:472:ASP:OD2	4:4:473:VAL:N	2.55	0.40
6:7:432:SER:OG	6:7:433:TRP:N	2.53	0.40
7:A:1429:C:H3'	7:A:1430:A:C5'	2.52	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	
1	0	209/218 (96%)	207 (99%)	2 (1%)	0	100	100
2	1	255/323 (79%)	252 (99%)	3 (1%)	0	100	100
3	3	68/199 (34%)	68 (100%)	0	0	100	100
4	4	558/689 (81%)	552 (99%)	6 (1%)	0	100	100
5	6	122/343 (36%)	119 (98%)	3 (2%)	0	100	100
6	7	396/456 (87%)	389 (98%)	7 (2%)	0	100	100
8	B	218/296 (74%)	217 (100%)	1 (0%)	0	100	100
9	C	122/167 (73%)	119 (98%)	3 (2%)	0	100	100
10	D	228/430 (53%)	224 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	E	106/125 (85%)	104 (98%)	2 (2%)	0	100	100
12	F	204/242 (84%)	202 (99%)	2 (1%)	0	100	100
13	G	288/396 (73%)	286 (99%)	1 (0%)	1 (0%)	41	68
14	H	126/201 (63%)	124 (98%)	2 (2%)	0	100	100
15	I	135/194 (70%)	130 (96%)	5 (4%)	0	100	100
16	J	105/138 (76%)	101 (96%)	4 (4%)	0	100	100
17	K	98/128 (77%)	97 (99%)	1 (1%)	0	100	100
18	L	159/257 (62%)	157 (99%)	2 (1%)	0	100	100
19	M	113/137 (82%)	113 (100%)	0	0	100	100
20	N	107/130 (82%)	106 (99%)	1 (1%)	0	100	100
21	O	188/258 (73%)	185 (98%)	3 (2%)	0	100	100
22	P	94/142 (66%)	94 (100%)	0	0	100	100
23	Q	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
24	R	289/360 (80%)	285 (99%)	4 (1%)	0	100	100
25	S	131/190 (69%)	130 (99%)	1 (1%)	0	100	100
26	T	162/173 (94%)	161 (99%)	1 (1%)	0	100	100
27	U	172/205 (84%)	172 (100%)	0	0	100	100
28	V	355/414 (86%)	348 (98%)	7 (2%)	0	100	100
29	W	96/187 (51%)	95 (99%)	1 (1%)	0	100	100
30	X	350/398 (88%)	342 (98%)	8 (2%)	0	100	100
31	Y	119/395 (30%)	118 (99%)	1 (1%)	0	100	100
32	Z	67/106 (63%)	65 (97%)	2 (3%)	0	100	100
All	All	5724/7984 (72%)	5645 (99%)	78 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	G	249	THR

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	
1	0	184/190 (97%)	183 (100%)	1 (0%)	88	96
2	1	239/291 (82%)	239 (100%)	0	100	100
3	3	65/166 (39%)	65 (100%)	0	100	100
4	4	506/609 (83%)	504 (100%)	2 (0%)	91	96
5	6	107/288 (37%)	107 (100%)	0	100	100
6	7	340/385 (88%)	339 (100%)	1 (0%)	92	97
8	B	194/249 (78%)	194 (100%)	0	100	100
9	C	111/143 (78%)	111 (100%)	0	100	100
10	D	196/357 (55%)	196 (100%)	0	100	100
11	E	91/107 (85%)	91 (100%)	0	100	100
12	F	183/209 (88%)	183 (100%)	0	100	100
13	G	254/342 (74%)	253 (100%)	1 (0%)	91	96
14	H	120/180 (67%)	120 (100%)	0	100	100
15	I	105/147 (71%)	105 (100%)	0	100	100
16	J	92/118 (78%)	92 (100%)	0	100	100
17	K	90/113 (80%)	90 (100%)	0	100	100
18	L	151/226 (67%)	151 (100%)	0	100	100
19	M	94/113 (83%)	93 (99%)	1 (1%)	73	90
20	N	95/115 (83%)	95 (100%)	0	100	100
21	O	171/230 (74%)	171 (100%)	0	100	100
22	P	87/123 (71%)	87 (100%)	0	100	100
23	Q	78/79 (99%)	78 (100%)	0	100	100
24	R	261/318 (82%)	261 (100%)	0	100	100
25	S	115/164 (70%)	115 (100%)	0	100	100
26	T	151/157 (96%)	151 (100%)	0	100	100
27	U	150/174 (86%)	150 (100%)	0	100	100
28	V	323/364 (89%)	323 (100%)	0	100	100
29	W	85/158 (54%)	85 (100%)	0	100	100
30	X	311/351 (89%)	310 (100%)	1 (0%)	92	97
31	Y	113/357 (32%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Z	63/95 (66%)	63 (100%)	0	100	100
All	All	5125/6918 (74%)	5118 (100%)	7 (0%)	93	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	107	GLN
4	4	164	ARG
4	4	167	LYS
6	7	139	ARG
13	G	379	ARG
19	M	29	ARG
30	X	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	285	ASN
5	6	90	HIS
5	6	165	HIS
6	7	49	HIS
6	7	112	HIS
6	7	398	HIS
6	7	400	HIS
6	7	412	HIS
10	D	280	HIS
11	E	58	HIS
12	F	127	HIS
23	Q	41	HIS
30	X	140	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	880/955 (92%)	203 (23%)	4 (0%)

All (203) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	650	U
7	A	651	A
7	A	680	U
7	A	688	A
7	A	689	U
7	A	704	U
7	A	721	U
7	A	722	C
7	A	735	A
7	A	736	C
7	A	737	C
7	A	739	C
7	A	741	A
7	A	753	A
7	A	761	A
7	A	766	G
7	A	769	G
7	A	772	A
7	A	773	U
7	A	777	G
7	A	782	A
7	A	791	G
7	A	794	U
7	A	796	G
7	A	807	A
7	A	829	C
7	A	830	U
7	A	831	U
7	A	832	U
7	A	835	C
7	A	851	A
7	A	860	A
7	A	861	U
7	A	866	A
7	A	868	C
7	A	871	A
7	A	886	C
7	A	889	G
7	A	893	G
7	A	902	G
7	A	903	U
7	A	919	A
7	A	931	C

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Mol	Chain	Res	Type
7	A	938	A
7	A	939	A
7	A	942	A
7	A	954	C
7	A	967	A
7	A	970	A
7	A	971	A
7	A	972	G
7	A	976	A
7	A	992	U
7	A	993	A
7	A	1001	C
7	A	1002	C
7	A	1011	C
7	A	1012	A
7	A	1014	A
7	A	1015	A
7	A	1031	G
7	A	1036	A
7	A	1041	A
7	A	1042	U
7	A	1052	C
7	A	1053	A
7	A	1060	A
7	A	1061	A
7	A	1081	U
7	A	1082	A
7	A	1103	A
7	A	1105	C
7	A	1106	C
7	A	1111	C
7	A	1117	A
7	A	1119	U
7	A	1120	C
7	A	1121	A
7	A	1137	A
7	A	1151	C
7	A	1152	A
7	A	1160	A
7	A	1167	A
7	A	1175	G
7	A	1178	G

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Mol	Chain	Res	Type
7	A	1179	G
7	A	1181	G
7	A	1182	C
7	A	1184	U
7	A	1185	C
7	A	1186	A
7	A	1187	U
7	A	1188	A
7	A	1189	U
7	A	1190	C
7	A	1191	C
7	A	1198	A
7	A	1200	G
7	A	1206	G
7	A	1215	U
7	A	1217	G
7	A	1218	A
7	A	1219	U
7	A	1220	A
7	A	1221	A
7	A	1223	C
7	A	1224	C
7	A	1225	C
7	A	1226	C
7	A	1229	U
7	A	1240	A
7	A	1241	C
7	A	1243	U
7	A	1246	U
7	A	1247	G
7	A	1248	C
7	A	1250	C
7	A	1251	A
7	A	1254	C
7	A	1258	A
7	A	1259	U
7	A	1260	A
7	A	1261	C
7	A	1264	C
7	A	1265	C
7	A	1284	U
7	A	1290	C

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Mol	Chain	Res	Type
7	A	1291	U
7	A	1294	A
7	A	1296	A
7	A	1297	G
7	A	1299	A
7	A	1323	G
7	A	1327	G
7	A	1331	A
7	A	1332	A
7	A	1333	G
7	A	1334	G
7	A	1338	A
7	A	1339	G
7	A	1342	C
7	A	1343	A
7	A	1344	U
7	A	1346	A
7	A	1350	G
7	A	1353	A
7	A	1354	A
7	A	1355	G
7	A	1357	A
7	A	1358	A
7	A	1365	A
7	A	1367	A
7	A	1368	U
7	A	1378	C
7	A	1385	C
7	A	1386	U
7	A	1387	A
7	A	1392	A
7	A	1397	U
7	A	1402	A
7	A	1404	A
7	A	1406	U
7	A	1416	A
7	A	1419	G
7	A	1420	U
7	A	1421	G
7	A	1422	G
7	A	1427	A
7	A	1430	A

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Mol	Chain	Res	Type
7	A	1434	A
7	A	1435	A
7	A	1440	G
7	A	1441	A
7	A	1448	U
7	A	1449	G
7	A	1463	G
7	A	1464	G
7	A	1467	C
7	A	1468	U
7	A	1470	A
7	A	1471	A
7	A	1475	C
7	A	1492	A
7	A	1512	A
7	A	1515	G
7	A	1519	A
7	A	1522	U
7	A	1525	C
7	A	1526	U
7	A	1527	A
7	A	1533	C
7	A	1536	A
7	A	1537	C
7	A	1538	G
7	A	1539	C
7	A	1543	U
7	A	1545	U
7	A	1549	G
7	A	1558	A
7	A	1572	A
7	A	1594	G
7	A	1595	G
7	A	1598	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1151	C
7	A	1219	U
7	A	1354	A
7	A	1434	A

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

3 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
23	AYA	Q	2	23	6,7,8	1.28	1 (16%)	5,8,10	1.30	1 (20%)
7	MA6	A	1584	7	19,26,27	1.09	1 (5%)	18,38,41	2.10	3 (16%)
7	MA6	A	1583	7	19,26,27	1.09	1 (5%)	18,38,41	2.07	4 (22%)

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
23	AYA	Q	2	23	-	0/4/6/8	-
7	MA6	A	1584	7	-	0/7/29/30	0/3/3/3
7	MA6	A	1583	7	-	2/7/29/30	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1584	MA6	C5-N7	3.42	1.52	1.39
7	A	1583	MA6	C5-N7	3.39	1.52	1.39
23	Q	2	AYA	CA-N	-2.62	1.43	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1583	MA6	C4-C5-N7	-5.62	103.54	109.40
7	A	1584	MA6	C4-C5-N7	-5.62	103.55	109.40
7	A	1584	MA6	N3-C2-N1	-4.94	120.95	128.68
7	A	1583	MA6	N3-C2-N1	-4.93	120.97	128.68
7	A	1584	MA6	C1'-N9-C4	-4.10	119.44	126.64
7	A	1583	MA6	C1'-N9-C4	-3.63	120.26	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	2	AYA	CB-CA-N	2.68	112.59	109.61
7	A	1583	MA6	N1-C6-N6	2.21	119.38	117.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1583	MA6	C3'-C4'-C5'-O5'
7	A	1583	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 35 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	$\# Z > 2$
39	FES	P	201	22,11	0,4,4	-	-	-		
39	FES	T	201	26,19	0,4,4	-	-	-		
40	ATP	X	501	36	26,33,33	0.66	0	31,52,52	1.08	2 (6%)
37	NAD	A	1733	36	42,48,48	2.39	15 (35%)	50,73,73	1.71	10 (20%)
41	GDP	X	503	-	24,30,30	3.38	12 (50%)	30,47,47	2.19	8 (26%)
34	SAM	7	502	-	24,29,29	1.17	3 (12%)	23,42,42	1.57	4 (17%)
33	SF4	7	501	6	0,12,12	-	-	-		

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
39	FES	P	201	22,11	-	-	0/1/1/1
39	FES	T	201	26,19	-	-	0/1/1/1
40	ATP	X	501	36	-	3/18/38/38	0/3/3/3
37	NAD	A	1733	36	-	1/26/62/62	0/5/5/5
41	GDP	X	503	-	-	8/12/32/32	0/3/3/3
34	SAM	7	502	-	-	2/12/33/33	0/3/3/3
33	SF4	7	501	6	-	-	0/6/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	503	GDP	O6-C6	9.24	1.42	1.23
41	X	503	GDP	C2-N1	7.53	1.56	1.37
37	A	1733	NAD	C7N-N7N	6.98	1.46	1.33
41	X	503	GDP	C2-N3	5.25	1.45	1.33
41	X	503	GDP	C2-N2	5.21	1.46	1.34
37	A	1733	NAD	O4D-C1D	5.15	1.48	1.41
37	A	1733	NAD	O4B-C1B	4.90	1.47	1.41
37	A	1733	NAD	C2N-N1N	3.94	1.39	1.35
41	X	503	GDP	C6-N1	3.89	1.43	1.37
34	7	502	SAM	C2-N3	3.82	1.38	1.32
37	A	1733	NAD	C4N-C3N	3.51	1.45	1.39
37	A	1733	NAD	C6A-N6A	3.42	1.46	1.34
37	A	1733	NAD	C5A-N7A	3.33	1.51	1.39
37	A	1733	NAD	C2D-C1D	-3.33	1.48	1.53
41	X	503	GDP	C5-C4	-2.94	1.35	1.43
41	X	503	GDP	C2'-C3'	-2.87	1.45	1.53
37	A	1733	NAD	O7N-C7N	-2.87	1.18	1.24
41	X	503	GDP	O4'-C1'	2.76	1.44	1.41
37	A	1733	NAD	C5N-C4N	2.64	1.44	1.38
41	X	503	GDP	C5-C6	-2.56	1.42	1.47
41	X	503	GDP	PA-O5'	2.35	1.68	1.59
37	A	1733	NAD	C2B-C1B	-2.29	1.50	1.53
34	7	502	SAM	C2-N1	2.28	1.38	1.33
41	X	503	GDP	PB-O3B	-2.28	1.46	1.54
37	A	1733	NAD	C3N-C7N	2.20	1.53	1.50
37	A	1733	NAD	C2D-C3D	-2.18	1.47	1.53
34	7	502	SAM	OXT-C	-2.12	1.23	1.30
41	X	503	GDP	PB-O2B	-2.11	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	A	1733	NAD	C4A-N3A	-2.10	1.32	1.35
37	A	1733	NAD	PA-O2A	-2.01	1.45	1.55

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	X	503	GDP	C8-N7-C5	7.02	116.36	102.99
37	A	1733	NAD	C4A-C5A-N7A	-5.57	103.59	109.40
34	7	502	SAM	N3-C2-N1	-5.43	120.19	128.68
37	A	1733	NAD	C1B-N9A-C4A	-4.93	117.98	126.64
41	X	503	GDP	C2-N1-C6	-4.82	116.22	125.10
37	A	1733	NAD	N3A-C2A-N1A	-4.38	121.83	128.68
41	X	503	GDP	C3'-C2'-C1'	3.77	106.65	100.98
37	A	1733	NAD	C3B-C2B-C1B	3.74	106.61	100.98
37	A	1733	NAD	C3D-C2D-C1D	3.04	105.55	100.98
41	X	503	GDP	O3B-PB-O3A	2.71	113.74	104.64
41	X	503	GDP	O2B-PB-O3A	2.70	113.69	104.64
41	X	503	GDP	PA-O3A-PB	-2.69	123.58	132.83
34	7	502	SAM	OXT-C-O	-2.40	118.65	124.09
34	7	502	SAM	C3'-C2'-C1'	2.37	104.54	100.98
40	X	501	ATP	C5-C6-N6	2.33	123.89	120.35
37	A	1733	NAD	C2B-C3B-C4B	2.32	107.14	102.64
41	X	503	GDP	O2A-PA-O1A	-2.27	101.03	112.24
37	A	1733	NAD	O2N-PN-O1N	-2.19	101.39	112.24
37	A	1733	NAD	C3N-C7N-N7N	2.15	120.33	117.75
37	A	1733	NAD	PN-O3-PA	-2.14	125.49	132.83
41	X	503	GDP	C5-C6-N1	2.12	117.70	113.95
34	7	502	SAM	OXT-C-CA	2.12	120.59	113.38
37	A	1733	NAD	O2A-PA-O1A	-2.04	102.17	112.24
40	X	501	ATP	PB-O3B-PG	2.03	139.79	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	7	502	SAM	CB-CG-SD-CE
40	X	501	ATP	PB-O3B-PG-O2G
41	X	503	GDP	PA-O3A-PB-O3B
41	X	503	GDP	C5'-O5'-PA-O1A
41	X	503	GDP	C5'-O5'-PA-O2A
41	X	503	GDP	PB-O3A-PA-O2A
41	X	503	GDP	C4'-C5'-O5'-PA

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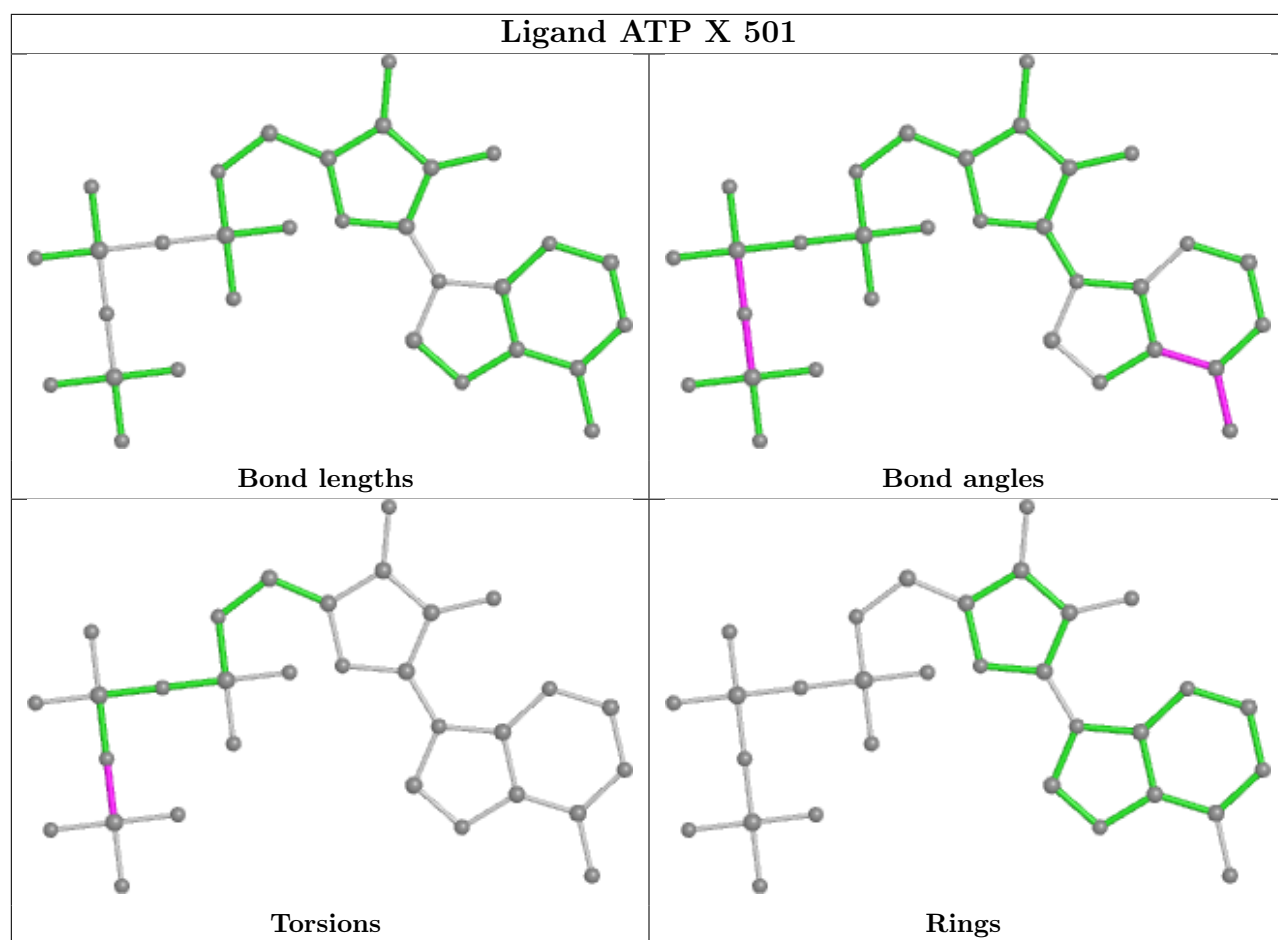
Mol	Chain	Res	Type	Atoms
40	X	501	ATP	PB-O3B-PG-O3G
41	X	503	GDP	PA-O3A-PB-O2B
41	X	503	GDP	C5'-O5'-PA-O3A
41	X	503	GDP	O4'-C4'-C5'-O5'
37	A	1733	NAD	C5B-O5B-PA-O1A
40	X	501	ATP	PB-O3B-PG-O1G
34	7	502	SAM	CB-CG-SD-C5'

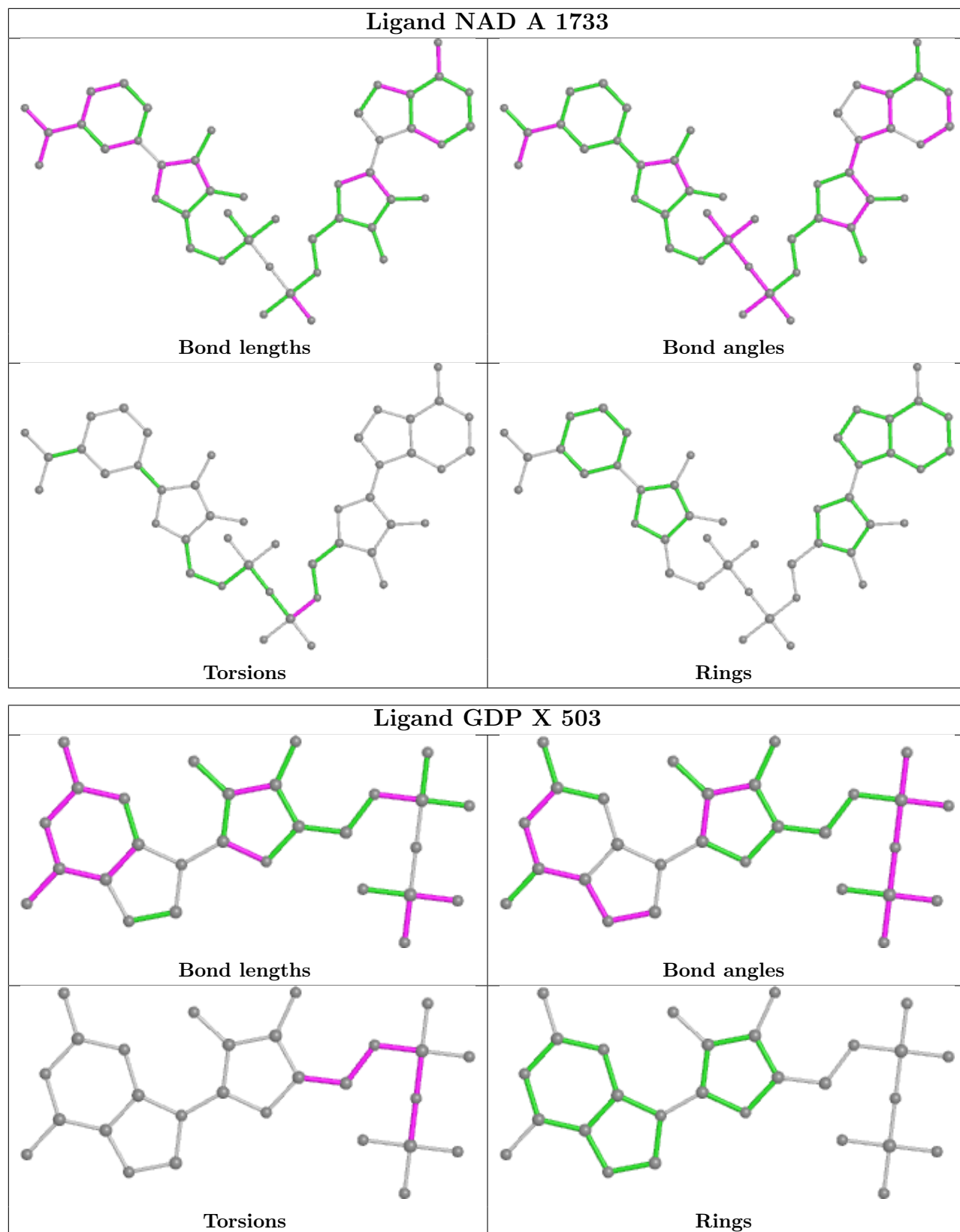
There are no ring outliers.

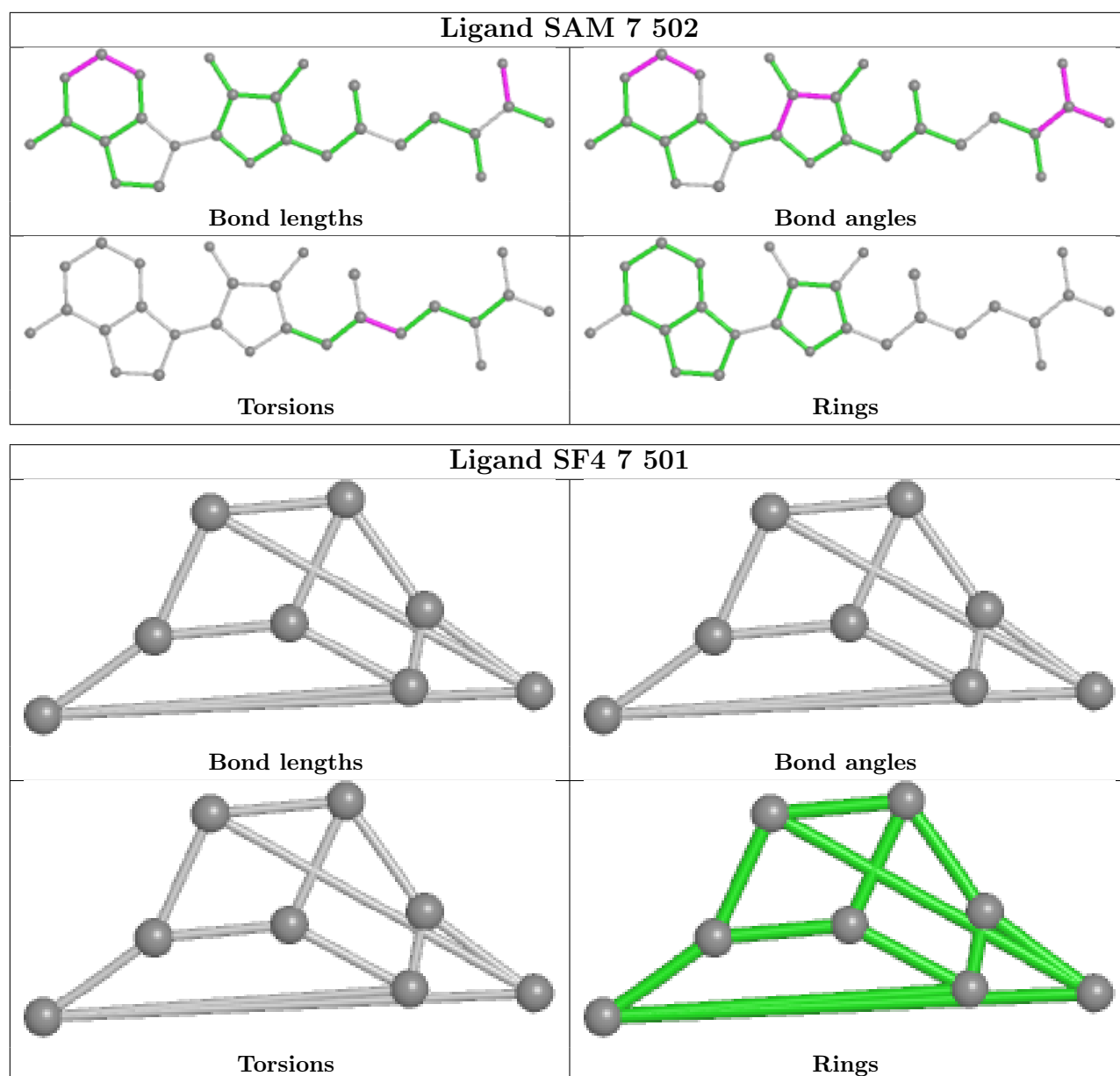
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	A	1733	NAD	1	0
41	X	503	GDP	1	0
34	7	502	SAM	2	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.

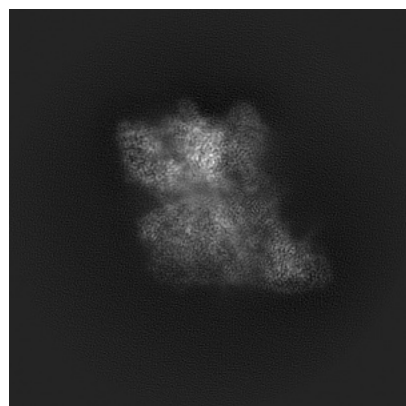
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26970. These allow visual inspection of the internal detail of the map and identification of artifacts.

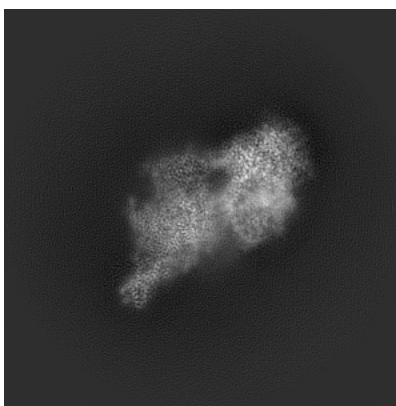
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

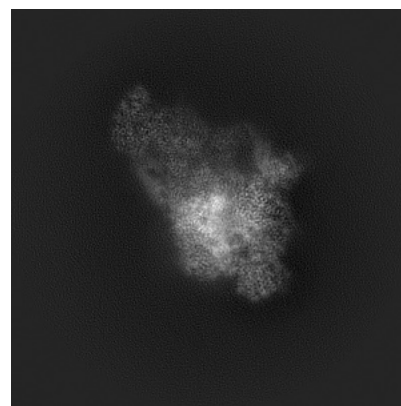
6.1.1 Primary map



X

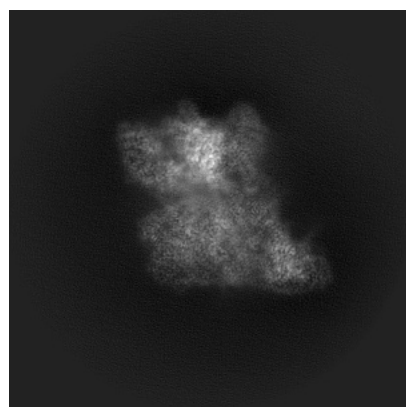


Y

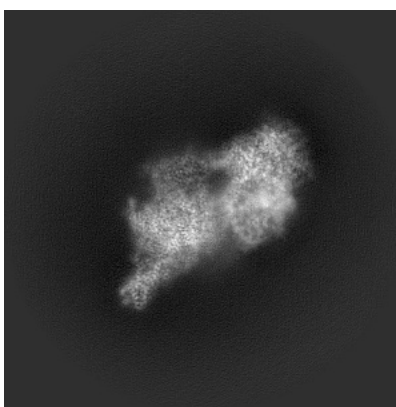


Z

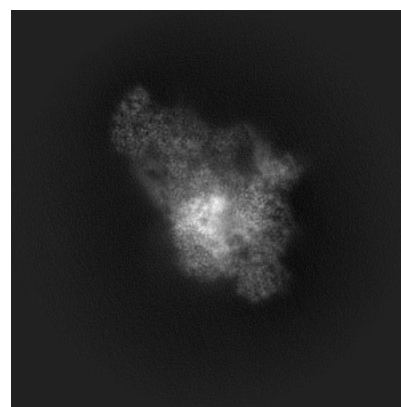
6.1.2 Raw map



X



Y

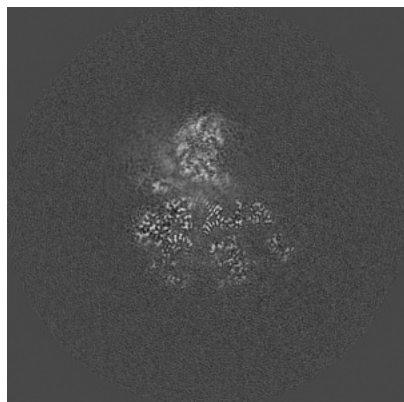


Z

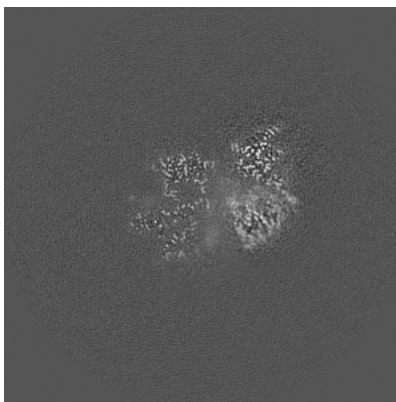
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

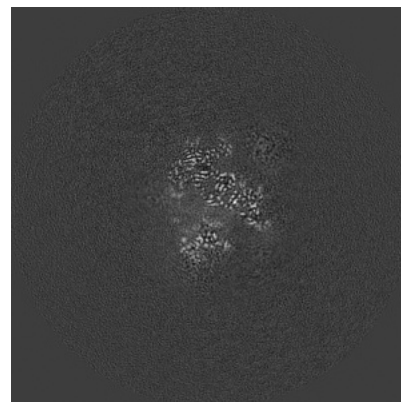
6.2.1 Primary map



X Index: 200

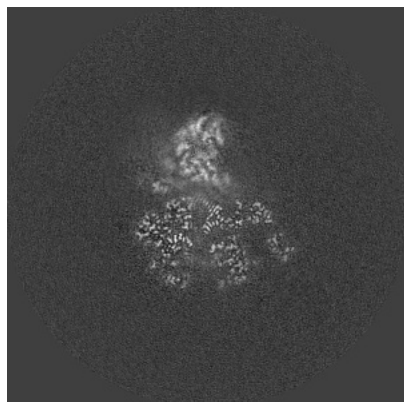


Y Index: 200

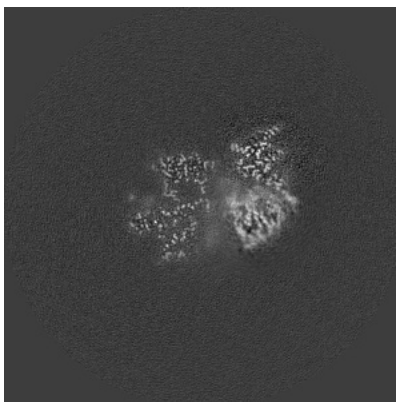


Z Index: 200

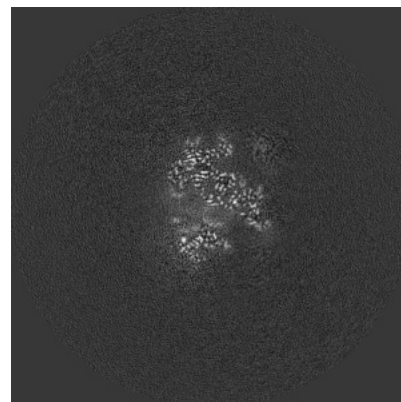
6.2.2 Raw map



X Index: 200



Y Index: 200

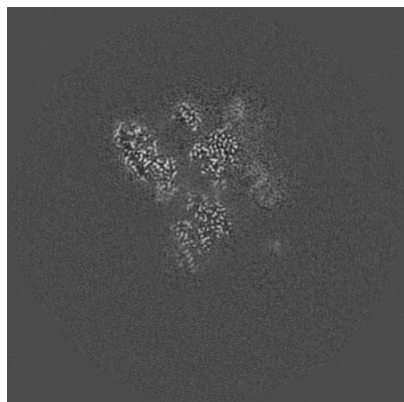


Z Index: 200

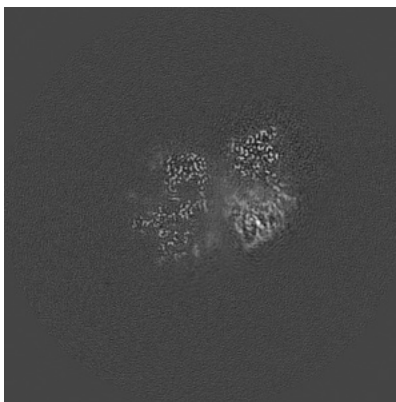
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

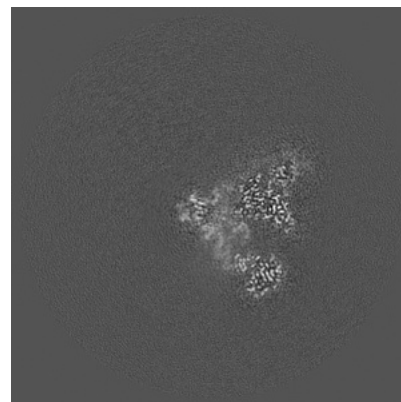
6.3.1 Primary map



X Index: 245

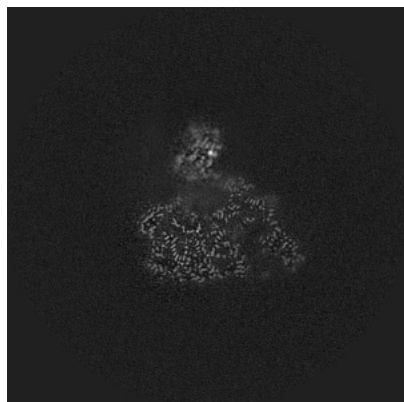


Y Index: 202

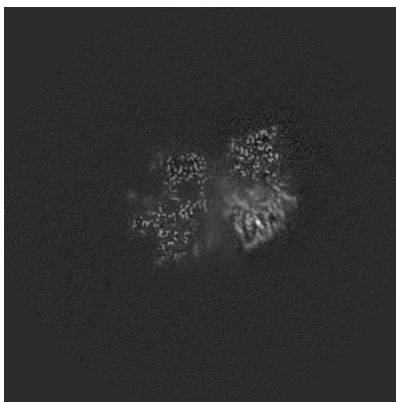


Z Index: 261

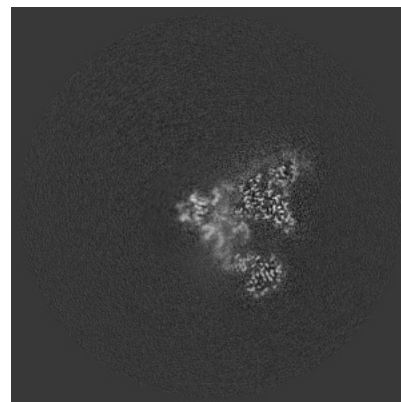
6.3.2 Raw map



X Index: 185



Y Index: 202



Z Index: 261

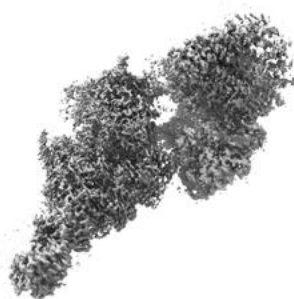
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

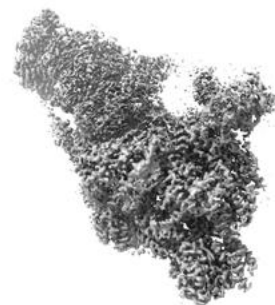
6.4.1 Primary map



X



Y



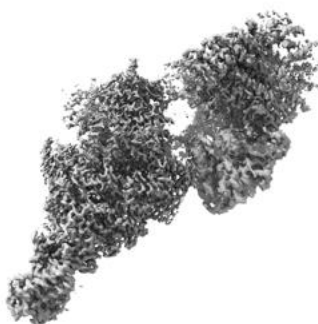
Z

The images above show the 3D surface view of the map at the recommended contour level 7.66. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

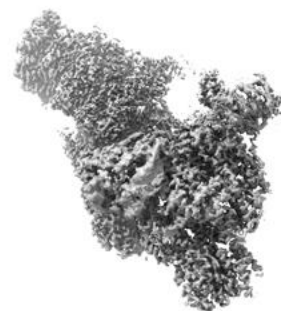
6.4.2 Raw map



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.

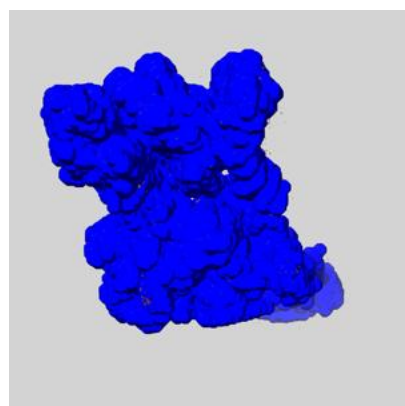
6.5 Mask visualisation [i](#)

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

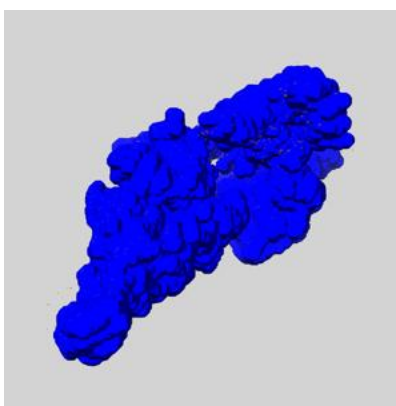
A mask typically either:

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

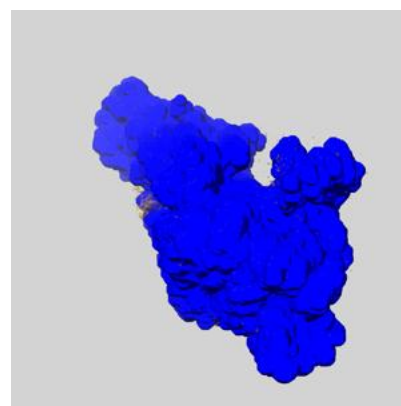
6.5.1 emd_26970_msk_1.map [i](#)



X



Y

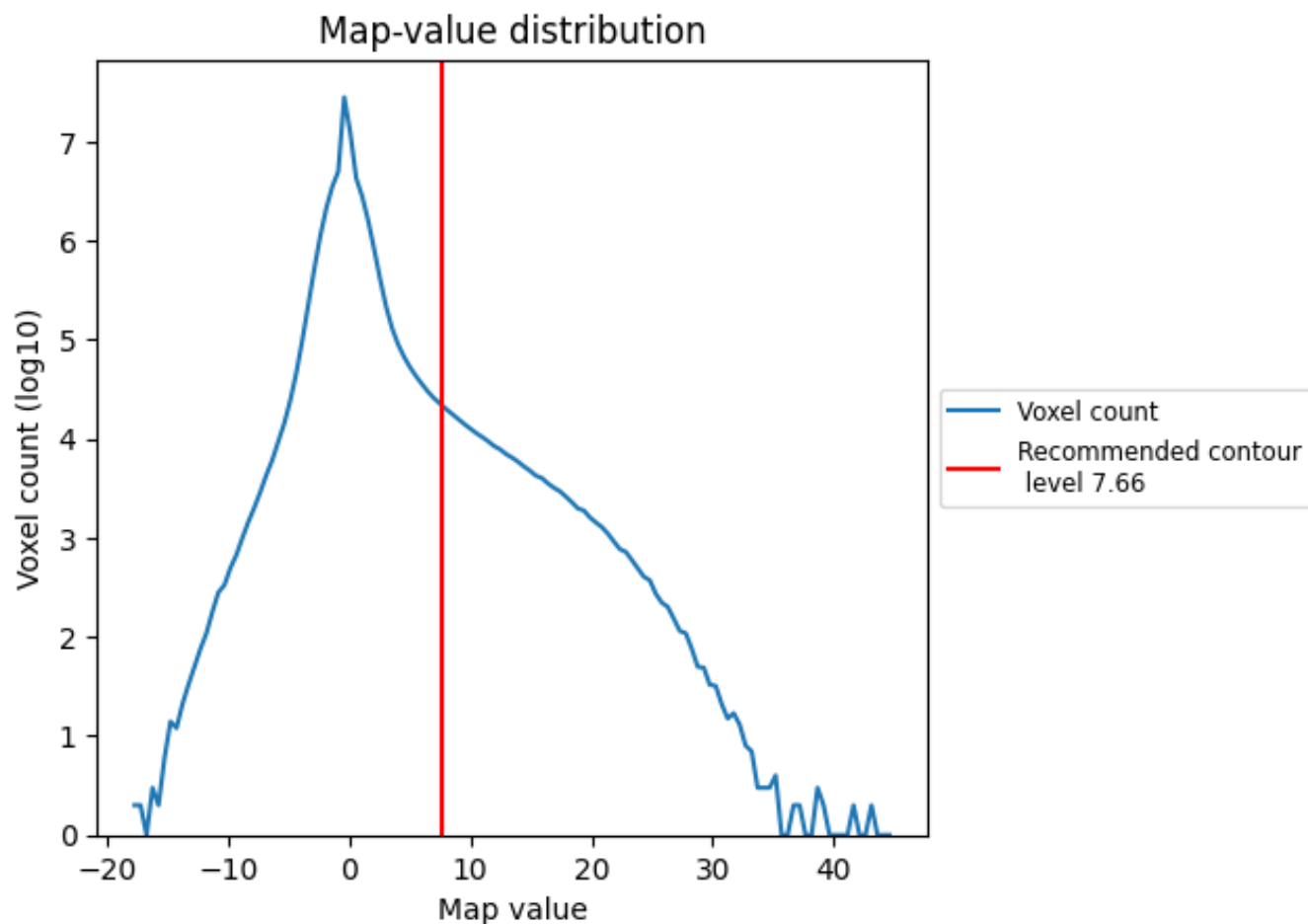


Z

7 Map analysis [i](#)

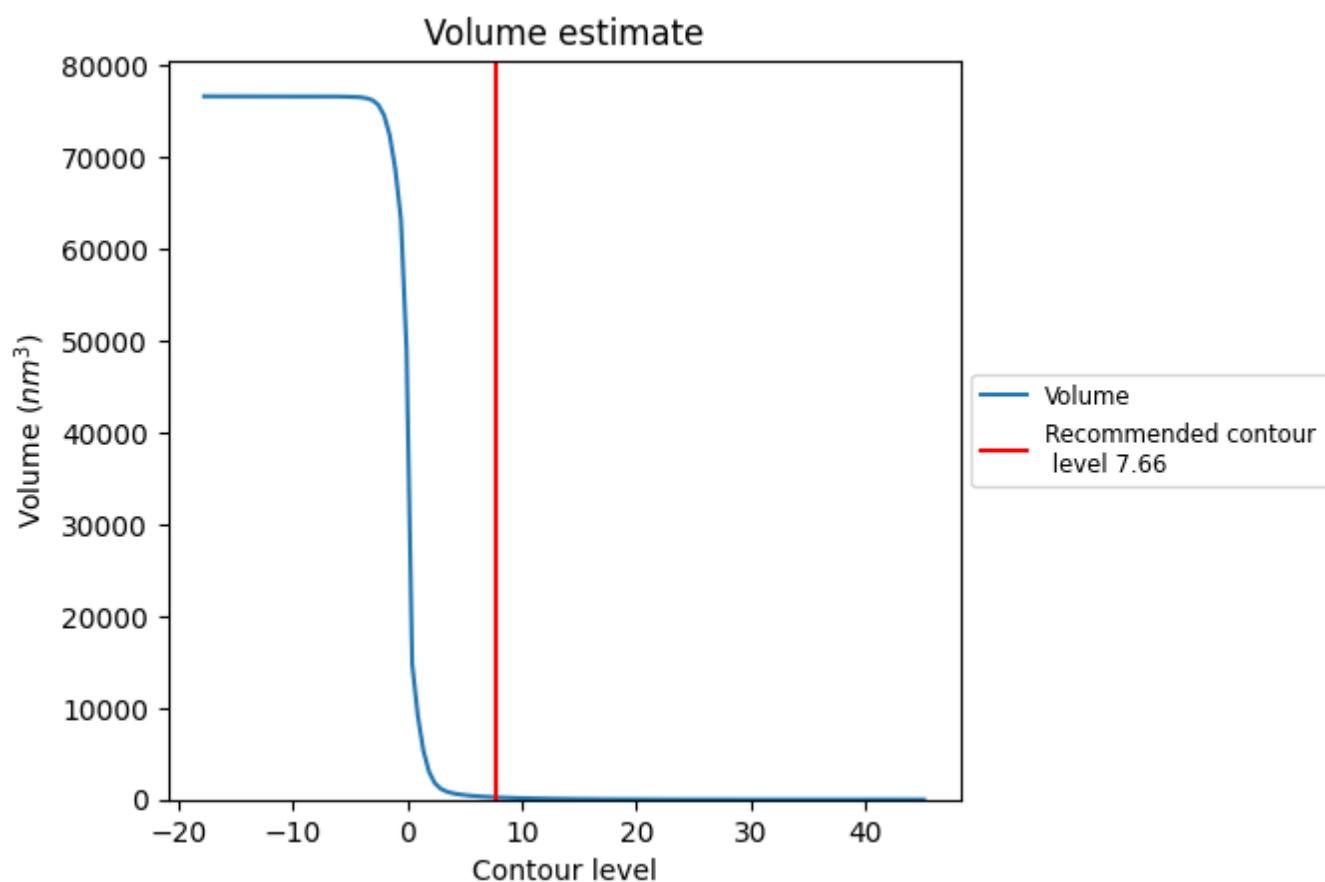
This section contains the results of statistical analysis of the map.

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.

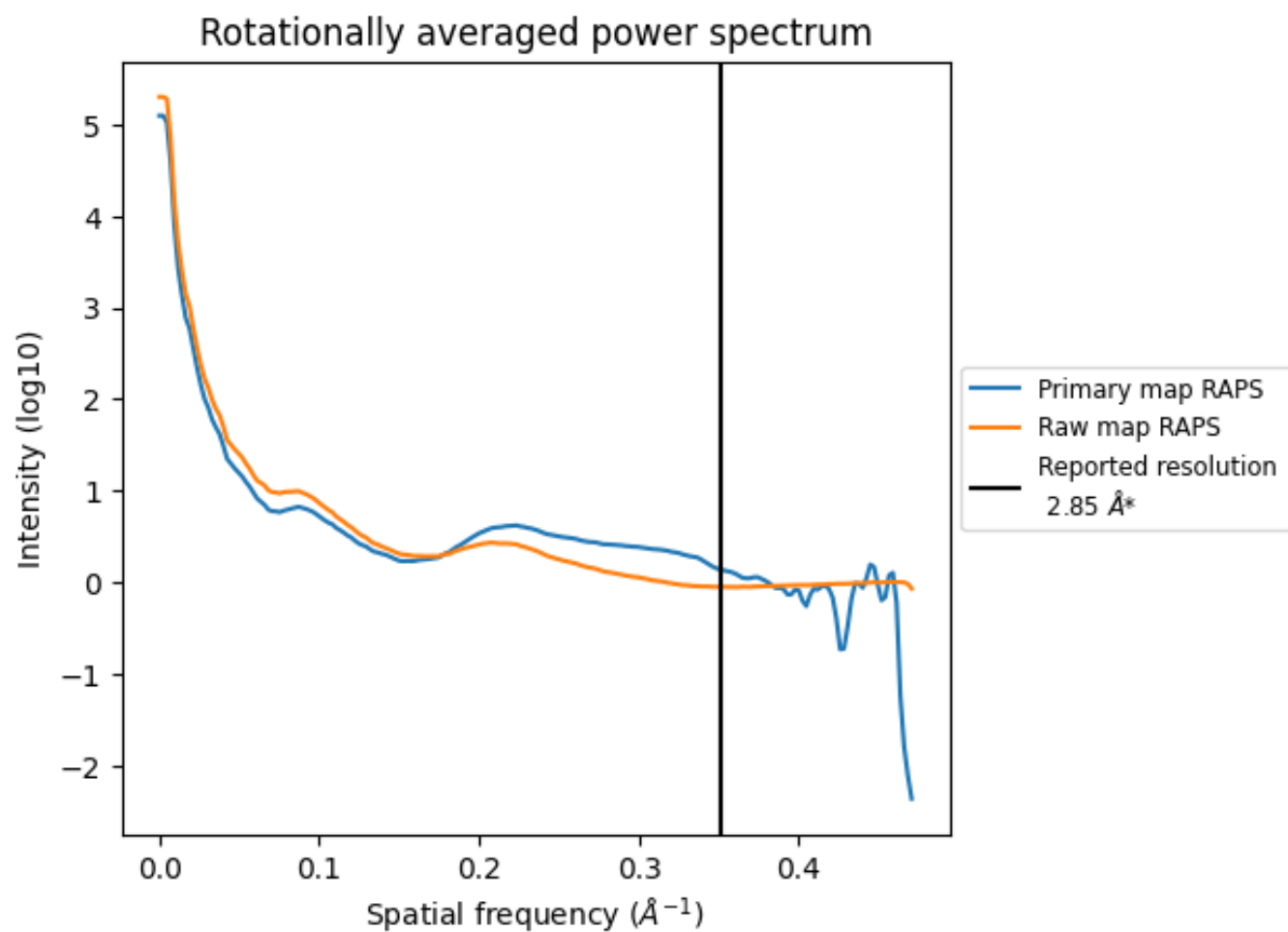
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm³; this corresponds to an approximate mass of 228 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 ⓘ

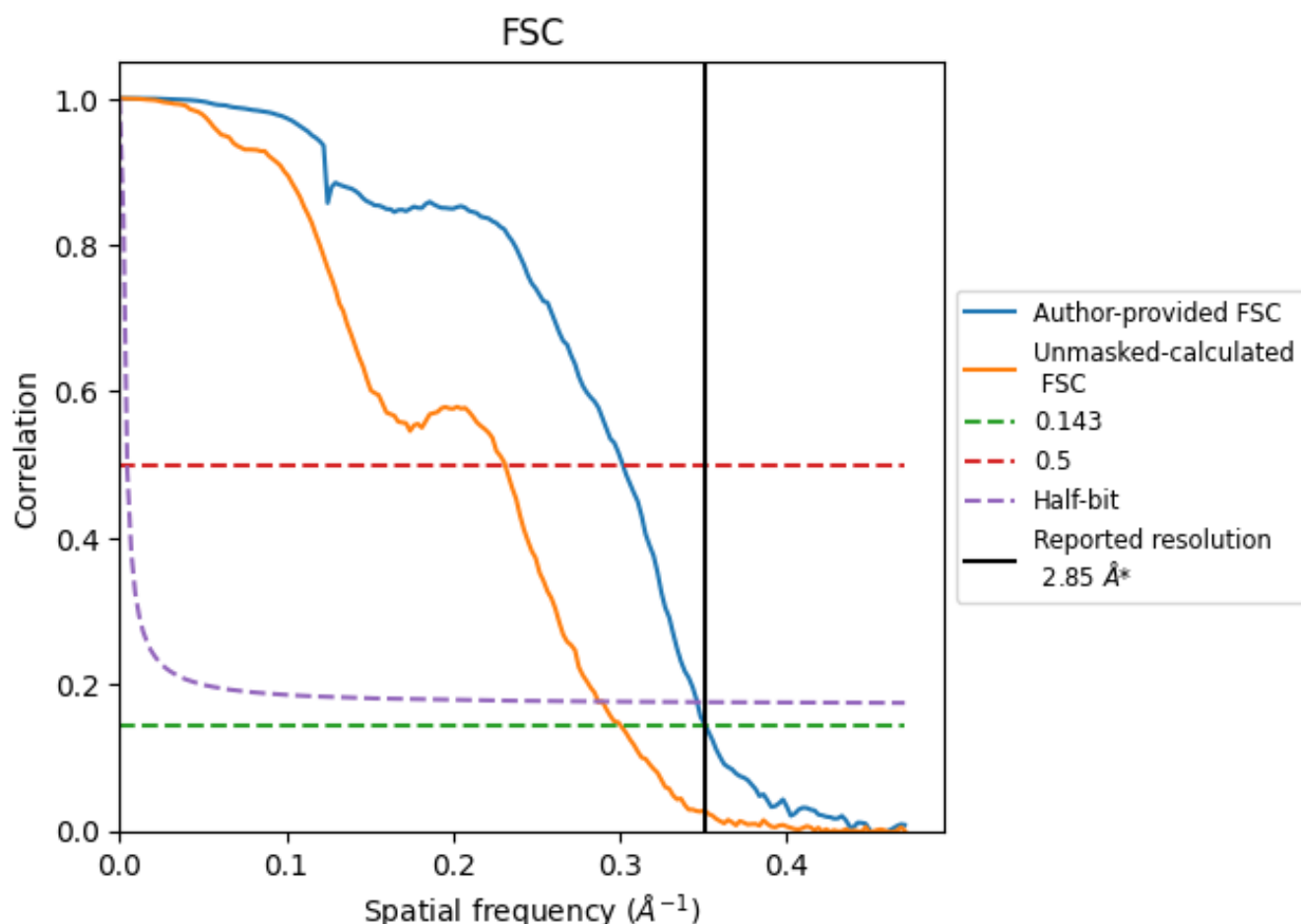


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 Å⁻¹

8.2 Resolution estimates [i](#)

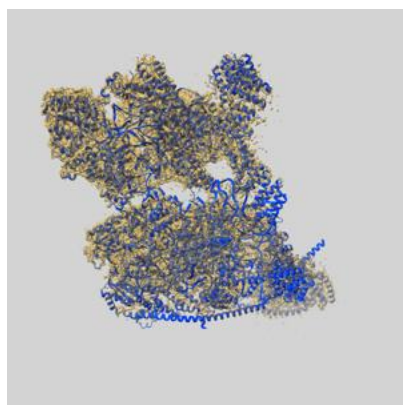
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.31	2.89
Unmasked-calculated*	3.33	4.33	3.48

*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 3.33 differs from the reported value 2.85 by more than 10 %

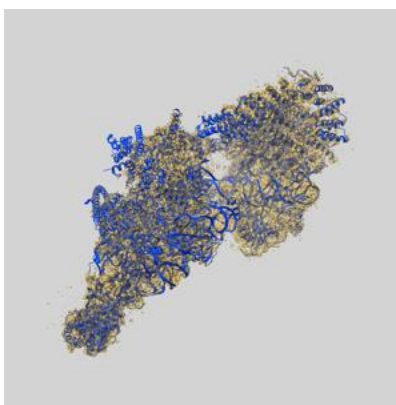
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26970 and PDB model 8CST. Per-residue inclusion information can be found in section [3](#) on page [13](#).

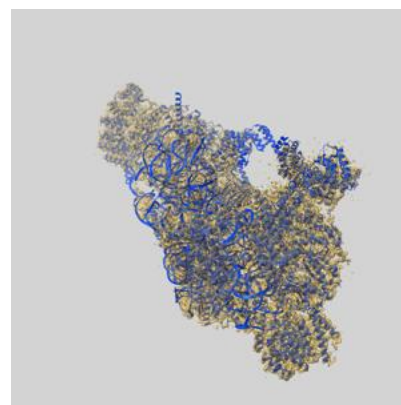
9.1 Map-model overlay [i](#)



X



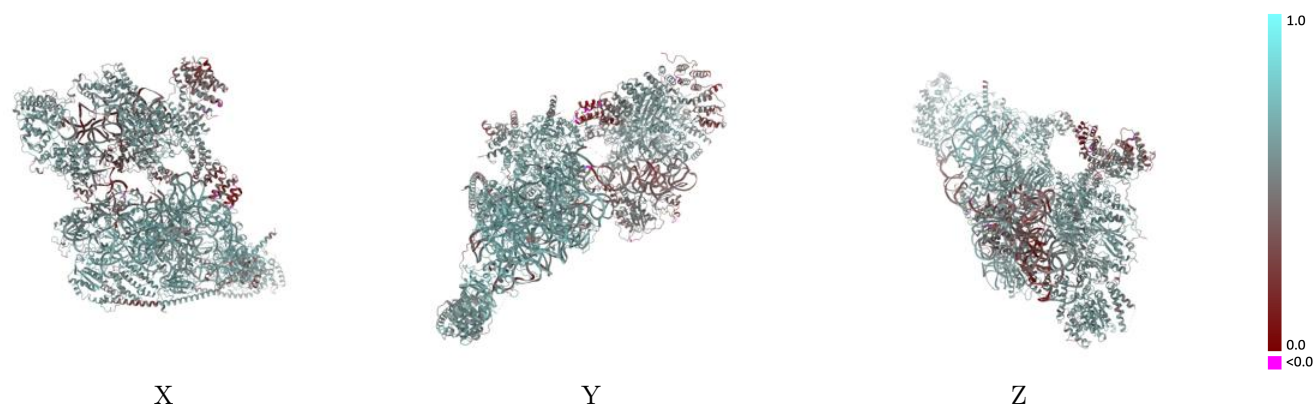
Y



Z

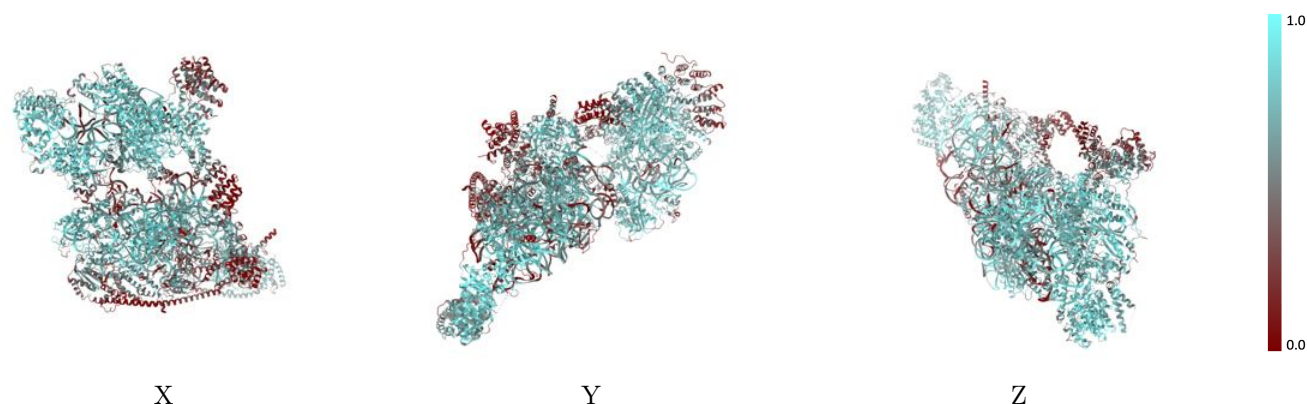
The images above show the 3D surface view of the map at the recommended contour level 7.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



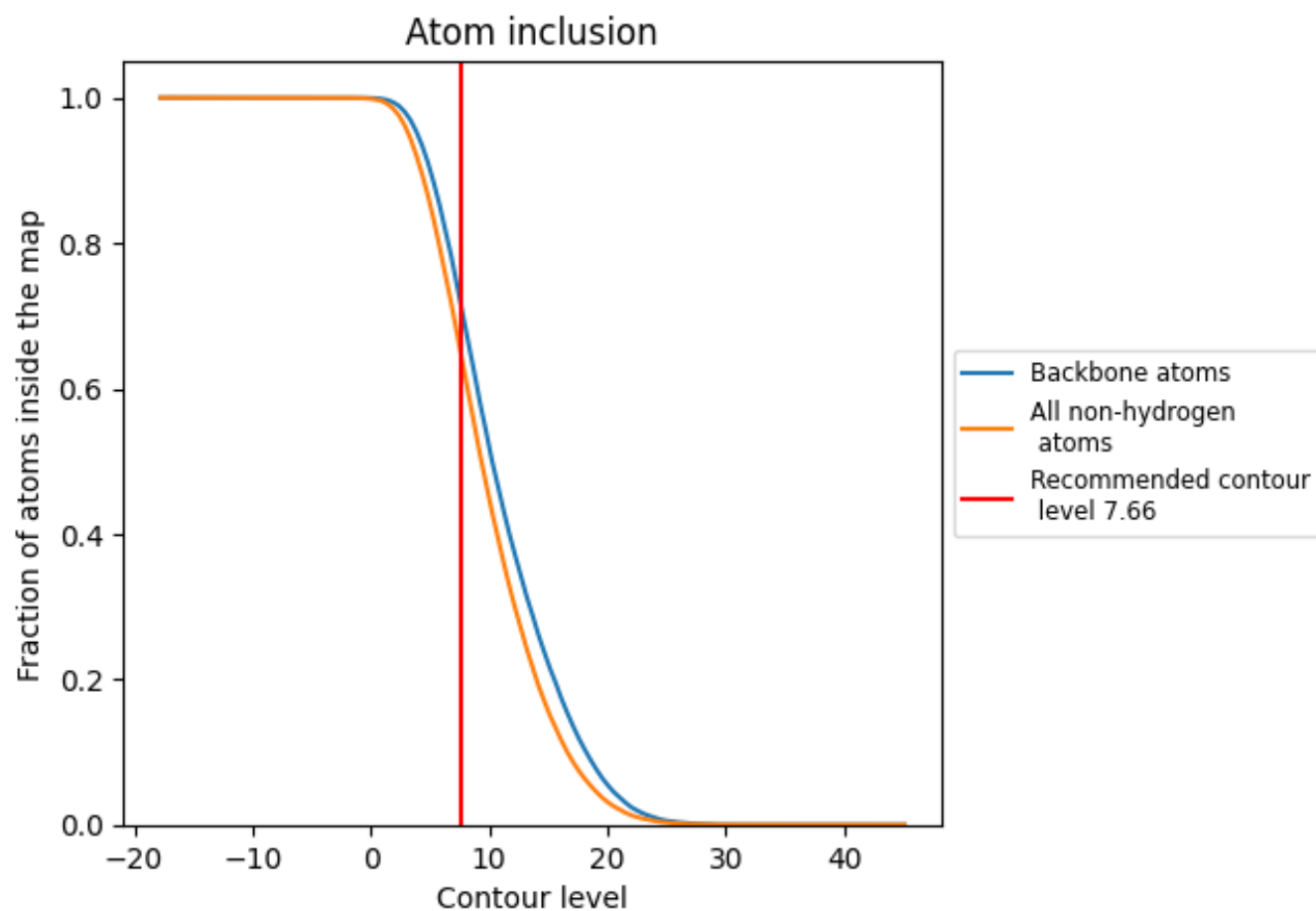
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7.66).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 64% 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 (7.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6444	 0.5550
0	 0.7031	 0.6050
1	 0.7629	 0.5690
3	 0.3782	 0.5800
4	 0.4772	 0.4270
6	 0.6882	 0.5540
7	 0.7132	 0.4110
A	 0.6908	 0.5370
B	 0.7961	 0.6320
C	 0.8205	 0.5830
D	 0.6009	 0.6190
E	 0.4748	 0.6170
F	 0.6997	 0.5180
G	 0.6670	 0.5520
H	 0.7735	 0.5800
I	 0.7722	 0.5800
J	 0.4132	 0.6050
K	 0.8007	 0.5820
L	 0.4981	 0.6210
M	 0.6659	 0.6480
N	 0.5571	 0.6430
O	 0.4977	 0.6250
P	 0.6047	 0.6310
Q	 0.7910	 0.6150
R	 0.3262	 0.5820
S	 0.5404	 0.5760
T	 0.5102	 0.6340
U	 0.3383	 0.5690
V	 0.7072	 0.5800
W	 0.6446	 0.6080
X	 0.8044	 0.5770
Y	 0.6696	 0.5370
Z	 0.7425	 0.5680

