



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 03:48 PM UTC

PDB ID : 8CSU / pdb_00008csu
EMDB ID : EMD-26971
Title : Human mitochondrial small subunit assembly intermediate (State C*)
Authors : Harper, N.J.; Burnside, C.; Klinge, S.
Deposited on : 2022-05-13
Resolution : 3.03 Å(reported)
Based on initial models : 6RW4, 2C2N, 6AAX

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:

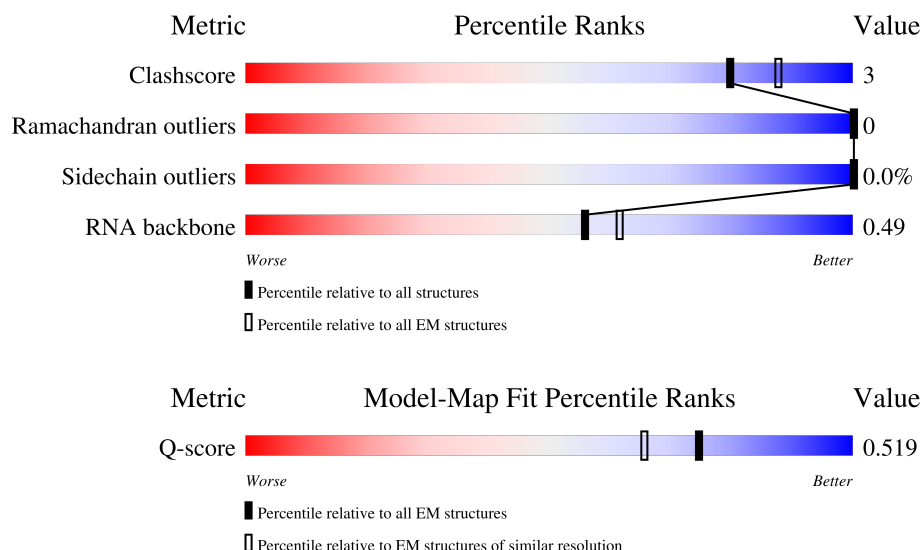
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.03 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	13929 (2.53 - 3.53)

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	25% 90% 6% .
2	1	323	11% 76% 20% .
3	3	199	23% 20% 77% .

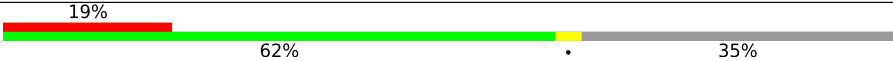
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Mol	Chain	Length	Quality of chain
4	4	689	
5	5	346	
6	6	343	
7	7	456	
8	A	955	
9	B	296	
10	C	167	
11	D	430	
12	E	125	
13	F	242	
14	G	396	
15	H	201	
16	I	194	
17	J	138	
18	K	128	
19	L	257	
20	M	137	
21	N	130	
22	O	258	
23	P	142	
24	Q	87	
25	R	360	
26	S	190	
27	T	173	
28	U	205	

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Mol	Chain	Length	Quality of chain
29	V	414	
30	W	187	
31	X	398	
32	Y	395	
33	Z	106	

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 68661 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	45	Total	C	N	O	0	0
			395	254	81	60		

- 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 Dimethyladenosine transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	319	Total	C	N	O	S	0	0
			2568	1648	458	451	11		

- Molecule 6 is a protein called Putative ribosome-binding factor A, mitochondrial.

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

- Molecule 7 is a protein called Methyltransferase-like protein 17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	414	Total	C	N	O	S	0	0
			3276	2087	601	572	16		

- Molecule 8 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	881	Total	C	N	O	P	0	0
			18715	8390	3366	6078	881		

- Molecule 9 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 10 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 11 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 12 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 13 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 14 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 15 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 16 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 17 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 18 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 19 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 20 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 21 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 22 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 23 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 24 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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 25 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 26 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 27 is a protein called 28S ribosomal protein S25, mitochondrial.

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

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

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

- Molecule 29 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 30 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 31 is a protein called 28S ribosomal protein S29, mitochondrial.

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

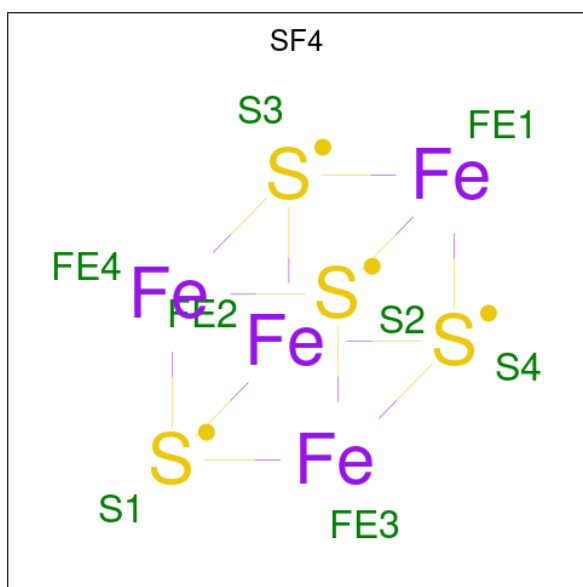
- Molecule 32 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 33 is a protein called 28S ribosomal protein S33, mitochondrial.

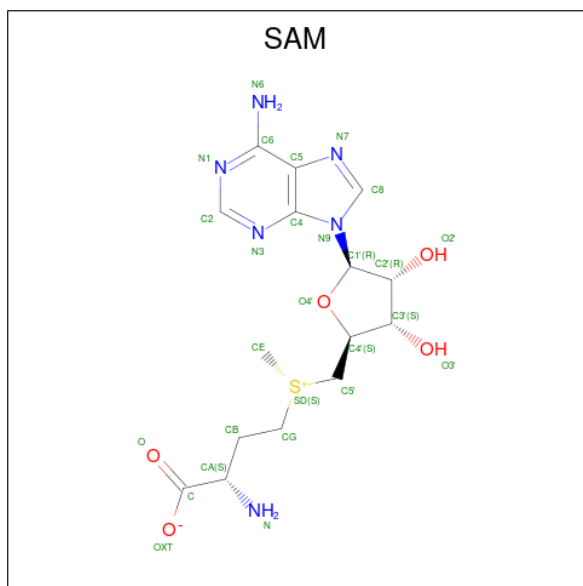
Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	69	Total	C	N	O	S	0	0
			581	377	101	100	3		

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	7	1	Total	Fe	S	0
			8	4	4	

- Molecule 35 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	7	1	Total	C	N	O	S	0
			27	15	6	5	1	

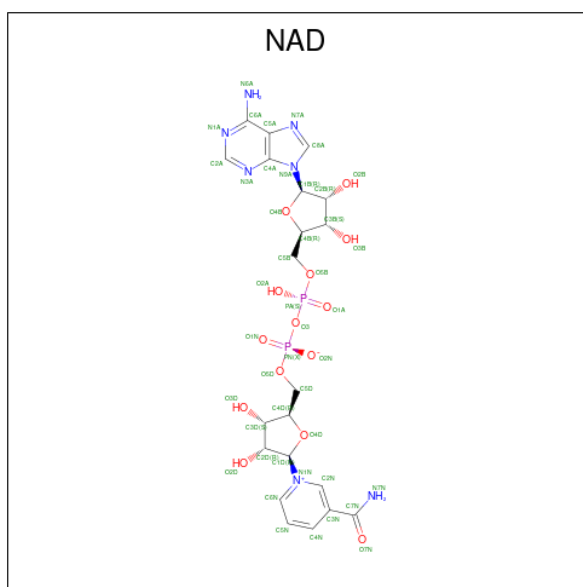
- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
36	A	5	Total	K	0
			5	5	

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

Mol	Chain	Residues	Atoms		AltConf
37	A	24	Total	Mg	0
			24	24	
37	B	1	Total	Mg	0
			1	1	
37	X	1	Total	Mg	0
			1	1	

- Molecule 38 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

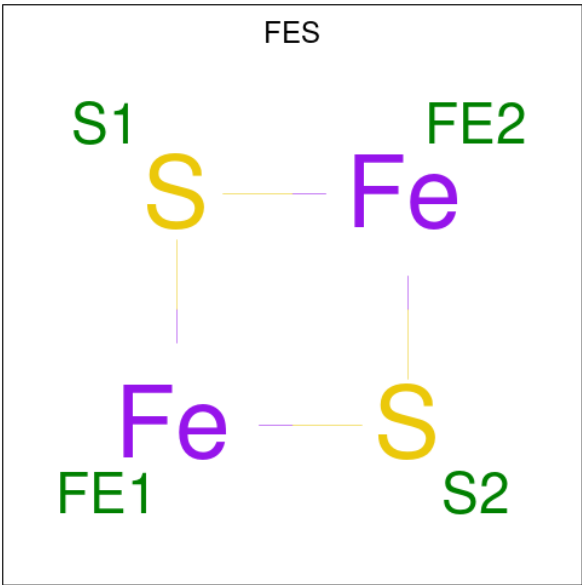


Mol	Chain	Residues	Atoms					AltConf
38	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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

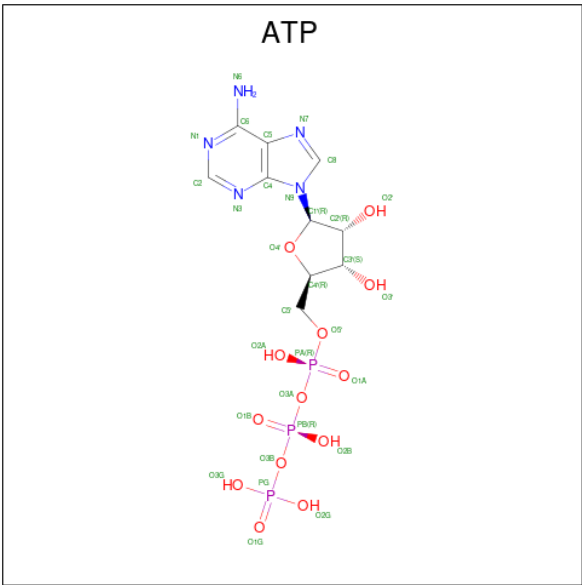
Mol	Chain	Residues	Atoms		AltConf
39	O	1	Total	Zn	0
			1	1	

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



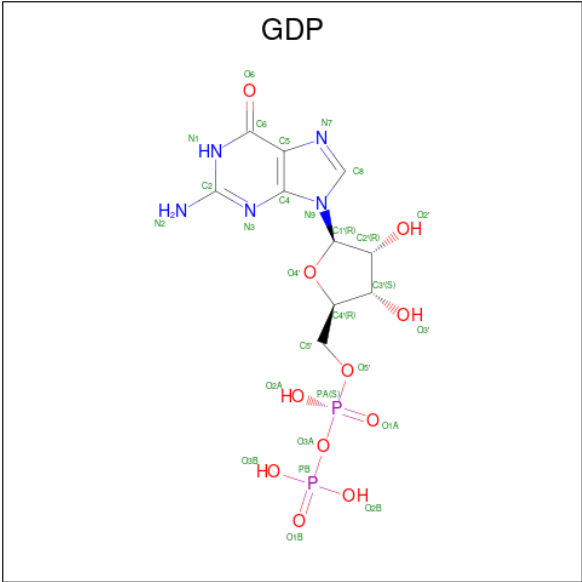
Mol	Chain	Residues	Atoms			AltConf
40	P	1	Total	Fe	S	0
			4	2	2	
40	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 41 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

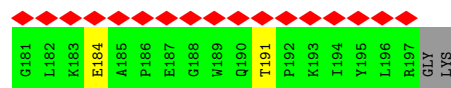


Mol	Chain	Residues	Atoms					AltConf
41	X	1	Total	C	N	O	P	0
			31	10	5	13	3	

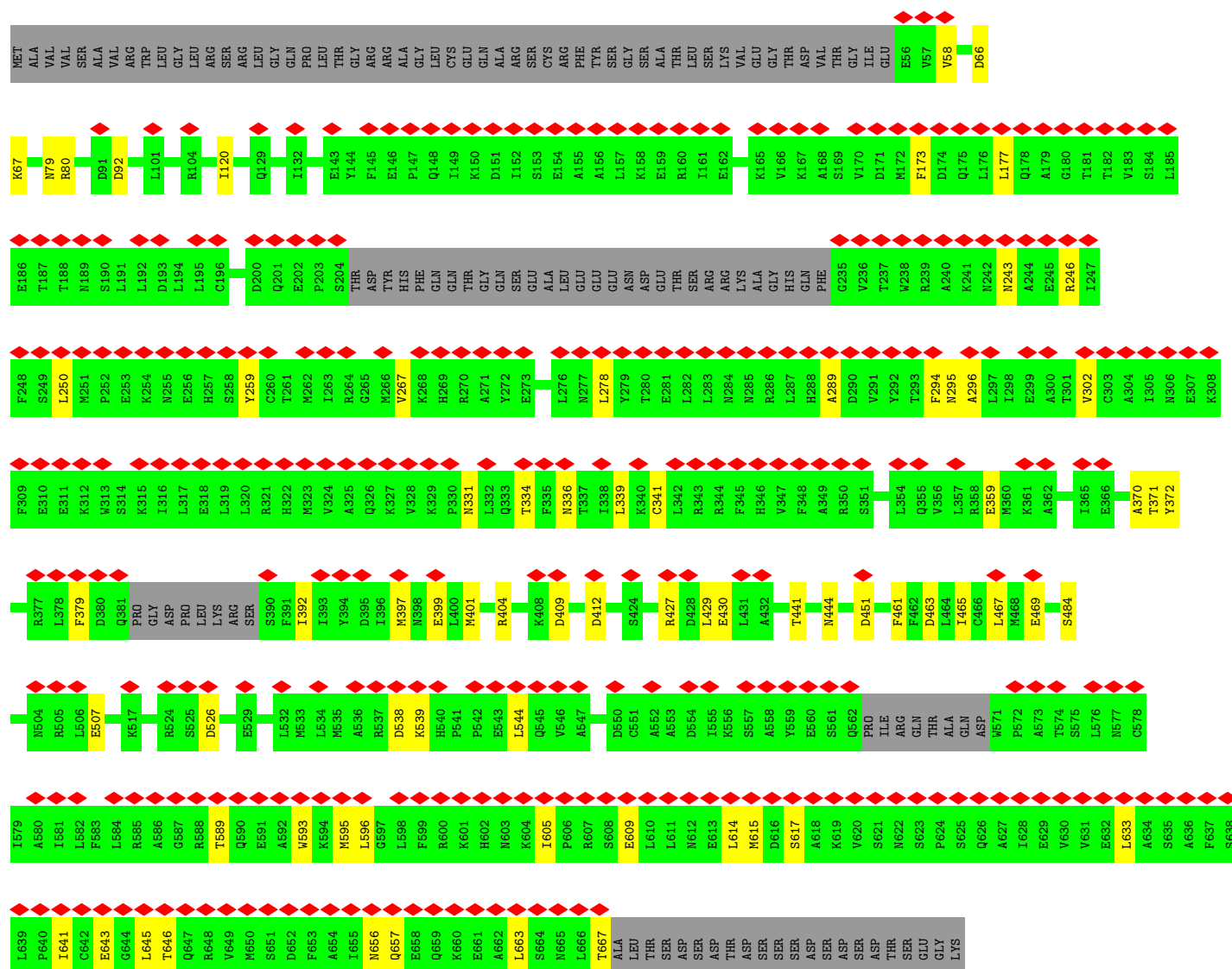
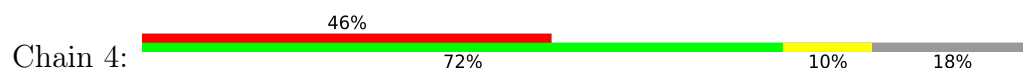
- Molecule 42 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



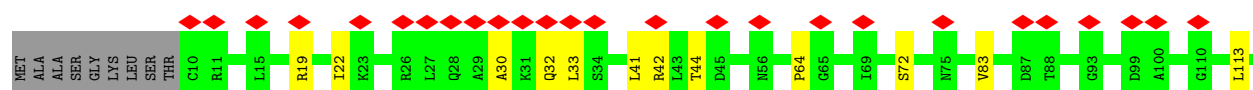
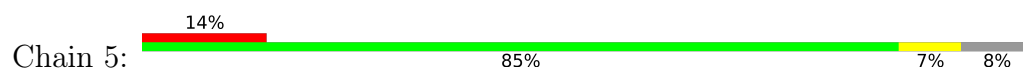
Mol	Chain	Residues	Atoms					AltConf
42	X	1	Total	C	N	O	P	0
			28	10	5	11	2	

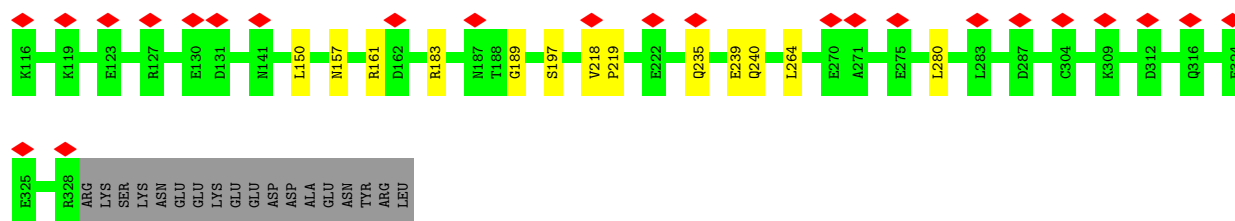


• Molecule 4: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

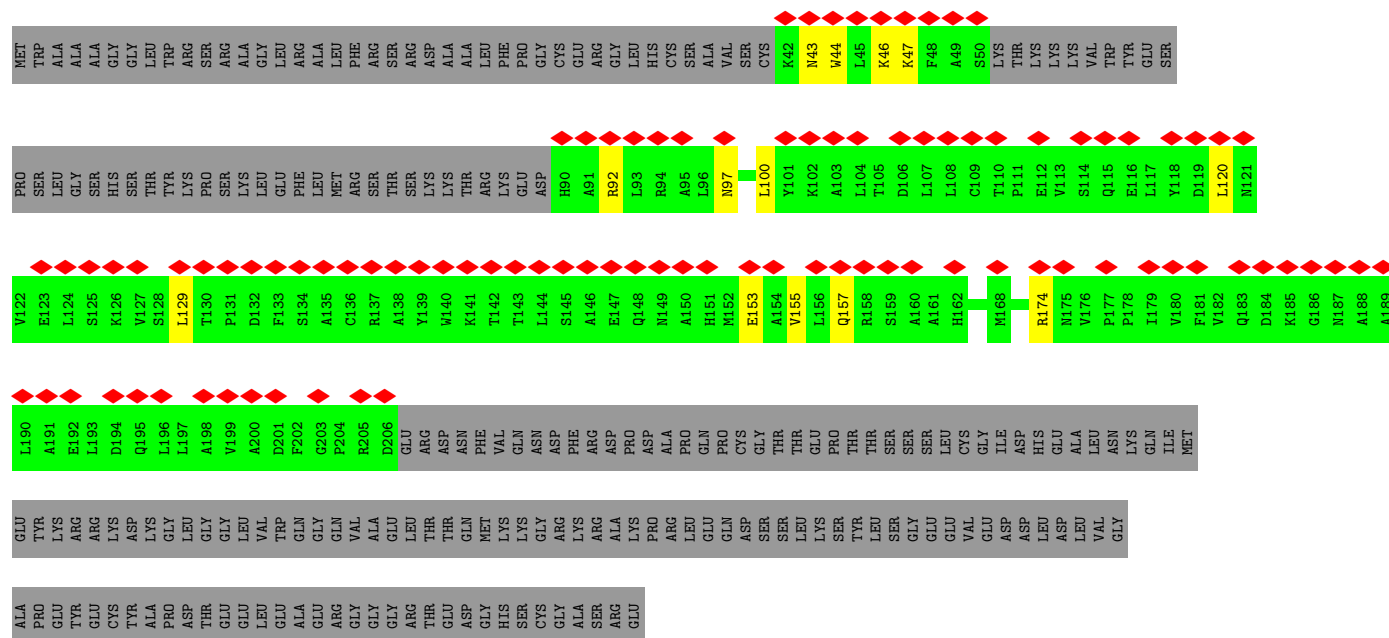


• Molecule 5: Dimethyladenosine transferase 1, mitochondrial

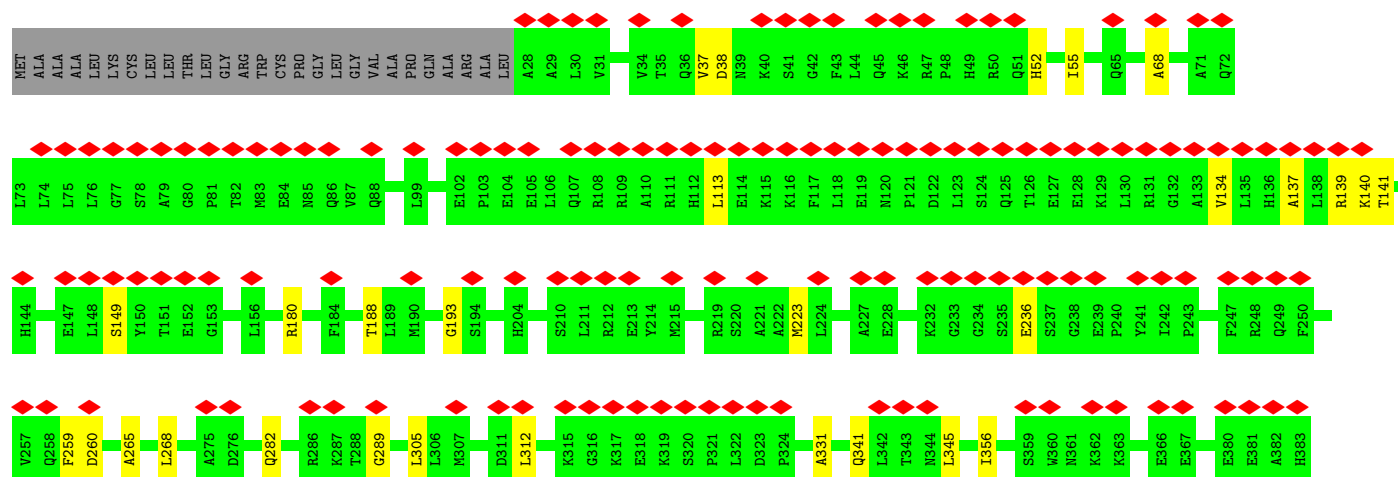
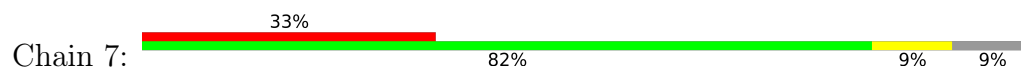




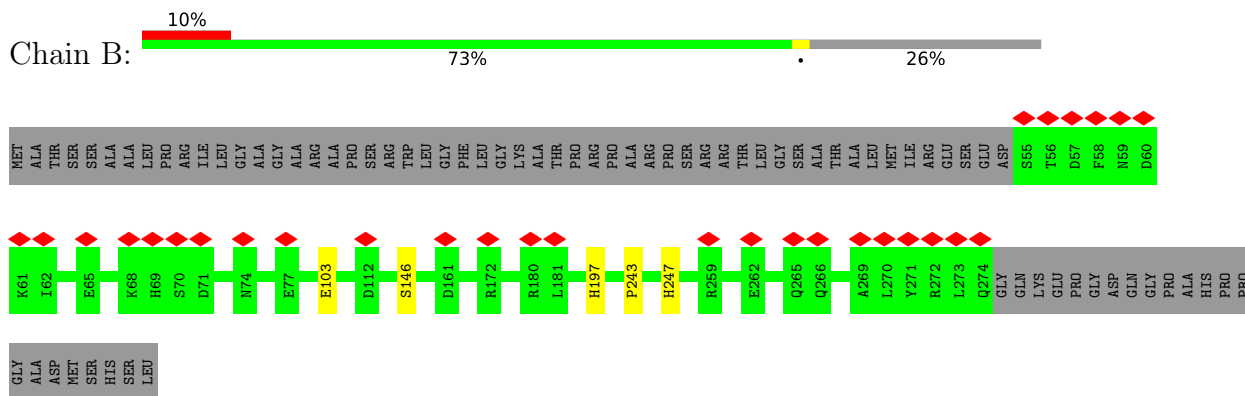
- Molecule 6: Putative ribosome-binding factor A, mitochondrial



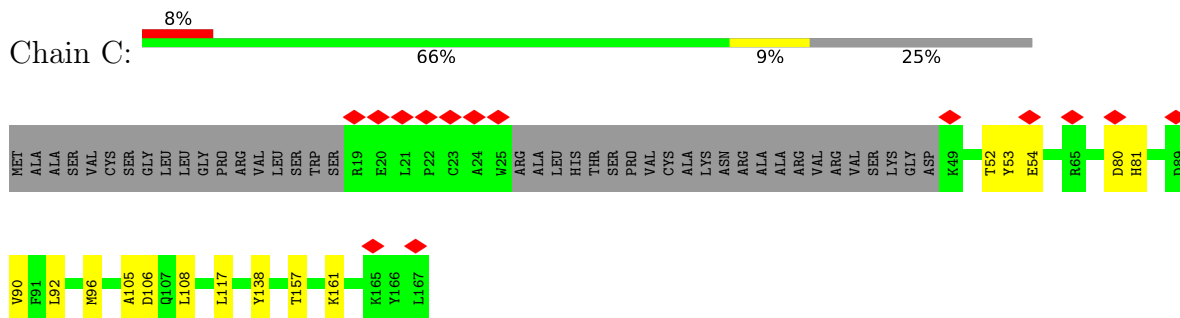
- Molecule 7: Methyltransferase-like protein 17, mitochondrial



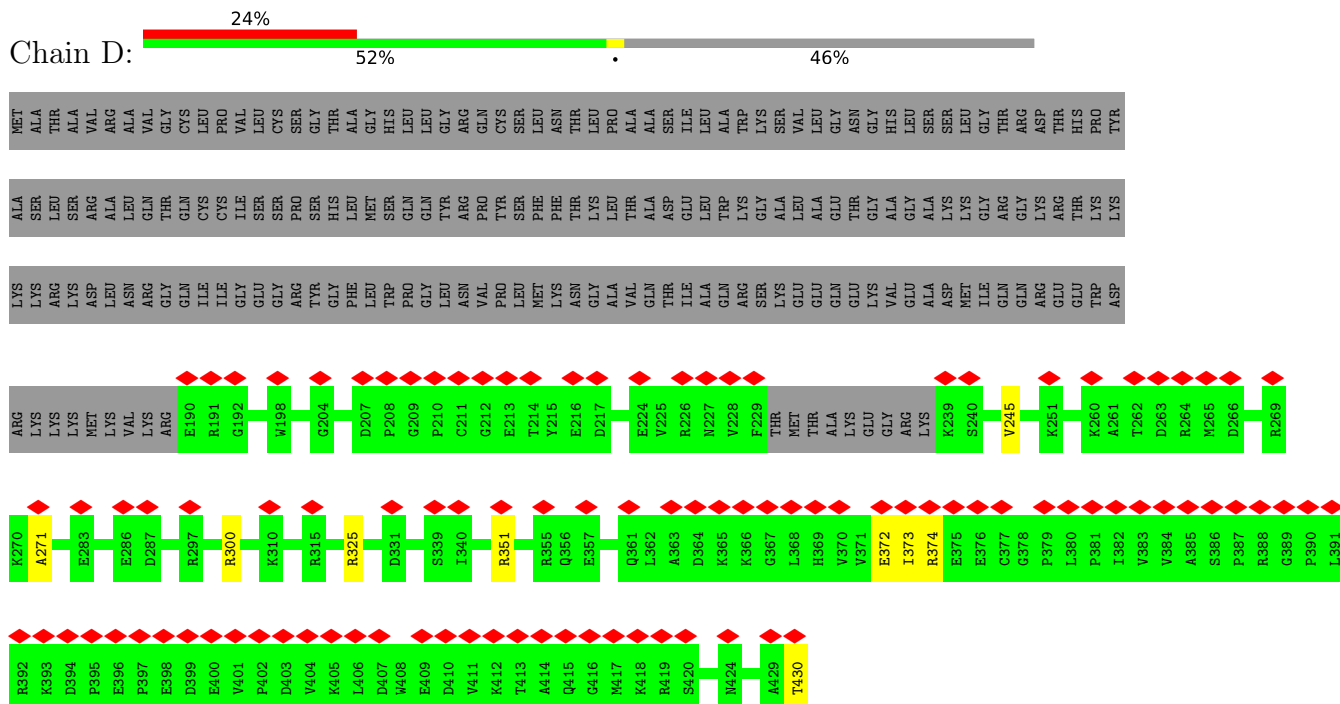




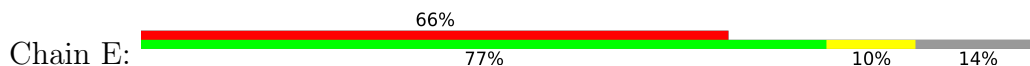
- Molecule 10: 28S ribosomal protein S24, mitochondrial

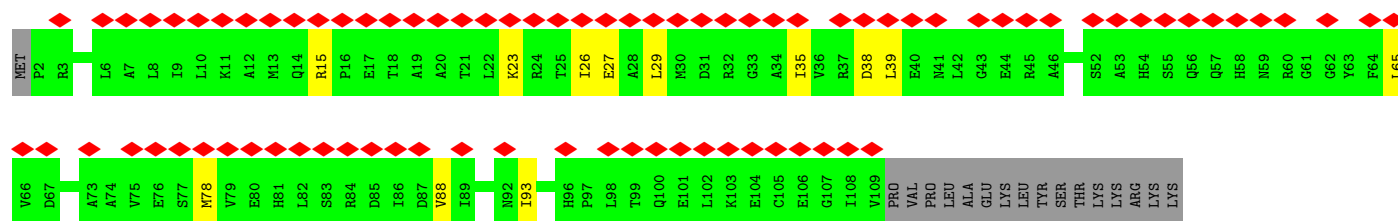


- Molecule 11: 28S ribosomal protein S5, mitochondrial

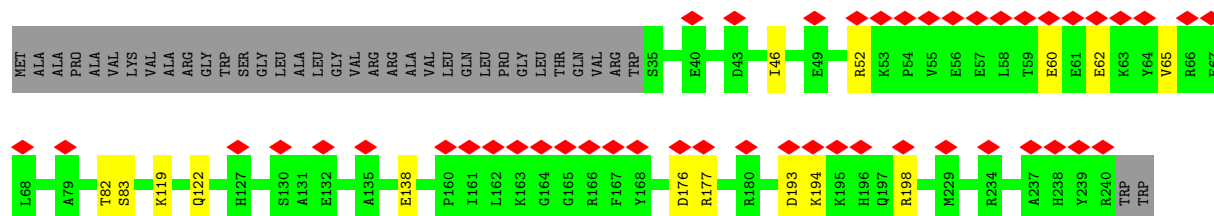
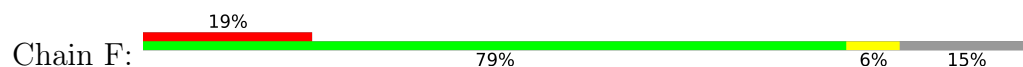


- Molecule 12: 28S ribosomal protein S6, mitochondrial

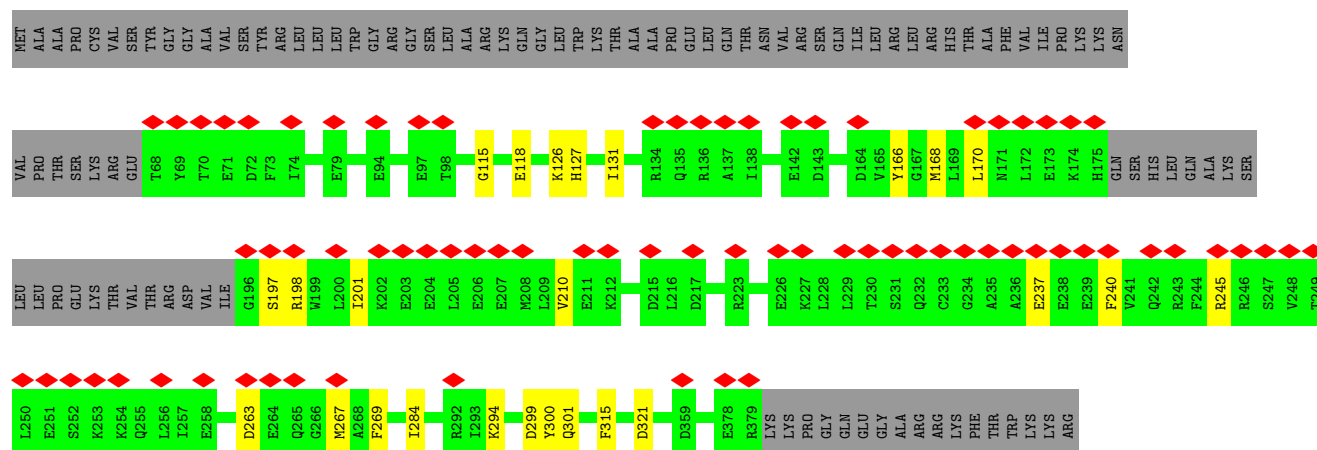




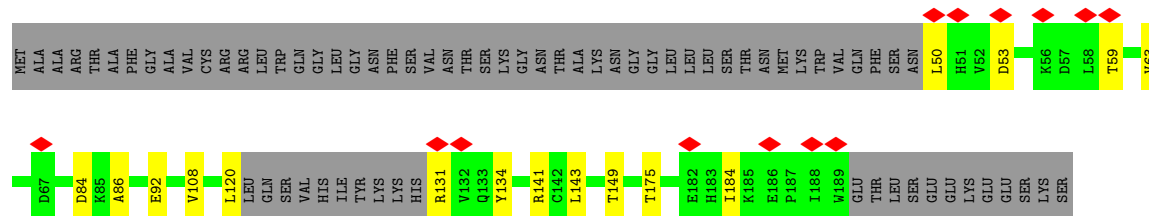
- Molecule 13: 28S ribosomal protein S7, mitochondrial



- Molecule 14: 28S ribosomal protein S9, mitochondrial

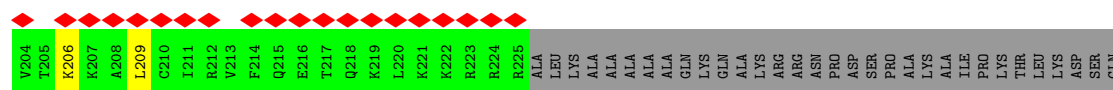


- Molecule 15: 28S ribosomal protein S10, mitochondrial

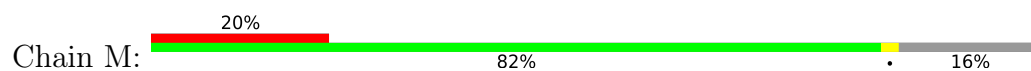


- Molecule 16: 28S ribosomal protein S11, mitochondrial

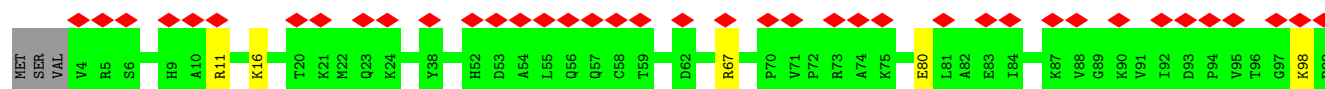
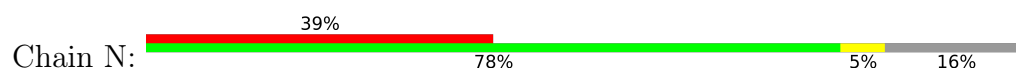




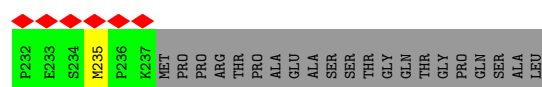
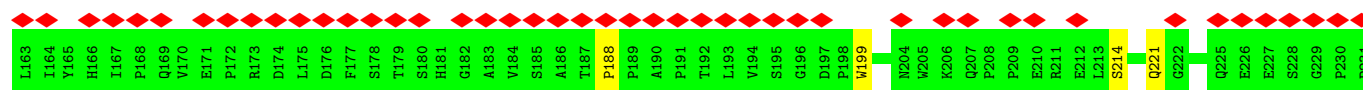
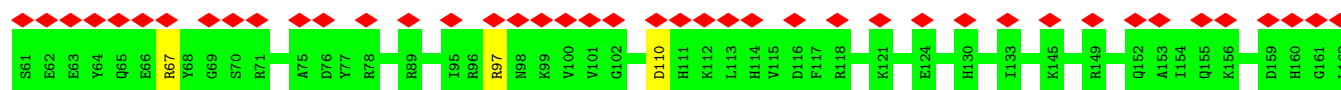
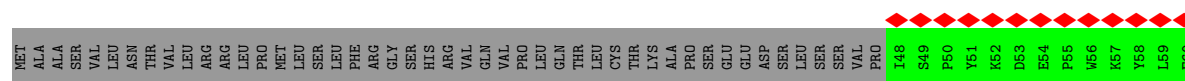
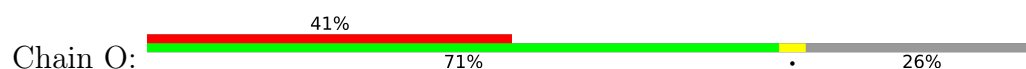
- Molecule 20: 28S ribosomal protein S16, mitochondrial



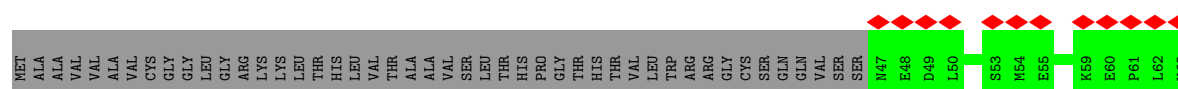
- Molecule 21: 28S ribosomal protein S17, mitochondrial

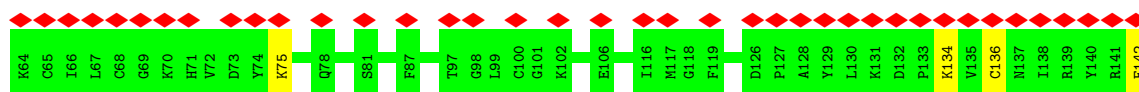


- Molecule 22: 28S ribosomal protein S18b, mitochondrial

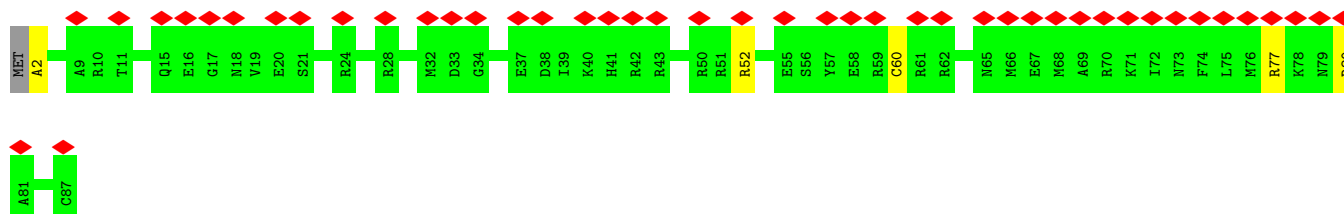
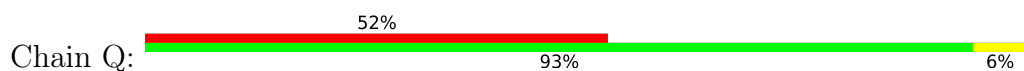


- Molecule 23: 28S ribosomal protein S18c, mitochondrial

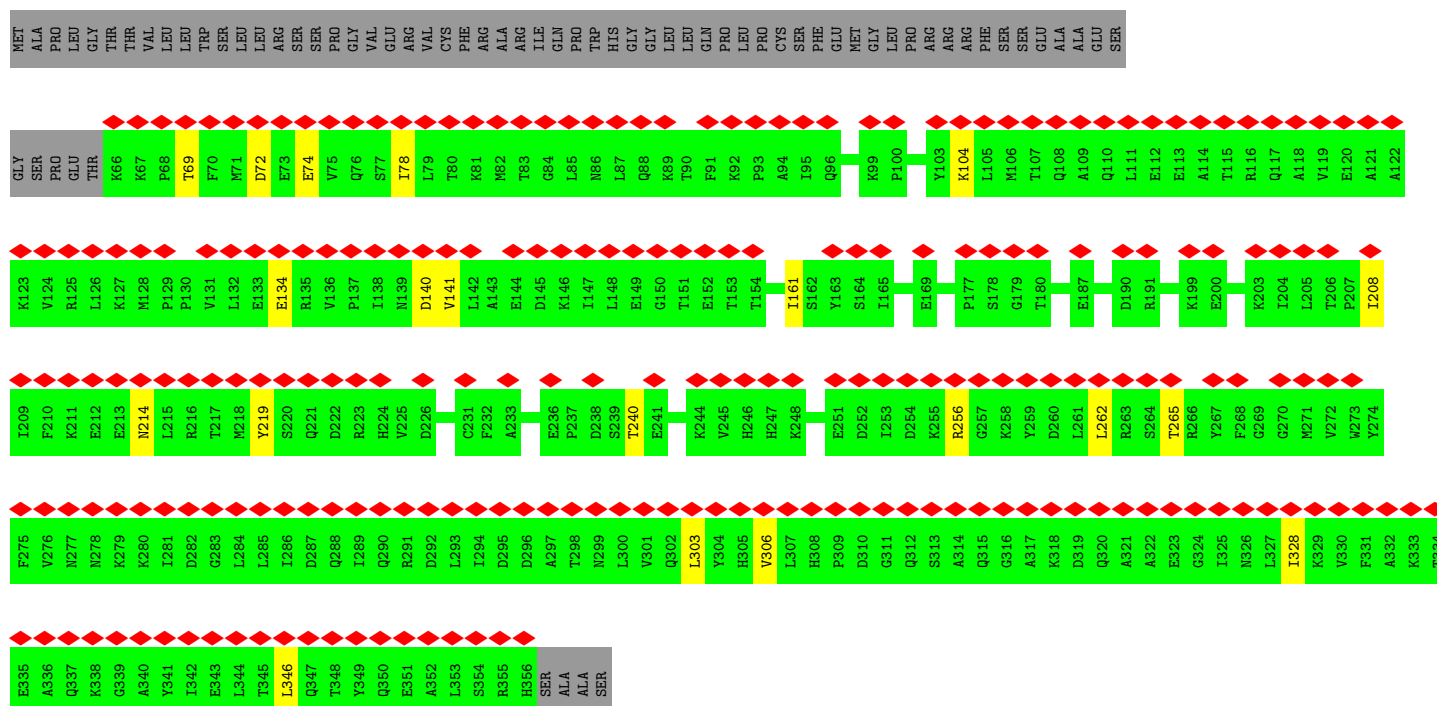
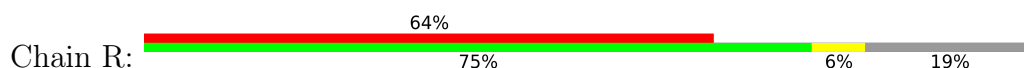




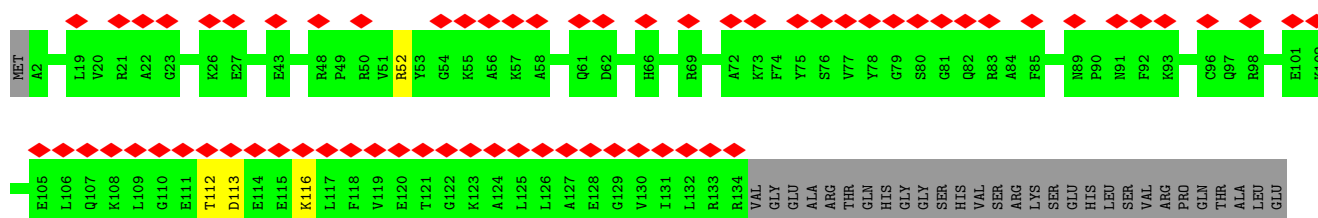
- Molecule 24: 28S ribosomal protein S21, mitochondrial



- Molecule 25: 28S ribosomal protein S22, mitochondrial



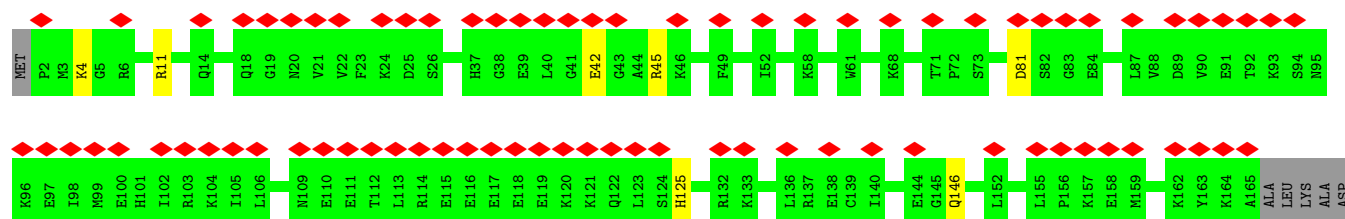
- Molecule 26: 28S ribosomal protein S23, mitochondrial



GLU ASN
GLU THR
GLN LYS
GLU VAL
PRO PRO
GLN ASP
GLN HIS
LEU LEU
ALA ALA
PRO PRO
ALA ALA
ASP GLN
SER SER
GLY GLY
LEU LEU
PRO PRO

- Molecule 27: 28S ribosomal protein S25, mitochondrial

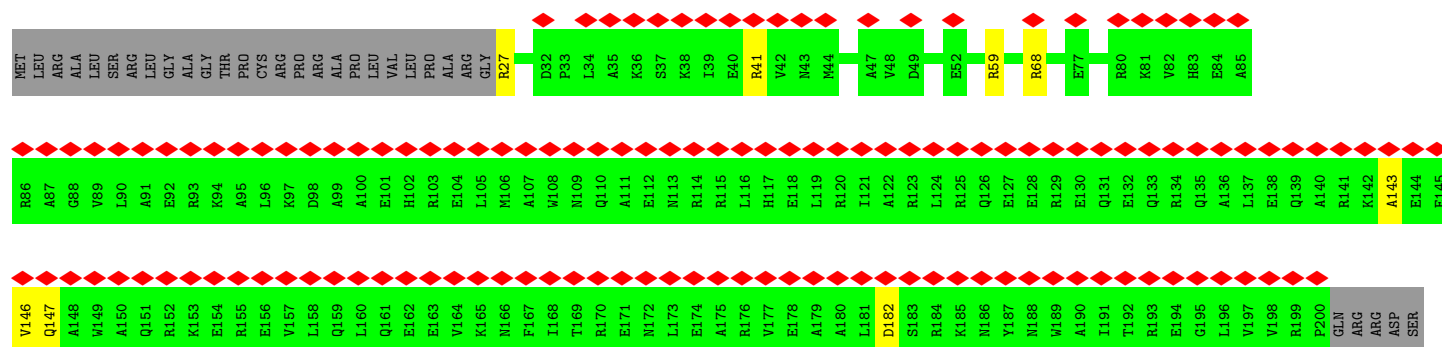
Chain T:



ALA
GLN
ASP

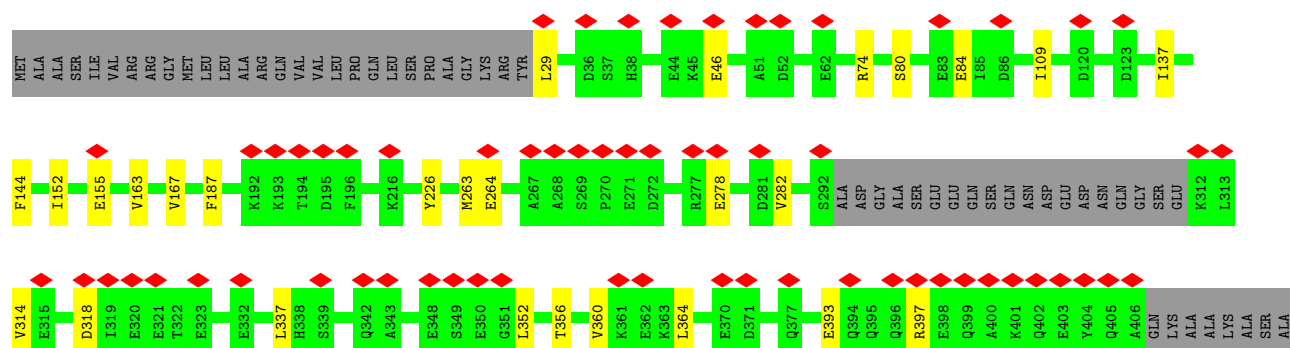
- Molecule 28: 28S ribosomal protein S26, mitochondrial

Chain U:



- Molecule 29: 28S ribosomal protein S27, mitochondrial

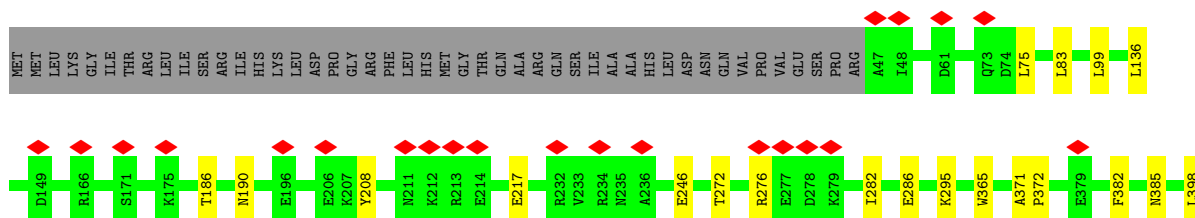
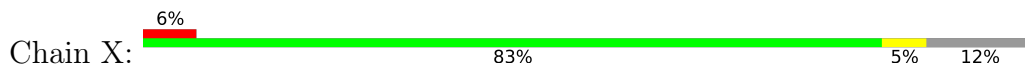
Chain V:



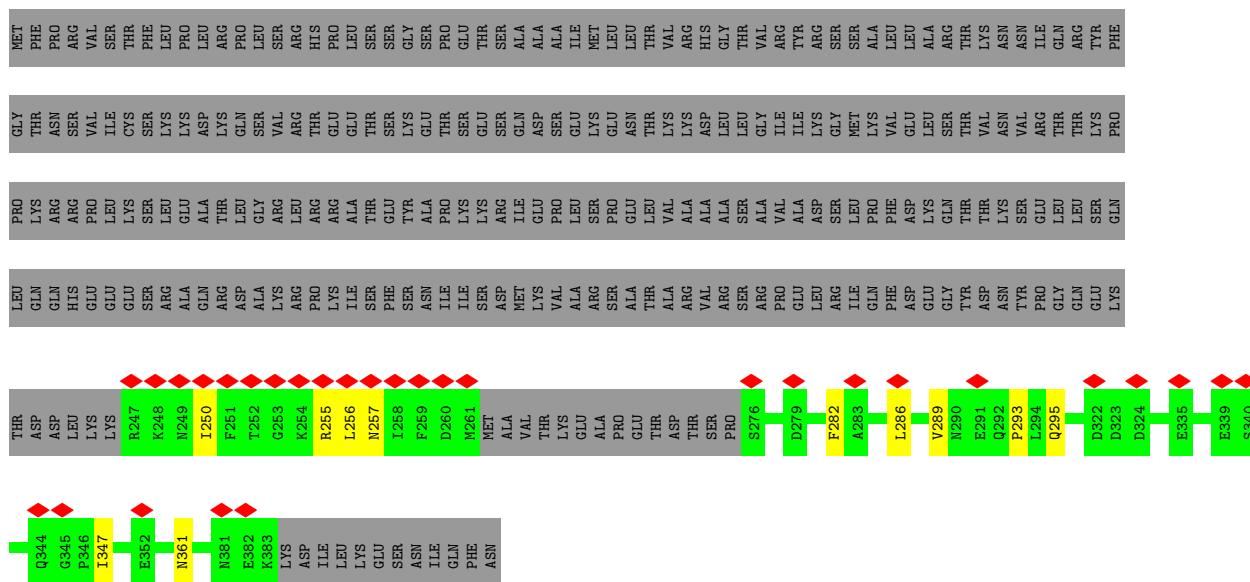
- Molecule 30: 28S ribosomal protein S28, mitochondrial

Chain W:

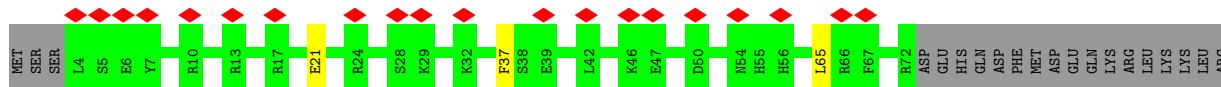
- Molecule 31: 28S ribosomal protein S29, mitochondrial



- Molecule 32: 28S ribosomal protein S31, mitochondrial



- Molecule 33: 28S ribosomal protein S33, mitochondrial



GLY
LYS
GLU
LYS
PRO
LYS
LYS
GLY
GLU
GLY
LYS
ARG
ALA
ALA
LYS
ARG
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33642	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	45.490	Depositor
Minimum map value	-21.701	Depositor
Average map value	0.031	Depositor
Map value standard deviation	1.227	Depositor
Recommended contour level	9	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, ZN, SAM, SF4, AYA, FES, ATP, GDP, MG, K

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	0.14	0/1800	0.33	0/2440
2	1	0.16	0/2143	0.35	0/2902
3	3	0.14	0/402	0.34	0/533
4	4	0.17	0/4686	0.38	0/6335
5	5	0.16	0/2624	0.40	0/3552
6	6	0.14	0/1012	0.34	0/1371
7	7	0.15	0/3368	0.33	0/4572
8	A	0.12	0/20931	0.29	0/32577
9	B	0.13	0/1832	0.32	0/2480
10	C	0.18	0/1074	0.40	0/1456
11	D	0.13	0/1877	0.36	0/2523
12	E	0.13	0/872	0.34	0/1177
13	F	0.14	0/1734	0.34	0/2327
14	G	0.14	0/2446	0.33	0/3283
15	H	0.16	0/1086	0.41	0/1473
16	I	0.16	0/1039	0.35	0/1400
17	J	0.13	0/855	0.33	0/1148
18	K	0.13	0/863	0.32	0/1159
19	L	0.14	0/1387	0.30	0/1853
20	M	0.13	0/934	0.33	0/1255
21	N	0.13	0/877	0.31	0/1187
22	O	0.13	0/1624	0.30	0/2210
23	P	0.13	0/791	0.31	0/1062
24	Q	0.11	0/748	0.27	0/994
25	R	0.12	0/2429	0.29	0/3280
26	S	0.16	0/1127	0.32	0/1518
27	T	0.12	0/1375	0.31	0/1847
28	U	0.16	0/1490	0.34	0/1999
29	V	0.15	0/3007	0.33	0/4062
30	W	0.13	0/787	0.28	0/1060
31	X	0.15	0/2921	0.37	0/3954
32	Y	0.15	0/1073	0.34	0/1444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.15	0/596	0.38	0/801
All	All	0.14	0/71810	0.33	0/101234

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
17	J	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	J	72	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1754	0	1754	14	0
2	1	2098	0	2115	12	0
3	3	395	0	432	6	0
4	4	4585	0	4595	56	0
5	5	2568	0	2655	17	0
6	6	994	0	1004	13	0
7	7	3276	0	3286	27	0
8	A	18715	0	9495	80	0
9	B	1789	0	1781	3	0
10	C	1042	0	1033	11	0
11	D	1838	0	1858	6	0
12	E	858	0	871	10	0
13	F	1696	0	1749	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	G	2395	0	2364	20	0
15	H	1064	0	1089	16	0
16	I	1019	0	1059	3	0
17	J	839	0	887	3	0
18	K	847	0	875	8	0
19	L	1363	0	1442	8	0
20	M	913	0	943	3	0
21	N	859	0	922	5	0
22	O	1570	0	1533	7	0
23	P	774	0	801	4	0
24	Q	744	0	758	4	0
25	R	2382	0	2405	11	0
26	S	1100	0	1103	3	0
27	T	1344	0	1359	5	0
28	U	1468	0	1478	9	0
29	V	2946	0	2942	18	0
30	W	775	0	791	2	0
31	X	2849	0	2843	13	0
32	Y	1043	0	996	8	0
33	Z	581	0	590	3	0
34	7	8	0	0	0	0
35	7	27	0	22	3	0
36	A	5	0	0	0	0
37	A	24	0	0	0	0
37	B	1	0	0	0	0
37	X	1	0	0	0	0
38	A	44	0	26	1	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	0	12	0	0
42	X	28	0	12	1	0
All	All	68661	0	59880	337	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 3.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:615:MET:HE1	4:4:645:LEU:HD22	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1199:G:H21	8:A:1423:A:H62	1.19	0.90
8:A:1251:A:N6	8:A:1341:C:O2'	2.07	0.87
6:6:153:GLU:O	6:6:157:GLN:NE2	2.11	0.84
8:A:1013:A:O2'	8:A:1014:A:O5'	1.96	0.83
8:A:1429:C:OP1	8:A:1432:U:O2'	1.98	0.82
7:7:394:LYS:NZ	7:7:429:ARG:O	2.13	0.81
6:6:46:LYS:NZ	8:A:1124:A:OP1	2.13	0.79
13:F:119:LYS:NZ	31:X:365:TRP:O	2.14	0.79
8:A:1384:A:N7	13:F:198:ARG:NH1	2.33	0.77
1:0:48:ARG:NH2	8:A:701:G:O6	2.21	0.74
21:N:98:LYS:NZ	21:N:112:SER:OG	2.18	0.73
18:K:31:ASP:OD1	18:K:32:TRP:N	2.22	0.72
10:C:105:ALA:O	10:C:161:LYS:NZ	2.18	0.72
1:0:19:ARG:NH1	8:A:808:C:OP1	2.23	0.71
7:7:37:VAL:HG23	7:7:424:LEU:HD22	1.73	0.70
6:6:43:ASN:ND2	8:A:1125:A:OP1	2.25	0.70
8:A:1154:A:O2'	8:A:1155:G:O5'	2.07	0.70
13:F:52:ARG:NH2	14:G:321:ASP:OD1	2.23	0.69
5:5:113:LEU:HD23	5:5:150:LEU:HD23	1.73	0.69
8:A:899:G:O2'	8:A:907:A:N1	2.24	0.68
8:A:1330:C:O2'	8:A:1332:A:OP1	2.10	0.68
5:5:183:ARG:O	5:5:197:SER:OG	2.08	0.68
7:7:113:LEU:HD21	7:7:137:ALA:HB3	1.76	0.68
8:A:1046:A:O2'	8:A:1048:C:OP2	2.11	0.67
4:4:596:LEU:HD22	4:4:633:LEU:HD22	1.75	0.67
4:4:302:VAL:HG21	4:4:341:CYS:HB3	1.75	0.67
8:A:702:C:OP1	8:A:848:U:O2'	2.13	0.67
4:4:615:MET:CE	4:4:645:LEU:HD22	2.25	0.67
8:A:738:A:O2'	8:A:739:C:O2	2.13	0.66
8:A:1121:A:OP1	11:D:300:ARG:NH2	2.29	0.66
4:4:336:ASN:ND2	4:4:409:ASP:OD1	2.29	0.66
7:7:223:MET:SD	35:7:502:SAM:O3'	2.55	0.65
4:4:295:ASN:OD1	4:4:334:THR:HG22	1.97	0.65
2:1:131:THR:OG1	15:H:149:THR:OG1	2.14	0.65
8:A:1363:C:O2'	8:A:1448:U:O2	2.13	0.64
8:A:1400:U:O2'	8:A:1444:A:N3	2.27	0.64
1:0:49:ARG:NH2	28:U:41:ARG:O	2.29	0.64
4:4:250:LEU:HD23	4:4:250:LEU:O	1.97	0.64
8:A:1358:A:O2'	8:A:1359:U:OP1	2.14	0.64
3:3:164:ARG:NH2	8:A:1501:A:OP1	2.30	0.64
8:A:942:A:N6	8:A:1047:A:OP2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:762:G:OP1	19:L:206:LYS:NZ	2.28	0.64
5:5:44:THR:HG1	5:5:72:SER:HG	1.46	0.64
14:G:263:ASP:OD2	14:G:267:MET:N	2.31	0.63
4:4:80:ARG:NH1	4:4:484:SER:OG	2.31	0.63
11:D:325:ARG:NH1	11:D:430:THR:OXT	2.32	0.63
7:7:140:LYS:O	7:7:141:THR:OG1	2.16	0.62
8:A:1444:A:N7	18:K:85:VAL:HG23	2.13	0.62
8:A:1190:C:H42	8:A:1464:G:H22	1.48	0.62
4:4:589:THR:HG22	4:4:593:TRP:NE1	2.15	0.62
4:4:404:ARG:NH1	15:H:59:THR:OG1	2.33	0.61
6:6:44:TRP:CD1	24:Q:60:CYS:HG	2.17	0.61
7:7:236:GLU:N	7:7:236:GLU:OE2	2.33	0.61
8:A:1199:G:N2	8:A:1423:A:H62	1.96	0.61
29:V:80:SER:N	29:V:84:GLU:OE1	2.32	0.61
7:7:38:ASP:HA	7:7:440:LEU:HD23	1.82	0.61
8:A:1443:U:O2'	8:A:1445:G:N7	2.27	0.61
2:1:244:THR:HG22	2:1:245:GLU:H	1.66	0.61
4:4:267:VAL:HG11	4:4:296:ALA:HB1	1.83	0.61
7:7:149:SER:OG	8:A:1178:G:O6	2.18	0.61
8:A:1118:A:O2'	11:D:351:ARG:NH2	2.33	0.61
5:5:235:GLN:NE2	5:5:239:GLU:OE2	2.35	0.60
8:A:1247:G:N2	8:A:1247:G:OP2	2.32	0.60
13:F:176:ASP:OD1	13:F:177:ARG:N	2.34	0.60
5:5:41:LEU:O	5:5:41:LEU:HD23	2.01	0.60
8:A:1191:C:H42	8:A:1463:G:H1	1.49	0.60
4:4:372:TYR:OH	4:4:399:GLU:OE1	2.19	0.60
7:7:140:LYS:NZ	8:A:1269:U:O2	2.35	0.60
14:G:294:LYS:NZ	14:G:299:ASP:OD2	2.28	0.59
12:E:29:LEU:HG	12:E:78:MET:HE2	1.84	0.59
4:4:614:LEU:O	4:4:617:SER:OG	2.17	0.59
8:A:1154:A:HO2'	8:A:1155:G:C5'	2.15	0.58
15:H:120:LEU:O	15:H:131:ARG:NH2	2.35	0.58
7:7:341:GLN:CD	7:7:410:MET:HE2	2.28	0.58
15:H:120:LEU:HD23	15:H:134:TYR:CD2	2.38	0.58
25:R:74:GLU:OE2	25:R:78:ILE:HD11	2.02	0.58
2:1:131:THR:HG1	15:H:149:THR:HG1	1.52	0.58
8:A:1199:G:H21	8:A:1423:A:N6	1.96	0.58
15:H:108:VAL:HG22	15:H:143:LEU:HD23	1.84	0.58
14:G:198:ARG:NH1	14:G:201:ILE:HG23	2.18	0.58
15:H:120:LEU:HD23	15:H:134:TYR:HD2	1.68	0.58
6:6:174:ARG:NH1	8:A:1571:U:O3'	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:143:ALA:O	28:U:146:VAL:HG12	2.03	0.57
7:7:418:ARG:NH2	8:A:1343:A:OP2	2.37	0.57
29:V:264:GLU:HG3	29:V:337:LEU:HD11	1.86	0.57
7:7:265:ALA:O	35:7:502:SAM:N	2.37	0.57
11:D:373:ILE:HD11	25:R:104:LYS:HD2	1.86	0.56
29:V:226:TYR:CE2	29:V:282:VAL:HG21	2.40	0.56
1:0:9:ARG:NE	8:A:805:C:O2	2.39	0.56
4:4:379:PHE:HE2	4:4:392:ILE:HG21	1.71	0.56
12:E:15:ARG:NH1	28:U:182:ASP:OD1	2.38	0.56
8:A:1559:G:OP2	8:A:1559:G:N2	2.34	0.56
24:Q:77:ARG:O	24:Q:80:ARG:NH2	2.38	0.56
1:0:166:TYR:O	22:O:199:TRP:NE1	2.35	0.55
21:N:67:ARG:NH1	21:N:80:GLU:OE1	2.38	0.55
9:B:103:GLU:OE2	26:S:52:ARG:NH2	2.39	0.55
8:A:1339:G:O2'	8:A:1344:U:O4	2.24	0.55
25:R:69:THR:OG1	25:R:72:ASP:OD2	2.24	0.55
16:I:71:SER:O	16:I:74:ARG:NH1	2.40	0.55
20:M:55:ASP:OD2	27:T:146:GLN:NE2	2.39	0.55
29:V:263:MET:HB3	29:V:337:LEU:HD13	1.89	0.55
26:S:112:THR:HG23	26:S:112:THR:O	2.07	0.54
3:3:154:ARG:NH1	5:5:189:GLY:O	2.39	0.54
18:K:29:TYR:CE1	18:K:38:VAL:HG21	2.43	0.54
8:A:871:A:OP2	22:O:97:ARG:NH1	2.40	0.54
29:V:187:PHE:CD2	29:V:356:THR:HG21	2.42	0.54
15:H:92:GLU:OE1	15:H:141:ARG:NH1	2.40	0.54
5:5:113:LEU:HD23	5:5:150:LEU:CD2	2.37	0.54
10:C:90:VAL:HG11	18:K:93:MET:HE1	1.89	0.54
10:C:96:MET:HB2	10:C:108:LEU:HD11	1.89	0.54
1:0:123:LYS:NZ	1:0:158:GLU:OE1	2.40	0.54
11:D:245:VAL:HG22	11:D:271:ALA:HB1	1.90	0.54
4:4:379:PHE:CD2	4:4:392:ILE:HD13	2.43	0.53
4:4:401:MET:HA	4:4:401:MET:HE2	1.89	0.53
3:3:173:LEU:HD22	19:L:209:LEU:HD23	1.90	0.53
13:F:119:LYS:NZ	31:X:398:LEU:OXT	2.31	0.53
32:Y:282:PHE:O	32:Y:286:LEU:HD23	2.09	0.53
6:6:100:LEU:HD12	6:6:129:LEU:HD21	1.91	0.53
8:A:1033:U:O2'	12:E:93:ILE:O	2.26	0.53
20:M:108:GLU:OE2	28:U:59:ARG:NH2	2.39	0.53
4:4:66:ASP:OD1	4:4:67:LYS:N	2.39	0.53
4:4:465:ILE:HG23	4:4:469:GLU:HG3	1.91	0.53
1:0:198:MET:HE1	28:U:68:ARG:HH22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:352:LEU:O	29:V:356:THR:HG23	2.08	0.53
2:1:103:LEU:HD22	10:C:106:ASP:OD2	2.09	0.53
8:A:1463:G:H2'	8:A:1464:G:H5'	1.91	0.53
25:R:328:ILE:CG2	25:R:346:LEU:HD11	2.39	0.53
8:A:700:A:N1	8:A:709:G:O2'	2.42	0.52
15:H:50:LEU:HD22	15:H:53:ASP:O	2.09	0.52
7:7:180:ARG:NH2	7:7:331:ALA:HB2	2.24	0.52
14:G:118:GLU:OE1	14:G:118:GLU:N	2.43	0.52
10:C:92:LEU:HD11	10:C:117:LEU:HD21	1.91	0.52
8:A:1013:A:HO2'	8:A:1014:A:P	2.32	0.52
8:A:1558:A:H4'	17:J:72:LYS:HG3	1.91	0.52
29:V:278:GLU:O	29:V:282:VAL:HG23	2.10	0.52
2:1:239:TRP:O	2:1:242:SER:OG	2.25	0.52
4:4:615:MET:HE1	4:4:645:LEU:CD2	2.35	0.51
5:5:42:ARG:NH1	8:A:1490:U:O2	2.43	0.51
7:7:259:PHE:O	7:7:289:GLY:N	2.42	0.51
7:7:415:LEU:HD22	7:7:428:ALA:HB2	1.93	0.51
4:4:441:THR:OG1	4:4:444:ASN:ND2	2.43	0.51
4:4:656:ASN:OD1	4:4:657:GLN:N	2.43	0.51
21:N:11:ARG:NH1	27:T:81:ASP:OD2	2.43	0.51
30:W:100:VAL:HG11	30:W:144:LEU:HD11	1.92	0.51
23:P:134:LYS:NZ	23:P:136:CYS:O	2.39	0.51
4:4:58:VAL:HG23	4:4:58:VAL:O	2.11	0.51
4:4:379:PHE:CE2	4:4:392:ILE:HG21	2.45	0.51
4:4:643:GLU:O	4:4:646:THR:OG1	2.22	0.51
8:A:1293:C:N4	24:Q:80:ARG:O	2.40	0.51
11:D:372:GLU:OE2	11:D:374:ARG:NE	2.44	0.51
14:G:210:VAL:HG12	14:G:210:VAL:O	2.10	0.51
7:7:68:ALA:HA	7:7:356:ILE:HD11	1.93	0.50
26:S:113:ASP:OD1	26:S:116:LYS:NZ	2.44	0.50
6:6:47:LYS:NZ	8:A:1596:A:OP2	2.28	0.50
4:4:595:MET:HE3	4:4:595:MET:HA	1.93	0.50
8:A:781:A:O2'	38:A:1730:NAD:N7N	2.42	0.50
4:4:427:ARG:HH21	4:4:467:LEU:HD23	1.75	0.50
4:4:646:THR:HG22	4:4:663:LEU:HD11	1.92	0.50
14:G:126:LYS:HB2	14:G:131:ILE:HD11	1.94	0.50
8:A:1523:A:O2'	8:A:1527:A:N1	2.43	0.49
2:1:253:TRP:O	2:1:256:SER:OG	2.25	0.49
6:6:92:ARG:NH2	8:A:1081:U:O2	2.45	0.49
25:R:219:TYR:O	25:R:256:ARG:NH2	2.42	0.49
33:Z:21:GLU:OE2	33:Z:21:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:430:GLU:OE1	4:4:430:GLU:N	2.45	0.49
6:6:97:ASN:OD1	6:6:129:LEU:HD23	2.12	0.49
13:F:122:GLN:NE2	13:F:138:GLU:O	2.41	0.49
4:4:429:LEU:HD21	4:4:469:GLU:OE2	2.13	0.49
25:R:208:ILE:O	25:R:214:ASN:ND2	2.45	0.49
4:4:243:ASN:OD1	4:4:246:ARG:NH2	2.45	0.49
4:4:538:ASP:OD2	4:4:539:LYS:N	2.45	0.49
8:A:1106:C:O2'	8:A:1108:C:OP2	2.26	0.49
14:G:197:SER:OG	14:G:245:ARG:NH2	2.46	0.49
32:Y:255:ARG:O	32:Y:257:ASN:ND2	2.46	0.49
25:R:134:GLU:OE2	25:R:240:THR:OG1	2.25	0.48
5:5:64:PRO:HG3	5:5:83:VAL:HG13	1.94	0.48
8:A:1389:G:N2	8:A:1416:A:N7	2.61	0.48
31:X:295:LYS:NZ	42:X:503:GDP:O3A	2.46	0.48
4:4:507:GLU:HA	4:4:544:LEU:HD11	1.95	0.48
14:G:115:GLY:N	15:H:84:ASP:OD1	2.46	0.48
8:A:1495:C:H42	8:A:1554:G:H1	1.60	0.48
12:E:26:ILE:HD11	12:E:39:LEU:HD22	1.95	0.48
14:G:126:LYS:CB	14:G:131:ILE:HD11	2.42	0.48
7:7:345:LEU:HD21	8:A:1259:U:C1'	2.44	0.48
10:C:80:ASP:OD1	10:C:81:HIS:N	2.45	0.48
22:O:67:ARG:NH1	22:O:110:ASP:OD2	2.47	0.48
14:G:168:MET:HE1	14:G:240:PHE:CD1	2.49	0.48
1:0:175:ILE:HG21	22:O:188:PRO:HD2	1.96	0.48
1:0:198:MET:CE	28:U:68:ARG:HH22	2.27	0.48
14:G:237:GLU:OE1	14:G:237:GLU:N	2.43	0.48
8:A:762:G:P	19:L:206:LYS:HZ3	2.36	0.47
31:X:99:LEU:HD21	31:X:136:LEU:HD22	1.95	0.47
3:3:176:ILE:HD11	19:L:206:LYS:HE3	1.96	0.47
8:A:1466:C:O2'	8:A:1467:C:OP1	2.25	0.47
4:4:461:PHE:CZ	4:4:465:ILE:HD11	2.50	0.47
12:E:65:LEU:HD11	23:P:75:LYS:CD	2.45	0.47
7:7:193:GLY:O	35:7:502:SAM:N	2.48	0.47
15:H:184:ILE:O	15:H:184:ILE:HG22	2.15	0.47
4:4:359:GLU:OE2	32:Y:256:LEU:HG	2.15	0.47
7:7:113:LEU:HD23	7:7:134:VAL:HG13	1.97	0.47
7:7:188:THR:OG1	7:7:260:ASP:N	2.41	0.47
18:K:75:ILE:HD12	18:K:78:LEU:HD12	1.97	0.47
4:4:609:GLU:N	4:4:609:GLU:OE1	2.45	0.46
7:7:345:LEU:HD21	8:A:1259:U:H1'	1.96	0.46
15:H:120:LEU:HD12	18:K:108:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:893:G:N7	17:J:78:ARG:NH1	2.63	0.46
13:F:60:GLU:OE1	13:F:60:GLU:N	2.49	0.46
15:H:84:ASP:OD2	15:H:86:ALA:N	2.47	0.46
9:B:243:PRO:O	9:B:247:HIS:ND1	2.42	0.46
13:F:62:GLU:O	13:F:65:VAL:HG12	2.15	0.46
21:N:103:THR:O	21:N:103:THR:HG22	2.15	0.46
12:E:23:LYS:NZ	12:E:27:GLU:OE2	2.38	0.46
31:X:208:TYR:OH	31:X:246:GLU:OE2	2.20	0.46
8:A:843:G:N2	8:A:846:A:OP2	2.42	0.46
14:G:300:TYR:OH	31:X:382:PHE:O	2.21	0.46
8:A:893:G:OP2	17:J:79:LYS:NZ	2.49	0.46
4:4:331:ASN:OD1	4:4:334:THR:HG23	2.15	0.45
13:F:46:ILE:O	13:F:46:ILE:HG22	2.17	0.45
32:Y:293:PRO:O	32:Y:295:GLN:NE2	2.39	0.45
3:3:184:GLU:OE2	3:3:184:GLU:N	2.49	0.45
4:4:370:ALA:N	4:4:412:ASP:OD1	2.44	0.45
7:7:268:LEU:HB2	7:7:305:LEU:HD21	1.98	0.45
8:A:1190:C:N4	8:A:1464:G:H22	2.14	0.45
2:1:254:GLU:OE1	2:1:254:GLU:N	2.48	0.45
32:Y:347:ILE:HD12	32:Y:347:ILE:H	1.81	0.45
6:6:174:ARG:NH2	8:A:1572:A:OP2	2.49	0.45
6:6:120:LEU:CD1	6:6:155:VAL:HG21	2.47	0.45
7:7:282:GLN:HG2	7:7:312:LEU:HD21	1.97	0.45
4:4:92:ASP:OD1	10:C:157:THR:N	2.46	0.45
7:7:394:LYS:O	7:7:395:ARG:NH1	2.45	0.45
1:0:110:ASP:OD1	1:0:110:ASP:N	2.50	0.44
8:A:712:C:H42	28:U:27:ARG:HB2	1.82	0.44
9:B:146:SER:OG	9:B:197:HIS:ND1	2.34	0.44
14:G:127:HIS:O	14:G:131:ILE:HD12	2.17	0.44
18:K:66:ILE:HD12	18:K:66:ILE:H	1.81	0.44
4:4:173:PHE:CE2	4:4:177:LEU:HD11	2.53	0.44
4:4:596:LEU:HD22	4:4:633:LEU:CD2	2.47	0.44
8:A:1571:U:O2'	16:I:193:LYS:NZ	2.30	0.44
31:X:186:THR:O	31:X:190:ASN:ND2	2.51	0.44
4:4:267:VAL:HG11	4:4:296:ALA:CB	2.46	0.44
4:4:392:ILE:HG22	32:Y:250:ILE:HG21	1.99	0.44
31:X:217:GLU:N	31:X:217:GLU:OE1	2.50	0.44
1:0:37:ASP:O	1:0:41:LEU:N	2.49	0.44
29:V:187:PHE:HD2	29:V:356:THR:HG21	1.82	0.44
4:4:79:ASN:HB3	15:H:50:LEU:HD12	1.98	0.44
25:R:140:ASP:OD1	25:R:141:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T:4:LYS:O	27:T:11:ARG:NH1	2.51	0.44
30:W:114:ILE:HG21	30:W:142:LEU:HD11	2.00	0.44
8:A:760:A:N1	8:A:780:C:O2'	2.47	0.43
29:V:46:GLU:OE2	29:V:74:ARG:NE	2.40	0.43
31:X:272:THR:OG1	31:X:282:ILE:O	2.34	0.43
1:0:42:THR:HG22	1:0:49:ARG:HG2	1.99	0.43
3:3:173:LEU:HD12	3:3:191:THR:HG23	1.99	0.43
4:4:339:LEU:CD1	4:4:371:THR:HG23	2.48	0.43
8:A:1260:A:N6	8:A:1330:C:H41	2.16	0.43
22:O:214:SER:OG	29:V:318:ASP:OD2	2.25	0.43
28:U:143:ALA:O	28:U:147:GLN:OE1	2.36	0.43
29:V:29:LEU:HD23	29:V:152:ILE:HG21	1.99	0.43
29:V:155:GLU:O	29:V:155:GLU:HG3	2.18	0.43
12:E:35:ILE:HD12	19:L:97:MET:HE2	2.00	0.43
14:G:166:TYR:CE1	14:G:170:LEU:HD11	2.54	0.43
25:R:262:LEU:O	25:R:265:THR:OG1	2.23	0.43
29:V:144:PHE:CD1	29:V:167:VAL:HG22	2.52	0.43
7:7:432:SER:OG	7:7:433:TRP:N	2.52	0.43
14:G:198:ARG:HH12	14:G:201:ILE:HG23	1.83	0.43
7:7:52:HIS:O	7:7:55:ILE:HG22	2.19	0.43
8:A:1077:U:O2'	8:A:1078:A:OP1	2.27	0.43
13:F:46:ILE:HG23	14:G:315:PHE:CZ	2.54	0.43
32:Y:286:LEU:O	32:Y:289:VAL:HG22	2.19	0.43
19:L:65:ASP:OD1	19:L:65:ASP:N	2.52	0.43
2:1:107:LYS:NZ	10:C:54:GLU:OE2	2.51	0.43
19:L:181:ILE:HG23	19:L:185:LEU:HD12	2.00	0.43
29:V:393:GLU:OE2	29:V:397:ARG:HD2	2.19	0.43
12:E:88:VAL:HG23	12:E:88:VAL:O	2.19	0.43
4:4:641:ILE:HG22	4:4:645:LEU:HG	2.00	0.42
2:1:152:ASP:OD1	15:H:175:THR:OG1	2.24	0.42
5:5:239:GLU:O	5:5:240:GLN:NE2	2.52	0.42
5:5:264:LEU:HD12	5:5:280:LEU:HD21	2.01	0.42
13:F:193:ASP:OD1	13:F:194:LYS:N	2.52	0.42
8:A:1362:G:H8	8:A:1362:G:P	2.42	0.42
12:E:38:ASP:OD1	12:E:39:LEU:N	2.52	0.42
1:0:29:ARG:NH2	8:A:1530:A:OP1	2.53	0.42
23:P:142:GLU:OE1	23:P:142:GLU:N	2.52	0.42
27:T:42:GLU:OE1	27:T:45:ARG:NH2	2.43	0.42
13:F:82:THR:HG22	13:F:83:SER:N	2.34	0.42
31:X:75:LEU:HD11	31:X:83:LEU:HD11	2.00	0.42
5:5:157:ASN:O	5:5:161:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:589:THR:HG22	4:4:593:TRP:HE1	1.84	0.42
4:4:120:ILE:HD12	10:C:138:TYR:HE1	1.85	0.42
5:5:218:VAL:HB	5:5:219:PRO:HD3	2.02	0.42
8:A:1367:A:N6	8:A:1387:A:O2'	2.52	0.42
8:A:1592:U:OP2	24:Q:52:ARG:NH2	2.48	0.42
31:X:276:ARG:NH2	31:X:286:GLU:OE1	2.51	0.42
4:4:605:ILE:O	4:4:605:ILE:HG13	2.20	0.41
5:5:32:GLN:HG3	5:5:32:GLN:O	2.20	0.41
6:6:100:LEU:CD1	6:6:129:LEU:HD21	2.49	0.41
4:4:463:ASP:O	4:4:467:LEU:HD13	2.19	0.41
8:A:1248:C:O2'	8:A:1251:A:O2'	2.10	0.41
14:G:269:PHE:CD2	14:G:284:ILE:HG23	2.54	0.41
2:1:244:THR:HG22	2:1:245:GLU:N	2.32	0.41
4:4:289:ALA:HB3	4:4:294:PHE:CE1	2.55	0.41
1:0:198:MET:HE1	28:U:68:ARG:NH2	2.33	0.41
2:1:95:VAL:HG12	14:G:131:ILE:HG22	2.02	0.41
4:4:451:ASP:OD1	4:4:451:ASP:N	2.53	0.41
7:7:139:ARG:NE	8:A:1270:U:O2'	2.51	0.41
10:C:52:THR:HG22	10:C:53:TYR:N	2.34	0.41
19:L:116:VAL:HG12	19:L:126:GLU:HG3	2.02	0.41
31:X:371:ALA:HB3	31:X:372:PRO:HD3	2.01	0.41
2:1:292:TYR:O	2:1:296:VAL:HG23	2.21	0.41
25:R:303:LEU:HA	25:R:306:VAL:HG12	2.01	0.41
32:Y:361:ASN:ND2	33:Z:37:PHE:O	2.53	0.41
4:4:646:THR:HG21	4:4:667:THR:CG2	2.51	0.41
5:5:44:THR:OG1	5:5:72:SER:OG	2.24	0.41
8:A:1254:C:H42	18:K:36:ARG:HH21	1.67	0.41
12:E:65:LEU:HD11	23:P:75:LYS:HD2	2.02	0.41
29:V:360:VAL:HG13	29:V:364:LEU:HD22	2.03	0.41
4:4:526:ASP:N	4:4:526:ASP:OD1	2.54	0.41
8:A:1140:A:H2	8:A:1163:C:H42	1.69	0.41
10:C:138:TYR:OH	33:Z:65:LEU:HD22	2.20	0.41
14:G:301:GLN:OE1	31:X:385:ASN:ND2	2.43	0.41
15:H:63:VAL:O	15:H:63:VAL:HG13	2.21	0.41
29:V:109:ILE:HG23	29:V:137:ILE:HG23	2.02	0.41
8:A:1066:C:O2'	16:I:187:ARG:O	2.38	0.41
25:R:161:ILE:O	27:T:125:HIS:NE2	2.51	0.41
29:V:163:VAL:O	29:V:167:VAL:HG23	2.21	0.41
5:5:19:ARG:HH22	5:5:30:ALA:HB2	1.86	0.40
6:6:47:LYS:HZ1	8:A:1596:A:P	2.37	0.40
8:A:950:A:OP1	21:N:16:LYS:NZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:221:GLN:NE2	29:V:314:VAL:O	2.53	0.40
4:4:397:MET:HG3	4:4:401:MET:HE3	2.02	0.40
5:5:22:ILE:HD13	5:5:33:LEU:HD13	2.02	0.40
8:A:992:U:O2'	8:A:994:A:OP2	2.29	0.40
8:A:1195:U:H2'	8:A:1196:A:O4'	2.22	0.40
20:M:114:ARG:NH1	22:O:235:MET:SD	2.95	0.40
4:4:259:TYR:CD1	4:4:278:LEU:HD11	2.57	0.40
4:4:429:LEU:HD11	4:4:469:GLU:OE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	209/218 (96%)	204 (98%)	5 (2%)	0	100	100
2	1	255/323 (79%)	250 (98%)	5 (2%)	0	100	100
3	3	43/199 (22%)	43 (100%)	0	0	100	100
4	4	558/689 (81%)	551 (99%)	7 (1%)	0	100	100
5	5	317/346 (92%)	308 (97%)	9 (3%)	0	100	100
6	6	122/343 (36%)	119 (98%)	3 (2%)	0	100	100
7	7	412/456 (90%)	403 (98%)	9 (2%)	0	100	100
9	B	218/296 (74%)	217 (100%)	1 (0%)	0	100	100
10	C	122/167 (73%)	120 (98%)	2 (2%)	0	100	100
11	D	228/430 (53%)	225 (99%)	3 (1%)	0	100	100
12	E	106/125 (85%)	105 (99%)	1 (1%)	0	100	100
13	F	204/242 (84%)	201 (98%)	3 (2%)	0	100	100
14	G	288/396 (73%)	281 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	H	126/201 (63%)	124 (98%)	2 (2%)	0	100	100
16	I	135/194 (70%)	131 (97%)	4 (3%)	0	100	100
17	J	106/138 (77%)	103 (97%)	3 (3%)	0	100	100
18	K	98/128 (77%)	96 (98%)	2 (2%)	0	100	100
19	L	159/257 (62%)	159 (100%)	0	0	100	100
20	M	113/137 (82%)	113 (100%)	0	0	100	100
21	N	107/130 (82%)	107 (100%)	0	0	100	100
22	O	188/258 (73%)	186 (99%)	2 (1%)	0	100	100
23	P	94/142 (66%)	93 (99%)	1 (1%)	0	100	100
24	Q	84/87 (97%)	84 (100%)	0	0	100	100
25	R	289/360 (80%)	286 (99%)	3 (1%)	0	100	100
26	S	131/190 (69%)	130 (99%)	1 (1%)	0	100	100
27	T	162/173 (94%)	161 (99%)	1 (1%)	0	100	100
28	U	172/205 (84%)	169 (98%)	3 (2%)	0	100	100
29	V	355/414 (86%)	351 (99%)	4 (1%)	0	100	100
30	W	96/187 (51%)	95 (99%)	1 (1%)	0	100	100
31	X	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
32	Y	119/395 (30%)	119 (100%)	0	0	100	100
33	Z	67/106 (63%)	65 (97%)	2 (3%)	0	100	100
All	All	6033/8330 (72%)	5944 (98%)	89 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	184 (100%)	0	100	100
2	1	239/291 (82%)	239 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	40/166 (24%)	40 (100%)	0	100	100
4	4	506/609 (83%)	506 (100%)	0	100	100
5	5	286/309 (93%)	286 (100%)	0	100	100
6	6	107/288 (37%)	107 (100%)	0	100	100
7	7	354/385 (92%)	354 (100%)	0	100	100
9	B	194/249 (78%)	194 (100%)	0	100	100
10	C	111/143 (78%)	111 (100%)	0	100	100
11	D	196/357 (55%)	196 (100%)	0	100	100
12	E	91/107 (85%)	91 (100%)	0	100	100
13	F	183/209 (88%)	183 (100%)	0	100	100
14	G	254/342 (74%)	254 (100%)	0	100	100
15	H	120/180 (67%)	120 (100%)	0	100	100
16	I	105/147 (71%)	104 (99%)	1 (1%)	68	81
17	J	93/118 (79%)	93 (100%)	0	100	100
18	K	90/113 (80%)	90 (100%)	0	100	100
19	L	151/226 (67%)	151 (100%)	0	100	100
20	M	94/113 (83%)	94 (100%)	0	100	100
21	N	95/115 (83%)	95 (100%)	0	100	100
22	O	171/230 (74%)	171 (100%)	0	100	100
23	P	87/123 (71%)	87 (100%)	0	100	100
24	Q	78/79 (99%)	78 (100%)	0	100	100
25	R	261/318 (82%)	261 (100%)	0	100	100
26	S	115/164 (70%)	115 (100%)	0	100	100
27	T	151/157 (96%)	151 (100%)	0	100	100
28	U	150/174 (86%)	150 (100%)	0	100	100
29	V	323/364 (89%)	323 (100%)	0	100	100
30	W	85/158 (54%)	85 (100%)	0	100	100
31	X	311/351 (89%)	311 (100%)	0	100	100
32	Y	113/357 (32%)	113 (100%)	0	100	100
33	Z	63/95 (66%)	63 (100%)	0	100	100
All	All	5401/7227 (75%)	5400 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	I	178	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	26	ASN
1	0	108	ASN
1	0	111	HIS
1	0	145	HIS
2	1	231	HIS
4	4	257	HIS
4	4	444	ASN
4	4	489	HIS
5	5	95	GLN
5	5	171	GLN
5	5	229	HIS
5	5	235	GLN
5	5	272	GLN
5	5	321	ASN
6	6	171	GLN
7	7	60	HIS
7	7	98	HIS
7	7	146	GLN
7	7	175	HIS
7	7	185	GLN
7	7	187	GLN
7	7	383	HIS
7	7	398	HIS
7	7	400	HIS
9	B	130	ASN
10	C	57	HIS
11	D	280	HIS
11	D	302	HIS
11	D	361	GLN
11	D	415	GLN
12	E	58	HIS
13	F	134	GLN
13	F	146	HIS
13	F	224	HIS
14	G	139	GLN
14	G	156	GLN

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Mol	Chain	Res	Type
15	H	147	HIS
16	I	87	HIS
17	J	105	HIS
22	O	166	HIS
22	O	169	GLN
22	O	223	HIS
23	P	71	HIS
23	P	95	HIS
25	R	299	ASN
25	R	308	HIS
27	T	37	HIS
28	U	61	GLN
28	U	62	HIS
29	V	122	GLN
29	V	224	GLN
31	X	180	GLN
31	X	257	HIS
31	X	291	HIS
31	X	358	GLN
32	Y	303	GLN
33	Z	55	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	A	874/955 (91%)	211 (24%)	6 (0%)

All (211) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	650	U
8	A	651	A
8	A	664	G
8	A	680	U
8	A	688	A
8	A	689	U
8	A	704	U
8	A	721	U
8	A	722	C
8	A	730	A
8	A	736	C

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Mol	Chain	Res	Type
8	A	737	C
8	A	739	C
8	A	740	G
8	A	741	A
8	A	745	A
8	A	753	A
8	A	761	A
8	A	766	G
8	A	769	G
8	A	772	A
8	A	773	U
8	A	777	G
8	A	791	G
8	A	794	U
8	A	796	G
8	A	807	A
8	A	830	U
8	A	831	U
8	A	832	U
8	A	835	C
8	A	851	A
8	A	860	A
8	A	861	U
8	A	866	A
8	A	868	C
8	A	871	A
8	A	883	U
8	A	886	C
8	A	889	G
8	A	893	G
8	A	902	G
8	A	903	U
8	A	919	A
8	A	923	A
8	A	931	C
8	A	938	A
8	A	939	A
8	A	954	C
8	A	955	A
8	A	967	A
8	A	970	A
8	A	971	A

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Mol	Chain	Res	Type
8	A	972	G
8	A	992	U
8	A	993	A
8	A	1001	C
8	A	1002	C
8	A	1011	C
8	A	1012	A
8	A	1014	A
8	A	1015	A
8	A	1042	U
8	A	1052	C
8	A	1060	A
8	A	1061	A
8	A	1077	U
8	A	1078	A
8	A	1080	A
8	A	1081	U
8	A	1103	A
8	A	1105	C
8	A	1111	C
8	A	1117	A
8	A	1119	U
8	A	1120	C
8	A	1121	A
8	A	1126	A
8	A	1137	A
8	A	1151	C
8	A	1152	A
8	A	1155	G
8	A	1160	A
8	A	1167	A
8	A	1175	G
8	A	1177	C
8	A	1178	G
8	A	1179	G
8	A	1181	G
8	A	1182	C
8	A	1184	U
8	A	1185	C
8	A	1186	A
8	A	1187	U
8	A	1188	A

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Mol	Chain	Res	Type
8	A	1189	U
8	A	1190	C
8	A	1191	C
8	A	1197	G
8	A	1198	A
8	A	1200	G
8	A	1201	A
8	A	1202	G
8	A	1203	C
8	A	1213	A
8	A	1215	U
8	A	1217	G
8	A	1242	C
8	A	1245	U
8	A	1246	U
8	A	1247	G
8	A	1248	C
8	A	1249	U
8	A	1250	C
8	A	1251	A
8	A	1255	U
8	A	1258	A
8	A	1259	U
8	A	1261	C
8	A	1264	C
8	A	1284	U
8	A	1287	A
8	A	1290	C
8	A	1291	U
8	A	1294	A
8	A	1296	A
8	A	1297	G
8	A	1299	A
8	A	1330	C
8	A	1331	A
8	A	1332	A
8	A	1333	G
8	A	1338	A
8	A	1342	C
8	A	1343	A
8	A	1344	U
8	A	1350	G

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Mol	Chain	Res	Type
8	A	1354	A
8	A	1359	U
8	A	1361	G
8	A	1362	G
8	A	1364	U
8	A	1367	A
8	A	1368	U
8	A	1369	U
8	A	1376	C
8	A	1378	C
8	A	1382	A
8	A	1385	C
8	A	1386	U
8	A	1387	A
8	A	1392	A
8	A	1397	U
8	A	1404	A
8	A	1405	C
8	A	1406	U
8	A	1416	A
8	A	1419	G
8	A	1420	U
8	A	1421	G
8	A	1422	G
8	A	1424	U
8	A	1427	A
8	A	1429	C
8	A	1430	A
8	A	1448	U
8	A	1449	G
8	A	1463	G
8	A	1464	G
8	A	1467	C
8	A	1468	U
8	A	1470	A
8	A	1471	A
8	A	1474	G
8	A	1477	U
8	A	1493	C
8	A	1494	C
8	A	1495	C
8	A	1511	C

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Mol	Chain	Res	Type
8	A	1512	A
8	A	1513	A
8	A	1514	A
8	A	1518	C
8	A	1519	A
8	A	1520	U
8	A	1525	C
8	A	1526	U
8	A	1527	A
8	A	1532	C
8	A	1533	C
8	A	1535	U
8	A	1537	C
8	A	1538	G
8	A	1539	C
8	A	1543	U
8	A	1544	A
8	A	1549	G
8	A	1556	C
8	A	1557	A
8	A	1558	A
8	A	1559	G
8	A	1560	U
8	A	1564	A
8	A	1572	A
8	A	1574	G
8	A	1577	U
8	A	1582	G
8	A	1583	A
8	A	1585	A
8	A	1594	G
8	A	1595	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1077	U
8	A	1151	C
8	A	1254	C
8	A	1330	C
8	A	1358	A
8	A	1536	A

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
24	AYA	Q	2	24	6,7,8	1.26	1 (16%)	6,8,10	1.14	1 (16%)

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
24	AYA	Q	2	24	-	0/5/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	2	AYA	CA-N	-2.33	1.44	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	2	AYA	CB-CA-N	2.49	112.49	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 32 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	ATP	X	501	37	32,33,33	0.32	0	48,52,52	0.69	0
40	FES	T	201	20,27	0,4,4	-	-	-	-	-
35	SAM	7	502	-	27,29,29	1.09	5 (18%)	34,42,42	1.99	9 (26%)
40	FES	P	201	12,23	0,4,4	-	-	-	-	-
34	SF4	7	501	7	0,12,12	-	-	-	-	-
38	NAD	A	1730	37	46,48,48	3.09	17 (36%)	64,73,73	2.73	18 (28%)
42	GDP	X	503	-	29,30,30	3.29	10 (34%)	45,47,47	2.33	14 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	ATP	X	501	37	-	4/22/38/38	0/3/3/3
40	FES	T	201	20,27	-	-	0/1/1/1
35	SAM	7	502	-	-	4/17/33/33	0/3/3/3
40	FES	P	201	12,23	-	-	0/1/1/1
34	SF4	7	501	7	-	-	0/6/5/5
38	NAD	A	1730	37	-	2/30/62/62	0/5/5/5
42	GDP	X	503	-	-	3/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	X	503	GDP	O6-C6	9.77	1.42	1.23
42	X	503	GDP	C2-N1	7.68	1.56	1.37
42	X	503	GDP	PA-O3A	7.28	1.67	1.59
38	A	1730	NAD	C7N-N7N	7.18	1.46	1.33
38	A	1730	NAD	PN-O3	7.17	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A	1730	NAD	PA-O3	7.13	1.67	1.59
38	A	1730	NAD	C5A-N7A	7.10	1.52	1.39
38	A	1730	NAD	O4D-C1D	5.75	1.48	1.40
38	A	1730	NAD	C8A-N9A	-5.73	1.27	1.37
42	X	503	GDP	C2-N3	5.31	1.46	1.33
42	X	503	GDP	C2-N2	5.25	1.46	1.34
38	A	1730	NAD	C6A-N6A	4.84	1.46	1.34
38	A	1730	NAD	C2N-N1N	4.35	1.39	1.35
38	A	1730	NAD	C4N-C3N	4.05	1.45	1.39
38	A	1730	NAD	C4A-N9A	-3.82	1.29	1.37
38	A	1730	NAD	C5A-C4A	3.78	1.45	1.39
38	A	1730	NAD	C5N-C4N	3.46	1.44	1.38
38	A	1730	NAD	O7N-C7N	-2.87	1.18	1.24
42	X	503	GDP	C2'-C3'	-2.82	1.45	1.53
42	X	503	GDP	C6-N1	2.64	1.43	1.38
35	7	502	SAM	C2-N3	2.52	1.38	1.33
38	A	1730	NAD	O4B-C1B	2.51	1.47	1.42
35	7	502	SAM	C2-N1	2.49	1.38	1.33
42	X	503	GDP	PA-O5'	2.44	1.68	1.59
38	A	1730	NAD	C3N-C7N	2.31	1.54	1.50
42	X	503	GDP	PB-O3B	-2.30	1.46	1.54
38	A	1730	NAD	C8A-N7A	2.25	1.36	1.31
35	7	502	SAM	OXT-C	-2.23	1.23	1.30
38	A	1730	NAD	C2D-C3D	-2.17	1.47	1.53
42	X	503	GDP	PB-O2B	-2.17	1.46	1.54
35	7	502	SAM	C8-N7	2.09	1.35	1.31
35	7	502	SAM	C5-N7	-2.04	1.35	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	1730	NAD	C4A-N9A-C8A	13.63	120.05	105.74
42	X	503	GDP	N9-C8-N7	-6.87	100.66	113.40
42	X	503	GDP	C8-N7-C5	6.81	116.40	104.26
38	A	1730	NAD	N3A-C4A-N9A	6.61	138.41	127.17
38	A	1730	NAD	C5A-C4A-N3A	-6.18	118.21	126.72
38	A	1730	NAD	C4A-C5A-N7A	-6.13	103.58	110.58
35	7	502	SAM	N3-C2-N1	-5.57	120.14	128.58
42	X	503	GDP	C2-N1-C6	-4.83	116.34	125.11
35	7	502	SAM	C5-C4-N3	-4.61	120.37	126.72
38	A	1730	NAD	N9A-C8A-N7A	-4.58	107.43	113.94
38	A	1730	NAD	N3A-C2A-N1A	-4.45	121.84	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	X	503	GDP	C8-N9-C4	4.17	113.84	106.03
38	A	1730	NAD	C4D-O4D-C1D	-4.01	106.25	109.92
38	A	1730	NAD	C4A-N9A-C1B	-3.80	117.75	126.63
35	7	502	SAM	N9-C8-N7	-3.74	108.63	113.94
42	X	503	GDP	C6-C5-C4	3.64	124.31	118.83
38	A	1730	NAD	C2A-N3A-C4A	3.57	120.54	111.83
35	7	502	SAM	C2-N3-C4	3.47	120.31	111.83
38	A	1730	NAD	C6A-C5A-N7A	3.39	138.63	132.09
35	7	502	SAM	C5-N7-C8	3.38	108.76	103.45
42	X	503	GDP	C4-C5-N7	-3.16	105.66	110.67
42	X	503	GDP	O2B-PB-O3A	2.98	114.62	104.64
35	7	502	SAM	N3-C4-N9	2.86	132.03	127.17
42	X	503	GDP	N9-C4-N3	2.77	131.49	125.95
42	X	503	GDP	C2-N3-C4	2.73	117.00	112.30
42	X	503	GDP	O3B-PB-O3A	2.72	113.75	104.64
35	7	502	SAM	OXT-C-O	-2.64	118.09	124.08
42	X	503	GDP	C3'-C2'-C1'	2.59	106.37	101.46
35	7	502	SAM	C4-C5-N7	-2.41	107.83	110.58
38	A	1730	NAD	O2A-PA-O1A	-2.38	101.36	112.44
38	A	1730	NAD	O2N-PN-O1N	-2.37	101.40	112.44
42	X	503	GDP	O2A-PA-O1A	-2.37	101.41	112.44
38	A	1730	NAD	C3B-C2B-C1B	2.34	105.89	101.46
38	A	1730	NAD	C2B-C3B-C4B	2.27	106.99	102.61
38	A	1730	NAD	C5A-C4A-N9A	-2.23	103.38	105.81
38	A	1730	NAD	C1B-N9A-C8A	-2.21	122.18	127.09
35	7	502	SAM	O4'-C1'-N9	2.11	112.13	108.09
42	X	503	GDP	C5-C4-N3	-2.09	125.06	128.39
42	X	503	GDP	O6-C6-C5	-2.08	121.03	126.53
38	A	1730	NAD	C2D-C3D-C4D	2.08	106.62	102.61
38	A	1730	NAD	C3N-C7N-N7N	2.02	120.23	117.74

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	7	502	SAM	CB-CG-SD-CE
41	X	501	ATP	PB-O3B-PG-O2G
35	7	502	SAM	O-C-CA-CB
35	7	502	SAM	OXT-C-CA-CB
35	7	502	SAM	CB-CG-SD-C5'
38	A	1730	NAD	C5B-O5B-PA-O1A
42	X	503	GDP	O4'-C4'-C5'-O5'

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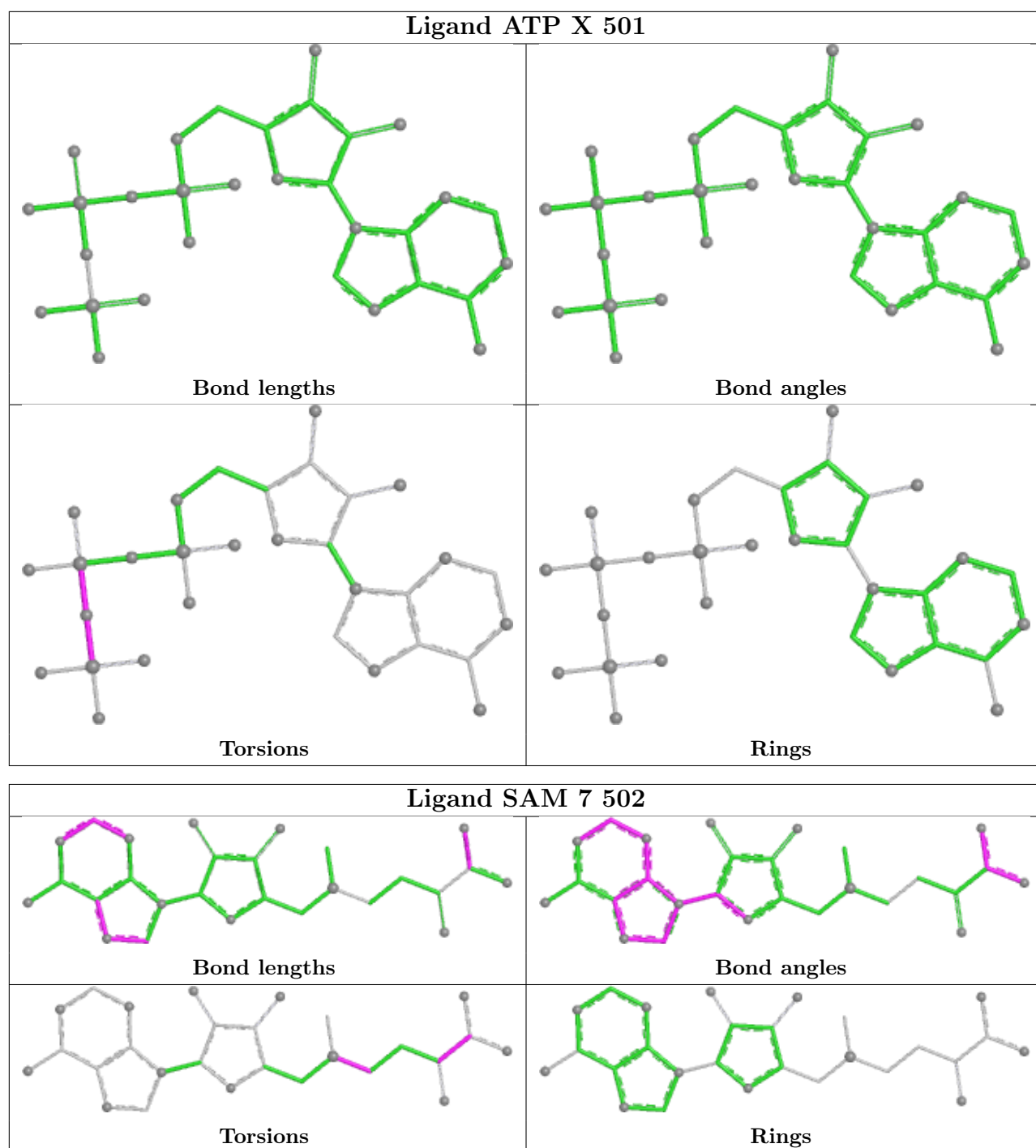
Mol	Chain	Res	Type	Atoms
38	A	1730	NAD	C4B-C5B-O5B-PA
41	X	501	ATP	PB-O3B-PG-O1G
41	X	501	ATP	PB-O3B-PG-O3G
41	X	501	ATP	PG-O3B-PB-O2B
42	X	503	GDP	PB-O3A-PA-O1A
42	X	503	GDP	PB-O3A-PA-O2A

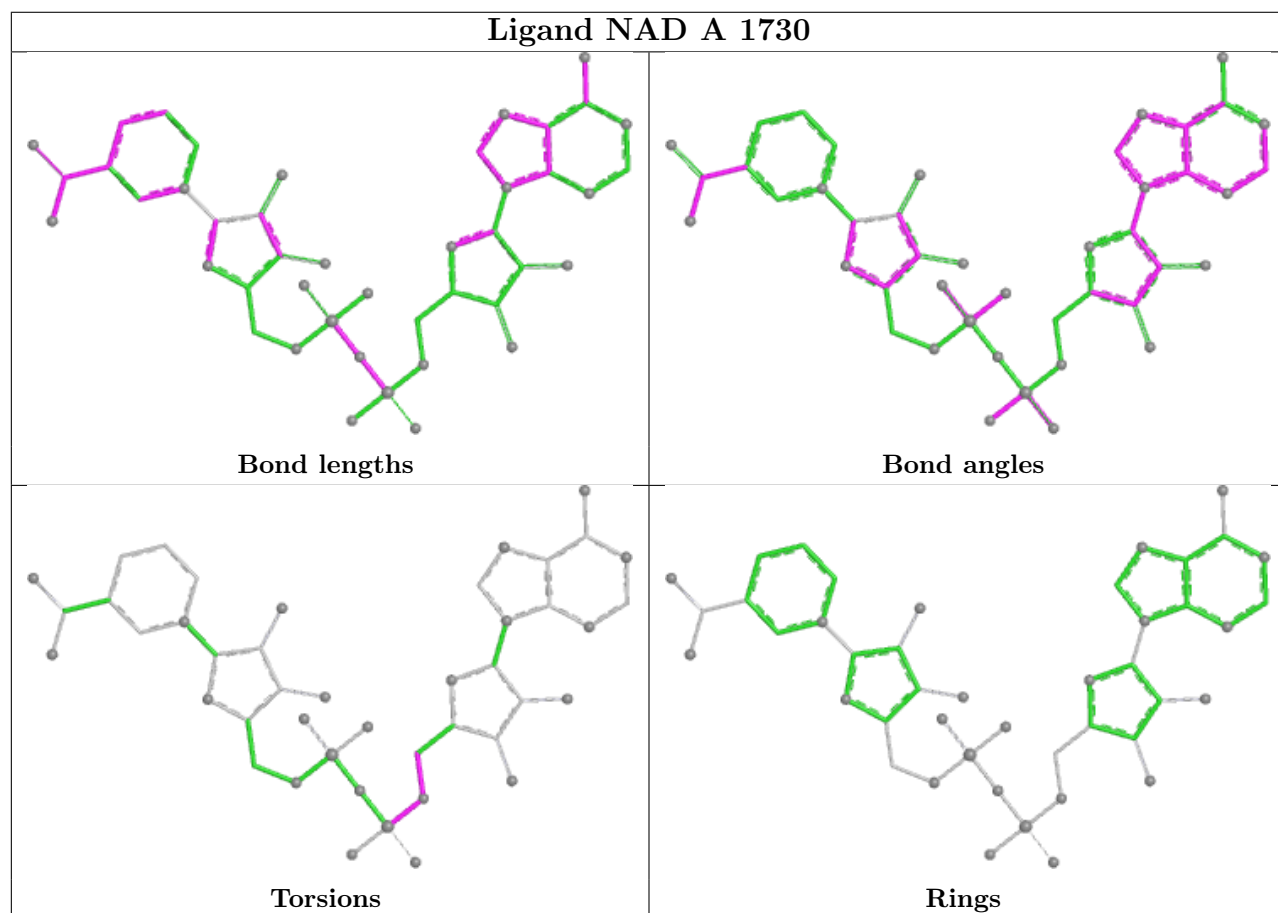
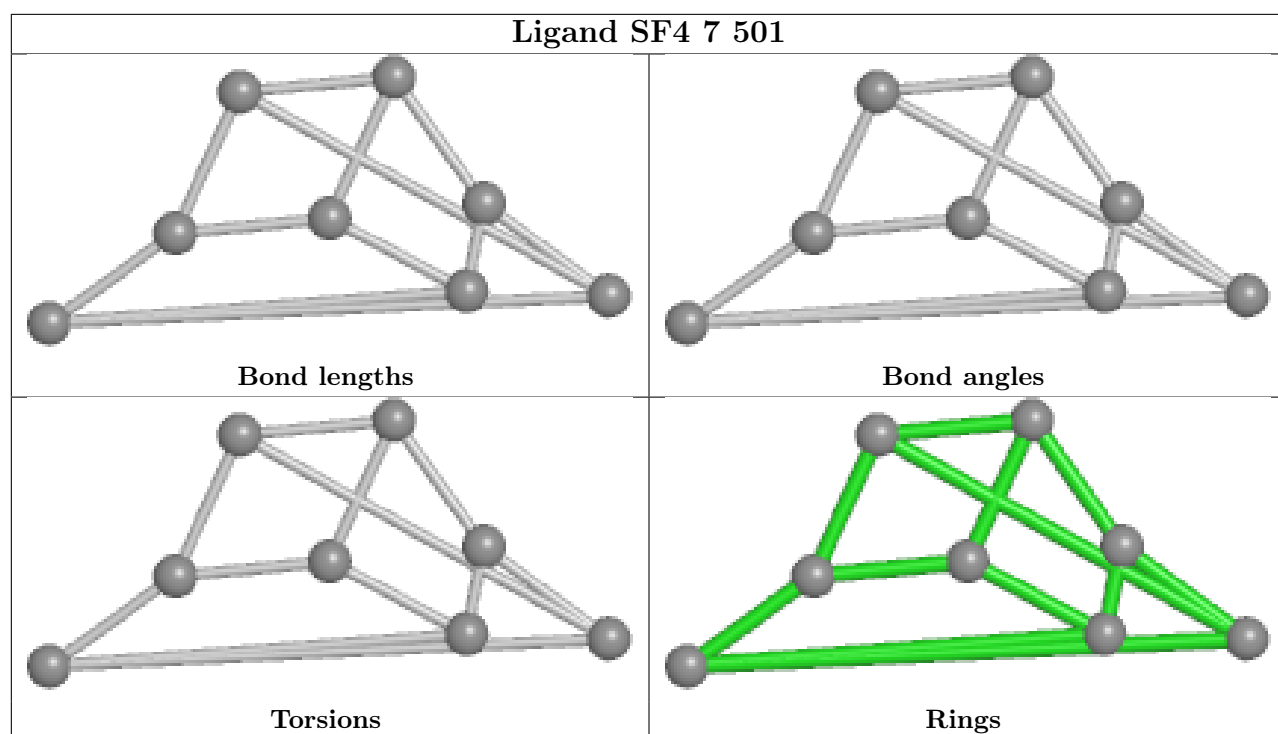
There are no ring outliers.

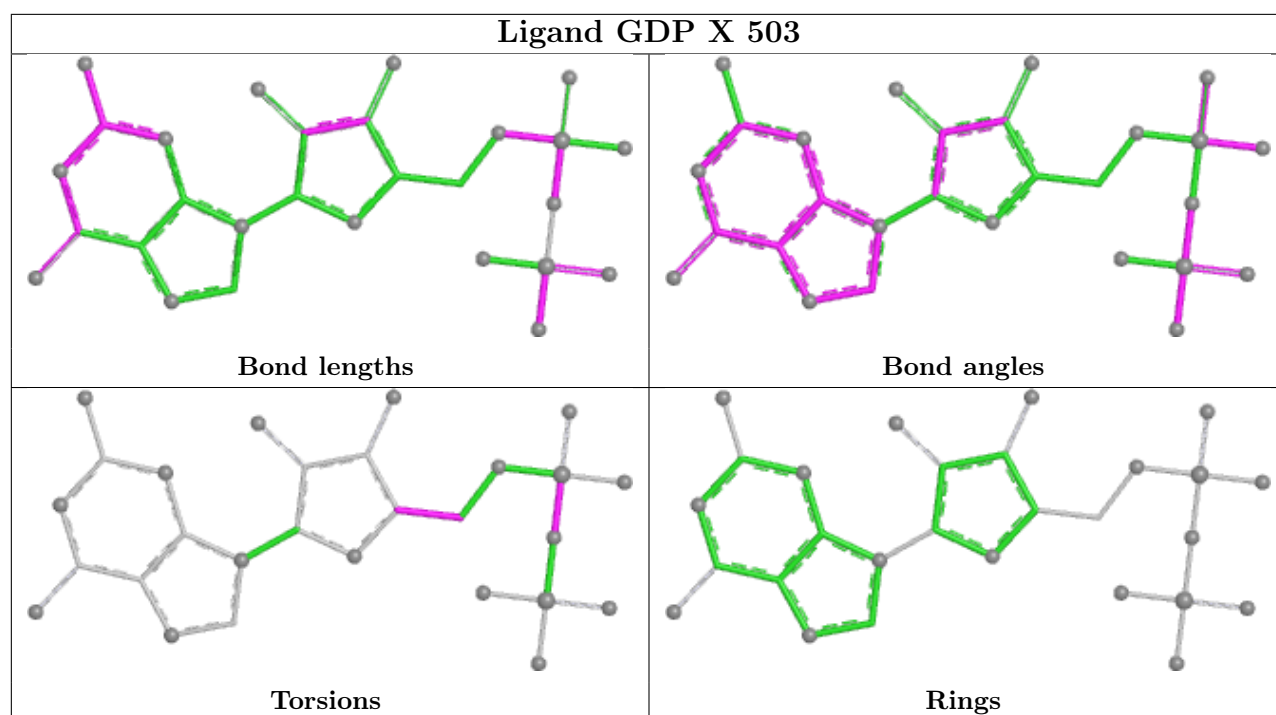
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	7	502	SAM	3	0
38	A	1730	NAD	1	0
42	X	503	GDP	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.

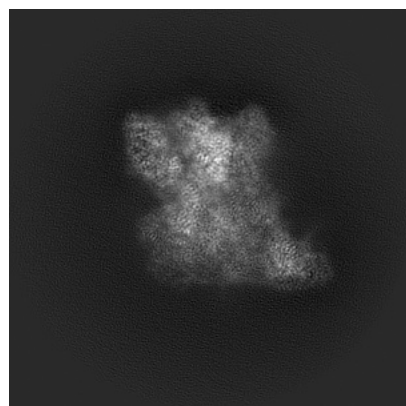
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26971. These allow visual inspection of the internal detail of the map and identification of artifacts.

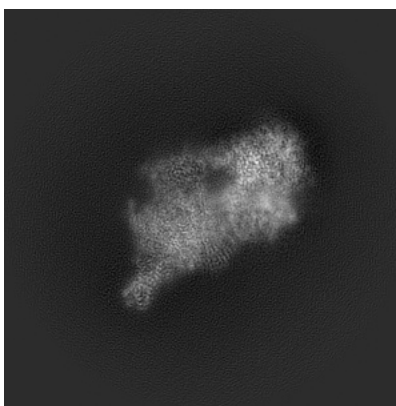
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

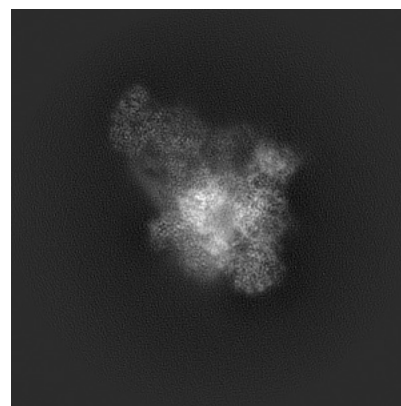
6.1.1 Primary map



X

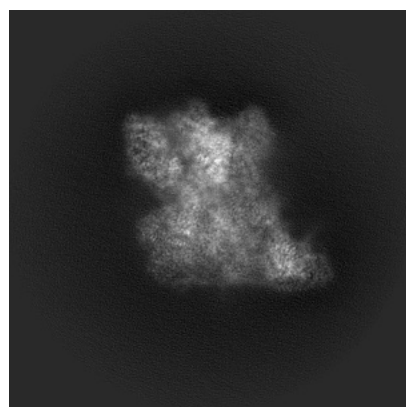


Y

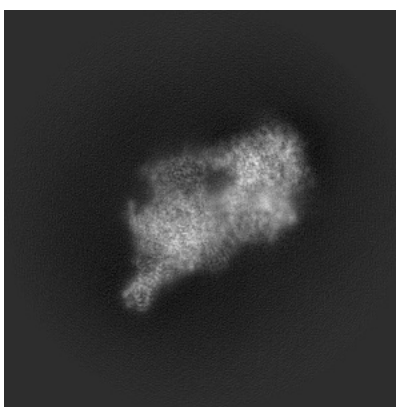


Z

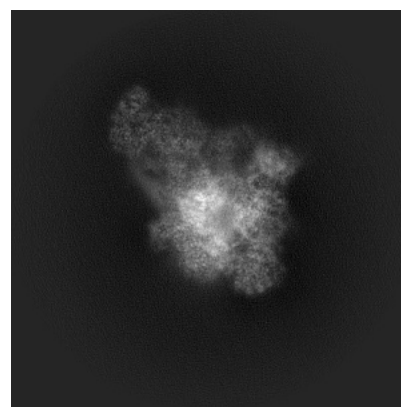
6.1.2 Raw map



X



Y

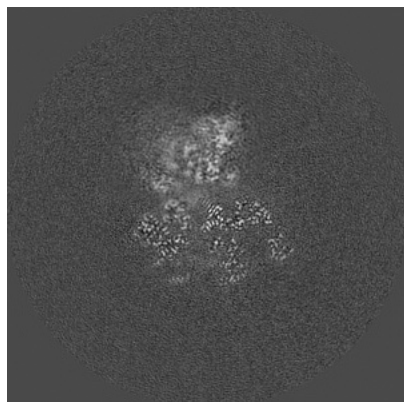


Z

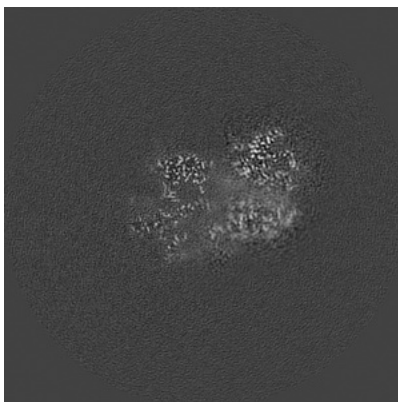
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

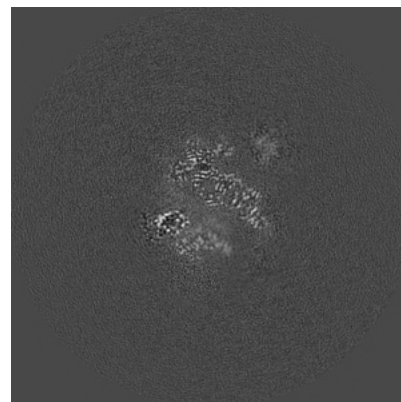
6.2.1 Primary map



X Index: 200

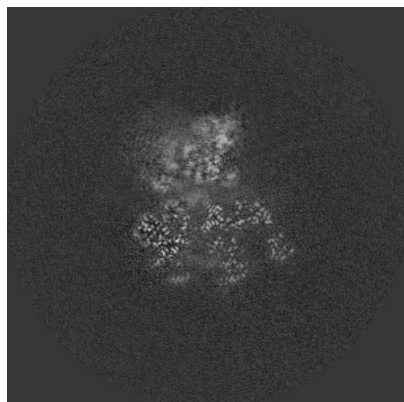


Y Index: 200

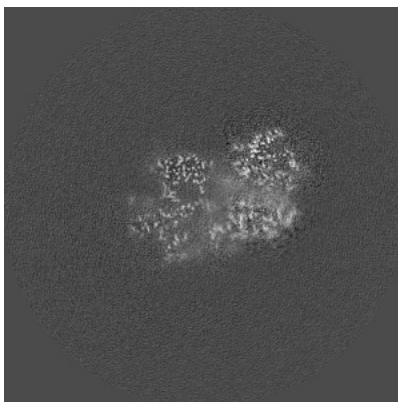


Z Index: 200

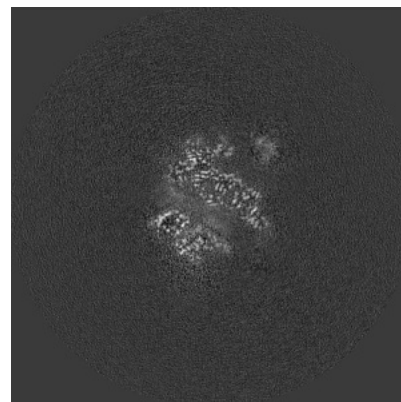
6.2.2 Raw map



X Index: 200



Y Index: 200

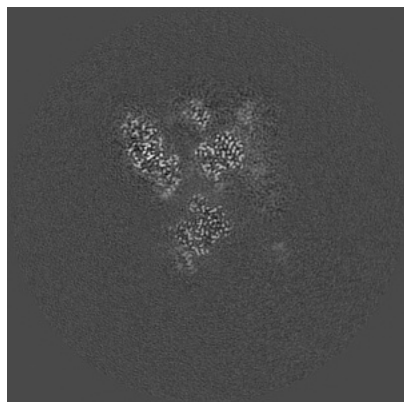


Z Index: 200

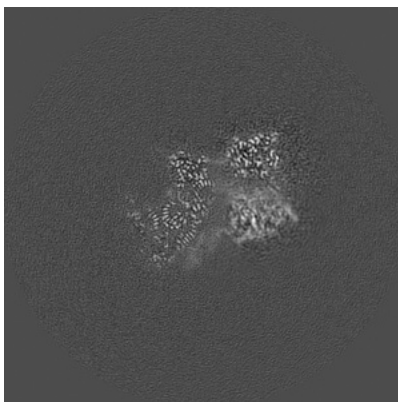
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

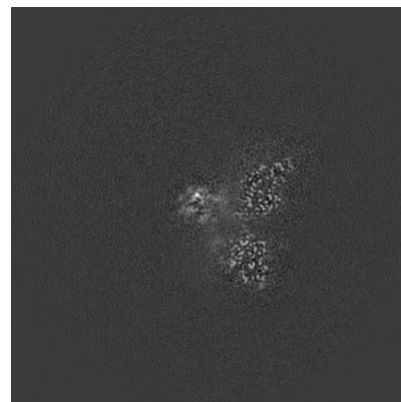
6.3.1 Primary map



X Index: 242

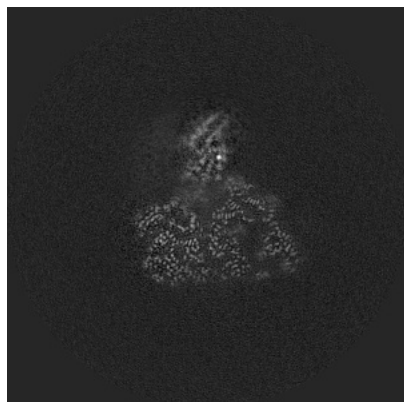


Y Index: 210

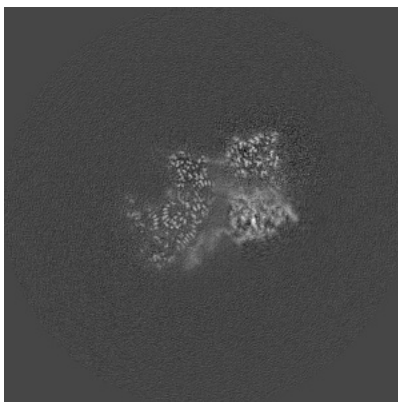


Z Index: 249

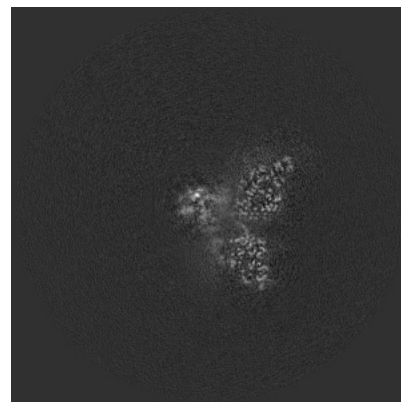
6.3.2 Raw map



X Index: 186



Y Index: 210

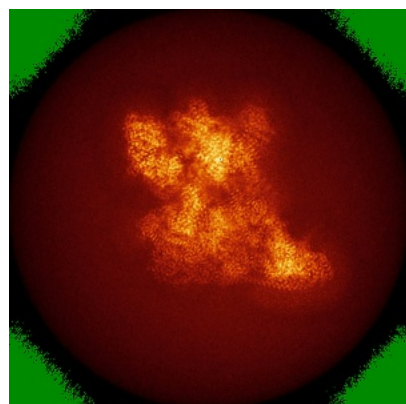


Z Index: 250

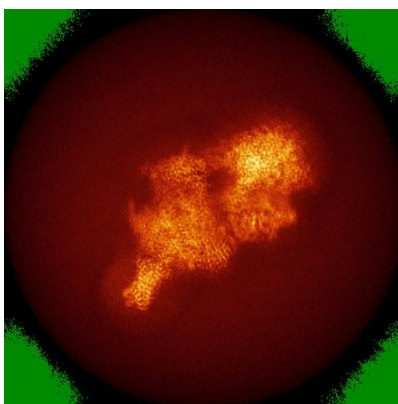
The images above show the largest variance slices of the map in three orthogonal directions.

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

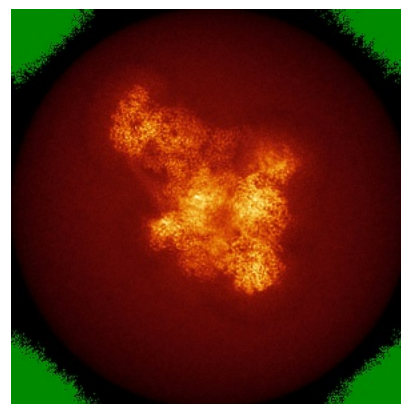
6.4.1 Primary map



X

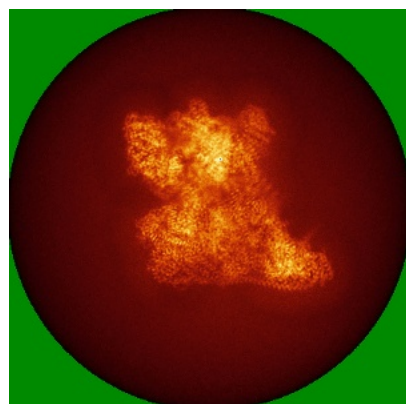


Y

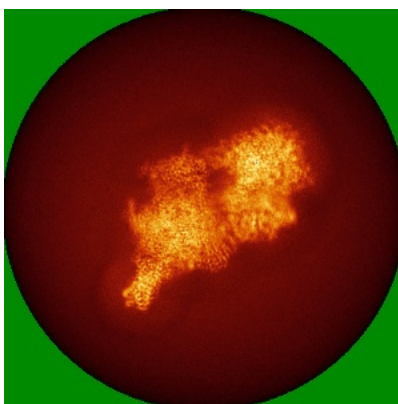


Z

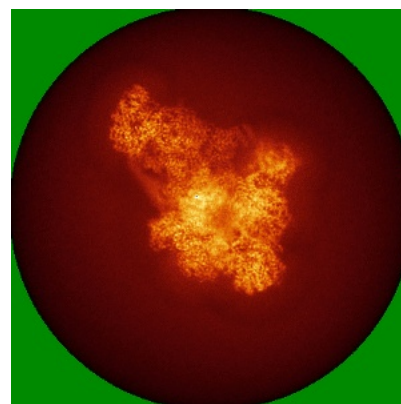
6.4.2 Raw map



X



Y

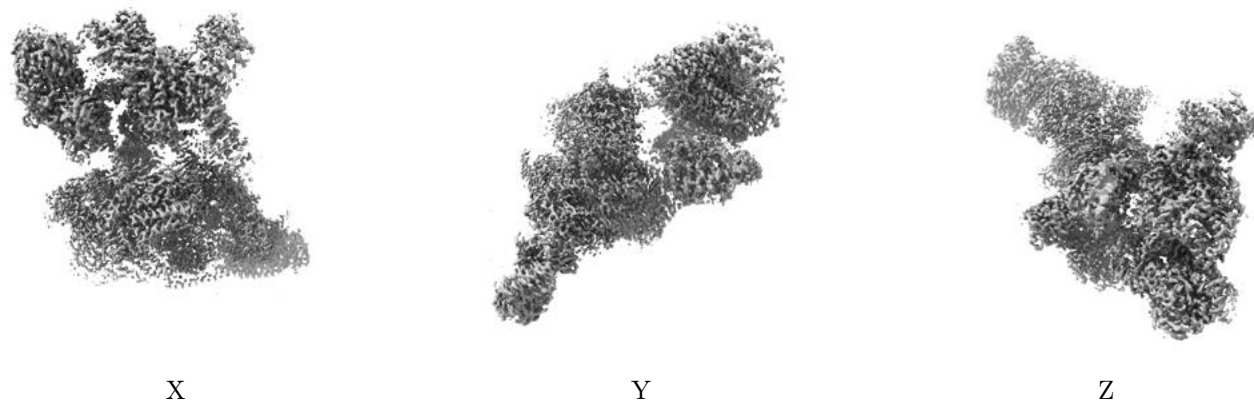


Z

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.

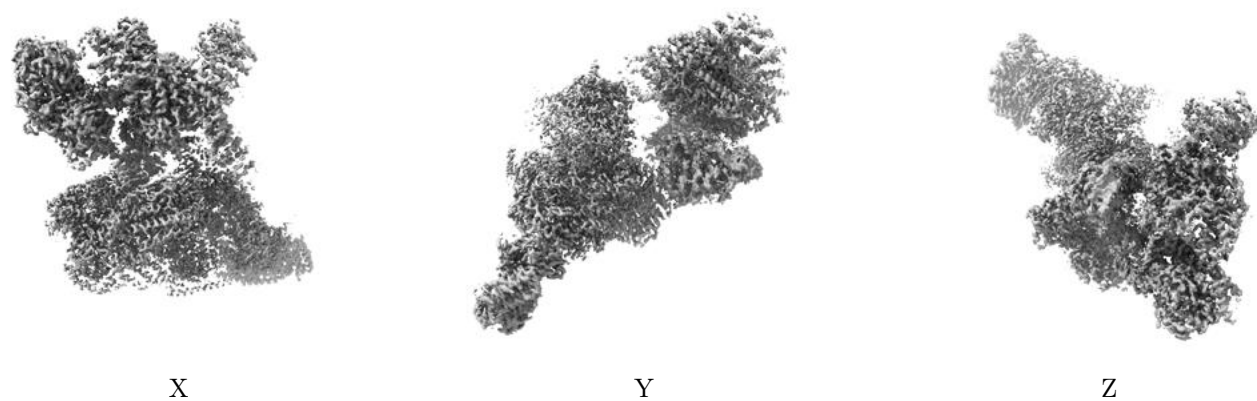
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 9.0. 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.

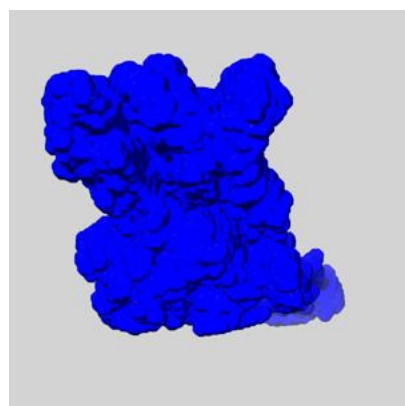
6.6 Mask visualisation [i](#)

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

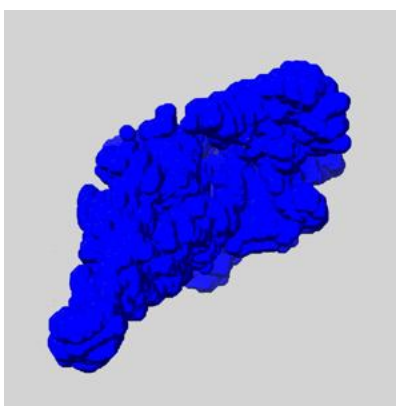
A mask typically either:

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

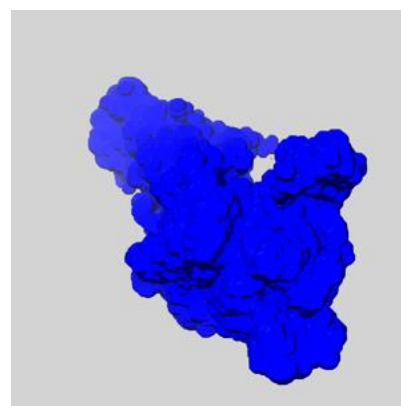
6.6.1 emd_26971_msk_1.map [i](#)



X



Y

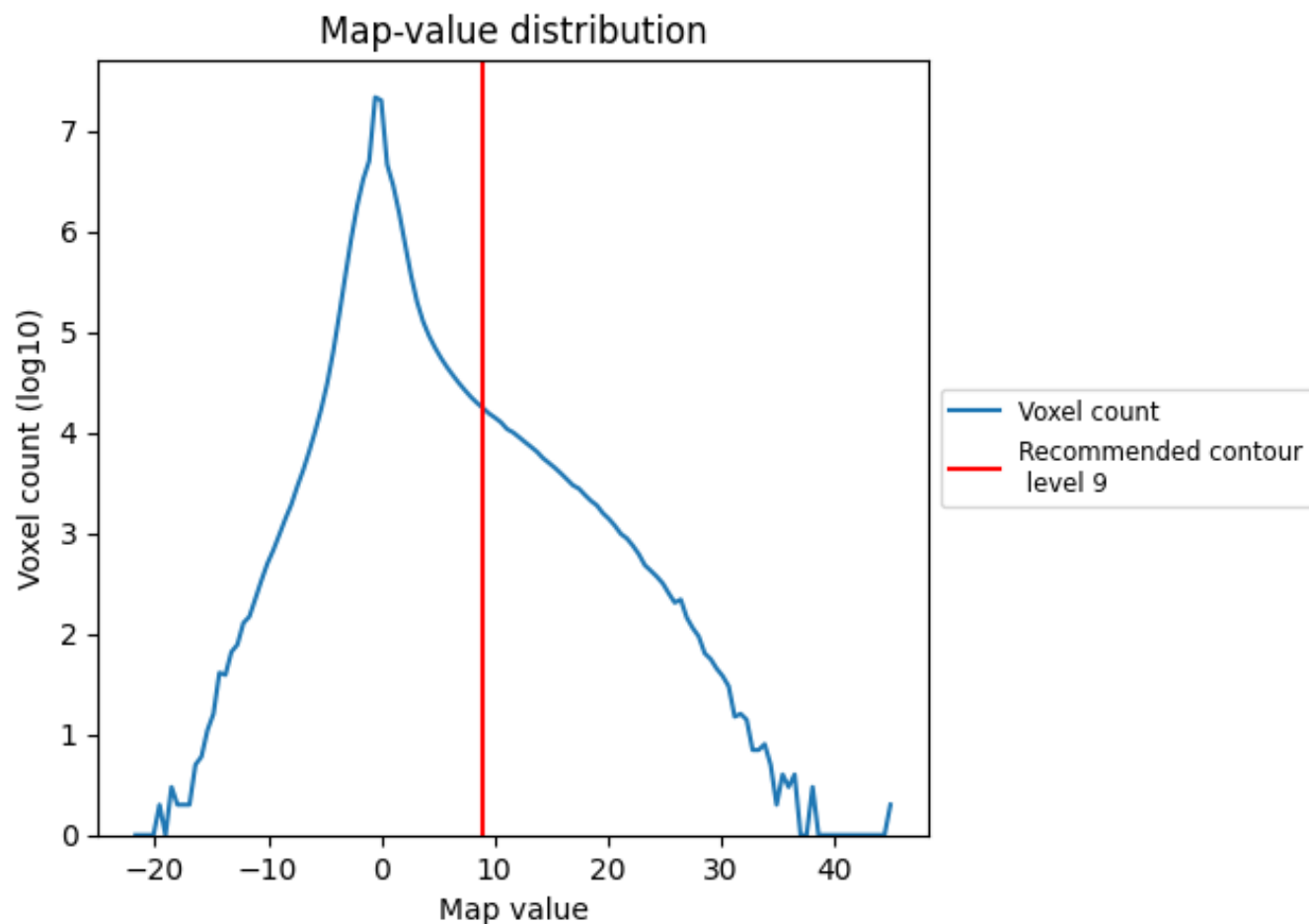


Z

7 Map analysis [i](#)

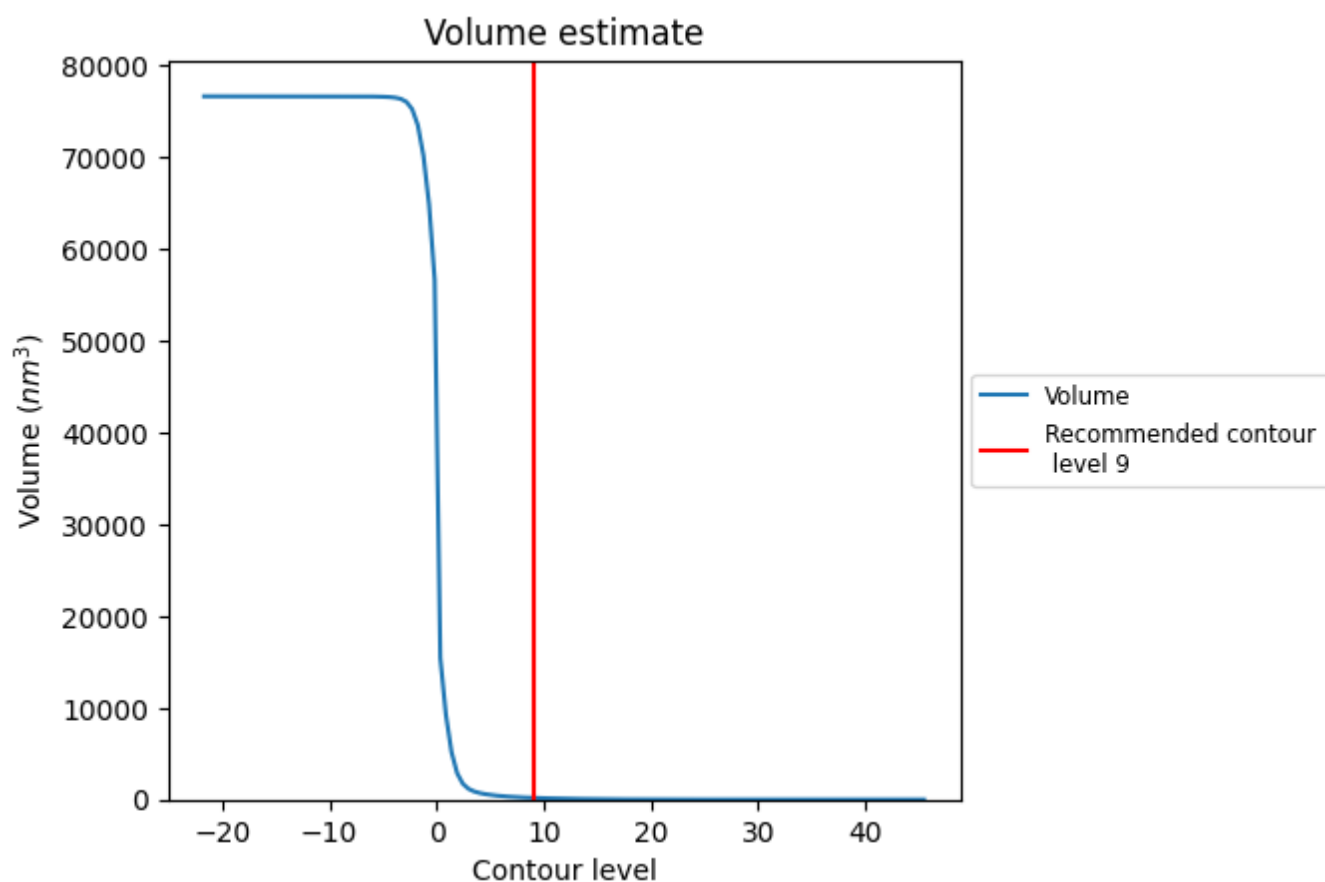
This section contains the results of statistical analysis of the map.

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.

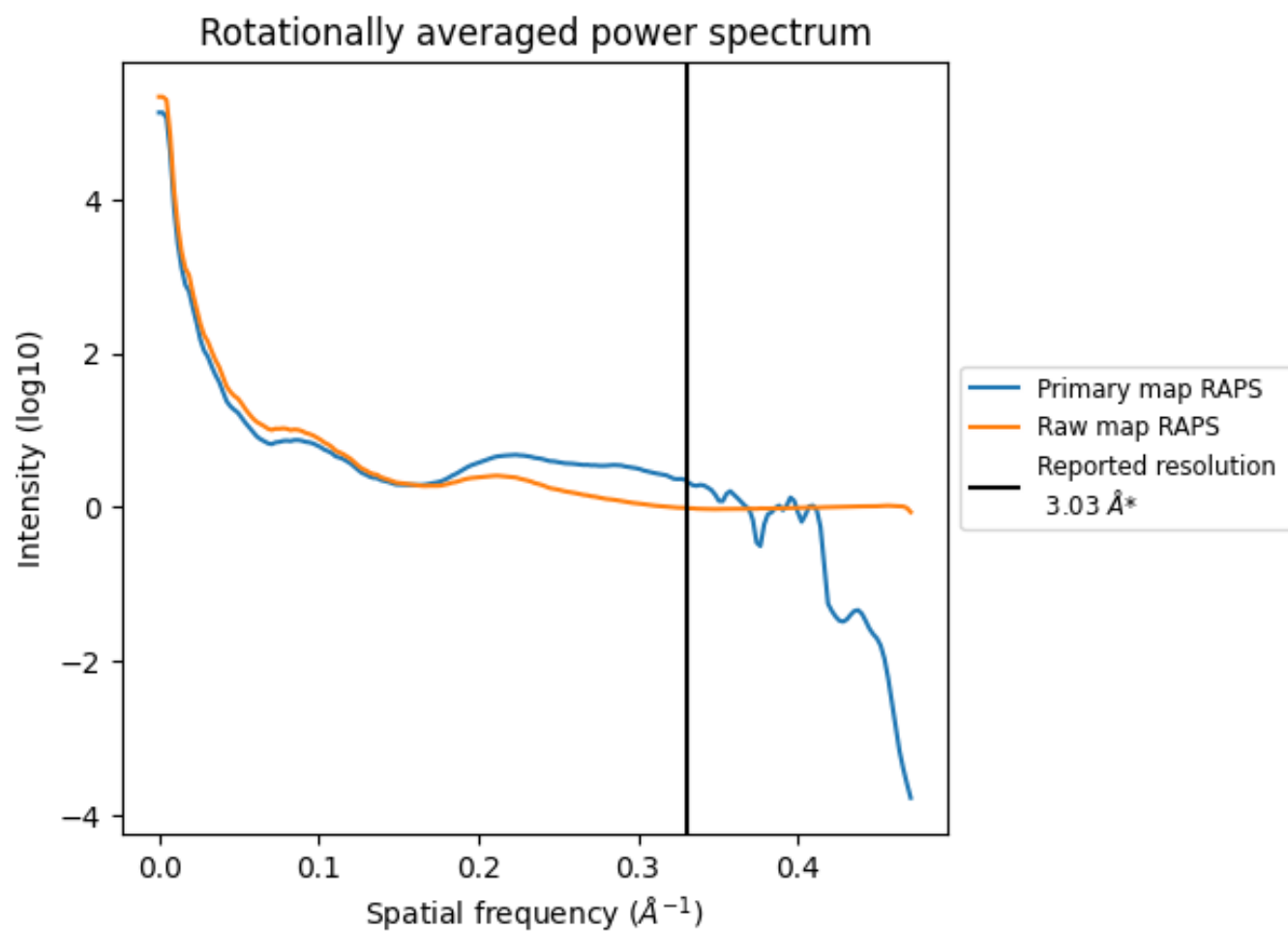
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 186 nm³; this corresponds to an approximate mass of 168 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 ⓘ

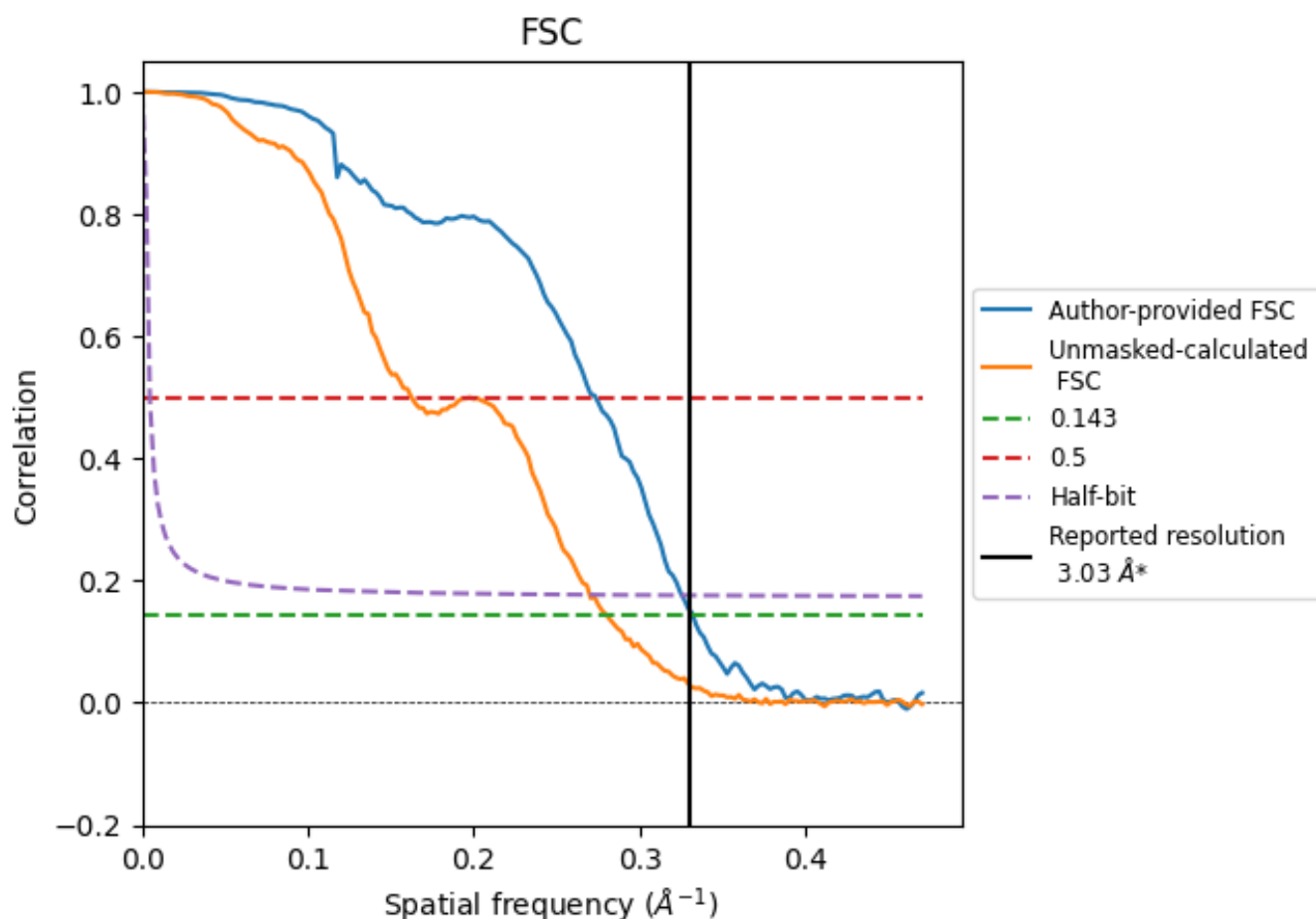


*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

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 $0.330 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

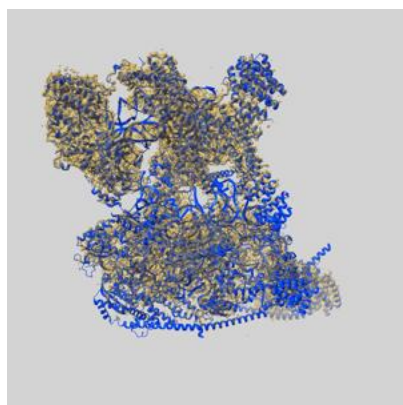
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.01	3.65	3.07
Unmasked-calculated*	3.57	6.15	3.70

*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 3.57 differs from the reported value 3.03 by more than 10 %

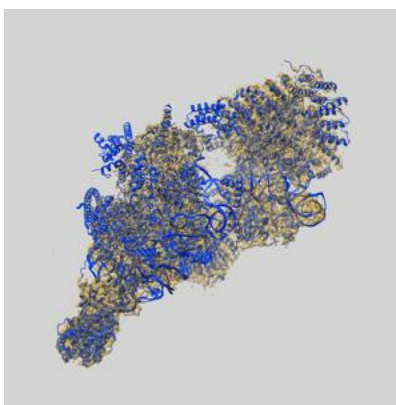
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26971 and PDB model 8CSU. Per-residue inclusion information can be found in section 3 on page 14.

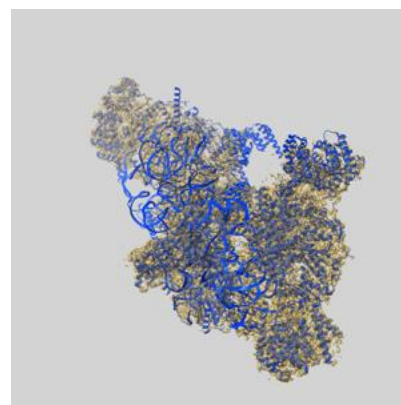
9.1 Map-model overlay [i](#)



X



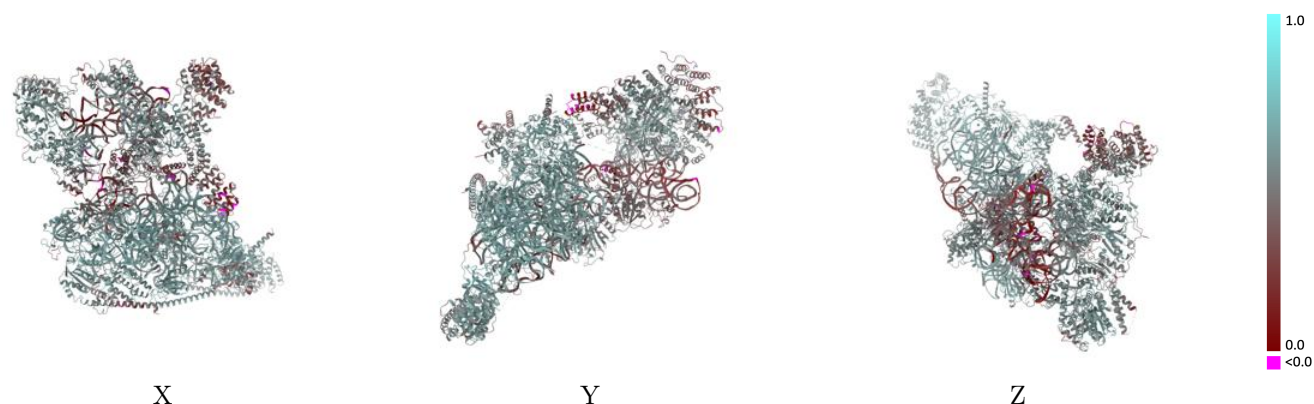
Y



Z

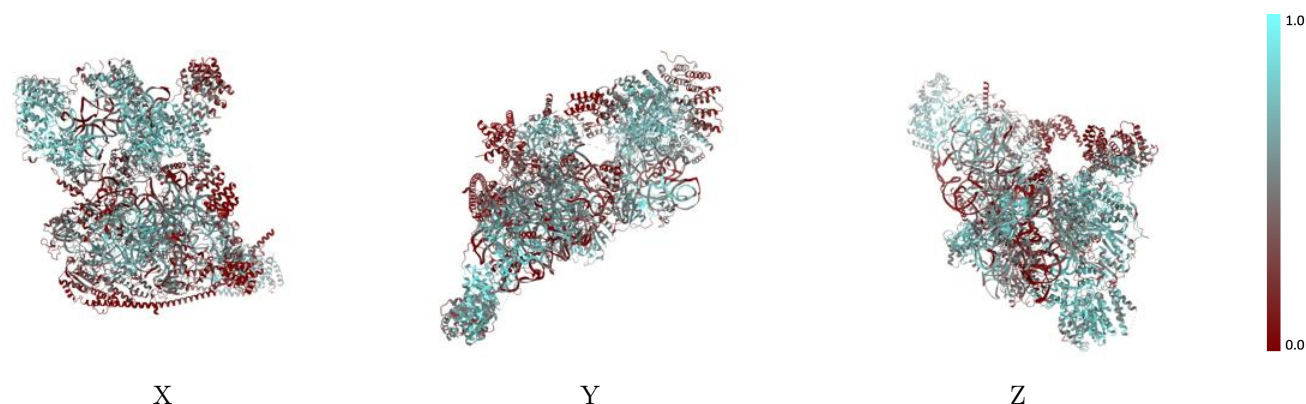
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



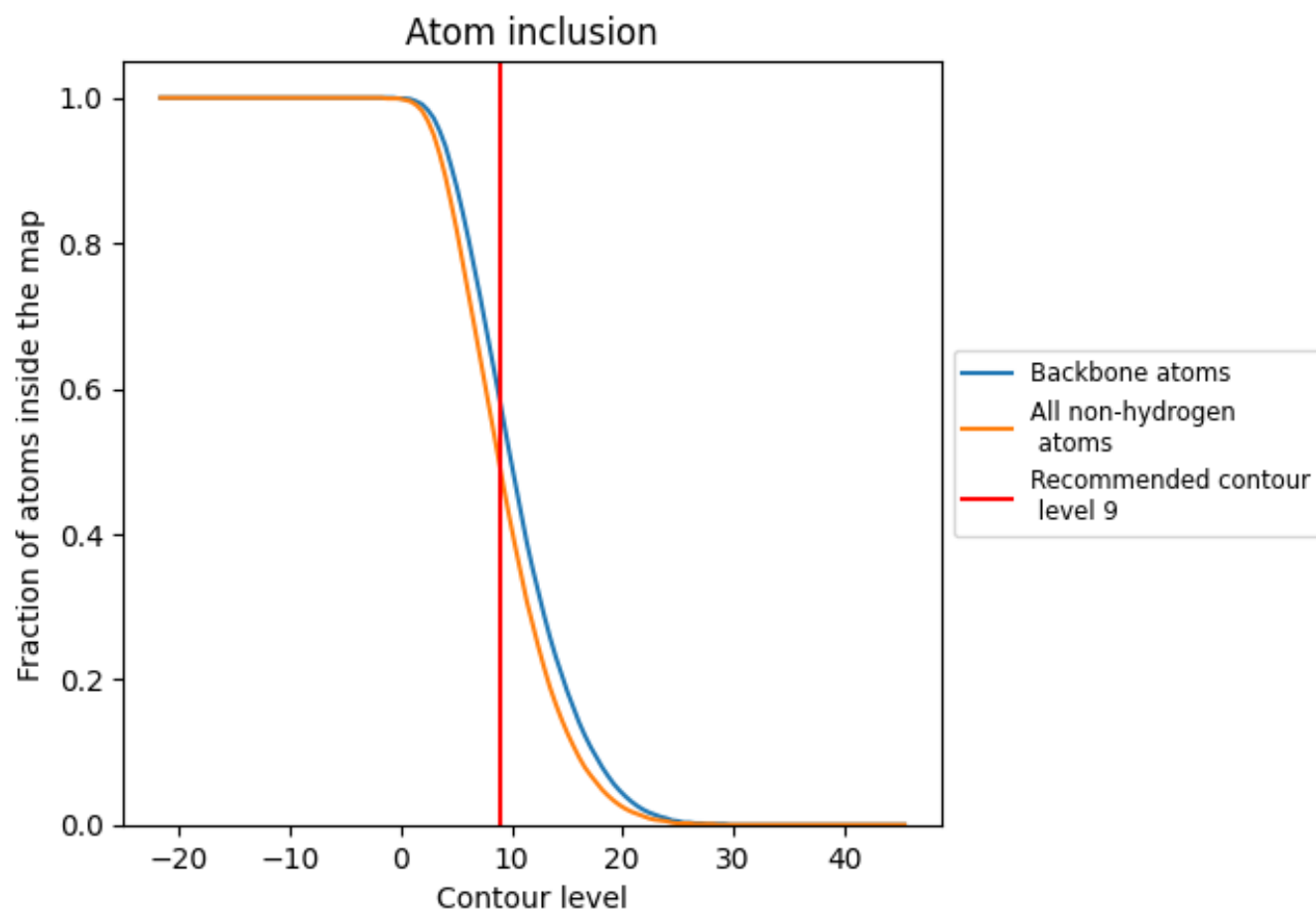
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 49% 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 (9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4880	0.5190
0	0.6250	0.5910
1	0.6460	0.5210
3	0.0240	0.4750
4	0.3840	0.4030
5	0.6370	0.5200
6	0.2450	0.4510
7	0.4860	0.3750
A	0.4910	0.4910
B	0.6740	0.6150
C	0.7020	0.5440
D	0.4380	0.6060
E	0.2490	0.5680
F	0.5910	0.5060
G	0.5750	0.5310
H	0.6470	0.5380
I	0.3980	0.5770
J	0.2380	0.5680
K	0.5030	0.4920
L	0.2600	0.5680
M	0.5750	0.6290
N	0.4240	0.6140
O	0.3750	0.6000
P	0.3640	0.5980
Q	0.4410	0.5880
R	0.2200	0.5550
S	0.4040	0.5550
T	0.3950	0.6080
U	0.2100	0.5390
V	0.6210	0.5600
W	0.5260	0.5980
X	0.7170	0.5520
Y	0.5750	0.5050
Z	0.5490	0.4930

