Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 03:21 AM EDT

PDB ID	:	8CSR / pdb_00008csr
EMDB ID	:	EMD-26968
Title	:	Human mitochondrial small subunit assembly intermediate (State C)
Authors	:	Harper, N.J.; Burnside, C.; Klinge, S.
Deposited on	:	2022-05-13
Resolution	:	2.54 Å(reported)
Based on initial models	:	2C2N, 6RW4, 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

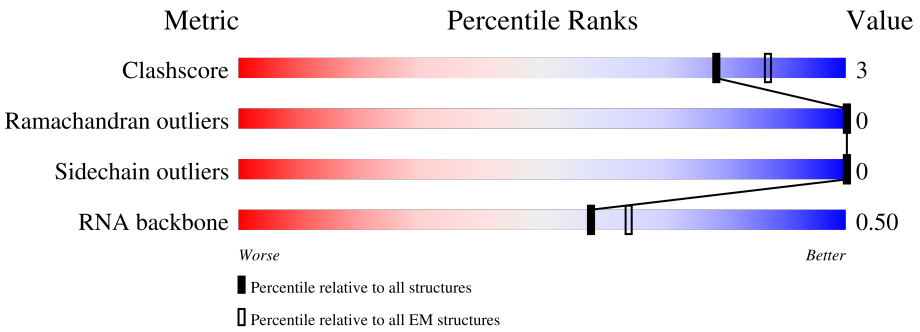
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

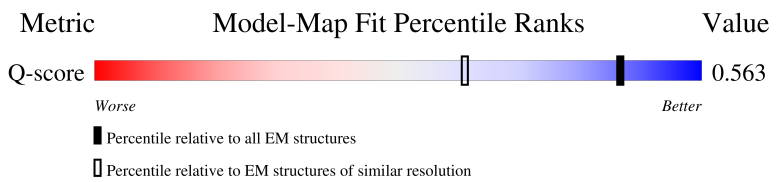
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.54 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	7403 (2.04 - 3.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	218	25% 92% 5% •
2	1	323	17% 70% 10% 20%
3	3	199	16% 21% • 77%

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Mol	Chain	Length	Quality of chain
4	4	689	37% 69% 13% 18%
5	5	346	10% 84% 8% 8%
6	6	343	12% 35% • 63%
7	7	456	5% 79% 9% 12%
8	8	390	• 77% 7% 16%
9	A	955	14% 64% 22% • 11%
10	B	296	9% 69% 6% 26%
11	C	167	10% 61% 14% 25%
12	D	430	12% 52% • 46%
13	E	125	13% 79% 7% 14%
14	F	242	8% 79% 6% 15%
15	G	396	20% 68% 5% 26%
16	H	201	15% 54% 10% 35%
17	I	194	• 69% • 29%
18	J	138	19% 76% • 22%
19	K	128	26% 21% 6% 73%
20	L	257	19% 57% 5% 37%
21	M	137	9% 82% • 16%
22	N	130	15% 82% • 16%
23	O	258	19% 71% • 26%
24	P	142	13% 62% 6% 32%
25	Q	87	9% 92% 7% •
26	R	360	33% 77% • 19%
27	S	190	25% 67% • 30%
28	T	173	20% 91% • 5%

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Mol	Chain	Length	Quality of chain
29	U	205	41% 82% • 15%
30	V	414	5% 83% • 13%
31	W	187	10% 48% 5% 48%
32	X	398	• 85% • 12%
33	Y	395	15% 25% 6% 69%
34	Z	106	45% 42% 10% 47%

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 69868 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
			Total	C	N	O	S		
1	0	211	1754	1108	333	308	5	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	45	395	254	81	60	0	0

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

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

- Molecule 5 is a protein called Dimethyladenosine transferase 1, mitochondrial.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	402	3179	2029	586	548	16	0	0

- Molecule 8 is a protein called Malonyl-CoA-acyl carrier protein transacylase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	326	2543	1617	463	446	17	0	0

- Molecule 9 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	A	853	18103	8118	3251	5881	853	0	0

- Molecule 10 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 11 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 12 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 13 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 14 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 15 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 16 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 17 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 18 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 19 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	K	35	296	182	67	47	0	0

- Molecule 20 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 21 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 22 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 23 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 24 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 25 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	86	744	460	150	126	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 26 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 27 is a protein called 28S ribosomal protein S23, mitochondrial.

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

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

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

- Molecule 29 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 30 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 31 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 32 is a protein called 28S ribosomal protein S29, mitochondrial.

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

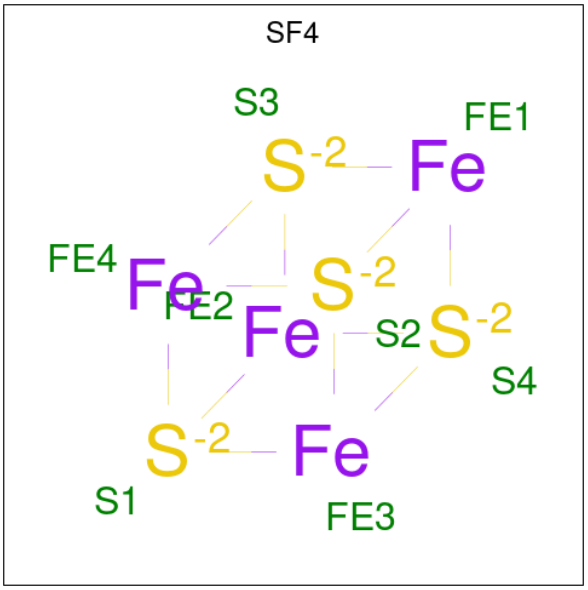
- Molecule 33 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Y	122	1032	670	171	188	3	0	0

- Molecule 34 is a protein called 28S ribosomal protein S33, mitochondrial.

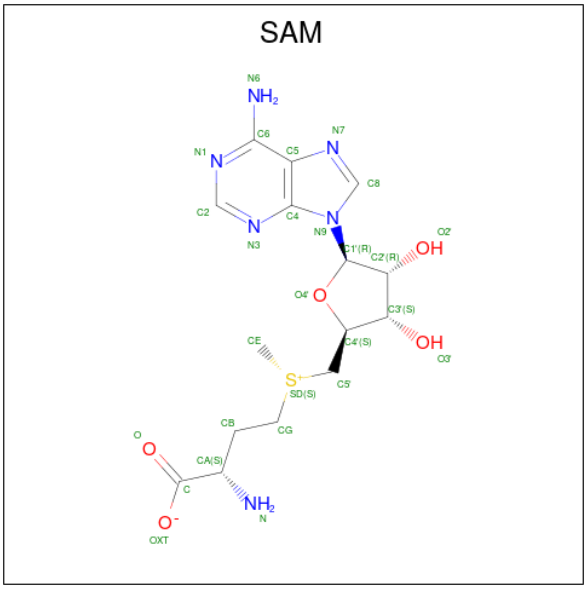
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Z	56	465	298	84	80	3	0	0

- Molecule 35 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
35	7	1	8	4	4	0

- Molecule 36 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
			Total	C	N	O	S	
36	7	1	27	15	6	5	1	0

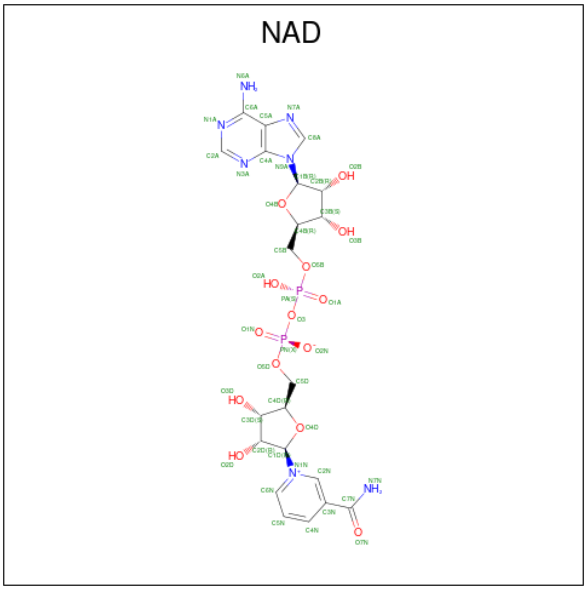
- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
38	A	29	29	29	0
38	B	1	1	1	0
38	X	1	1	1	0

- Molecule 39 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

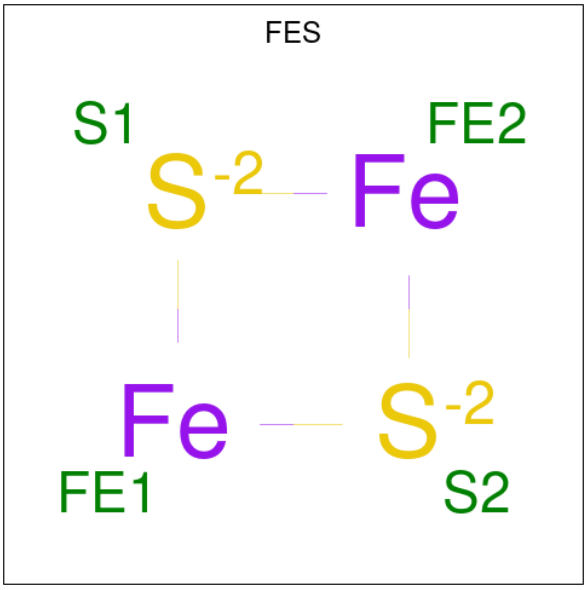


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	A	1	44	21	7	14	2	0

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

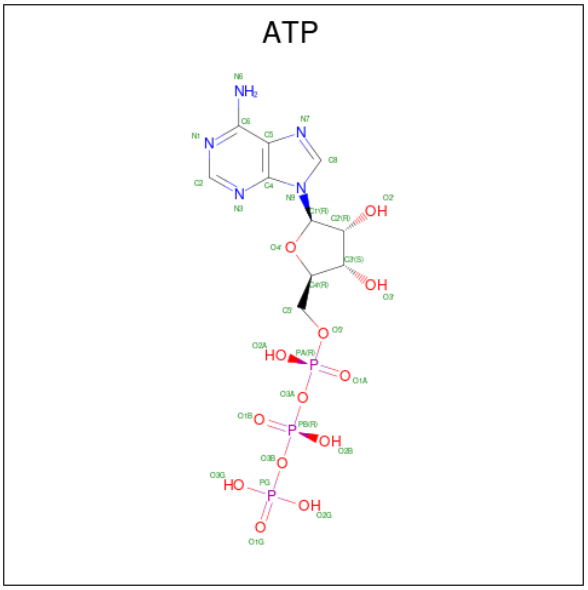
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
40	O	1	1	1	0

- Molecule 41 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



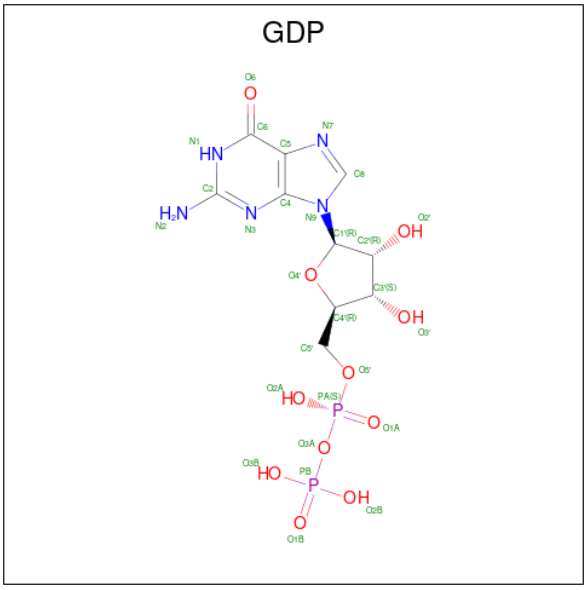
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
41	P	1	4	2	2	0
41	T	1	4	2	2	0

- Molecule 42 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 43 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 44 is water.

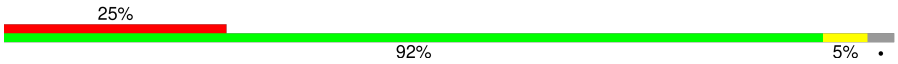
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
44	A	46	46	46	0

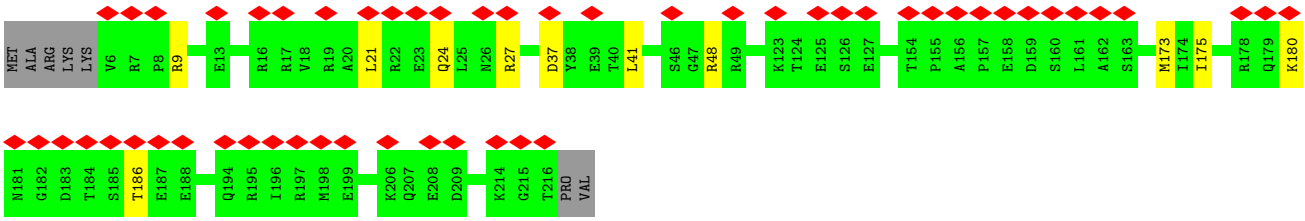
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 28S ribosomal protein S34, mitochondrial

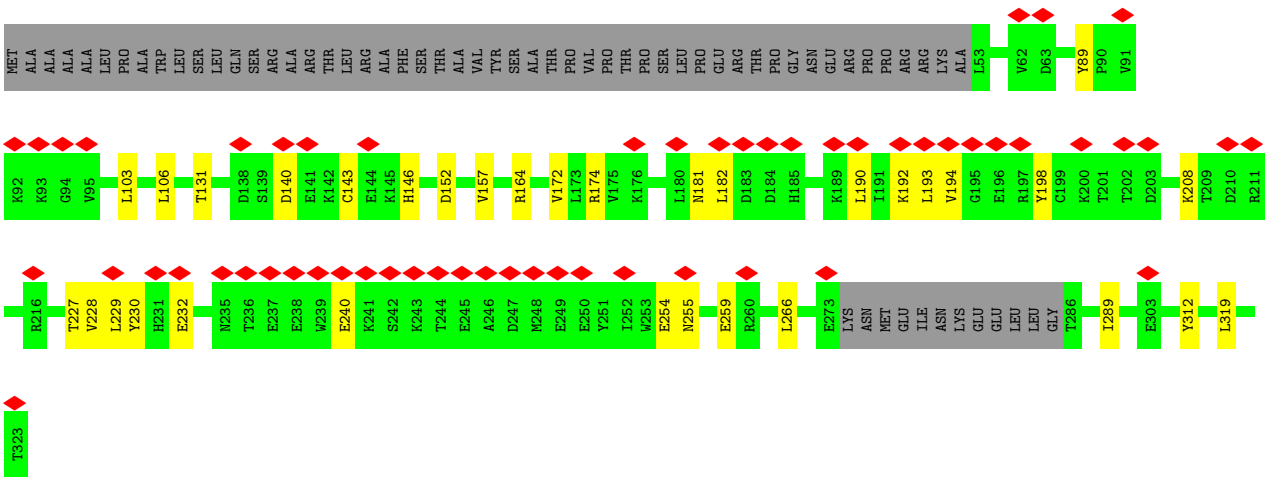
Chain 0:





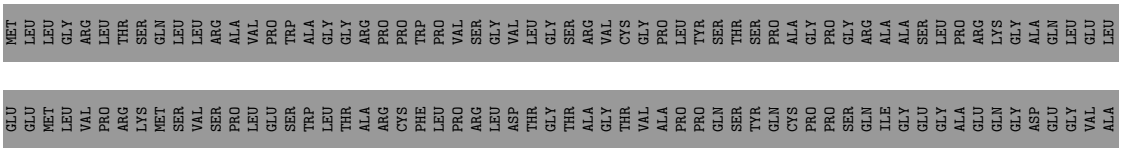
- Molecule 2: 28S ribosomal protein S35, mitochondrial

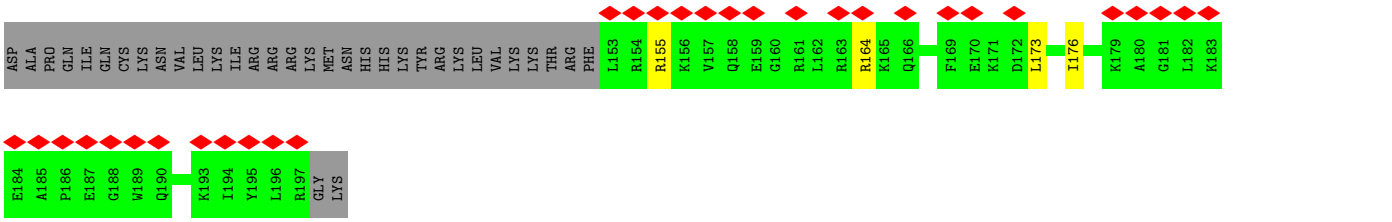
Chain 1:



- Molecule 3: Aurora kinase A-interacting protein

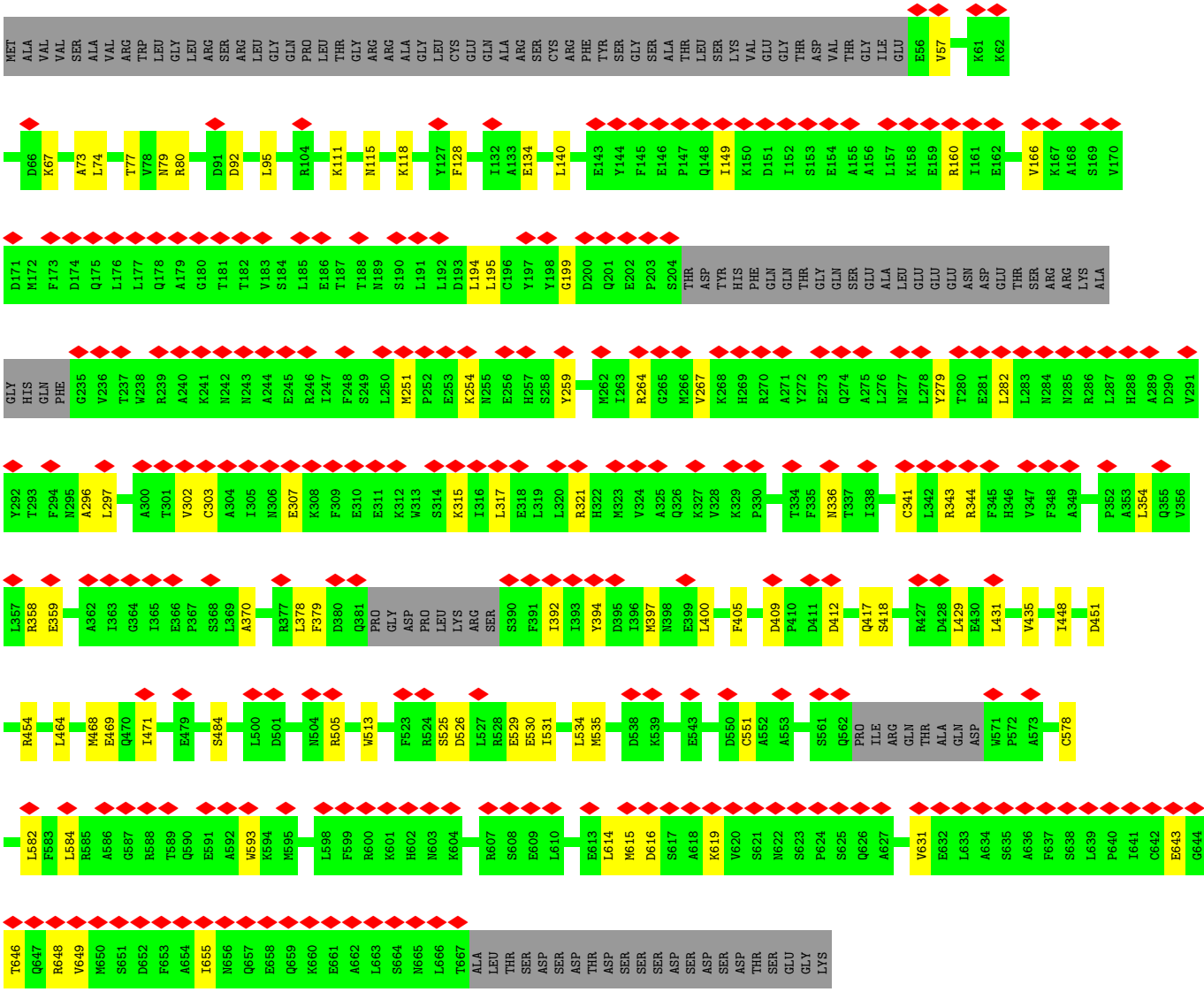
Chain 3:





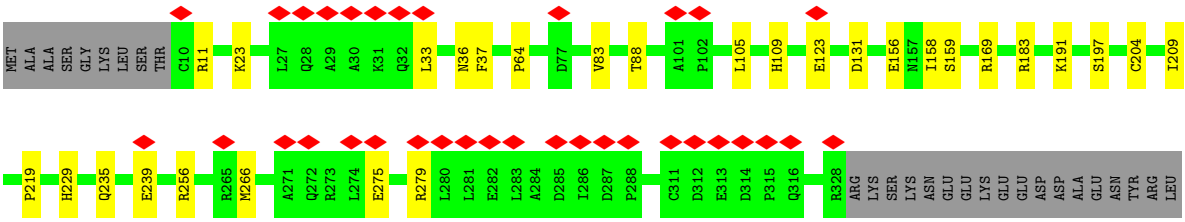
• Molecule 4: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain 4:



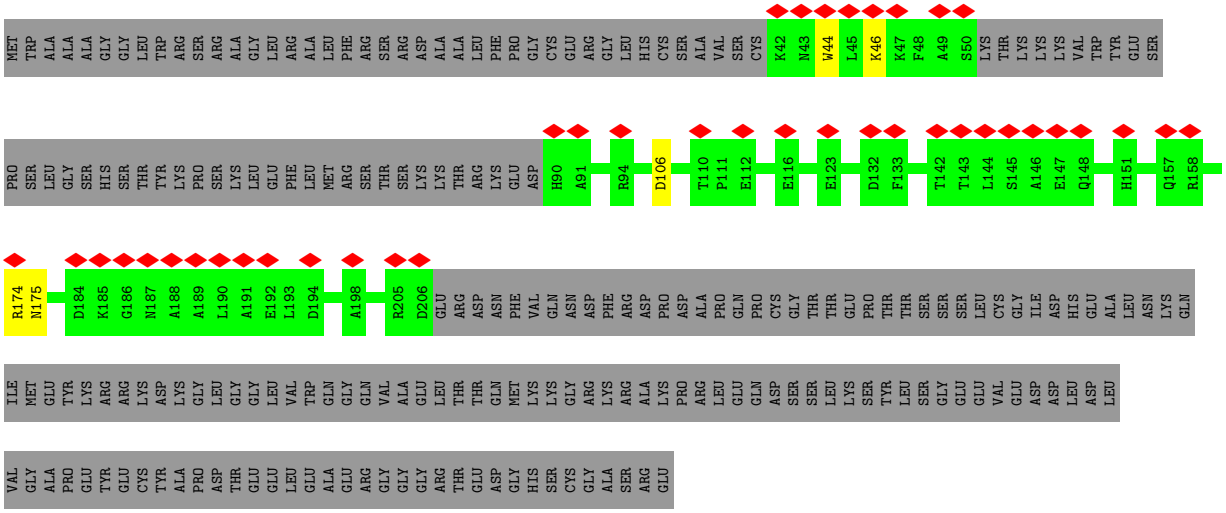
• Molecule 5: Dimethyladenosine transferase 1, mitochondrial

Chain 5:



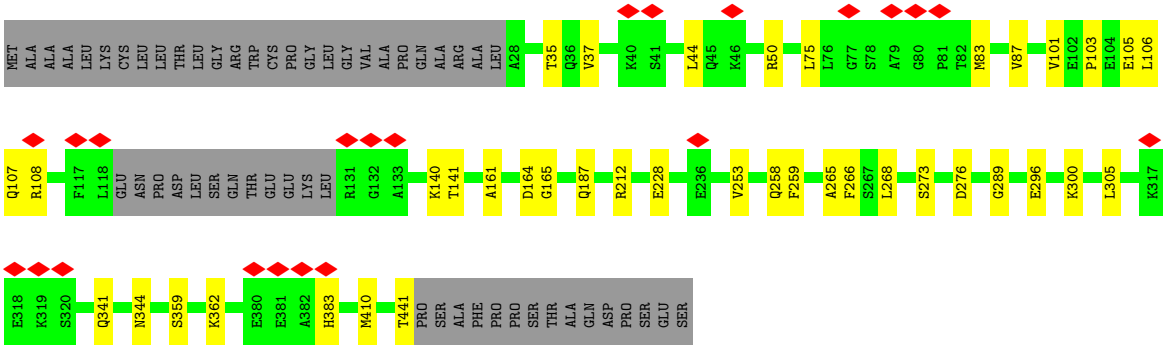
• Molecule 6: Putative ribosome-binding factor A, mitochondrial

Chain 6:



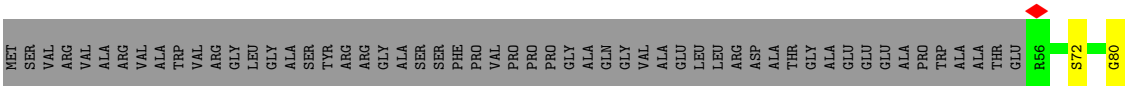
• Molecule 7: Methyltransferase-like protein 17, mitochondrial

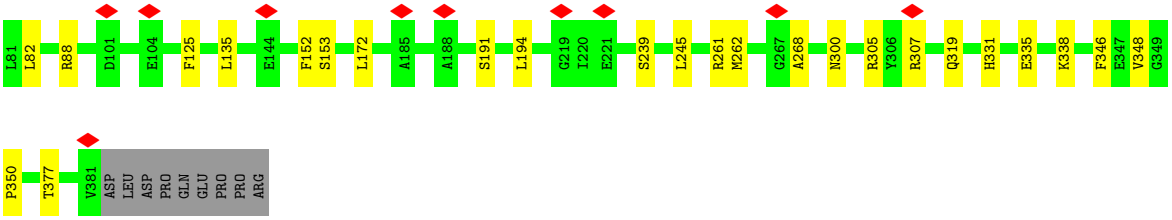
Chain 7:



• Molecule 8: Malonyl-CoA-acyl carrier protein transacylase, mitochondrial

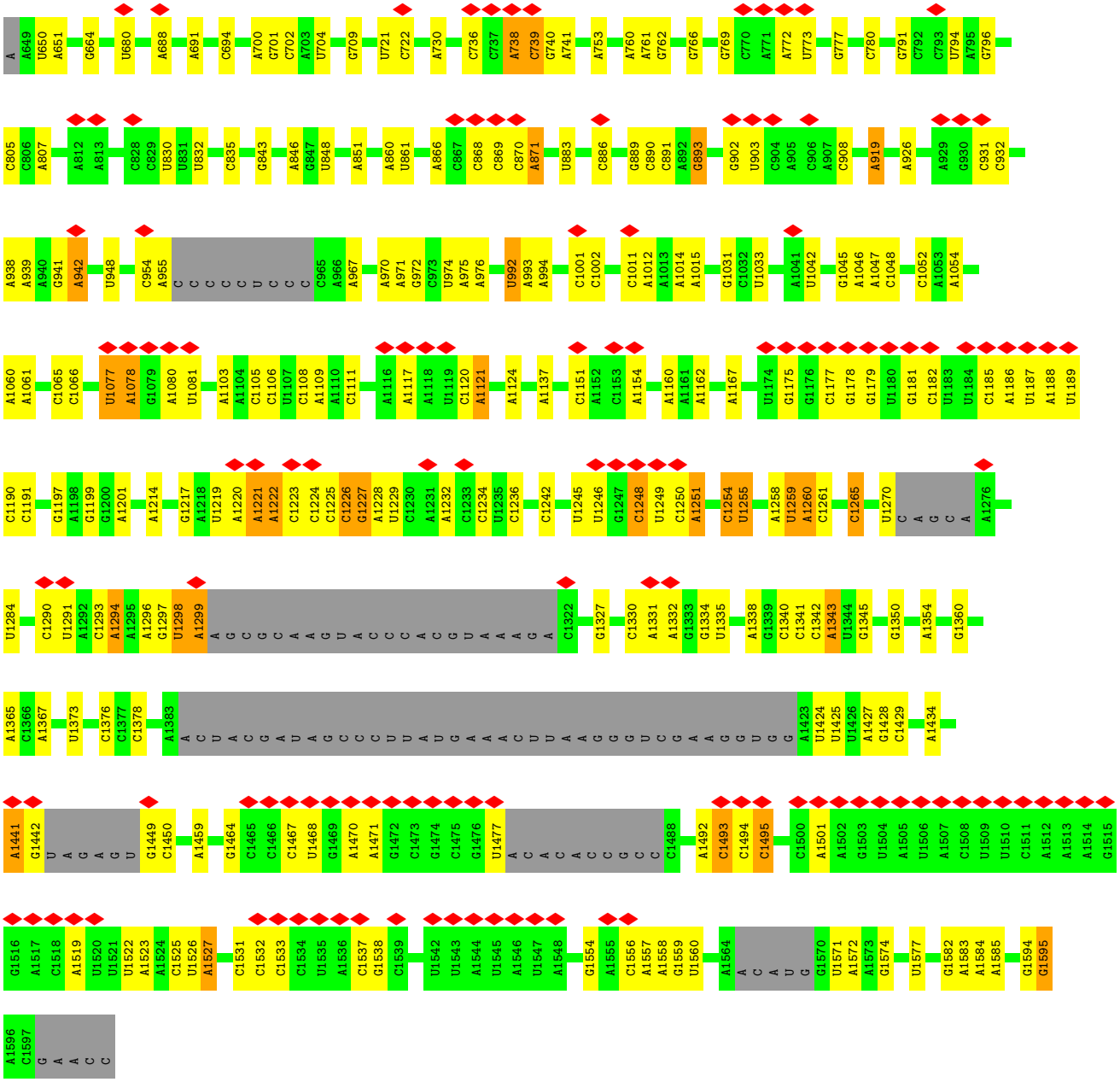
Chain 8:





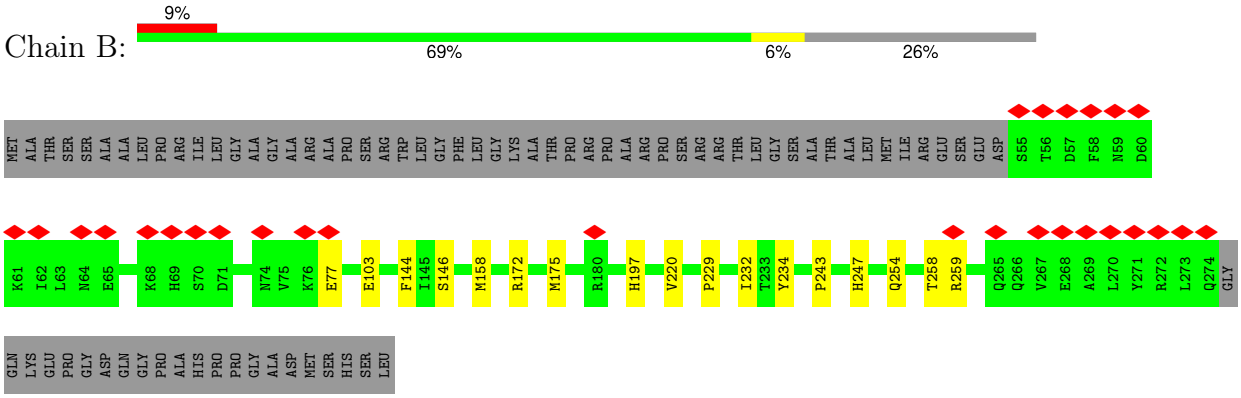
• Molecule 9: 12S mitochondrial rRNA

Chain A:



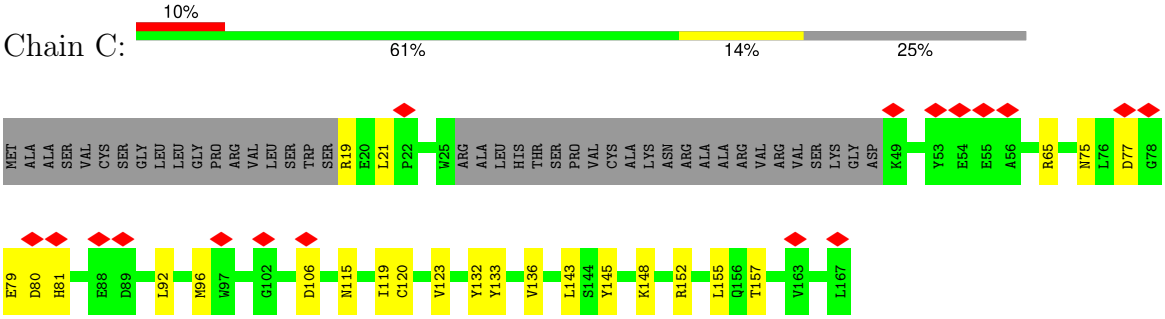
• Molecule 10: 28S ribosomal protein S2, mitochondrial

Chain B:



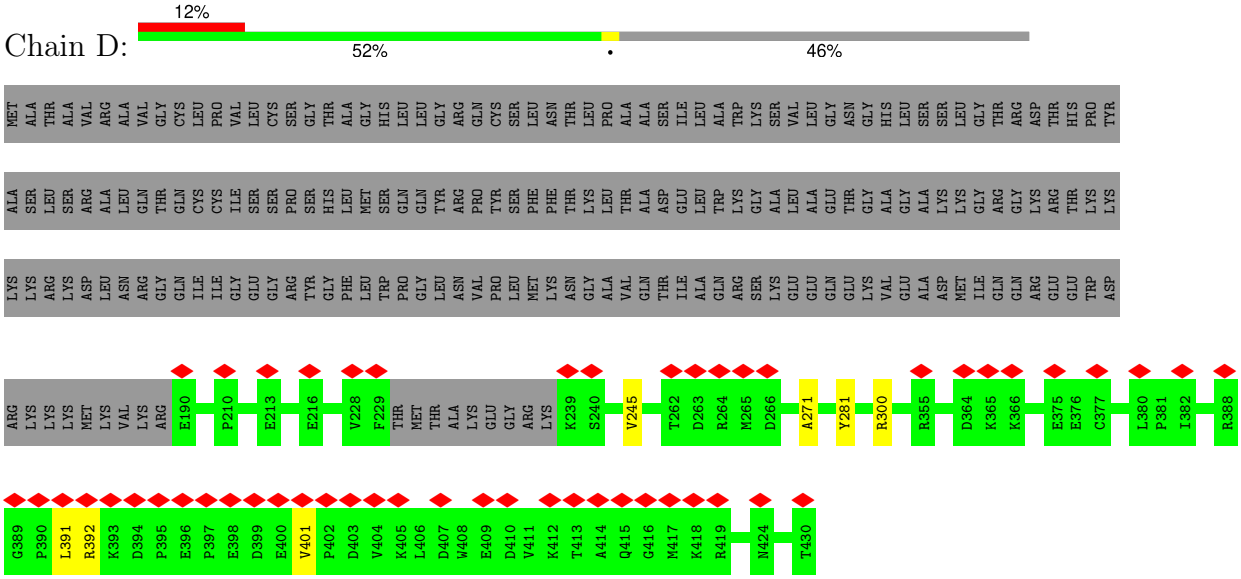
- Molecule 11: 28S ribosomal protein S24, mitochondrial

Chain C:



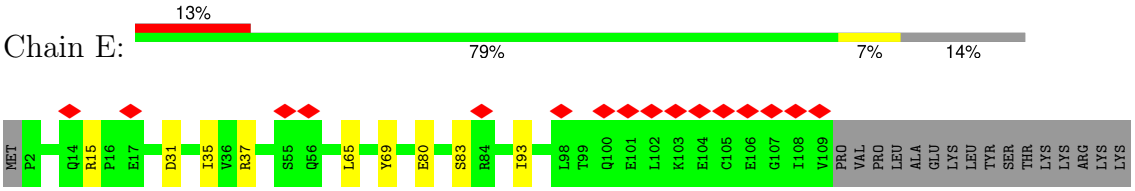
- Molecule 12: 28S ribosomal protein S5, mitochondrial

Chain D:



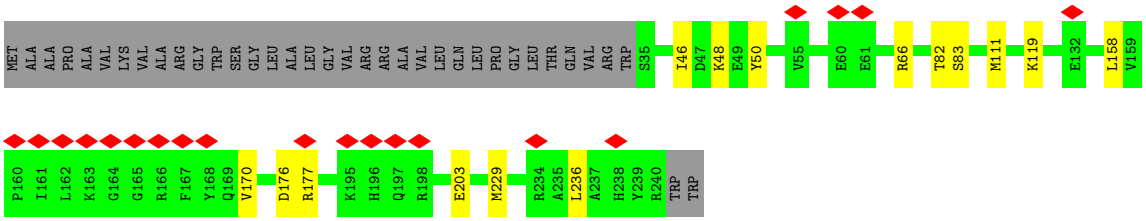
- Molecule 13: 28S ribosomal protein S6, mitochondrial

Chain E:



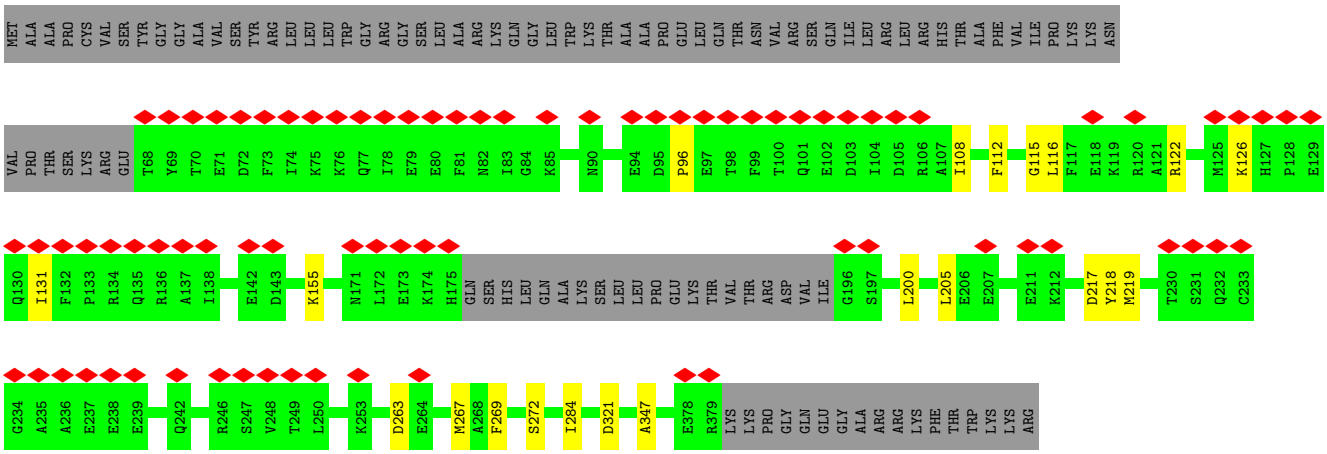
- Molecule 14: 28S ribosomal protein S7, mitochondrial

Chain F:



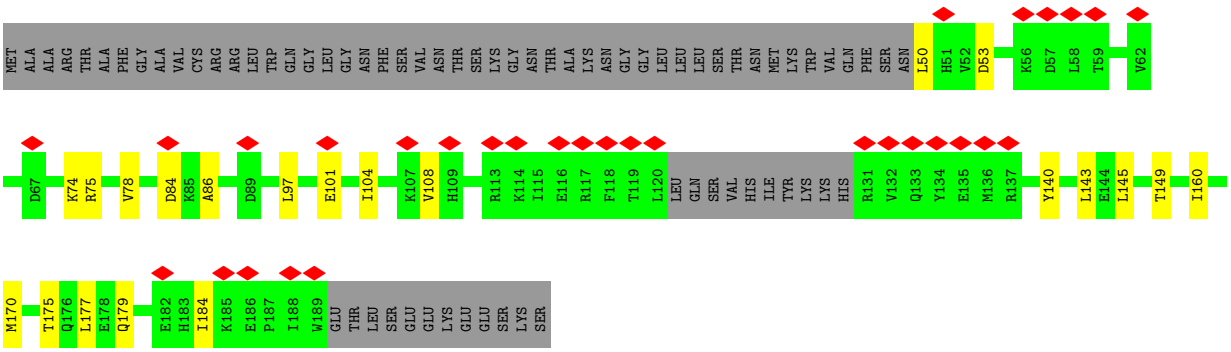
- Molecule 15: 28S ribosomal protein S9, mitochondrial

Chain G:



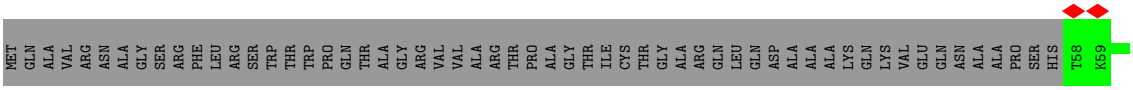
- Molecule 16: 28S ribosomal protein S10, mitochondrial

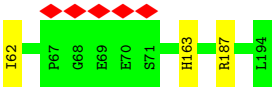
Chain H:



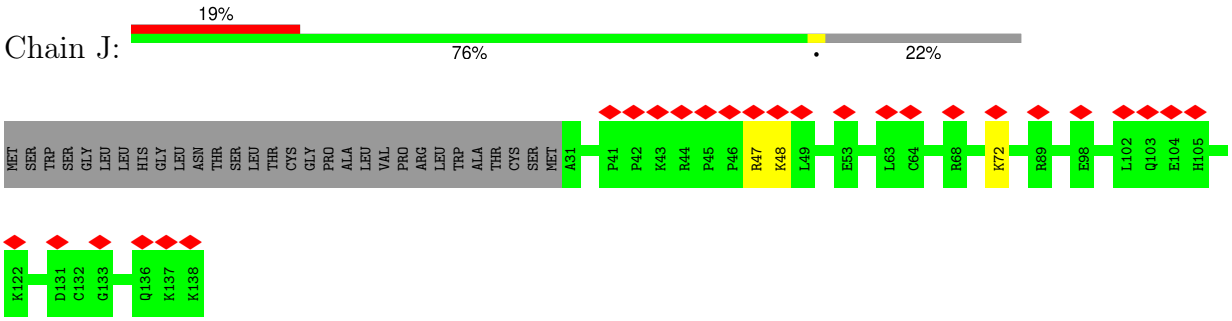
- Molecule 17: 28S ribosomal protein S11, mitochondrial

Chain I:

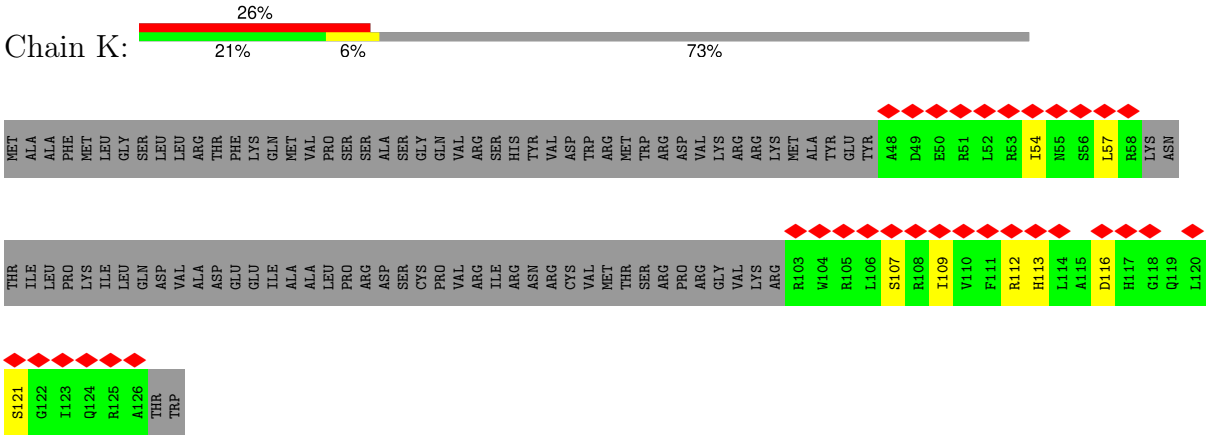




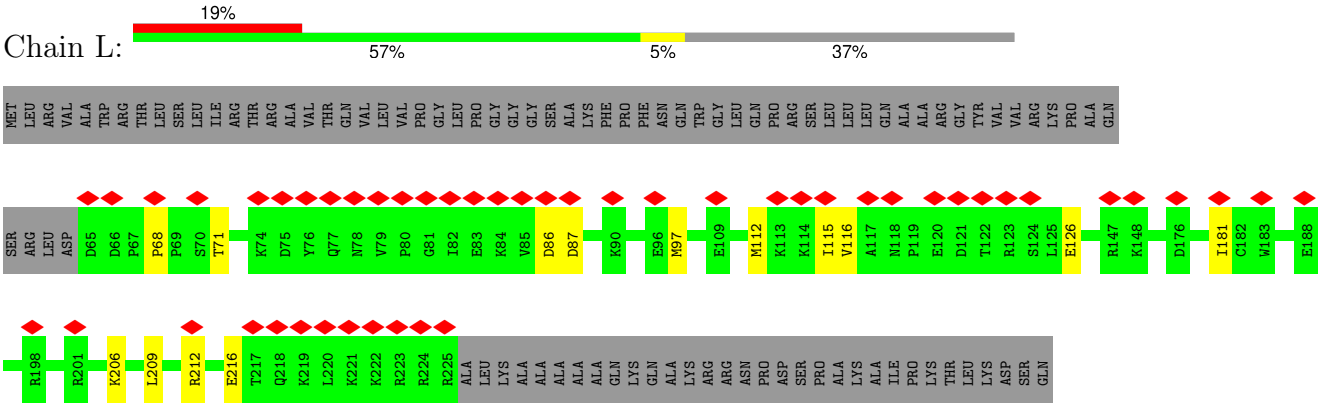
• Molecule 18: 28S ribosomal protein S12, mitochondrial



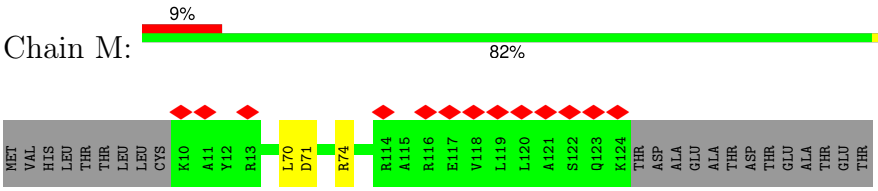
• Molecule 19: 28S ribosomal protein S14, mitochondrial



• Molecule 20: 28S ribosomal protein S15, mitochondrial

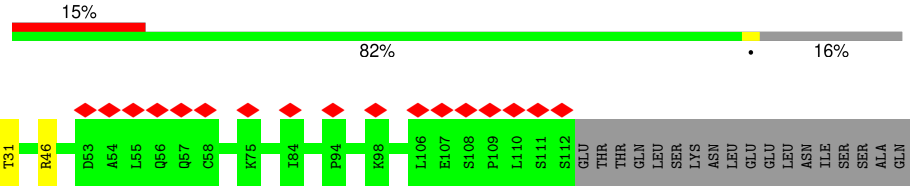


• Molecule 21: 28S ribosomal protein S16, mitochondrial



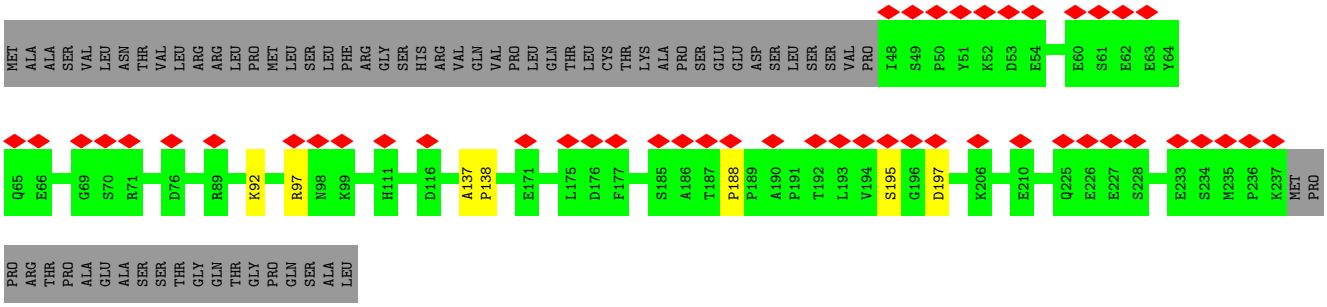
- Molecule 22: 28S ribosomal protein S17, mitochondrial

Chain N:



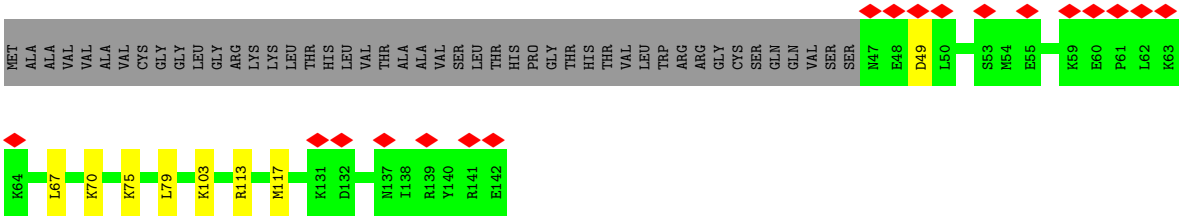
- Molecule 23: 28S ribosomal protein S18b, mitochondrial

Chain O:



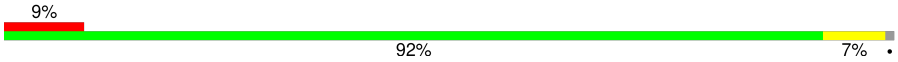
- Molecule 24: 28S ribosomal protein S18c, mitochondrial

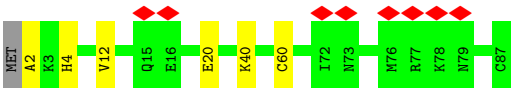
Chain P:



- Molecule 25: 28S ribosomal protein S21, mitochondrial

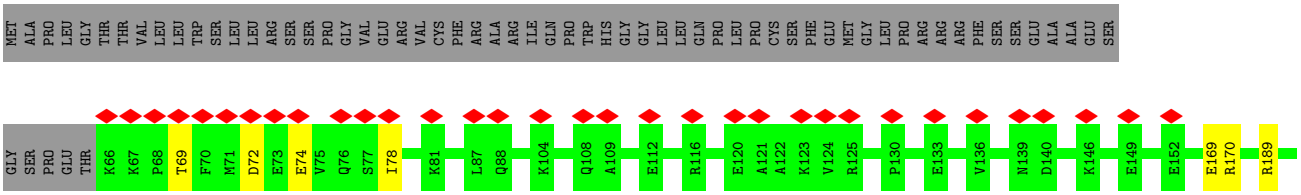
Chain Q:

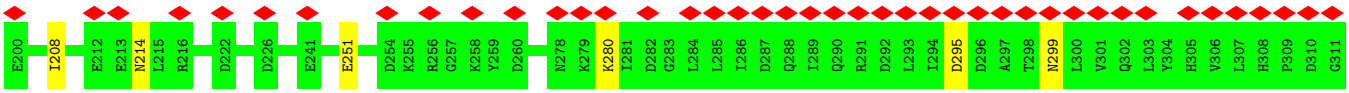


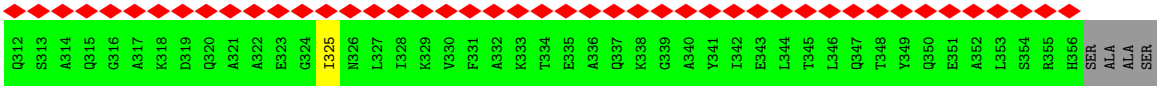


- Molecule 26: 28S ribosomal protein S22, mitochondrial

Chain R:

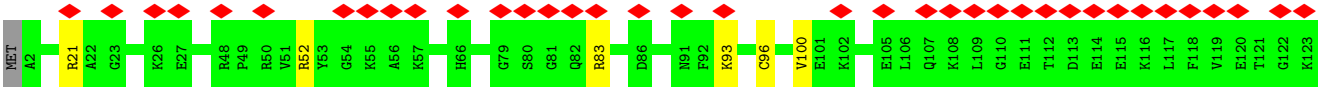


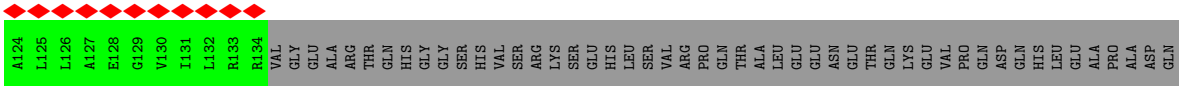


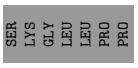


- Molecule 27: 28S ribosomal protein S23, mitochondrial

Chain S:

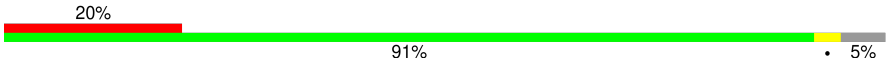


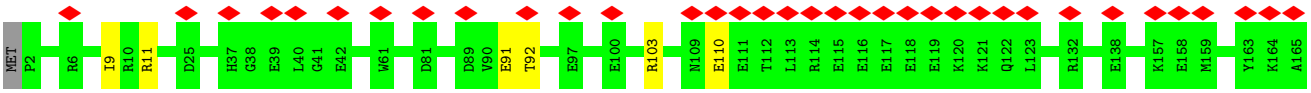




- Molecule 28: 28S ribosomal protein S25, mitochondrial

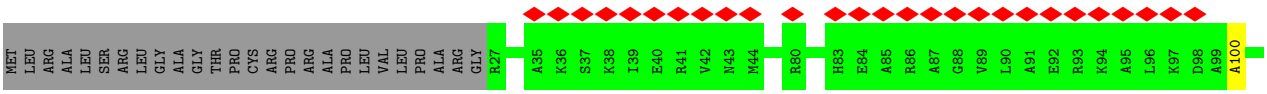
Chain T:

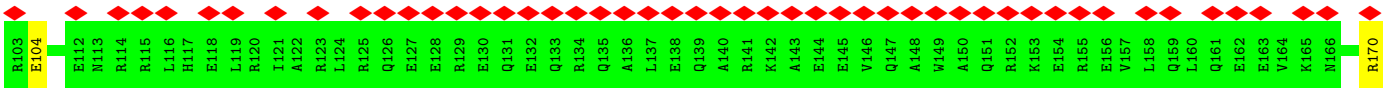


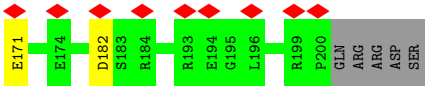


- Molecule 29: 28S ribosomal protein S26, mitochondrial

Chain U:

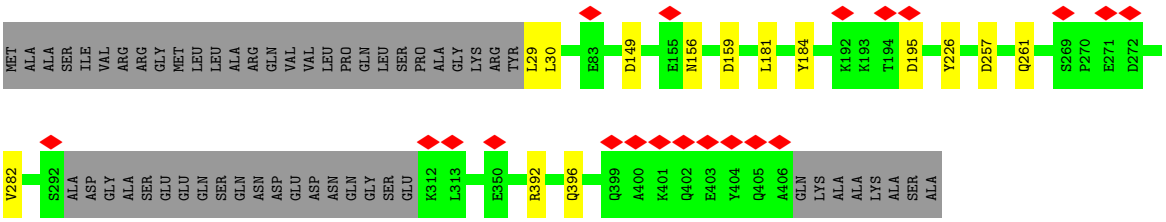




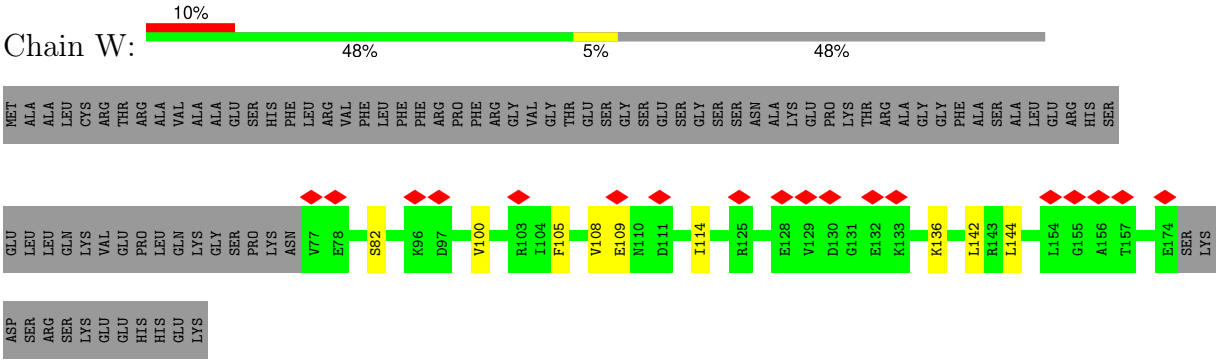


- Molecule 30: 28S ribosomal protein S27, mitochondrial

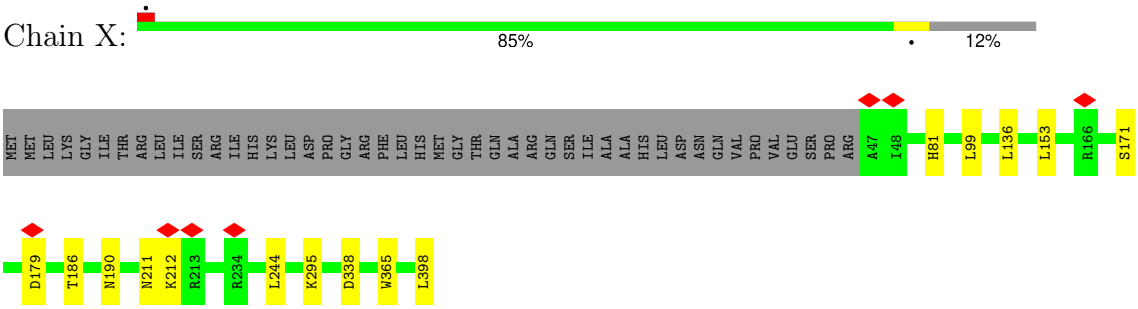
Chain V:



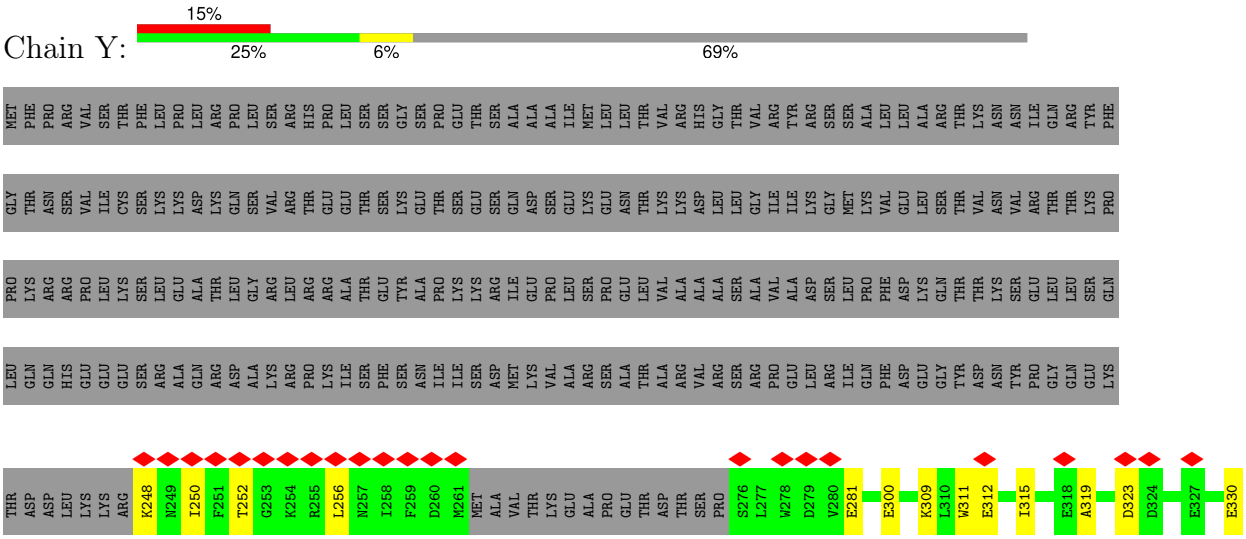
• Molecule 31: 28S ribosomal protein S28, mitochondrial

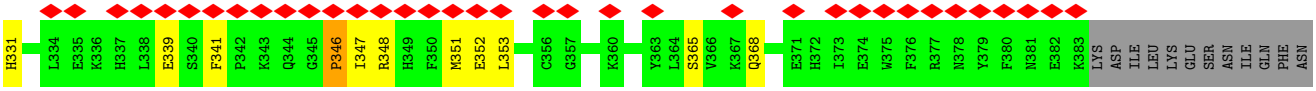


• Molecule 32: 28S ribosomal protein S29, mitochondrial



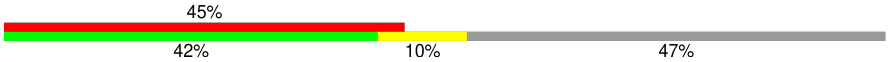
• Molecule 33: 28S ribosomal protein S31, mitochondrial

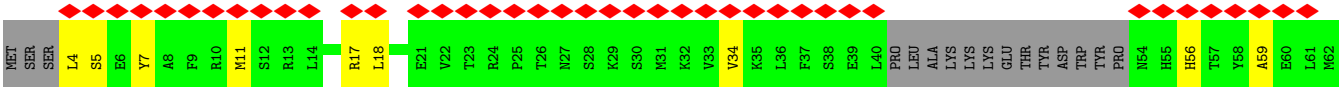


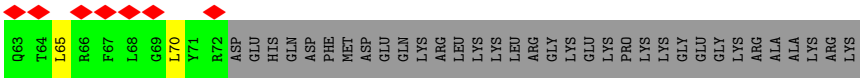


- Molecule 34: 28S ribosomal protein S33, mitochondrial

Chain Z:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	262363	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	57.818	Depositor
Minimum map value	-24.338	Depositor
Average map value	0.034	Depositor
Map value standard deviation	1.307	Depositor
Recommended contour level	8.5	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: AYA, MG, SAM, GDP, K, FES, SF4, NAD, ATP, ZN

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	0.15	0/1800	0.33	0/2440
2	1	0.19	0/2143	0.39	0/2902
3	3	0.15	0/402	0.35	0/533
4	4	0.17	0/4686	0.39	0/6335
5	5	0.16	0/2624	0.34	0/3552
6	6	0.13	0/1012	0.31	0/1371
7	7	0.19	0/3269	0.34	0/4436
8	8	0.18	0/2603	0.39	0/3520
9	A	0.15	0/20242	0.30	0/31497
10	B	0.14	0/1832	0.33	0/2480
11	C	0.19	0/1074	0.40	0/1456
12	D	0.14	0/1877	0.33	0/2523
13	E	0.14	0/872	0.35	0/1177
14	F	0.17	0/1734	0.36	0/2327
15	G	0.22	1/2446 (0.0%)	0.42	3/3283 (0.1%)
16	H	0.18	0/1086	0.43	0/1473
17	I	0.17	0/1039	0.35	0/1400
18	J	0.15	0/855	0.33	0/1148
19	K	0.15	0/299	0.32	0/397
20	L	0.15	0/1387	0.32	0/1853
21	M	0.14	0/934	0.31	0/1255
22	N	0.13	0/877	0.31	0/1187
23	O	0.13	0/1624	0.30	0/2210
24	P	0.15	0/791	0.31	0/1062
25	Q	0.15	0/748	0.33	0/994
26	R	0.13	0/2429	0.30	0/3280
27	S	0.15	0/1127	0.33	0/1518
28	T	0.17	0/1375	0.34	0/1847
29	U	0.15	0/1490	0.32	0/1999
30	V	0.19	0/3007	0.36	0/4062
31	W	0.13	0/787	0.29	0/1060
32	X	0.19	0/2921	0.35	0/3954

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Y	0.42	2/1062 (0.2%)	0.63	3/1430 (0.2%)
34	Z	0.17	0/473	0.45	0/631
All	All	0.17	3/72927 (0.0%)	0.34	6/102592 (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
18	J	0	1
30	V	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Y	346	PRO	CG-CD	-10.02	1.16	1.50
15	G	96	PRO	CG-CD	-5.78	1.31	1.50
33	Y	346	PRO	N-CD	5.34	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Y	346	PRO	N-CD-CG	-10.75	87.07	103.20
15	G	96	PRO	N-CD-CG	-10.28	87.79	103.20
33	Y	346	PRO	CA-N-CD	-9.89	98.15	112.00
15	G	96	PRO	CA-CB-CG	-7.92	89.45	104.50
33	Y	346	PRO	CA-CB-CG	-6.34	92.46	104.50
15	G	96	PRO	N-CA-CB	-5.43	97.52	103.39

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	J	72	LYS	Peptide
30	V	195	ASP	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	10	0
2	1	2098	0	2115	32	0
3	3	395	0	432	5	0
4	4	4585	0	4595	66	0
5	5	2568	0	2655	17	0
6	6	994	0	1004	5	0
7	7	3179	0	3195	27	0
8	8	2543	0	2561	19	0
9	A	18103	0	9198	56	0
10	B	1789	0	1781	9	0
11	C	1042	0	1033	25	0
12	D	1838	0	1858	5	0
13	E	858	0	871	8	0
14	F	1696	0	1749	11	0
15	G	2395	0	2364	12	0
16	H	1064	0	1089	21	0
17	I	1019	0	1059	3	0
18	J	839	0	887	2	0
19	K	296	0	304	6	0
20	L	1363	0	1442	13	0
21	M	913	0	943	2	0
22	N	859	0	922	1	0
23	O	1570	0	1533	5	0
24	P	774	0	801	7	0
25	Q	744	0	758	5	0
26	R	2382	0	2405	8	0
27	S	1100	0	1103	4	0
28	T	1344	0	1359	4	0
29	U	1468	0	1478	4	0
30	V	2946	0	2942	10	0
31	W	775	0	791	5	0
32	X	2849	0	2843	11	0
33	Y	1032	0	983	20	0
34	Z	465	0	475	9	0
35	7	8	0	0	0	0
36	7	27	0	22	2	0
37	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	29	0	0	0	0
38	B	1	0	0	0	0
38	X	1	0	0	0	0
39	A	44	0	26	0	0
40	O	1	0	0	0	0
41	P	4	0	0	0	0
41	T	4	0	0	0	0
42	X	31	0	12	0	0
43	X	28	0	12	1	0
44	A	46	0	0	1	0
All	All	69868	0	61354	358	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 (358) 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)
6:6:106:ASP:OD2	25:Q:40:LYS:NZ	2.10	0.84
11:C:80:ASP:OD1	11:C:81:HIS:N	2.14	0.80
4:4:379:PHE:CD2	4:4:392:ILE:HD13	2.18	0.79
6:6:46:LYS:NZ	9:A:1124:A:OP1	2.11	0.79
5:5:183:ARG:O	5:5:197:SER:OG	2.00	0.78
6:6:174:ARG:NH1	9:A:1571:U:O2'	2.15	0.78
3:3:155:ARG:NH1	9:A:1154:A:OP2	2.17	0.77
14:F:48:LYS:NZ	15:G:321:ASP:OD2	2.18	0.76
4:4:429:LEU:HD21	4:4:469:GLU:OE2	1.86	0.75
11:C:75:ASN:ND2	19:K:121:SER:O	2.19	0.75
9:A:762:G:OP1	20:L:206:LYS:NZ	2.19	0.74
7:7:105:GLU:OE1	7:7:108:ARG:NH2	2.20	0.74
2:1:192:LYS:NZ	34:Z:11:MET:SD	2.60	0.74
2:1:312:TYR:OH	32:X:338:ASP:OD1	2.04	0.74
4:4:643:GLU:O	4:4:646:THR:OG1	2.06	0.73
16:H:104:ILE:HG21	16:H:145:LEU:HD23	1.68	0.73
5:5:23:LYS:NZ	7:7:228:GLU:OE1	2.21	0.73
9:A:1559:G:N2	9:A:1559:G:OP2	2.18	0.73
7:7:140:LYS:NZ	9:A:1270:U:O2	2.21	0.72
4:4:80:ARG:NH1	4:4:484:SER:OG	2.23	0.72
4:4:95:LEU:O	11:C:133:TYR:OH	2.07	0.72
5:5:11:ARG:NH1	7:7:258:GLN:O	2.23	0.71
7:7:273:SER:OG	7:7:276:ASP:OD1	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:267:VAL:HG11	4:4:296:ALA:HB1	1.73	0.71
15:G:155:LYS:NZ	15:G:217:ASP:OD2	2.24	0.71
9:A:942:A:N6	9:A:1047:A:OP2	2.24	0.70
9:A:1226:C:O2'	9:A:1227:G:OP1	2.08	0.70
9:A:1248:C:HO2'	9:A:1251:A:HO2'	1.30	0.70
4:4:67:LYS:NZ	33:Y:312:GLU:OE2	2.18	0.69
9:A:919:A:OP1	23:O:92:LYS:NZ	2.23	0.69
14:F:119:LYS:NZ	32:X:365:TRP:O	2.20	0.69
6:6:44:TRP:CD1	25:Q:60:CYS:HG	2.12	0.68
20:L:86:ASP:OD1	20:L:87:ASP:N	2.26	0.68
20:L:115:ILE:HG21	20:L:181:ILE:HD13	1.75	0.68
32:X:171:SER:OG	32:X:179:ASP:OD1	2.09	0.68
14:F:50:TYR:O	14:F:66:ARG:NH2	2.27	0.68
4:4:530:GLU:O	4:4:534:LEU:HD13	1.95	0.68
8:8:152:PHE:O	8:8:300:ASN:ND2	2.26	0.67
10:B:172:ARG:HB2	10:B:175:MET:HE3	1.76	0.67
13:E:31:ASP:OD1	29:U:170:ARG:NH2	2.27	0.67
4:4:451:ASP:OD1	4:4:454:ARG:NH2	2.27	0.66
11:C:77:ASP:OD2	16:H:140:TYR:OH	2.12	0.66
32:X:295:LYS:NZ	43:X:503:GDP:O3A	2.27	0.66
4:4:471:ILE:HG21	4:4:505:ARG:HD3	1.77	0.66
15:G:115:GLY:N	16:H:84:ASP:OD1	2.28	0.65
28:T:103:ARG:NH2	28:T:110:GLU:OE2	2.30	0.65
4:4:303:CYS:SG	4:4:344:ARG:NH1	2.70	0.65
4:4:111:LYS:O	4:4:115:ASN:ND2	2.30	0.65
9:A:694:C:OP2	44:A:1801:HOH:O	2.14	0.65
15:G:272:SER:OG	15:G:347:ALA:O	2.15	0.65
9:A:1046:A:O2'	9:A:1048:C:OP2	2.13	0.65
13:E:80:GLU:O	13:E:83:SER:OG	2.14	0.65
1:0:48:ARG:NH2	9:A:701:G:O6	2.29	0.64
30:V:226:TYR:HE1	30:V:282:VAL:HG21	1.62	0.64
21:M:71:ASP:OD1	21:M:74:ARG:NH2	2.30	0.64
9:A:871:A:OP2	23:O:97:ARG:NH1	2.31	0.64
9:A:1265:C:OP1	19:K:107:SER:OG	2.11	0.64
4:4:92:ASP:OD1	11:C:157:THR:OG1	2.16	0.63
32:X:153:LEU:HD11	32:X:244:LEU:CD2	2.29	0.62
5:5:275:GLU:OE2	5:5:279:ARG:NH1	2.32	0.62
8:8:335:GLU:O	9:A:1227:G:N2	2.31	0.62
5:5:36:ASN:ND2	5:5:219:PRO:O	2.32	0.62
4:4:74:LEU:O	4:4:77:THR:OG1	2.14	0.62
4:4:302:VAL:HG21	4:4:341:CYS:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:266:LEU:HD11	2:1:289:ILE:HD11	1.80	0.62
7:7:300:LYS:NZ	7:7:344:ASN:O	2.30	0.62
7:7:37:VAL:HG11	7:7:44:LEU:HD11	1.81	0.62
3:3:164:ARG:NH2	9:A:1501:A:OP1	2.33	0.62
1:0:21:LEU:HD12	1:0:24:GLN:HE21	1.65	0.61
2:1:230:TYR:CD2	16:H:184:ILE:HG23	2.36	0.61
9:A:1121:A:OP1	12:D:300:ARG:NH2	2.32	0.61
2:1:143:CYS:SG	16:H:74:LYS:NZ	2.65	0.60
9:A:1259:U:O2'	9:A:1260:A:OP1	2.19	0.60
1:0:9:ARG:NE	9:A:805:C:O2	2.34	0.60
5:5:235:GLN:NE2	5:5:239:GLU:OE2	2.34	0.60
9:A:702:C:OP1	9:A:848:U:O2'	2.19	0.60
28:T:91:GLU:O	28:T:92:THR:OG1	2.18	0.60
2:1:227:THR:HA	16:H:184:ILE:HD11	1.83	0.60
4:4:140:LEU:HD13	11:C:148:LYS:HA	1.84	0.60
32:X:99:LEU:HD21	32:X:136:LEU:HD22	1.82	0.60
4:4:616:ASP:OD1	4:4:648:ARG:NH2	2.31	0.60
23:O:195:SER:OG	23:O:197:ASP:OD1	2.19	0.60
4:4:400:LEU:HD22	4:4:405:PHE:CZ	2.37	0.60
24:P:113:ARG:HG3	24:P:117:MET:HE3	1.83	0.59
32:X:211:ASN:OD1	32:X:212:LYS:N	2.36	0.59
33:Y:368:GLN:OE1	33:Y:368:GLN:N	2.35	0.59
30:V:156:ASN:ND2	30:V:159:ASP:OD2	2.35	0.59
8:8:194:LEU:CB	8:8:245:LEU:HD12	2.33	0.59
12:D:281:TYR:OH	27:S:21:ARG:NH1	2.36	0.59
33:Y:365:SER:OG	33:Y:368:GLN:OE1	2.21	0.58
4:4:343:ARG:HA	4:4:378:LEU:HD13	1.85	0.58
31:W:108:VAL:HG12	31:W:109:GLU:OE1	2.04	0.58
11:C:96:MET:HE3	11:C:143:LEU:HD11	1.86	0.58
9:A:1221:A:O2'	9:A:1222:A:OP2	2.20	0.58
1:0:24:GLN:O	1:0:27:ARG:NH1	2.37	0.58
2:1:232:GLU:OE1	34:Z:17:ARG:NH2	2.36	0.58
13:E:65:LEU:HD11	24:P:75:LYS:CD	2.34	0.58
11:C:136:VAL:CG2	11:C:155:LEU:HD11	2.35	0.57
4:4:379:PHE:HD2	4:4:392:ILE:HD13	1.67	0.57
20:L:126:GLU:HB2	20:L:181:ILE:HD11	1.87	0.57
2:1:146:HIS:O	16:H:179:GLN:NE2	2.35	0.57
9:A:738:A:O2'	9:A:739:C:O2	2.21	0.57
11:C:92:LEU:HD11	11:C:119:ILE:HD11	1.86	0.57
30:V:226:TYR:CE1	30:V:282:VAL:HG21	2.40	0.56
30:V:392:ARG:O	30:V:396:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y:353:LEU:HD21	34:Z:34:VAL:HG23	1.87	0.56
7:7:101:VAL:HB	11:C:21:LEU:HD21	1.88	0.56
33:Y:281:GLU:N	33:Y:281:GLU:OE1	2.39	0.56
7:7:50:ARG:NH1	9:A:1214:A:OP1	2.39	0.56
11:C:115:ASN:HD21	33:Y:311:TRP:CD1	2.24	0.56
2:1:143:CYS:SG	16:H:177:LEU:HD11	2.46	0.56
8:8:305:ARG:O	8:8:307:ARG:NH1	2.38	0.56
9:A:1106:C:O2'	9:A:1108:C:OP2	2.17	0.56
14:F:176:ASP:OD1	14:F:177:ARG:N	2.39	0.56
9:A:1523:A:O2'	9:A:1527:A:N1	2.36	0.55
11:C:132:TYR:O	11:C:136:VAL:HG23	2.06	0.55
16:H:84:ASP:OD2	16:H:86:ALA:N	2.40	0.55
9:A:700:A:N1	9:A:709:G:O2'	2.40	0.55
16:H:78:VAL:HG11	16:H:170:MET:HE2	1.89	0.54
32:X:153:LEU:HD11	32:X:244:LEU:HD23	1.89	0.54
16:H:50:LEU:HD22	16:H:53:ASP:O	2.07	0.54
30:V:30:LEU:HD12	30:V:149:ASP:HB2	1.88	0.54
8:8:194:LEU:HB3	8:8:245:LEU:HD12	1.88	0.54
33:Y:323:ASP:OD2	33:Y:331:HIS:NE2	2.40	0.54
13:E:15:ARG:NH2	29:U:182:ASP:OD1	2.41	0.54
1:0:180:LYS:NZ	26:R:169:GLU:OE1	2.41	0.54
7:7:75:LEU:HD22	7:7:83:MET:HE2	1.90	0.54
7:7:259:PHE:O	7:7:289:GLY:N	2.39	0.54
33:Y:330:GLU:OE1	33:Y:330:GLU:N	2.38	0.54
2:1:103:LEU:HD22	11:C:106:ASP:OD1	2.07	0.54
4:4:400:LEU:HD22	4:4:405:PHE:HZ	1.73	0.54
9:A:1495:C:H42	9:A:1554:G:H1	1.55	0.54
10:B:103:GLU:OE2	27:S:52:ARG:NH2	2.40	0.54
10:B:144:PHE:CE1	10:B:158:MET:HE1	2.43	0.54
33:Y:248:LYS:NZ	33:Y:252:THR:O	2.41	0.54
4:4:336:ASN:ND2	4:4:409:ASP:OD2	2.39	0.53
26:R:251:GLU:OE2	26:R:280:LYS:NZ	2.38	0.53
4:4:73:ALA:O	4:4:77:THR:HG23	2.09	0.53
26:R:74:GLU:OE2	26:R:78:ILE:HD11	2.09	0.53
2:1:106:LEU:HD21	11:C:120:CYS:HB3	1.91	0.53
2:1:152:ASP:OD1	16:H:175:THR:HG22	2.08	0.53
5:5:123:GLU:N	5:5:123:GLU:OE2	2.42	0.53
8:8:331:HIS:ND1	8:8:335:GLU:OE2	2.41	0.52
1:0:186:THR:O	1:0:186:THR:HG22	2.09	0.52
5:5:209:ILE:HD11	5:5:229:HIS:HB2	1.92	0.52
2:1:140:ASP:O	2:1:143:CYS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:267:VAL:HG11	4:4:296:ALA:CB	2.38	0.52
1:0:21:LEU:HD12	1:0:24:GLN:NE2	2.25	0.52
4:4:370:ALA:N	4:4:412:ASP:OD1	2.39	0.52
12:D:245:VAL:HG22	12:D:271:ALA:HB1	1.91	0.51
11:C:152:ARG:NH1	33:Y:300:GLU:OE1	2.43	0.51
15:G:263:ASP:OD1	15:G:267:MET:N	2.43	0.51
31:W:114:ILE:HG21	31:W:142:LEU:HD11	1.92	0.51
8:8:348:VAL:HG23	8:8:348:VAL:O	2.11	0.51
4:4:526:ASP:N	4:4:526:ASP:OD1	2.43	0.51
5:5:191:LYS:O	5:5:256:ARG:NH2	2.43	0.51
26:R:295:ASP:OD1	26:R:299:ASN:ND2	2.44	0.51
10:B:77:GLU:OE2	10:B:259:ARG:NH1	2.43	0.51
4:4:317:LEU:HD22	4:4:321:ARG:HH12	1.74	0.50
9:A:1248:C:O2'	9:A:1251:A:O2'	2.07	0.50
4:4:251:MET:O	4:4:254:LYS:NZ	2.24	0.50
7:7:107:GLN:NE2	11:C:19:ARG:O	2.44	0.50
13:E:65:LEU:HD11	24:P:75:LYS:HD2	1.93	0.50
1:0:37:ASP:O	1:0:41:LEU:N	2.44	0.50
2:1:106:LEU:HD21	11:C:120:CYS:CB	2.42	0.50
9:A:1219:U:O2'	9:A:1222:A:N7	2.44	0.50
12:D:391:LEU:HD23	12:D:392:ARG:O	2.12	0.50
3:3:176:ILE:HD11	20:L:206:LYS:HE3	1.94	0.50
8:8:194:LEU:HD13	8:8:262:MET:SD	2.52	0.50
9:A:932:C:N3	28:T:11:ARG:NH2	2.60	0.50
34:Z:56:HIS:O	34:Z:59:ALA:N	2.45	0.50
7:7:253:VAL:HG23	7:7:253:VAL:O	2.11	0.49
4:4:471:ILE:HG21	4:4:505:ARG:CD	2.41	0.49
8:8:72:SER:OG	8:8:350:PRO:O	2.29	0.49
4:4:513:TRP:CD1	4:4:531:ILE:HD13	2.47	0.49
4:4:645:LEU:O	4:4:649:VAL:HG23	2.13	0.49
16:H:78:VAL:CG1	16:H:170:MET:HE2	2.42	0.49
8:8:82:LEU:O	8:8:88:ARG:NE	2.45	0.49
4:4:307:GLU:OE2	4:4:315:LYS:NZ	2.46	0.49
8:8:153:SER:O	8:8:319:GLN:NE2	2.44	0.49
11:C:77:ASP:OD1	11:C:77:ASP:N	2.45	0.49
11:C:123:VAL:HG23	11:C:157:THR:HG22	1.95	0.49
14:F:158:LEU:HD11	14:F:229:MET:SD	2.53	0.49
16:H:108:VAL:HG22	16:H:143:LEU:CD2	2.43	0.49
30:V:29:LEU:HD11	30:V:184:TYR:CD2	2.48	0.49
9:A:974:U:O2'	9:A:975:A:N7	2.43	0.49
29:U:171:GLU:N	29:U:171:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:172:VAL:HG22	2:1:208:LYS:HG2	1.94	0.48
2:1:164:ARG:NH1	33:Y:319:ALA:O	2.46	0.48
3:3:173:LEU:HD22	20:L:209:LEU:CD2	2.43	0.48
2:1:240:GLU:OE1	34:Z:7:TYR:OH	2.32	0.48
16:H:160:ILE:HD12	16:H:170:MET:HE1	1.96	0.48
22:N:31:THR:HG22	22:N:46:ARG:HG2	1.94	0.48
7:7:187:GLN:OE1	7:7:212:ARG:NH2	2.46	0.48
7:7:341:GLN:CG	7:7:410:MET:HE2	2.44	0.48
9:A:1251:A:N6	9:A:1341:C:O2'	2.47	0.48
4:4:526:ASP:O	4:4:530:GLU:OE1	2.32	0.47
2:1:131:THR:HG1	16:H:149:THR:HG1	1.61	0.47
2:1:194:VAL:CG1	2:1:229:LEU:HD21	2.44	0.47
1:0:173:MET:HE1	21:M:70:LEU:CD1	2.44	0.47
14:F:119:LYS:NZ	32:X:398:LEU:OXT	2.32	0.47
4:4:394:TYR:CD1	4:4:431:LEU:HD21	2.49	0.47
5:5:156:GLU:O	5:5:159:SER:OG	2.22	0.47
4:4:267:VAL:CG1	4:4:296:ALA:HB1	2.43	0.47
4:4:354:LEU:HD13	33:Y:250:ILE:HD11	1.95	0.47
2:1:181:ASN:O	2:1:230:TYR:OH	2.25	0.47
4:4:57:VAL:HG23	4:4:57:VAL:O	2.14	0.47
4:4:95:LEU:HD21	11:C:132:TYR:HD2	1.79	0.47
4:4:578:CYS:O	4:4:582:LEU:HD23	2.15	0.47
5:5:131:ASP:O	5:5:169:ARG:NH1	2.48	0.47
10:B:146:SER:OG	10:B:197:HIS:ND1	2.37	0.47
17:I:62:ILE:HD11	25:Q:12:VAL:HG13	1.97	0.47
2:1:228:VAL:HG12	34:Z:18:LEU:CD1	2.44	0.47
4:4:118:LYS:NZ	11:C:145:TYR:OH	2.45	0.47
9:A:760:A:N1	9:A:780:C:O2'	2.43	0.47
24:P:49:ASP:OD2	31:W:82:SER:OG	2.21	0.47
4:4:354:LEU:O	4:4:358:ARG:NE	2.46	0.46
2:1:255:ASN:N	2:1:259:GLU:OE1	2.46	0.46
4:4:417:GLN:OE1	4:4:418:SER:N	2.47	0.46
9:A:976:A:OP1	25:Q:4:HIS:ND1	2.39	0.46
15:G:200:LEU:O	15:G:218:TYR:OH	2.27	0.46
30:V:392:ARG:HG2	30:V:396:GLN:HE22	1.79	0.46
2:1:254:GLU:OE1	2:1:254:GLU:N	2.48	0.46
4:4:149:ILE:O	4:4:160:ARG:NH1	2.41	0.46
24:P:70:LYS:O	24:P:103:LYS:NZ	2.47	0.46
4:4:195:LEU:O	4:4:199:GLY:N	2.47	0.46
7:7:383:HIS:O	7:7:383:HIS:ND1	2.49	0.46
4:4:259:TYR:HB3	4:4:282:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:157:VAL:HG22	33:Y:315:ILE:HG21	1.97	0.46
9:A:1033:U:O2'	13:E:93:ILE:O	2.33	0.46
33:Y:339:GLU:OE1	33:Y:339:GLU:N	2.42	0.46
3:3:173:LEU:HD22	20:L:209:LEU:HD23	1.97	0.46
4:4:619:LYS:HE3	4:4:648:ARG:HE	1.81	0.46
8:8:194:LEU:HB2	8:8:245:LEU:HD12	1.97	0.46
9:A:941:G:O2'	9:A:1109:A:OP2	2.28	0.46
20:L:68:PRO:O	20:L:71:THR:HG22	2.15	0.46
9:A:762:G:P	20:L:206:LYS:HZ3	2.33	0.45
4:4:535:MET:HE1	4:4:551:CYS:SG	2.56	0.45
5:5:266:MET:HE3	5:5:266:MET:HA	1.99	0.45
8:8:338:LYS:NZ	9:A:1365:A:OP2	2.37	0.45
2:1:152:ASP:OD2	2:1:174:ARG:NH1	2.42	0.45
9:A:1441:A:H2	9:A:1449:G:H22	1.65	0.45
20:L:212:ARG:O	20:L:216:GLU:OE1	2.33	0.45
30:V:29:LEU:HD12	30:V:181:LEU:HD23	1.98	0.45
8:8:239:SER:OG	8:8:268:ALA:HB1	2.16	0.45
33:Y:341:PHE:CE2	33:Y:351:MET:HE2	2.51	0.45
9:A:1343:A:O2'	9:A:1345:G:N7	2.44	0.45
4:4:279:TYR:CD2	4:4:297:LEU:HD13	2.51	0.45
7:7:266:PHE:O	36:7:502:SAM:HE3	2.17	0.45
9:A:1254:C:O2'	9:A:1255:U:OP2	2.35	0.45
23:O:137:ALA:HB3	23:O:138:PRO:HD3	1.99	0.45
2:1:131:THR:OG1	16:H:149:THR:OG1	2.27	0.45
4:4:79:ASN:HB3	16:H:50:LEU:HD12	1.99	0.45
9:A:992:U:O2'	9:A:994:A:OP2	2.33	0.45
16:H:108:VAL:HG22	16:H:143:LEU:HD23	1.98	0.45
9:A:1162:A:OP1	18:J:48:LYS:NZ	2.47	0.45
34:Z:4:LEU:HD23	34:Z:5:SER:O	2.17	0.44
20:L:116:VAL:HG12	20:L:126:GLU:HG3	1.98	0.44
4:4:140:LEU:HD21	33:Y:309:LYS:NZ	2.33	0.44
9:A:1492:A:O2'	9:A:1493:C:OP2	2.27	0.44
33:Y:248:LYS:NZ	33:Y:252:THR:OG1	2.35	0.44
9:A:1066:C:O2'	17:I:187:ARG:O	2.35	0.44
13:E:37:ARG:NH1	13:E:69:TYR:OH	2.51	0.44
15:G:200:LEU:HD11	15:G:205:LEU:HD13	2.00	0.44
29:U:100:ALA:O	29:U:104:GLU:OE1	2.35	0.44
34:Z:65:LEU:HD11	34:Z:70:LEU:HB2	1.98	0.44
7:7:268:LEU:HB2	7:7:305:LEU:HD21	1.99	0.44
8:8:125:PHE:CE2	8:8:172:LEU:HD22	2.53	0.44
11:C:79:GLU:OE1	11:C:79:GLU:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:112:MET:O	20:L:116:VAL:HG22	2.18	0.44
24:P:113:ARG:CG	24:P:117:MET:HE3	2.48	0.44
26:R:325:ILE:HD12	26:R:325:ILE:H	1.82	0.43
4:4:394:TYR:HD1	4:4:431:LEU:HD21	1.84	0.43
9:A:1226:C:HO2'	9:A:1227:G:P	2.36	0.43
30:V:257:ASP:O	30:V:261:GLN:HG3	2.19	0.43
32:X:186:THR:O	32:X:190:ASN:ND2	2.50	0.43
4:4:359:GLU:HG2	33:Y:256:LEU:HD12	2.01	0.43
8:8:80:GLY:O	8:8:377:THR:OG1	2.37	0.43
7:7:265:ALA:O	36:7:502:SAM:N	2.50	0.43
26:R:69:THR:N	26:R:72:ASP:OD2	2.45	0.43
7:7:87:VAL:HG13	7:7:161:ALA:HB2	1.99	0.43
4:4:525:SER:O	4:4:529:GLU:OE1	2.36	0.43
4:4:615:MET:HE1	4:4:631:VAL:HG23	1.99	0.43
7:7:359:SER:O	7:7:362:LYS:NZ	2.52	0.43
16:H:97:LEU:O	16:H:101:GLU:OE1	2.36	0.43
4:4:649:VAL:HG12	4:4:655:ILE:HD11	2.00	0.43
4:4:264:ARG:O	4:4:267:VAL:HG12	2.18	0.43
7:7:296:GLU:HG3	7:7:305:LEU:HD22	2.01	0.43
15:G:126:LYS:HB2	15:G:131:ILE:HD11	2.01	0.42
30:V:30:LEU:HD12	30:V:149:ASP:CB	2.48	0.42
24:P:67:LEU:HD21	24:P:79:LEU:HD11	2.00	0.42
4:4:593:TRP:CZ3	4:4:614:LEU:HD22	2.53	0.42
13:E:35:ILE:HD12	20:L:97:MET:HE2	2.01	0.42
31:W:100:VAL:HG11	31:W:144:LEU:HD11	2.01	0.42
7:7:164:ASP:OD1	7:7:165:GLY:N	2.52	0.42
9:A:1293:C:H3'	9:A:1294:A:H5'	2.00	0.42
14:F:111:MET:HA	14:F:111:MET:HE2	2.01	0.42
15:G:108:ILE:HD12	15:G:112:PHE:CD2	2.55	0.42
2:1:194:VAL:HG21	2:1:198:TYR:HB2	2.02	0.42
15:G:116:LEU:O	15:G:122:ARG:NE	2.51	0.42
14:F:203:GLU:OE1	14:F:203:GLU:N	2.50	0.42
15:G:218:TYR:HD2	15:G:219:MET:HE2	1.85	0.42
33:Y:346:PRO:HD2	33:Y:347:ILE:N	2.35	0.42
33:Y:348:ARG:NE	33:Y:352:GLU:OE2	2.53	0.42
2:1:182:LEU:HD11	2:1:190:LEU:HD22	2.02	0.42
2:1:289:ILE:HD13	2:1:319:LEU:HD21	2.02	0.42
4:4:194:LEU:C	4:4:194:LEU:HD23	2.45	0.42
6:6:175:ASN:HD21	9:A:1595:G:H22	1.67	0.42
7:7:35:THR:HG22	7:7:441:THR:C	2.45	0.42
9:A:948:U:OP2	9:A:1045:G:N1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:109:ILE:HG22	19:K:113:HIS:CD2	2.54	0.42
16:H:75:ARG:H	16:H:175:THR:HG1	1.68	0.42
10:B:243:PRO:O	10:B:247:HIS:ND1	2.51	0.42
5:5:64:PRO:HG2	5:5:83:VAL:CG1	2.50	0.41
4:4:448:ILE:HD12	4:4:454:ARG:HD3	2.02	0.41
5:5:83:VAL:HG21	5:5:105:LEU:HD11	2.01	0.41
27:S:83:ARG:NH2	27:S:93:LYS:O	2.53	0.41
2:1:89:TYR:HB2	11:C:65:ARG:HD2	2.02	0.41
27:S:96:CYS:O	27:S:100:VAL:HG23	2.20	0.41
4:4:464:LEU:HD23	4:4:468:MET:HE1	2.02	0.41
5:5:88:THR:HG22	5:5:109:HIS:CD2	2.55	0.41
7:7:103:PRO:O	7:7:106:LEU:N	2.51	0.41
26:R:208:ILE:O	26:R:214:ASN:ND2	2.51	0.41
2:1:193:LEU:HG	34:Z:11:MET:HE2	2.02	0.41
14:F:46:ILE:O	14:F:46:ILE:HG22	2.20	0.41
32:X:81:HIS:HD2	32:X:190:ASN:HB3	1.84	0.41
9:A:893:G:O2'	9:A:908:C:O2'	2.32	0.41
10:B:254:GLN:O	10:B:258:THR:HG23	2.20	0.41
19:K:54:ILE:HA	19:K:57:LEU:HD12	2.03	0.41
26:R:170:ARG:O	26:R:189:ARG:NH1	2.47	0.41
9:A:1298:U:H2'	9:A:1299:A:O4'	2.21	0.41
8:8:191:SER:HB2	8:8:268:ALA:HB2	2.02	0.41
8:8:194:LEU:HD12	8:8:261:ARG:C	2.46	0.41
9:A:843:G:N2	9:A:846:A:OP2	2.45	0.41
4:4:128:PHE:O	11:C:148:LYS:NZ	2.38	0.41
5:5:158:ILE:HD13	5:5:204:CYS:SG	2.61	0.41
10:B:220:VAL:HG22	10:B:234:TYR:HB2	2.03	0.41
17:I:163:HIS:NE2	25:Q:20:GLU:OE2	2.54	0.41
4:4:128:PHE:C	11:C:148:LYS:HZ1	2.26	0.41
5:5:33:LEU:HD21	5:5:37:PHE:HE2	1.85	0.41
12:D:401:VAL:HG13	28:T:9:ILE:HG21	2.02	0.41
14:F:82:THR:HG22	14:F:83:SER:N	2.35	0.41
14:F:170:VAL:HG23	14:F:236:LEU:O	2.21	0.41
7:7:140:LYS:O	7:7:141:THR:HG22	2.20	0.40
31:W:105:PHE:O	31:W:136:LYS:NZ	2.53	0.40
1:0:175:ILE:HG21	23:O:188:PRO:HD2	2.04	0.40
4:4:166:VAL:HG23	4:4:195:LEU:HD23	2.03	0.40
9:A:1077:U:O2'	9:A:1078:A:OP1	2.34	0.40
4:4:397:MET:HE1	4:4:435:VAL:HA	2.04	0.40
9:A:926:A:OP1	18:J:47:ARG:NH1	2.53	0.40
15:G:269:PHE:HD2	15:G:284:ILE:HG23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:268:LEU:CB	7:7:305:LEU:HD21	2.51	0.40
9:A:1265:C:H5"	19:K:109:ILE:HD13	2.03	0.40
19:K:112:ARG:O	19:K:116:ASP:N	2.40	0.40
2:1:164:ARG:NH2	4:4:134:GLU:OE2	2.53	0.40
4:4:584:LEU:HD21	4:4:614:LEU:HD23	2.03	0.40
8:8:135:LEU:HD11	8:8:346:PHE:CD1	2.57	0.40
10:B:229:PRO:HA	10:B:232:ILE:HD13	2.03	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%)	205 (98%)	4 (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%)	549 (98%)	9 (2%)	0	100	100
5	5	317/346 (92%)	311 (98%)	6 (2%)	0	100	100
6	6	122/343 (36%)	119 (98%)	3 (2%)	0	100	100
7	7	398/456 (87%)	386 (97%)	12 (3%)	0	100	100
8	8	324/390 (83%)	316 (98%)	8 (2%)	0	100	100
10	B	218/296 (74%)	217 (100%)	1 (0%)	0	100	100
11	C	122/167 (73%)	118 (97%)	4 (3%)	0	100	100
12	D	228/430 (53%)	224 (98%)	4 (2%)	0	100	100
13	E	106/125 (85%)	105 (99%)	1 (1%)	0	100	100
14	F	204/242 (84%)	201 (98%)	3 (2%)	0	100	100
15	G	288/396 (73%)	283 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	H	126/201 (63%)	122 (97%)	4 (3%)	0	100	100
17	I	135/194 (70%)	130 (96%)	5 (4%)	0	100	100
18	J	106/138 (77%)	103 (97%)	3 (3%)	0	100	100
19	K	31/128 (24%)	31 (100%)	0	0	100	100
20	L	159/257 (62%)	158 (99%)	1 (1%)	0	100	100
21	M	113/137 (82%)	113 (100%)	0	0	100	100
22	N	107/130 (82%)	106 (99%)	1 (1%)	0	100	100
23	O	188/258 (73%)	185 (98%)	3 (2%)	0	100	100
24	P	94/142 (66%)	94 (100%)	0	0	100	100
25	Q	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	R	289/360 (80%)	285 (99%)	4 (1%)	0	100	100
27	S	131/190 (69%)	131 (100%)	0	0	100	100
28	T	162/173 (94%)	161 (99%)	1 (1%)	0	100	100
29	U	172/205 (84%)	172 (100%)	0	0	100	100
30	V	355/414 (86%)	349 (98%)	6 (2%)	0	100	100
31	W	96/187 (51%)	93 (97%)	3 (3%)	0	100	100
32	X	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
33	Y	118/395 (30%)	117 (99%)	1 (1%)	0	100	100
34	Z	52/106 (49%)	47 (90%)	5 (10%)	0	100	100
All	All	6260/8720 (72%)	6152 (98%)	108 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	342/385 (89%)	342 (100%)	0	100	100
8	8	270/317 (85%)	270 (100%)	0	100	100
10	B	194/249 (78%)	194 (100%)	0	100	100
11	C	111/143 (78%)	111 (100%)	0	100	100
12	D	196/357 (55%)	196 (100%)	0	100	100
13	E	91/107 (85%)	91 (100%)	0	100	100
14	F	183/209 (88%)	183 (100%)	0	100	100
15	G	254/342 (74%)	254 (100%)	0	100	100
16	H	120/180 (67%)	120 (100%)	0	100	100
17	I	105/147 (71%)	105 (100%)	0	100	100
18	J	93/118 (79%)	93 (100%)	0	100	100
19	K	30/113 (26%)	30 (100%)	0	100	100
20	L	151/226 (67%)	151 (100%)	0	100	100
21	M	94/113 (83%)	94 (100%)	0	100	100
22	N	95/115 (83%)	95 (100%)	0	100	100
23	O	171/230 (74%)	171 (100%)	0	100	100
24	P	87/123 (71%)	87 (100%)	0	100	100
25	Q	78/79 (99%)	78 (100%)	0	100	100
26	R	261/318 (82%)	261 (100%)	0	100	100
27	S	115/164 (70%)	115 (100%)	0	100	100
28	T	151/157 (96%)	151 (100%)	0	100	100
29	U	150/174 (86%)	150 (100%)	0	100	100
30	V	323/364 (89%)	323 (100%)	0	100	100
31	W	85/158 (54%)	85 (100%)	0	100	100
32	X	311/351 (89%)	311 (100%)	0	100	100
33	Y	112/357 (31%)	112 (100%)	0	100	100
34	Z	51/95 (54%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5586/7544 (74%)	5586 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	24	GLN
1	0	108	ASN
1	0	145	HIS
3	3	158	GLN
4	4	129	GLN
4	4	470	GLN
5	5	56	ASN
5	5	95	GLN
5	5	137	HIS
5	5	171	GLN
5	5	235	GLN
5	5	254	GLN
5	5	321	ASN
6	6	43	ASN
6	6	165	HIS
7	7	86	GLN
7	7	144	HIS
7	7	398	HIS
7	7	400	HIS
8	8	108	HIS
10	B	74	ASN
10	B	201	ASN
12	D	280	HIS
12	D	361	GLN
13	E	54	HIS
13	E	57	GLN
13	E	81	HIS
15	G	130	GLN
15	G	156	GLN
15	G	242	GLN
17	I	87	HIS
18	J	77	ASN
18	J	134	HIS
22	N	52	HIS
23	O	169	GLN

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Mol	Chain	Res	Type
24	P	71	HIS
26	R	277	ASN
26	R	278	ASN
28	T	35	ASN
28	T	63	GLN
29	U	62	HIS
30	V	131	ASN
30	V	145	ASN
30	V	188	HIS
30	V	237	GLN
30	V	396	GLN
32	X	176	GLN
32	X	291	HIS
32	X	363	ASN
33	Y	372	HIS
34	Z	56	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	A	845/955 (88%)	195 (23%)	4 (0%)

All (195) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	650	U
9	A	651	A
9	A	664	G
9	A	680	U
9	A	688	A
9	A	691	A
9	A	704	U
9	A	721	U
9	A	722	C
9	A	730	A
9	A	736	C
9	A	738	A
9	A	739	C
9	A	740	G
9	A	741	A
9	A	753	A

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Mol	Chain	Res	Type
9	A	761	A
9	A	766	G
9	A	769	G
9	A	772	A
9	A	773	U
9	A	777	G
9	A	791	G
9	A	794	U
9	A	796	G
9	A	807	A
9	A	830	U
9	A	832	U
9	A	835	C
9	A	851	A
9	A	860	A
9	A	861	U
9	A	866	A
9	A	868	C
9	A	869	C
9	A	870	C
9	A	871	A
9	A	883	U
9	A	886	C
9	A	889	G
9	A	890	C
9	A	891	C
9	A	893	G
9	A	902	G
9	A	903	U
9	A	919	A
9	A	931	C
9	A	938	A
9	A	939	A
9	A	942	A
9	A	954	C
9	A	955	A
9	A	967	A
9	A	970	A
9	A	971	A
9	A	972	G
9	A	992	U
9	A	993	A

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Mol	Chain	Res	Type
9	A	1001	C
9	A	1002	C
9	A	1011	C
9	A	1012	A
9	A	1014	A
9	A	1015	A
9	A	1031	G
9	A	1042	U
9	A	1052	C
9	A	1054	A
9	A	1060	A
9	A	1061	A
9	A	1065	C
9	A	1077	U
9	A	1078	A
9	A	1080	A
9	A	1081	U
9	A	1103	A
9	A	1105	C
9	A	1111	C
9	A	1117	A
9	A	1120	C
9	A	1121	A
9	A	1137	A
9	A	1151	C
9	A	1160	A
9	A	1167	A
9	A	1175	G
9	A	1177	C
9	A	1178	G
9	A	1179	G
9	A	1181	G
9	A	1182	C
9	A	1185	C
9	A	1186	A
9	A	1187	U
9	A	1188	A
9	A	1189	U
9	A	1190	C
9	A	1191	C
9	A	1197	G
9	A	1199	G

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Mol	Chain	Res	Type
9	A	1201	A
9	A	1217	G
9	A	1220	A
9	A	1221	A
9	A	1222	A
9	A	1223	C
9	A	1224	C
9	A	1225	C
9	A	1226	C
9	A	1227	G
9	A	1228	A
9	A	1229	U
9	A	1232	A
9	A	1234	C
9	A	1236	C
9	A	1242	C
9	A	1245	U
9	A	1246	U
9	A	1248	C
9	A	1249	U
9	A	1250	C
9	A	1251	A
9	A	1254	C
9	A	1255	U
9	A	1258	A
9	A	1259	U
9	A	1260	A
9	A	1261	C
9	A	1265	C
9	A	1284	U
9	A	1290	C
9	A	1291	U
9	A	1294	A
9	A	1296	A
9	A	1297	G
9	A	1298	U
9	A	1299	A
9	A	1327	G
9	A	1330	C
9	A	1331	A
9	A	1332	A
9	A	1334	G

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Mol	Chain	Res	Type
9	A	1335	U
9	A	1338	A
9	A	1340	C
9	A	1342	C
9	A	1343	A
9	A	1350	G
9	A	1354	A
9	A	1360	G
9	A	1367	A
9	A	1373	U
9	A	1376	C
9	A	1378	C
9	A	1424	U
9	A	1425	U
9	A	1427	A
9	A	1428	G
9	A	1429	C
9	A	1434	A
9	A	1441	A
9	A	1442	G
9	A	1450	C
9	A	1459	A
9	A	1464	G
9	A	1467	C
9	A	1468	U
9	A	1470	A
9	A	1471	A
9	A	1477	U
9	A	1493	C
9	A	1494	C
9	A	1495	C
9	A	1519	A
9	A	1522	U
9	A	1525	C
9	A	1526	U
9	A	1527	A
9	A	1532	C
9	A	1533	C
9	A	1537	C
9	A	1538	G
9	A	1556	C
9	A	1557	A

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Mol	Chain	Res	Type
9	A	1558	A
9	A	1560	U
9	A	1572	A
9	A	1574	G
9	A	1577	U
9	A	1582	G
9	A	1583	A
9	A	1584	A
9	A	1585	A
9	A	1594	G
9	A	1595	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	1077	U
9	A	1226	C
9	A	1330	C
9	A	1531	C

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

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	$\#\|Z\| > 2$
25	AYA	Q	2	25	6,7,8	1.24	1 (16%)	6,8,10	1.29	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
25	AYA	Q	2	25	-	0/5/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Q	2	AYA	CA-N	-2.34	1.44	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Q	2	AYA	CB-CA-N	2.84	112.88	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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 37 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	$\#\|Z\| > 2$
43	GDP	X	503	-	29,30,30	3.29	10 (34%)	45,47,47	2.35	15 (33%)
39	NAD	A	1735	38	46,48,48	3.07	18 (39%)	64,73,73	2.72	17 (26%)
41	FES	T	201	28,21	0,4,4	-	-	-		
42	ATP	X	501	38	32,33,33	0.60	1 (3%)	48,52,52	0.70	0
36	SAM	7	502	-	27,29,29	1.10	5 (18%)	34,42,42	2.01	8 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	SF4	7	501	7	0,12,12	-	-	-		
41	FES	P	201	24,13	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	NAD	A	1735	38	-	2/30/62/62	0/5/5/5
41	FES	P	201	24,13	-	-	0/1/1/1
41	FES	T	201	28,21	-	-	0/1/1/1
42	ATP	X	501	38	-	4/22/38/38	0/3/3/3
36	SAM	7	502	-	-	4/17/33/33	0/3/3/3
35	SF4	7	501	7	-	-	0/6/5/5
43	GDP	X	503	-	-	6/16/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	X	503	GDP	O6-C6	9.80	1.42	1.23
43	X	503	GDP	C2-N1	7.65	1.56	1.37
43	X	503	GDP	PA-O3A	7.40	1.67	1.59
39	A	1735	NAD	PN-O3	7.16	1.67	1.59
39	A	1735	NAD	C7N-N7N	7.13	1.46	1.33
39	A	1735	NAD	PA-O3	7.00	1.67	1.59
39	A	1735	NAD	C5A-N7A	6.96	1.51	1.39
39	A	1735	NAD	C8A-N9A	-5.82	1.27	1.37
39	A	1735	NAD	O4D-C1D	5.61	1.48	1.40
43	X	503	GDP	C2-N3	5.28	1.46	1.33
43	X	503	GDP	C2-N2	5.24	1.46	1.34
39	A	1735	NAD	C6A-N6A	4.81	1.46	1.34
39	A	1735	NAD	C2N-N1N	4.40	1.39	1.35
39	A	1735	NAD	C4N-C3N	3.98	1.45	1.39
39	A	1735	NAD	C4A-N9A	-3.87	1.29	1.37
39	A	1735	NAD	C5A-C4A	3.77	1.45	1.39
39	A	1735	NAD	C5N-C4N	3.35	1.44	1.38
39	A	1735	NAD	O7N-C7N	-2.89	1.18	1.24
43	X	503	GDP	C2'-C3'	-2.74	1.45	1.53
39	A	1735	NAD	O4B-C1B	2.56	1.47	1.42
43	X	503	GDP	C6-N1	2.52	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	7	502	SAM	C2-N3	2.50	1.38	1.33
36	7	502	SAM	C2-N1	2.48	1.38	1.33
43	X	503	GDP	PA-O5'	2.42	1.68	1.59
43	X	503	GDP	PB-O3B	-2.31	1.46	1.54
39	A	1735	NAD	C3N-C7N	2.29	1.54	1.50
36	7	502	SAM	OXT-C	-2.23	1.23	1.30
39	A	1735	NAD	C2D-C3D	-2.19	1.47	1.53
43	X	503	GDP	PB-O2B	-2.19	1.46	1.54
42	X	501	ATP	PA-O3A	-2.14	1.57	1.59
39	A	1735	NAD	C8A-N7A	2.11	1.35	1.31
36	7	502	SAM	C5-N7	-2.11	1.35	1.39
36	7	502	SAM	C8-N7	2.01	1.35	1.31
39	A	1735	NAD	PA-O2A	-2.01	1.46	1.55

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	A	1735	NAD	C4A-N9A-C8A	13.76	120.19	105.74
43	X	503	GDP	N9-C8-N7	-6.87	100.65	113.40
43	X	503	GDP	C8-N7-C5	6.87	116.49	104.26
39	A	1735	NAD	N3A-C4A-N9A	6.78	138.70	127.17
39	A	1735	NAD	C5A-C4A-N3A	-6.16	118.24	126.72
39	A	1735	NAD	C4A-C5A-N7A	-5.91	103.83	110.58
36	7	502	SAM	N3-C2-N1	-5.62	120.08	128.58
43	X	503	GDP	C2-N1-C6	-4.86	116.29	125.11
36	7	502	SAM	C5-C4-N3	-4.68	120.28	126.72
39	A	1735	NAD	N9A-C8A-N7A	-4.52	107.53	113.94
39	A	1735	NAD	N3A-C2A-N1A	-4.48	121.79	128.58
43	X	503	GDP	C8-N9-C4	4.12	113.75	106.03
39	A	1735	NAD	C4D-O4D-C1D	-3.84	106.41	109.92
36	7	502	SAM	N9-C8-N7	-3.74	108.62	113.94
43	X	503	GDP	C6-C5-C4	3.64	124.30	118.83
39	A	1735	NAD	C4A-N9A-C1B	-3.63	118.14	126.63
39	A	1735	NAD	C2A-N3A-C4A	3.53	120.45	111.83
36	7	502	SAM	C2-N3-C4	3.52	120.44	111.83
36	7	502	SAM	C5-N7-C8	3.35	108.72	103.45
39	A	1735	NAD	C6A-C5A-N7A	3.25	138.36	132.09
43	X	503	GDP	C4-C5-N7	-3.22	105.57	110.67
36	7	502	SAM	N3-C4-N9	2.96	132.19	127.17
43	X	503	GDP	C3'-C2'-C1'	2.95	107.05	101.46
43	X	503	GDP	O3B-PB-O3A	2.86	114.21	104.64
43	X	503	GDP	C2-N3-C4	2.77	117.07	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	7	502	SAM	OXT-C-O	-2.76	117.81	124.08
43	X	503	GDP	N9-C4-N3	2.76	131.47	125.95
43	X	503	GDP	O2B-PB-O3A	2.55	113.18	104.64
39	A	1735	NAD	C5A-C4A-N9A	-2.53	103.05	105.81
43	X	503	GDP	O2A-PA-O1A	-2.45	101.05	112.44
39	A	1735	NAD	C1B-N9A-C8A	-2.45	121.66	127.09
39	A	1735	NAD	O2N-PN-O1N	-2.39	101.30	112.44
36	7	502	SAM	C4-C5-N7	-2.35	107.90	110.58
43	X	503	GDP	C2'-C3'-C4'	2.30	107.05	102.61
39	A	1735	NAD	O2A-PA-O1A	-2.28	101.83	112.44
39	A	1735	NAD	C3N-C7N-N7N	2.24	120.50	117.74
39	A	1735	NAD	C3B-C2B-C1B	2.18	105.58	101.46
39	A	1735	NAD	C2B-C3B-C4B	2.15	106.77	102.61
43	X	503	GDP	C5-C4-N3	-2.13	125.00	128.39
43	X	503	GDP	O6-C6-C5	-2.01	121.22	126.53

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	7	502	SAM	CA-CB-CG-SD
36	7	502	SAM	CB-CG-SD-CE
42	X	501	ATP	PB-O3B-PG-O2G
43	X	503	GDP	PA-O3A-PB-O3B
43	X	503	GDP	C5'-O5'-PA-O3A
43	X	503	GDP	C5'-O5'-PA-O2A
36	7	502	SAM	N-CA-CB-CG
36	7	502	SAM	CB-CG-SD-C5'
39	A	1735	NAD	C5B-O5B-PA-O1A
43	X	503	GDP	C5'-O5'-PA-O1A
43	X	503	GDP	PB-O3A-PA-O2A
39	A	1735	NAD	C4B-C5B-O5B-PA
42	X	501	ATP	PB-O3B-PG-O3G
43	X	503	GDP	PA-O3A-PB-O2B
42	X	501	ATP	PG-O3B-PB-O2B
42	X	501	ATP	PA-O3A-PB-O2B

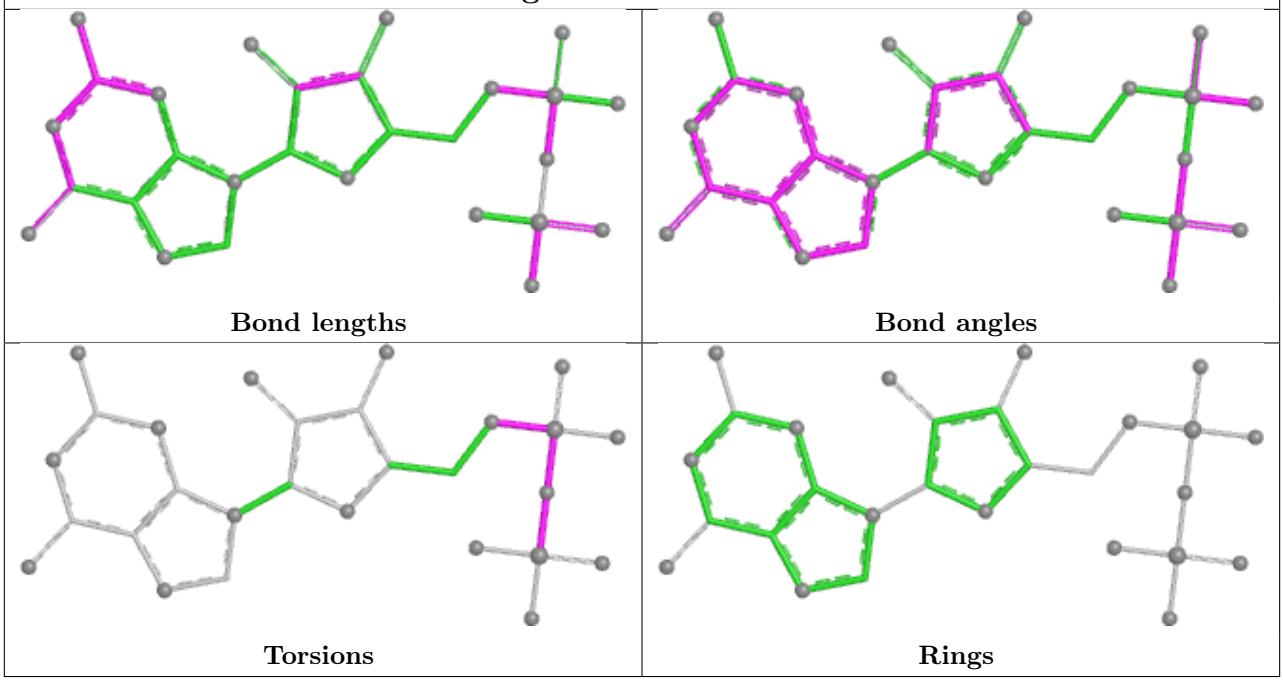
There are no ring outliers.

2 monomers are involved in 3 short contacts:

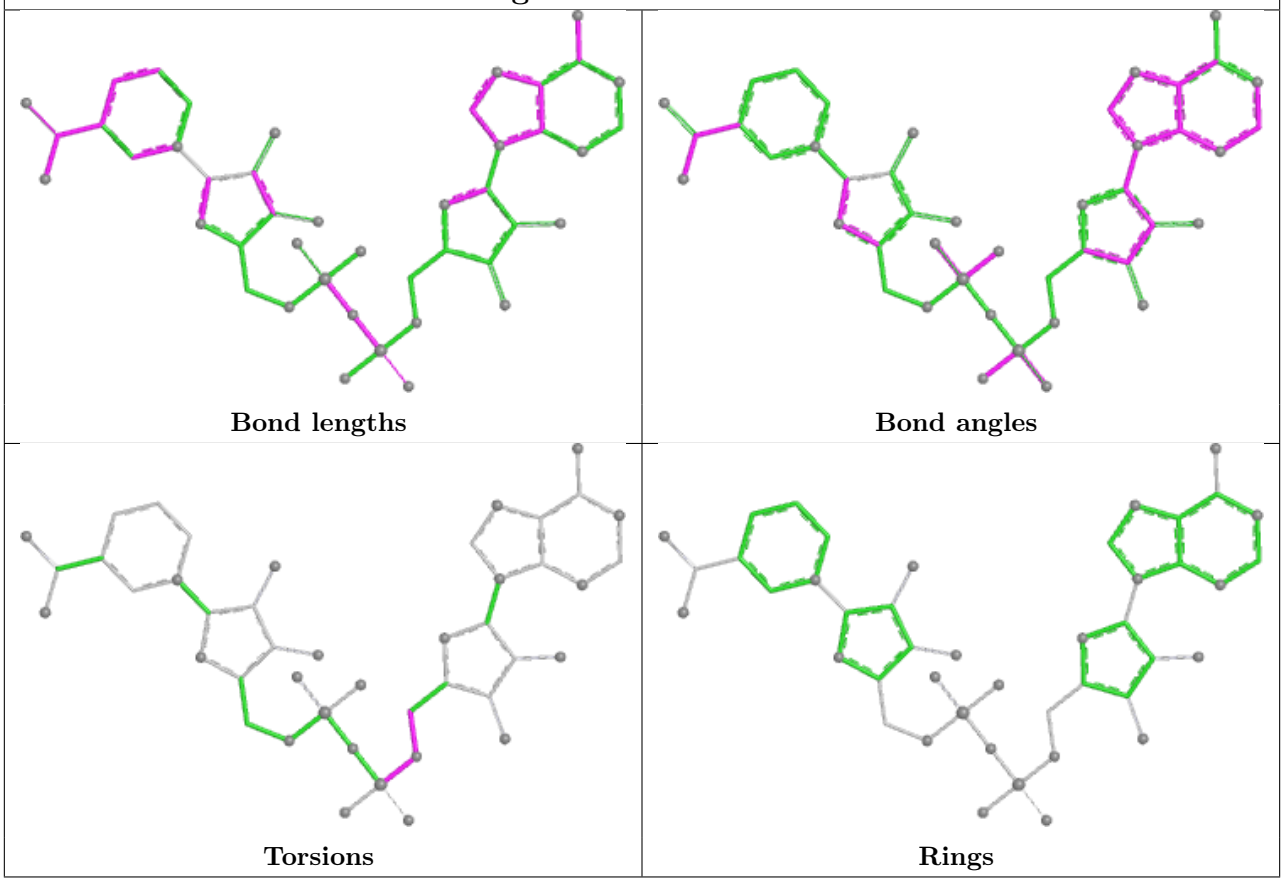
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	X	503	GDP	1	0
36	7	502	SAM	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

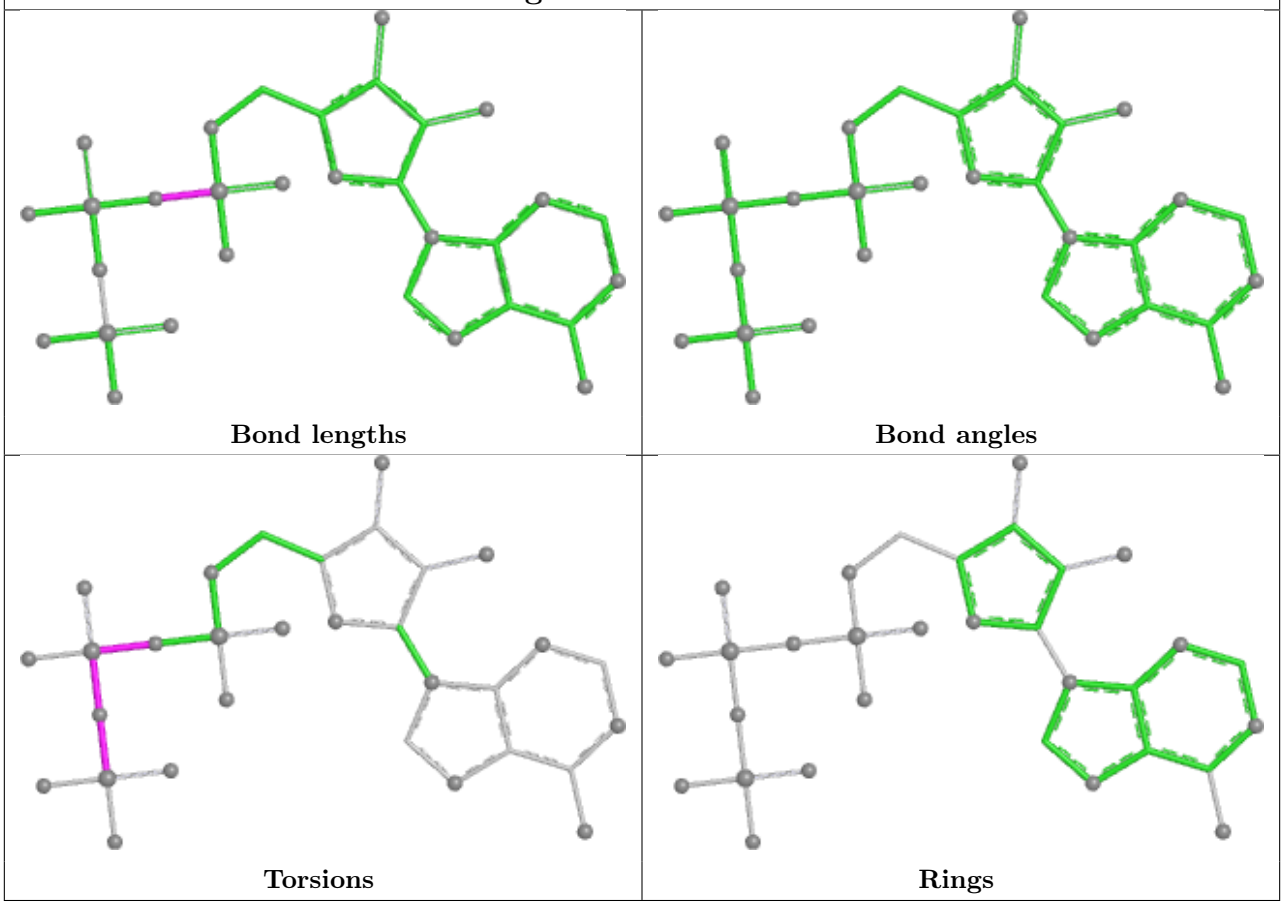
Ligand GDP X 503



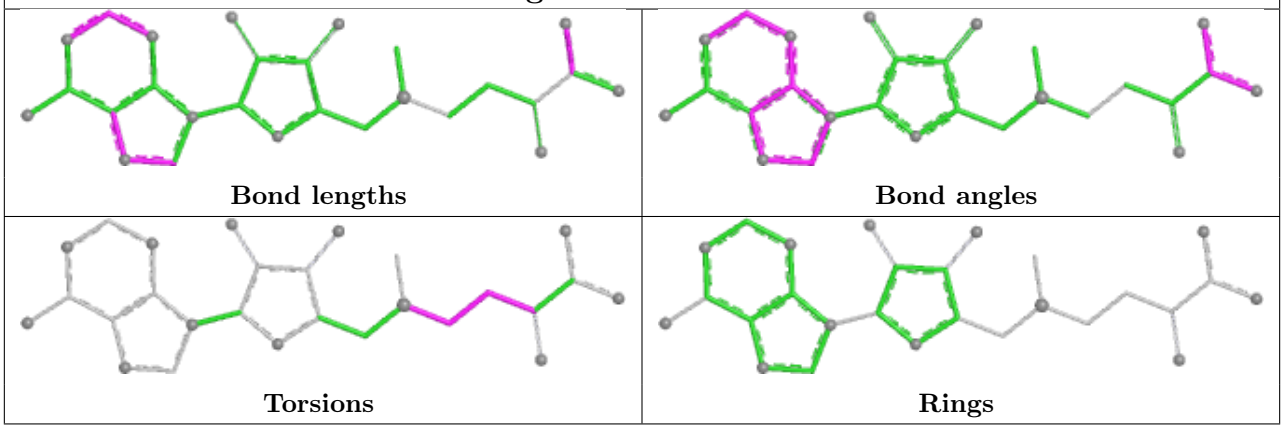
Ligand NAD A 1735

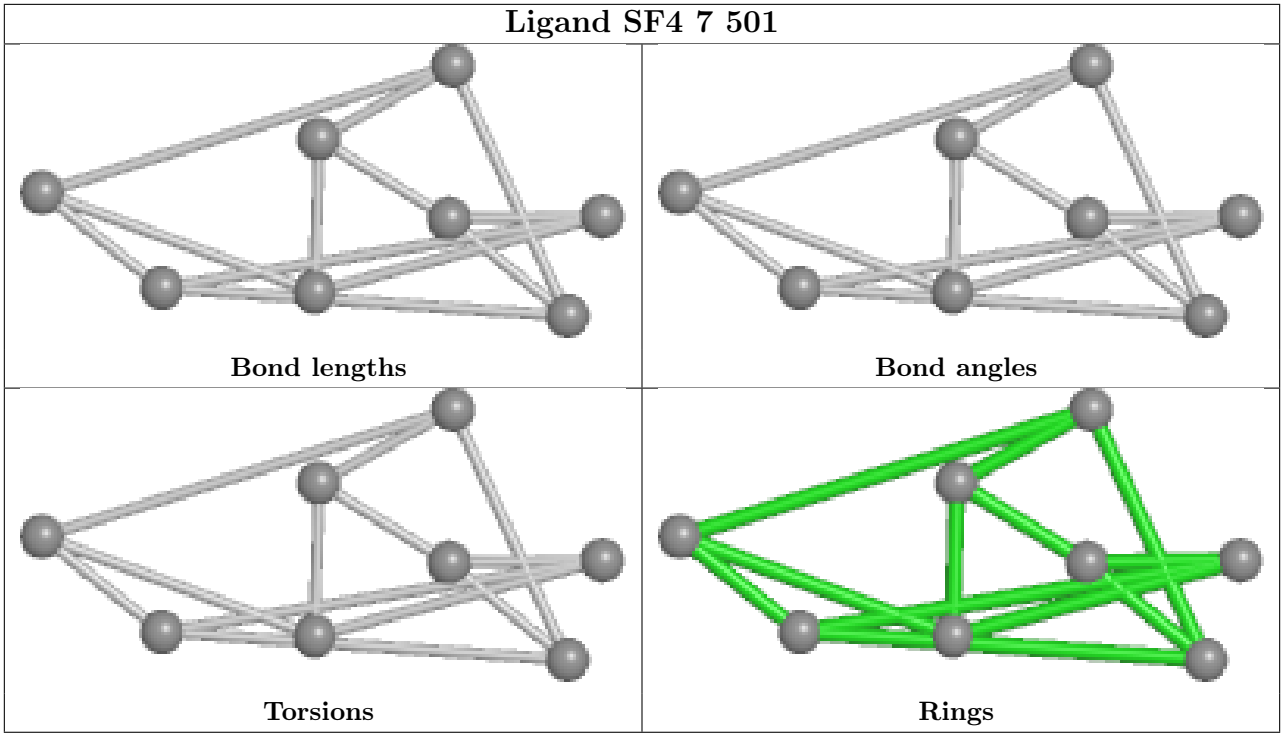


Ligand ATP X 501



Ligand SAM 7 502





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.

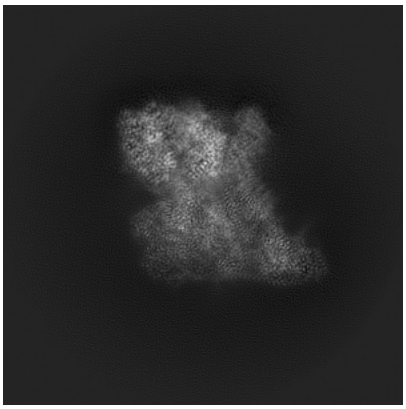
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26968. These allow visual inspection of the internal detail of the map and identification of artifacts.

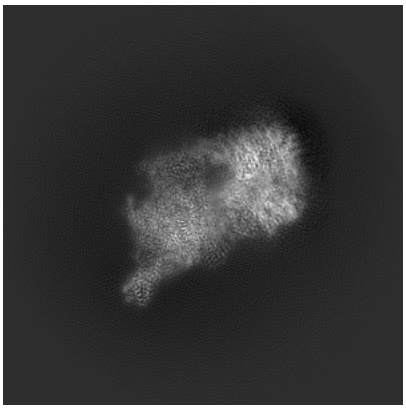
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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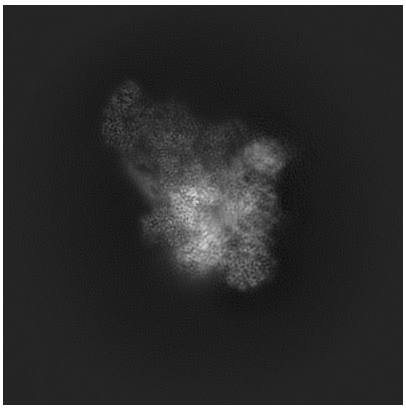
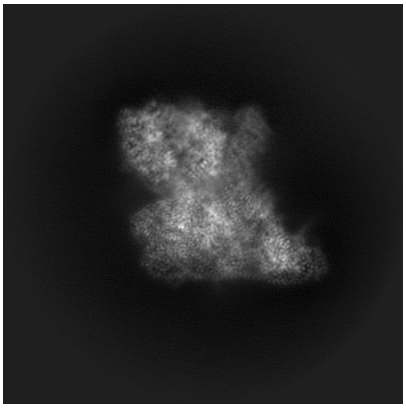


Z

6.1.2 Raw map



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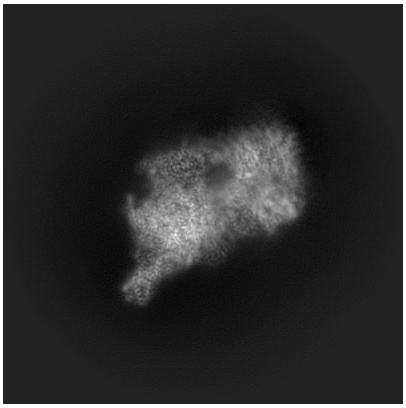

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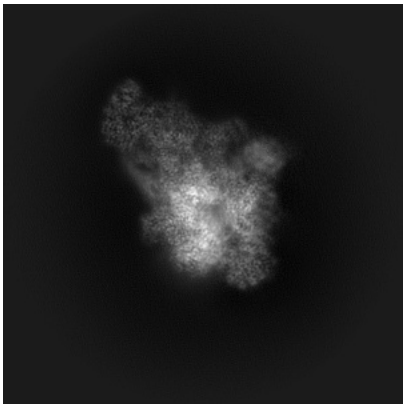
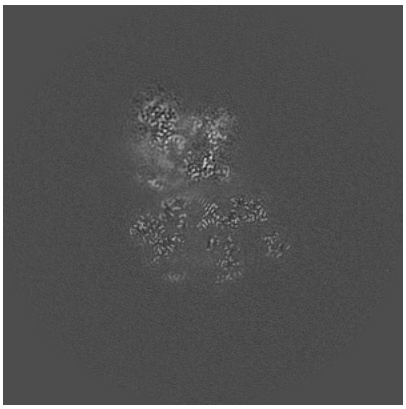


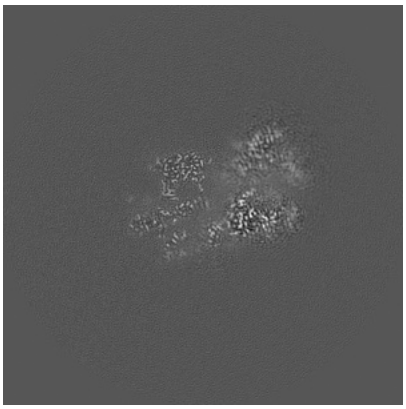
Z

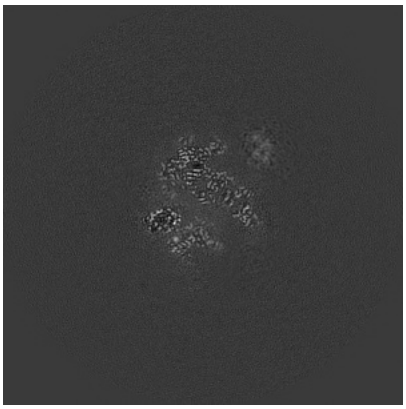
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

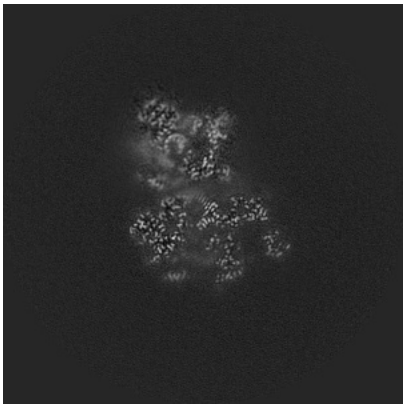
6.2.1 Primary map


X Index: 200


Y Index: 200


Z Index: 200

6.2.2 Raw map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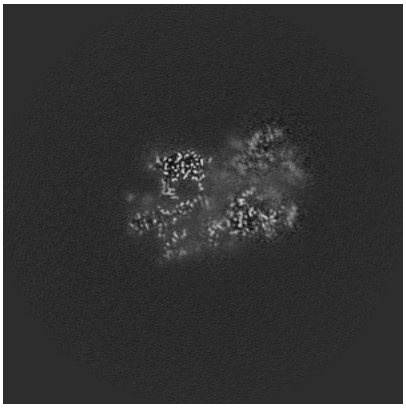
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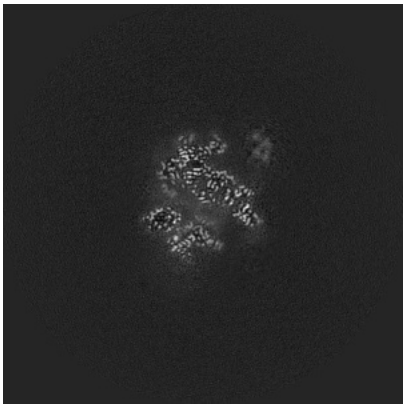
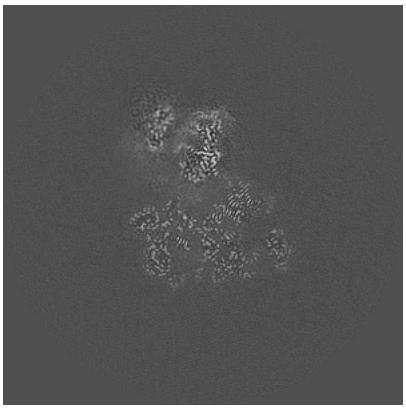
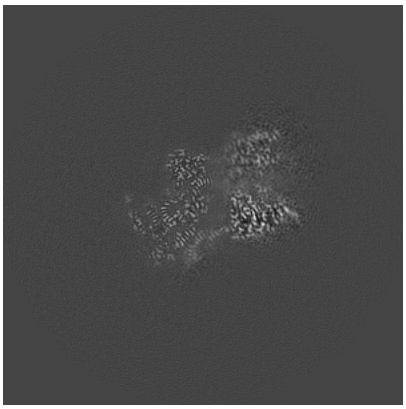

Z Index: 200

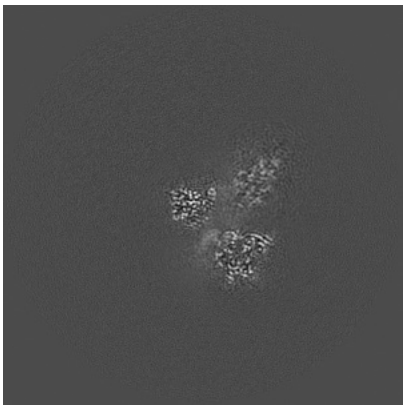
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

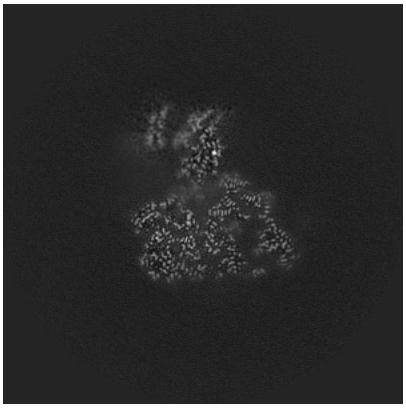
6.3.1 Primary map

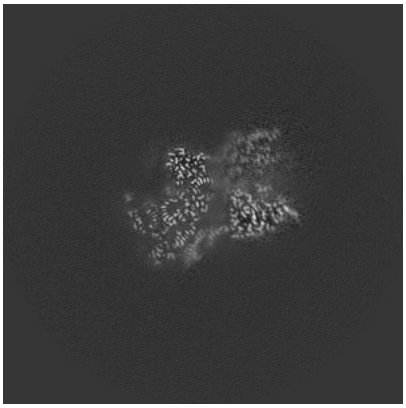

X Index: 191

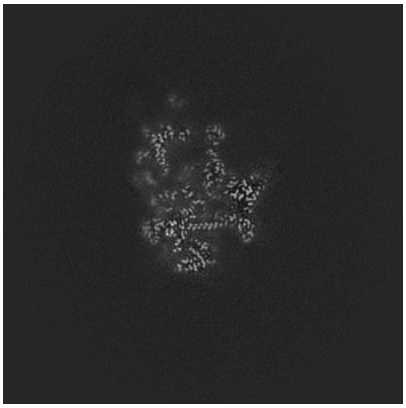

Y Index: 209


Z Index: 242

6.3.2 Raw map


X Index: 186

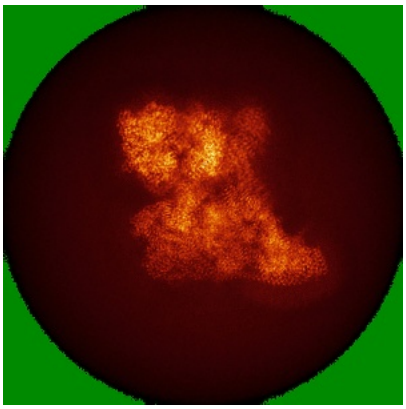

Y Index: 209

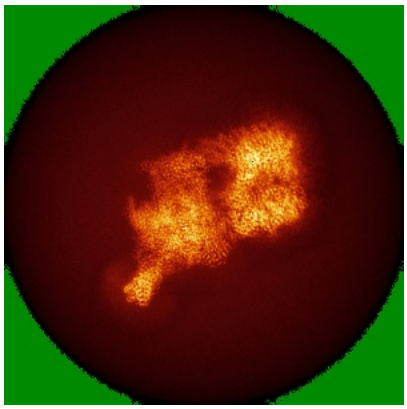

Z Index: 177

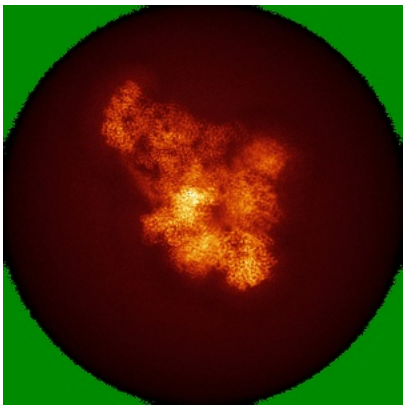
The images above show the largest variance slices of the map in three orthogonal directions.

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

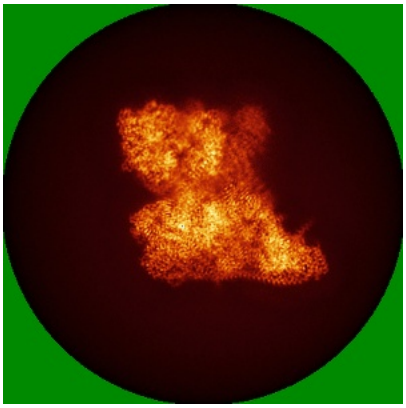
6.4.1 Primary map

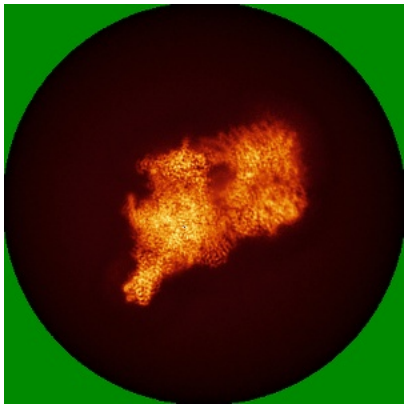

X

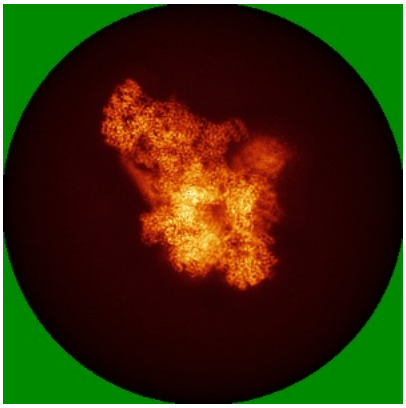

Y


Z

6.4.2 Raw map


X

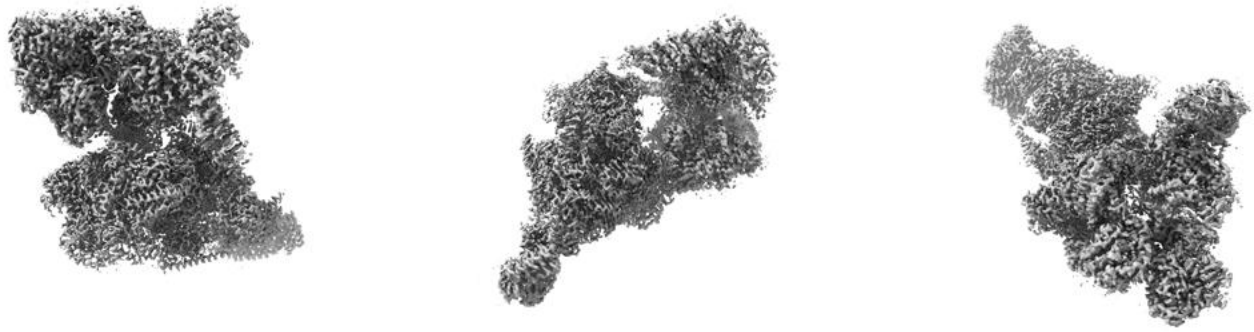

Y


Z

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

6.5 Orthogonal surface views (i)

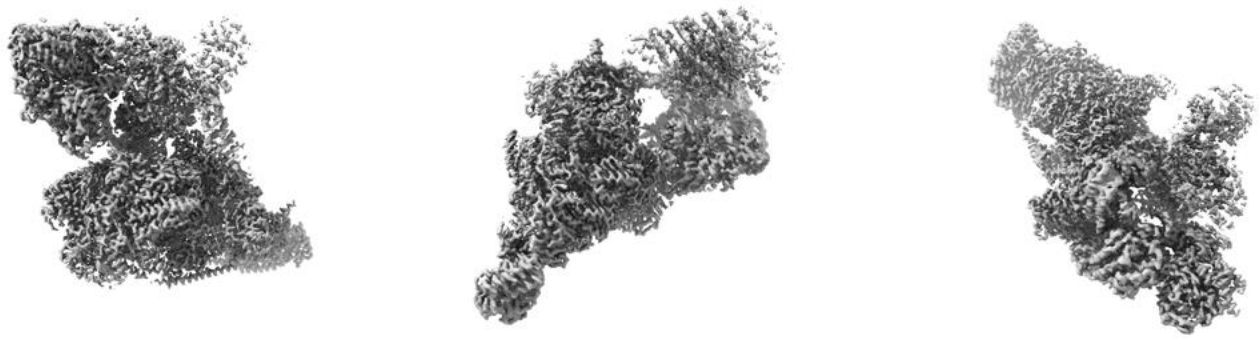
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 8.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

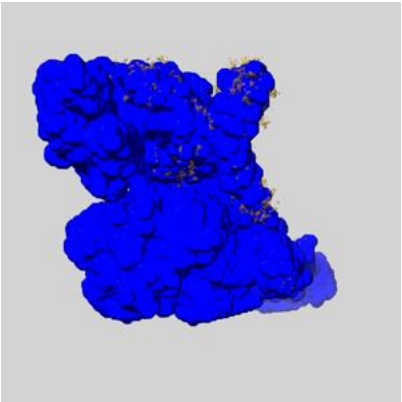
6.6 Mask visualisation (i)

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

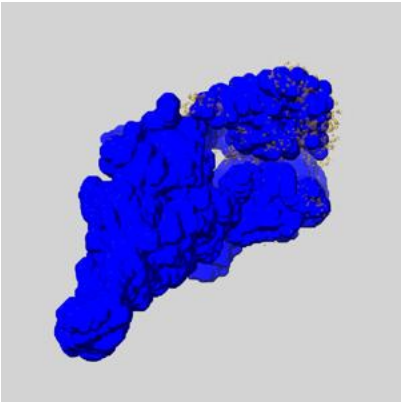
A mask typically either:

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

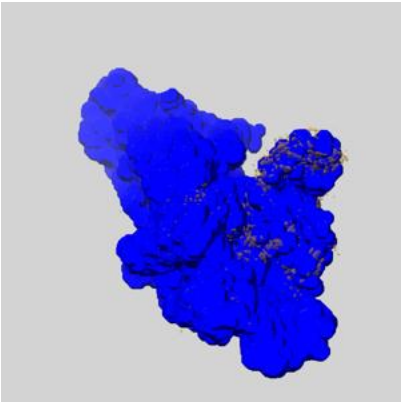
6.6.1 emd_26968_msk_1.map (i)



X



Y

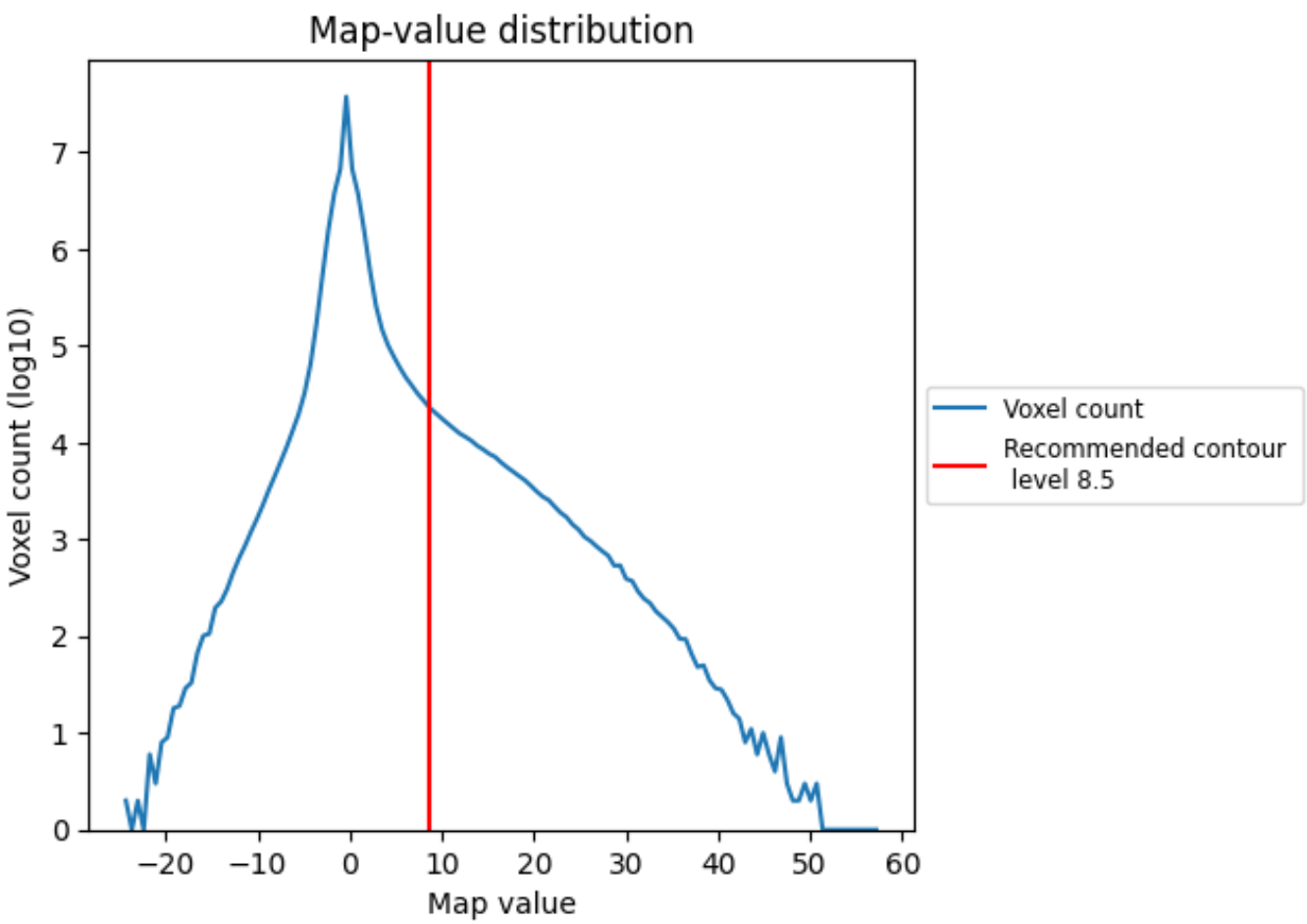


Z

7 Map analysis (i)

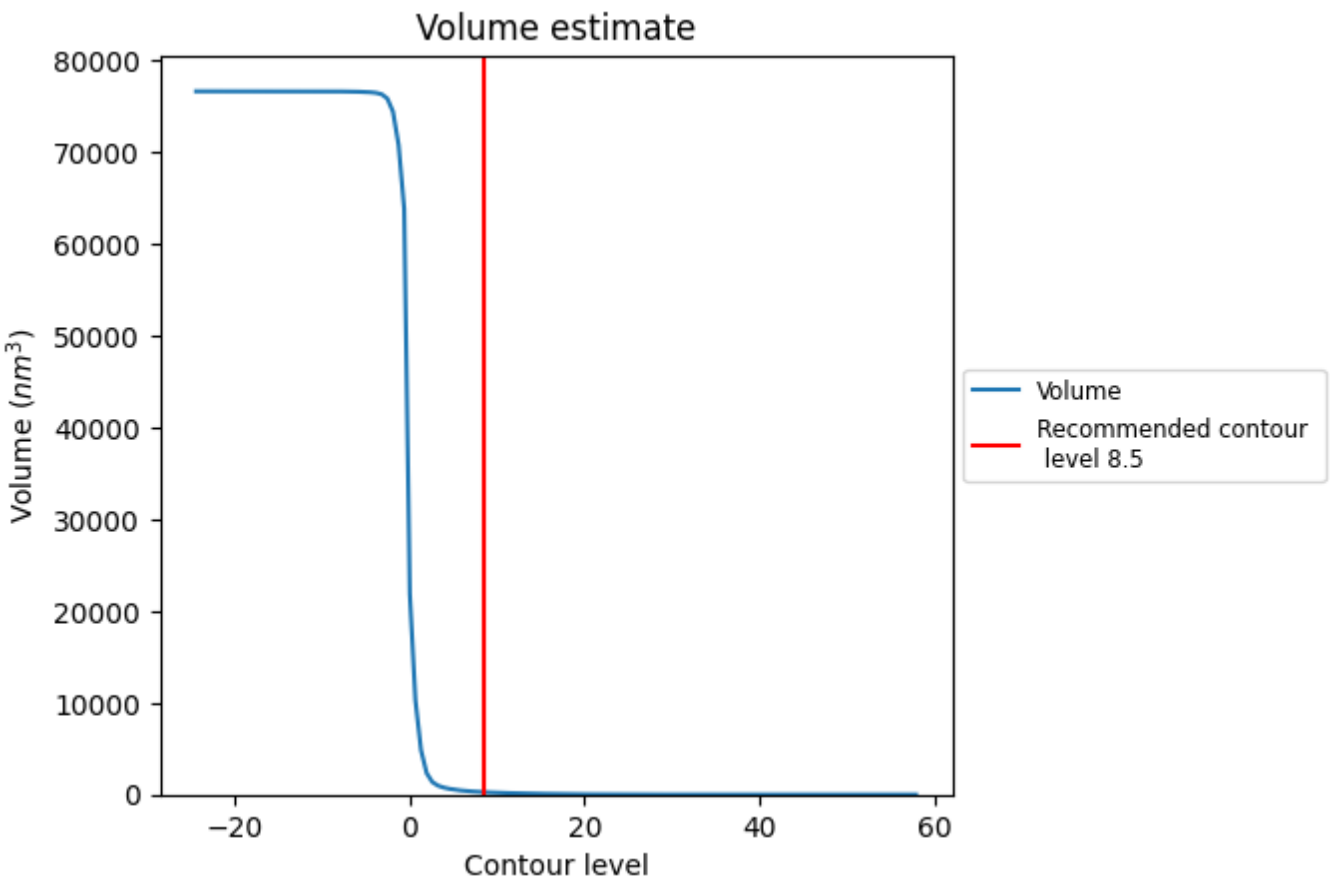
This section contains the results of statistical analysis of the map.

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.

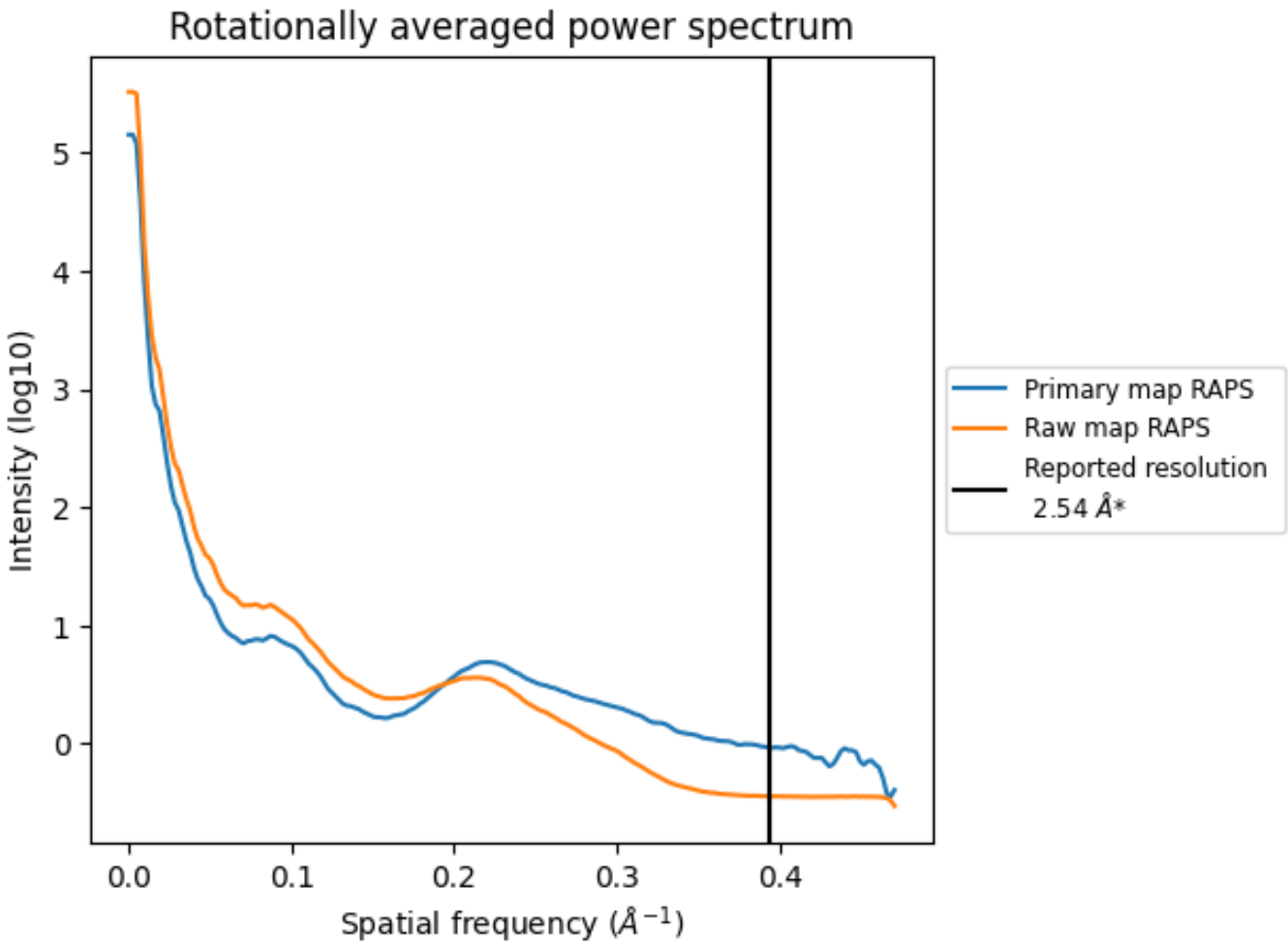
7.2 Volume estimate (i)



The volume at the recommended contour level is 261 nm^3; this corresponds to an approximate mass of 236 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

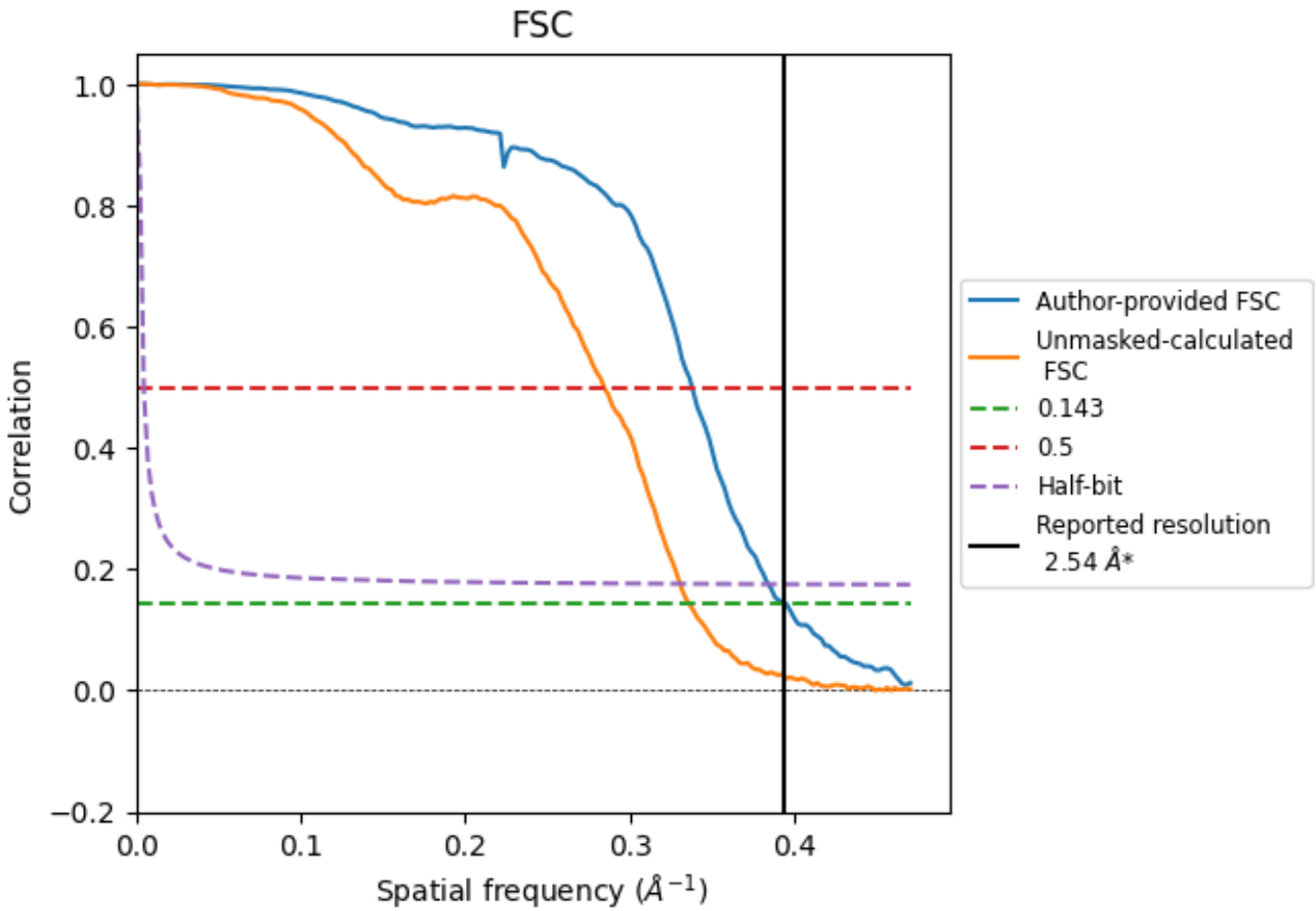


*Reported resolution corresponds to spatial frequency of 0.394 Å^{-1}

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 0.394 Å^{-1}

8.2 Resolution estimates (i)

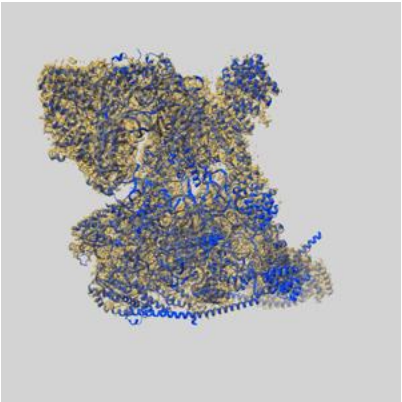
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.53	2.96	2.60
Unmasked-calculated*	2.97	3.51	3.02

*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 2.97 differs from the reported value 2.54 by more than 10 %

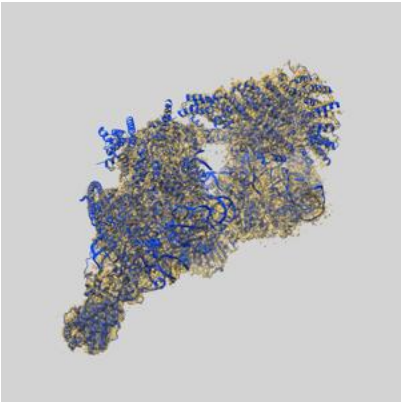
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26968 and PDB model 8CSR. Per-residue inclusion information can be found in section 3 on page 14.

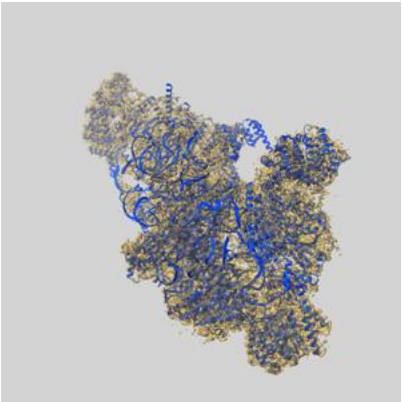
9.1 Map-model overlay (i)



X



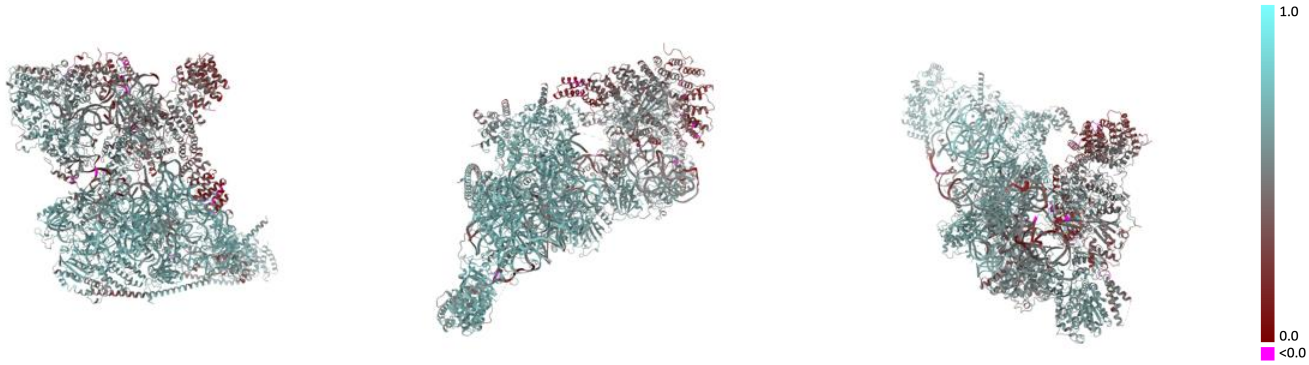
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

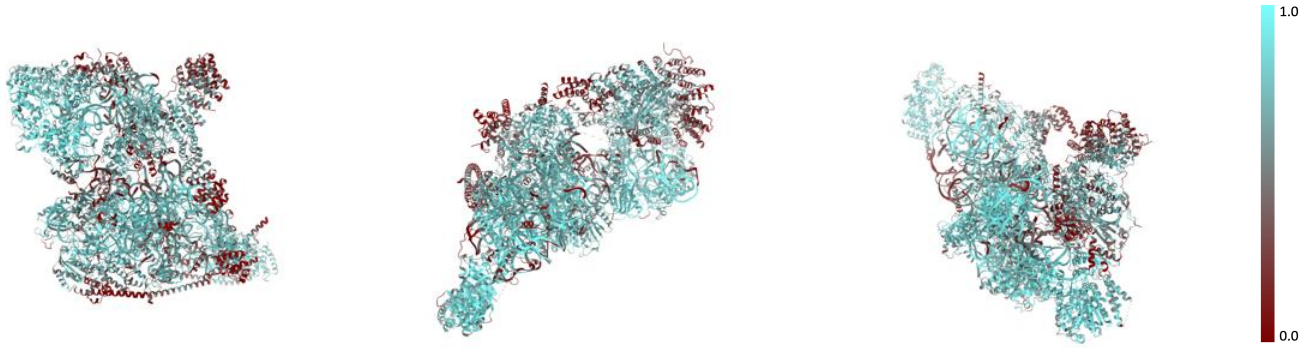
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

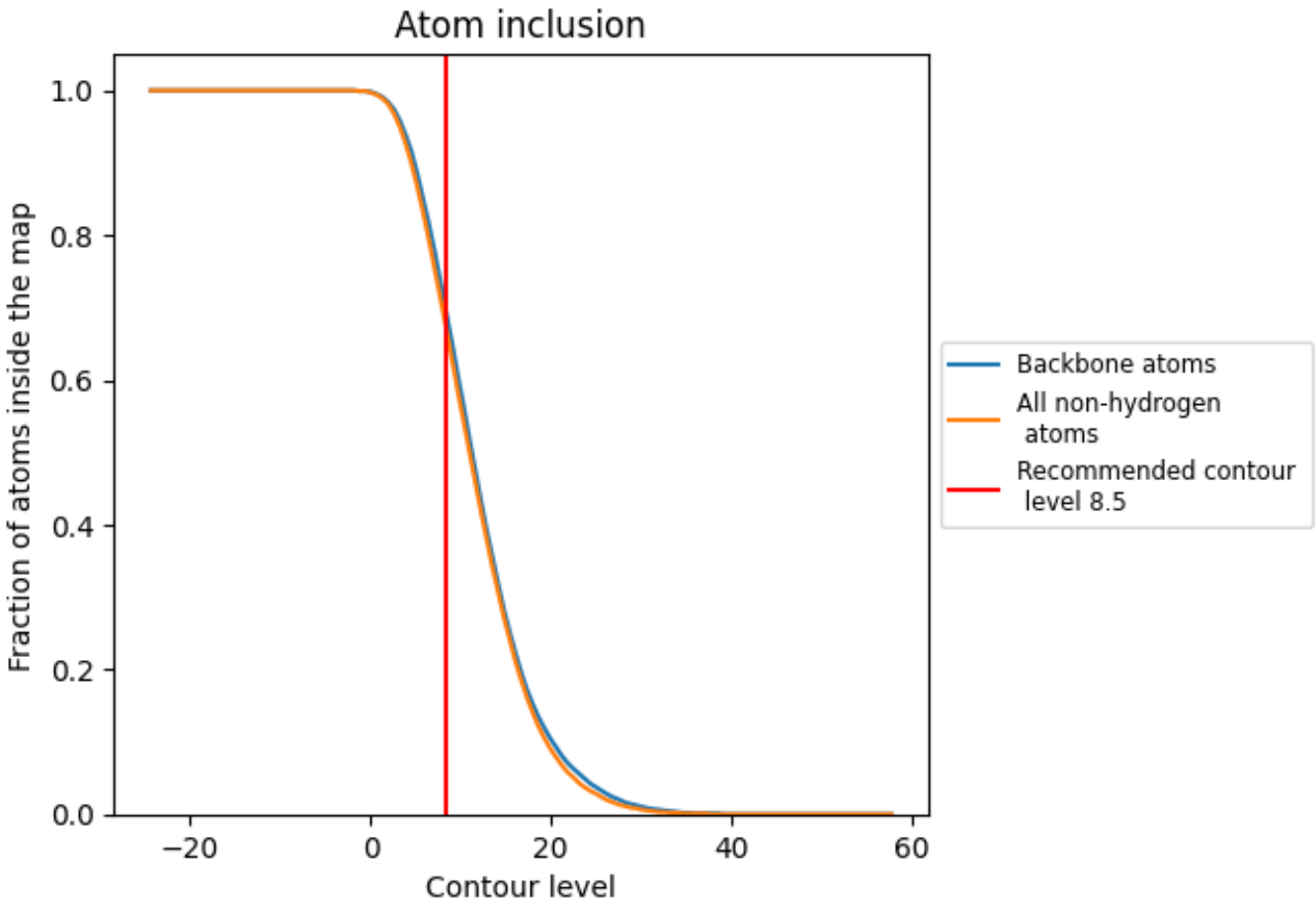
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8.5).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (8.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6660	0.5630
0	0.6440	0.6310
1	0.5770	0.4380
3	0.2770	0.5600
4	0.4490	0.3400
5	0.7610	0.6300
6	0.5220	0.5670
7	0.8320	0.5730
8	0.7850	0.4910
A	0.7420	0.5750
B	0.7650	0.6700
C	0.6440	0.4560
D	0.6800	0.6570
E	0.6500	0.6440
F	0.7530	0.5180
G	0.6260	0.5400
H	0.5680	0.4460
I	0.7550	0.6520
J	0.5640	0.6210
K	0.0750	0.2250
L	0.5220	0.6290
M	0.7950	0.6810
N	0.7000	0.6760
O	0.6210	0.6490
P	0.6870	0.6500
Q	0.7090	0.6490
R	0.4790	0.6140
S	0.5430	0.5900
T	0.6520	0.6460
U	0.4370	0.5940
V	0.7770	0.6170
W	0.6500	0.6580
X	0.8380	0.5820
Y	0.4270	0.3570
Z	0.1380	0.2860