Full wwPDB EM Validation Report ⓘ

Aug 23, 2026 – 11:32 am BST

PDB ID	:	9H54 / pdb_00009h54
EMDB ID	:	EMD-51876
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit in complex with NOA1 and partial RBFA (state N2)
Authors	:	Singh, V.; Shiriaev, D.; Khawaja, A.; Rorbach, J.
Deposited on	:	2024-10-22
Resolution	:	3.00 Å(reported)

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:

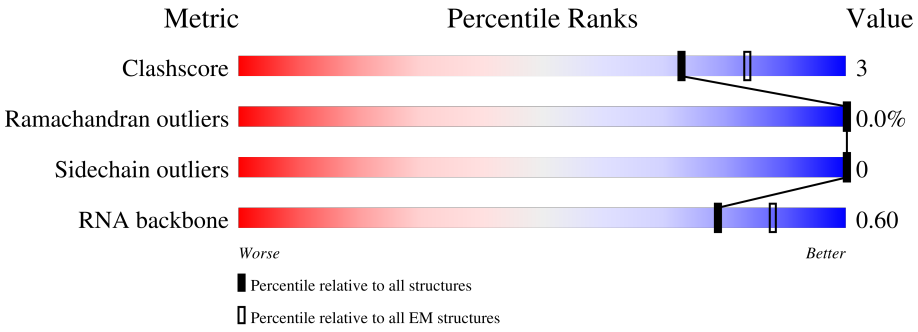
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

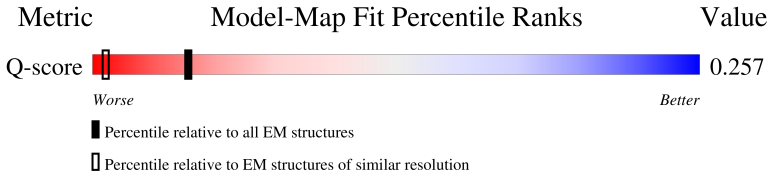
1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.





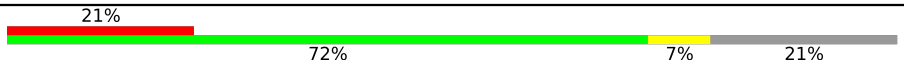
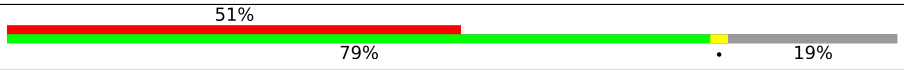
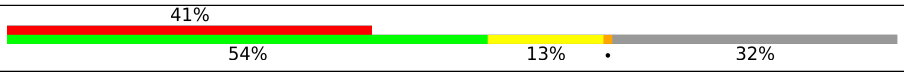
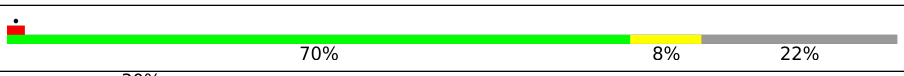
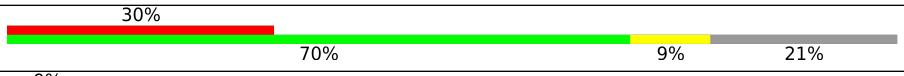
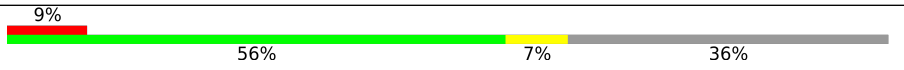
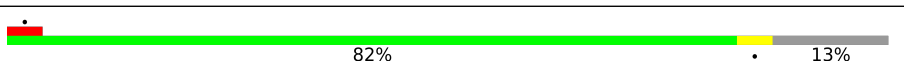
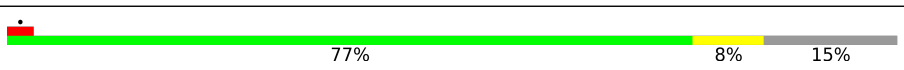
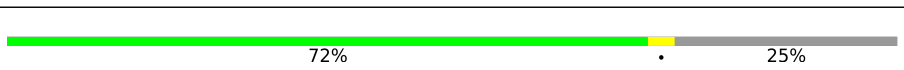
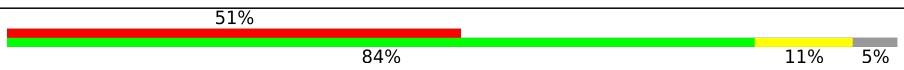
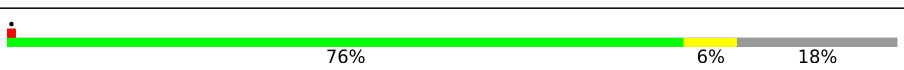
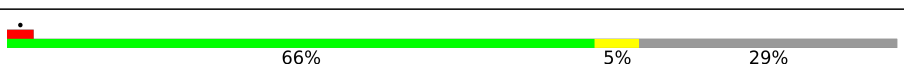
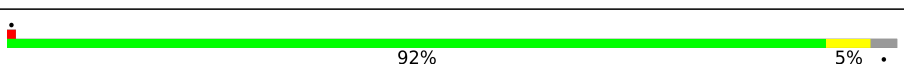
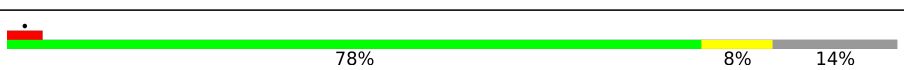
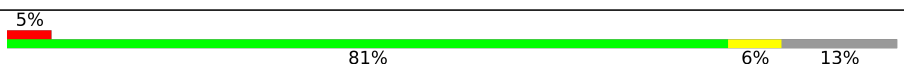
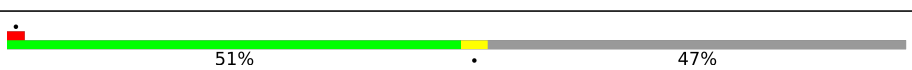
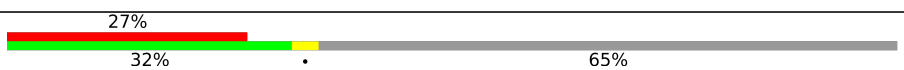
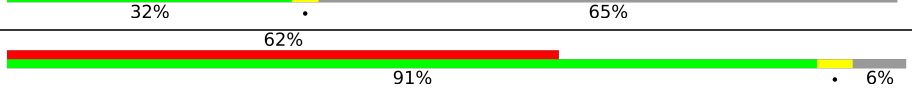
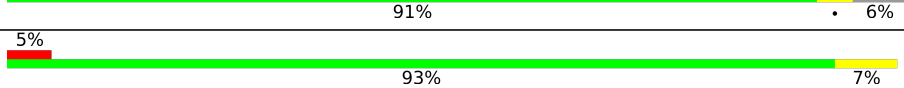
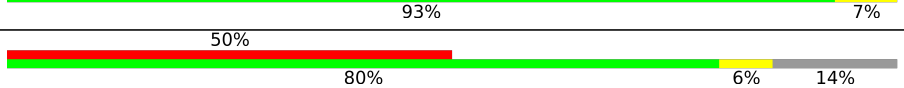
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	A	955	13% 67% 15% • 16%
2	B	296	• 73% • 24%
3	C	167	32% 65% 12% 23%

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Mol	Chain	Length	Quality of chain
4	D	430	
5	E	125	
6	F	242	
7	G	396	
8	H	201	
9	I	194	
10	J	138	
11	K	128	
12	L	257	
13	M	137	
14	N	130	
15	O	258	
16	P	142	
17	Q	87	
18	R	360	
19	S	190	
20	T	173	
21	U	205	
22	V	414	
23	W	187	
24	X	398	
25	Y	395	
26	Z	106	
27	0	215	
28	1	323	

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Mol	Chain	Length	Quality of chain
29	4	689	71% 76% 10% 14%
30	9	698	31% 50% 9% 41%
31	a	343	95%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	FES	P	201	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 122384 atoms, of which 57290 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	801	25644	7627	8633	3067	5516	801	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	225	3654	1164	1826	331	323	10	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	128	2099	677	1052	185	181	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	340	5479	1695	2775	512	484	13	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	109	1747	544	882	158	159	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	196	3296	1031	1677	292	285	11	1	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	313	Total	C	H	N	O	S	0	0
			5147	1637	2570	456	470	14		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	140	Total	C	H	N	O	S	0	0
			2343	745	1191	194	210	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	131	Total	C	H	N	O	S	0	0
			1964	609	998	178	175	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	108	Total	C	H	N	O	S	0	0
			1731	521	892	169	143	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	101	Total	C	H	N	O	S	0	0
			1751	537	889	179	141	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	164	Total	C	H	N	O	S	0	0
			2851	882	1467	256	239	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1914	594	972	185	157	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	110	Total	C	H	N	O	S	0	0
			1801	562	933	156	147	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	193	Total	C	H	N	O	S	0	0
			3158	1014	1566	294	277	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	97	Total	C	H	N	O	S	0	0
			1590	501	809	134	138	8		

- Molecule 17 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	83	Total	C	H	N	O	S	0	0
			1425	431	723	145	118	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	295	Total	C	H	N	O	S	0	0
			4845	1533	2436	413	455	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	135	Total	C	H	N	O	S	0	0
			2228	716	1117	198	196	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	176	Total	C	H	N	O	S	0	0
			2993	916	1505	301	267	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	362	Total	C	H	N	O	S	0	0
			5941	1904	2972	495	558	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	100	Total	C	H	N	O	S	0	0
			1595	498	806	141	146	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	352	Total	C	H	N	O	S	0	0
			5707	1822	2858	499	517	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	138	Total	C	H	N	O	S	0	0
			2293	753	1127	195	214	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	100	Total	C	H	N	O	S	0	0
			1701	534	862	153	148	4		

- Molecule 27 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	0	215	Total	C	H	N	O	S	0	0
			3589	1130	1802	339	313	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	278	Total	C	H	N	O	S	0	0
			4550	1430	2294	386	429	11		

- Molecule 29 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	590	Total	C	H	N	O	S	0	0
			9572	3056	4797	809	882	28		

- Molecule 30 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	9	415	Total	C	H	N	O	S	0	0
			6647	2103	3374	576	582	12		

- Molecule 31 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	16	Total	C	H	N	O	0	0
			182	82	58	18	24		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	40	Total	Mg	0
			40	40	
32	B	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
32	X	1	Total Mg 1 1	0

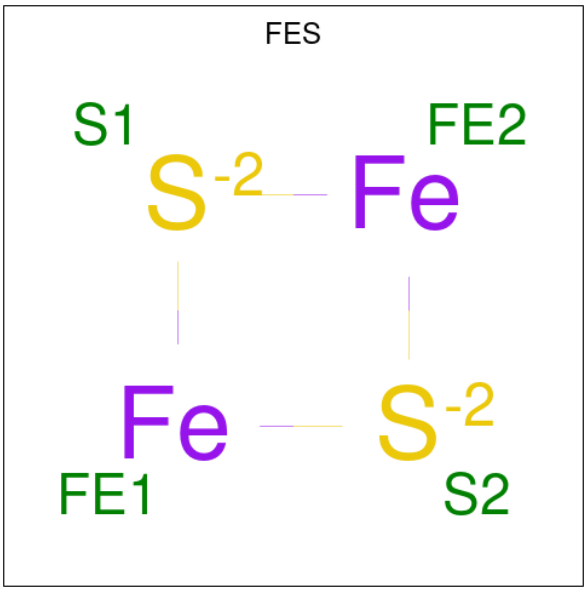
- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
33	A	11	Total K 11 11	0

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

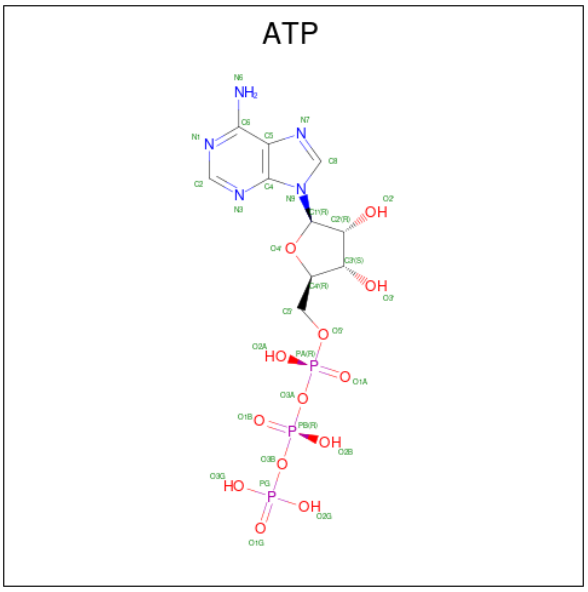
Mol	Chain	Residues	Atoms	AltConf
34	O	1	Total Zn 1 1	0

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



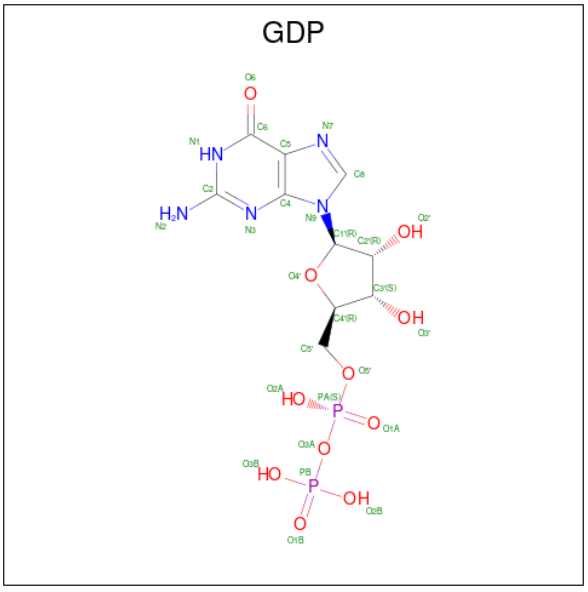
Mol	Chain	Residues	Atoms	AltConf
35	P	1	Total Fe S 4 2 2	0
35	T	1	Total Fe S 4 2 2	0

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
36	X	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 37 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						AltConf
37	X	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	
37	9	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

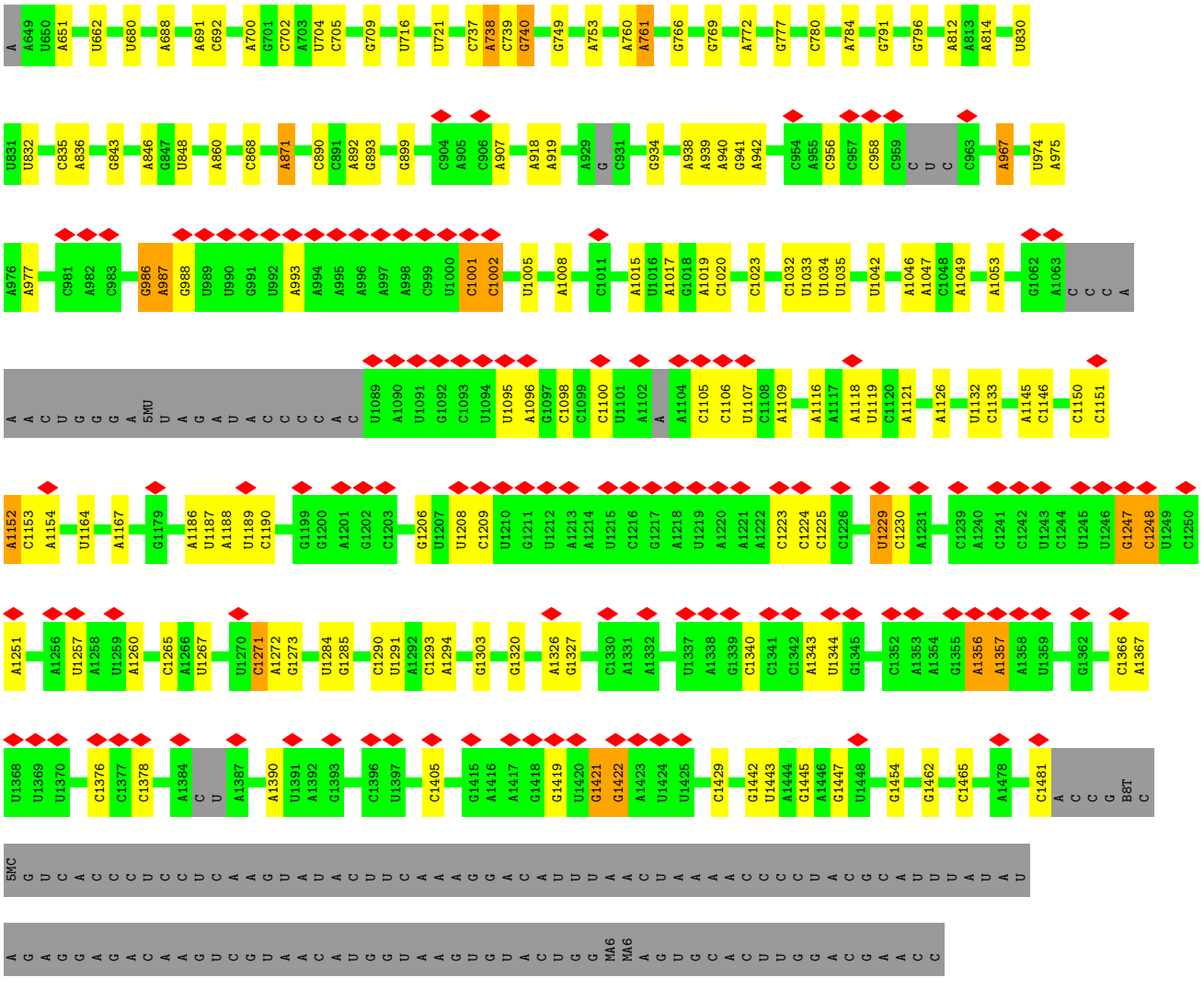
3 Residue-property plots (i)

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: 12S mitochondrial rRNA

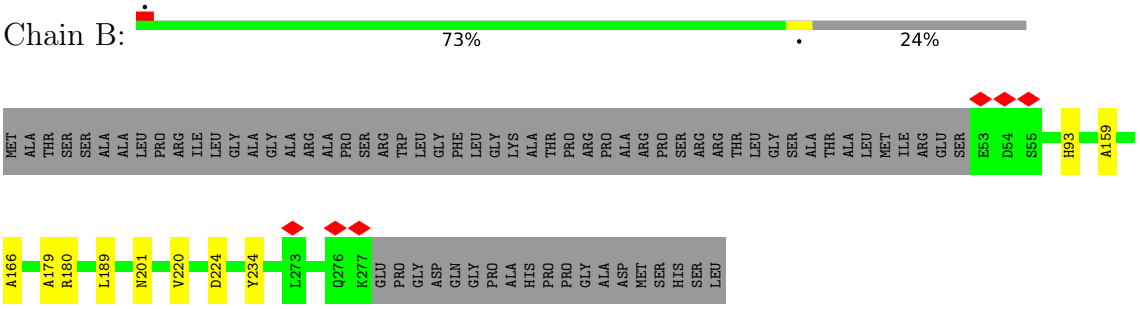
Chain A:





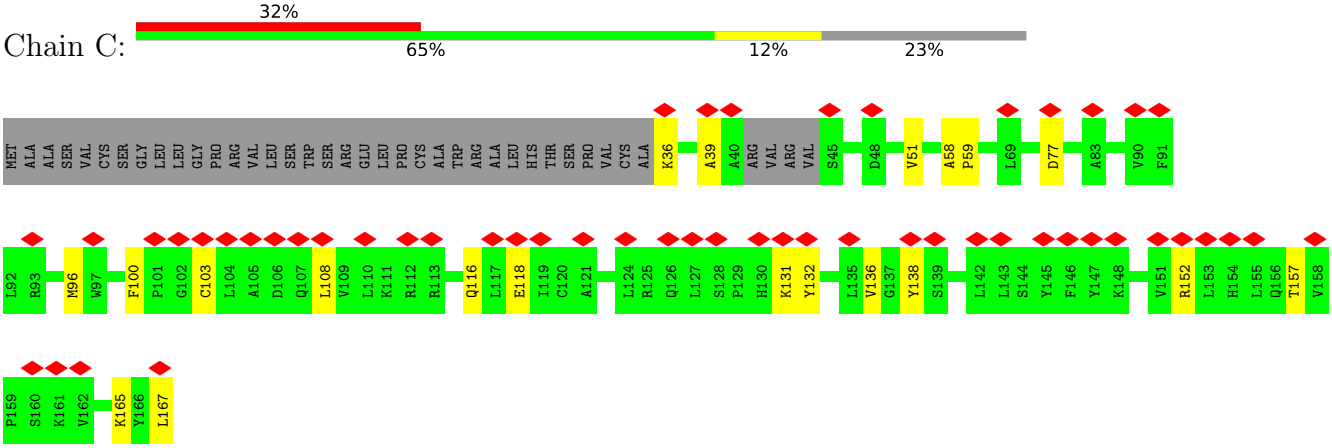
• Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:



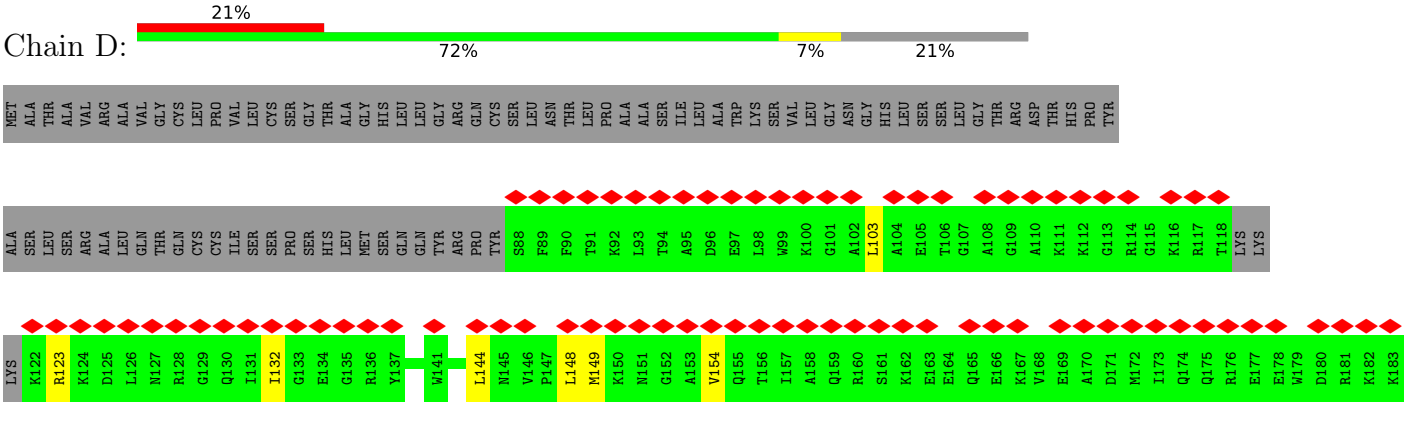
• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:



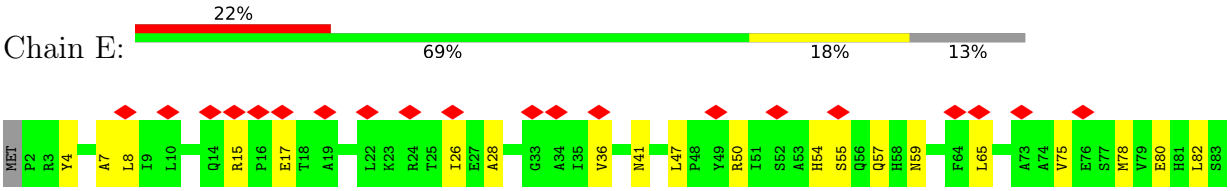
• Molecule 4: 28S ribosomal protein S5, mitochondrial

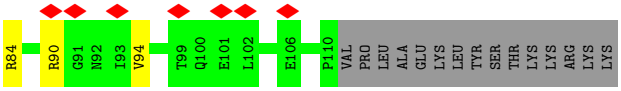
Chain D:



• Molecule 5: 28S ribosomal protein S6, mitochondrial

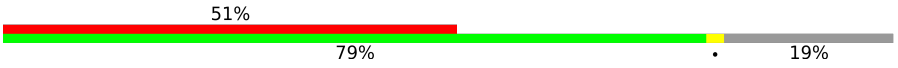
Chain E:

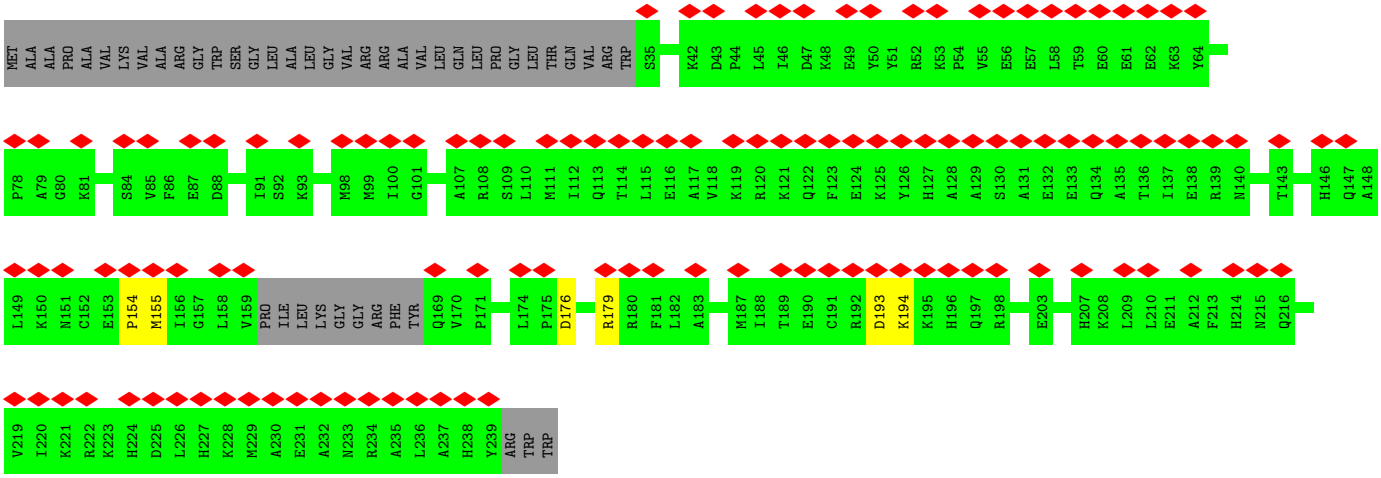




• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:

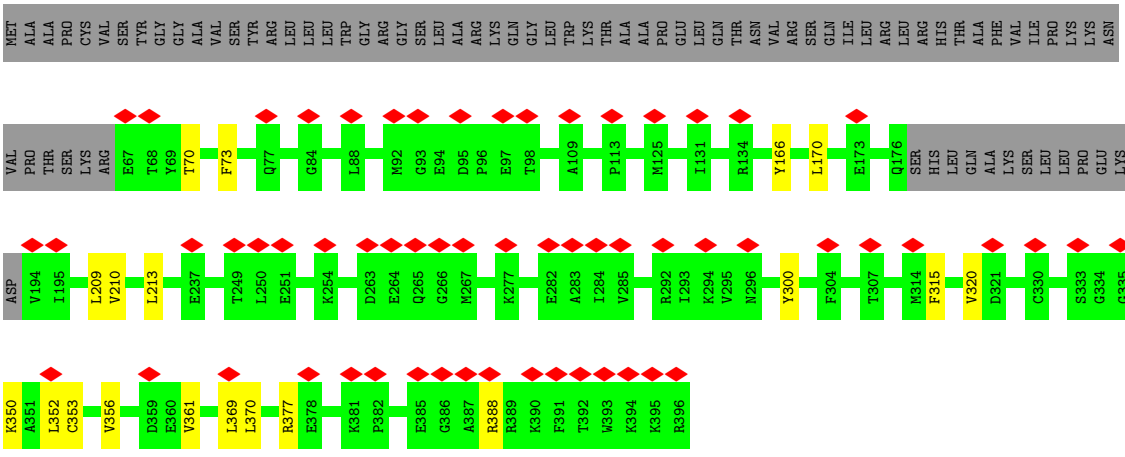




• Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G:

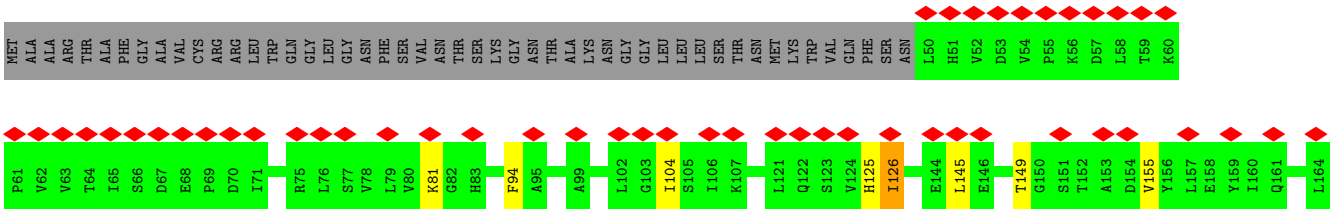


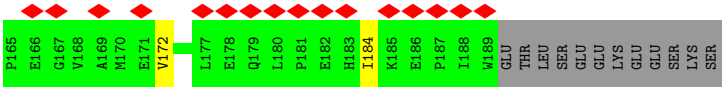


• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



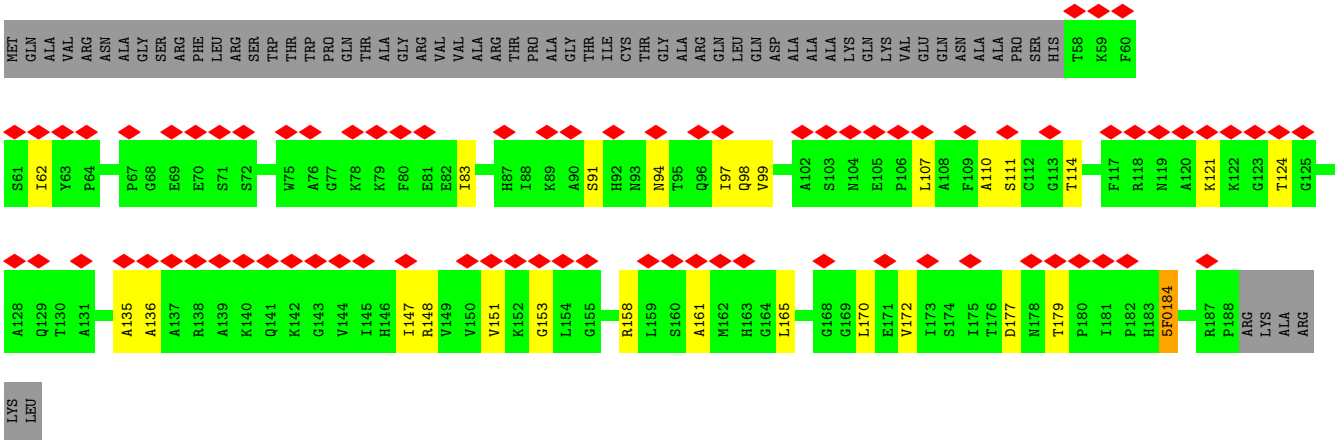




• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:

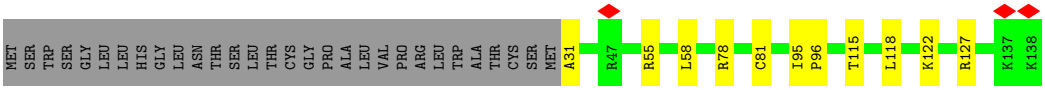




• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:

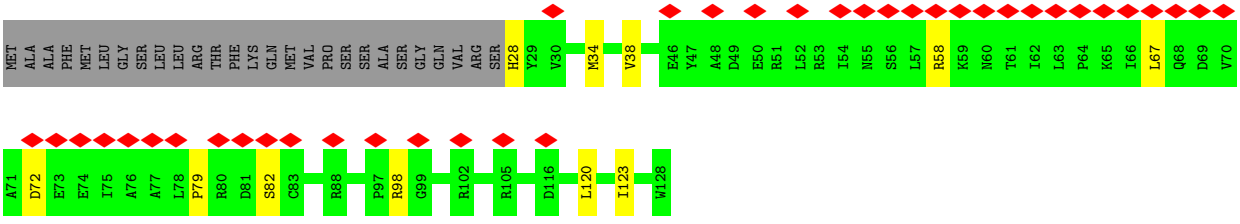




• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:

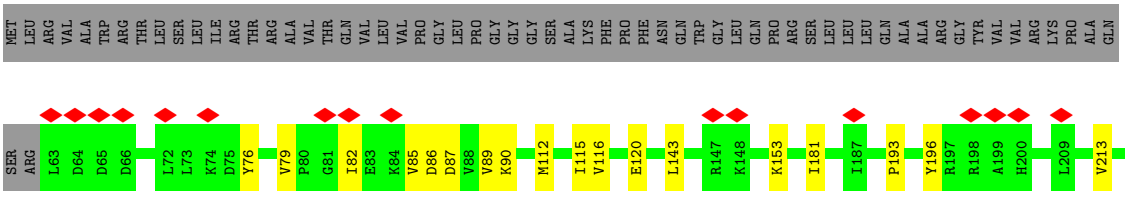


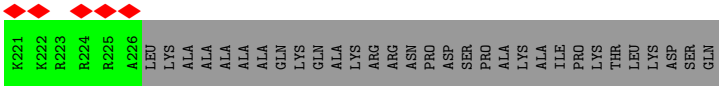


• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L:



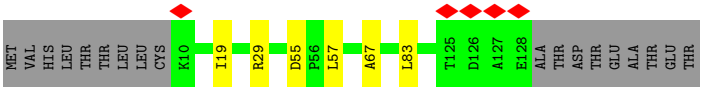




• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain M:

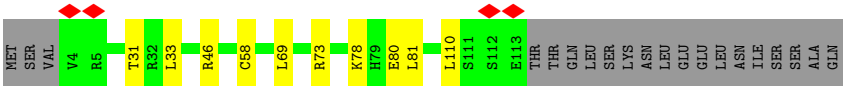




• Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain N:

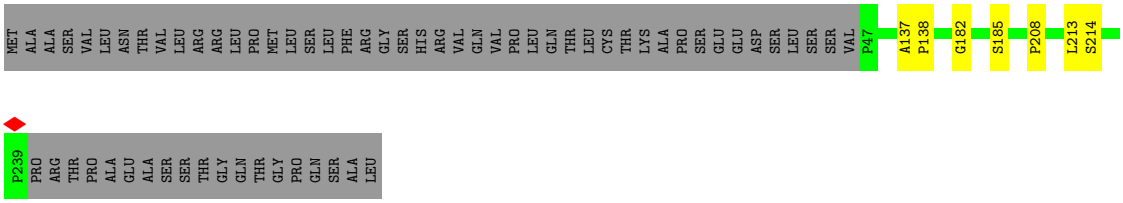




• Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain O:

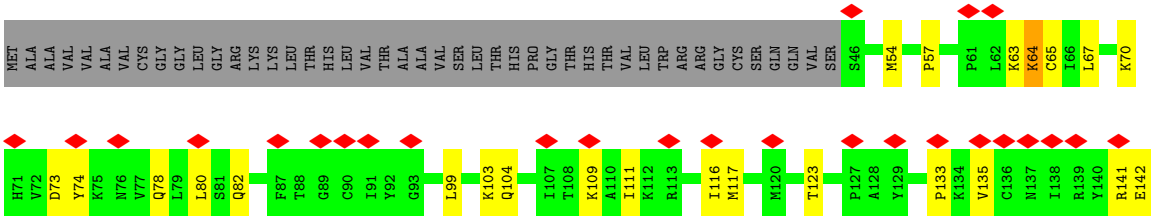




• Molecule 16: 28S ribosomal protein S18c, mitochondrial

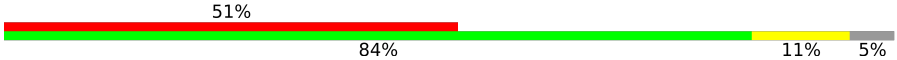
Chain P:

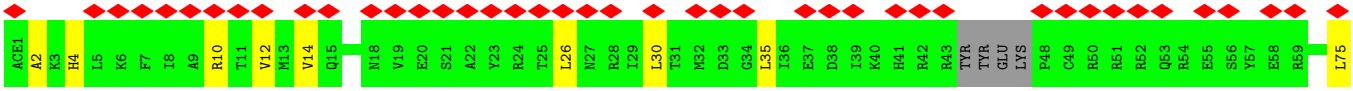




• Molecule 17: Small ribosomal subunit protein bS21m

Chain Q:

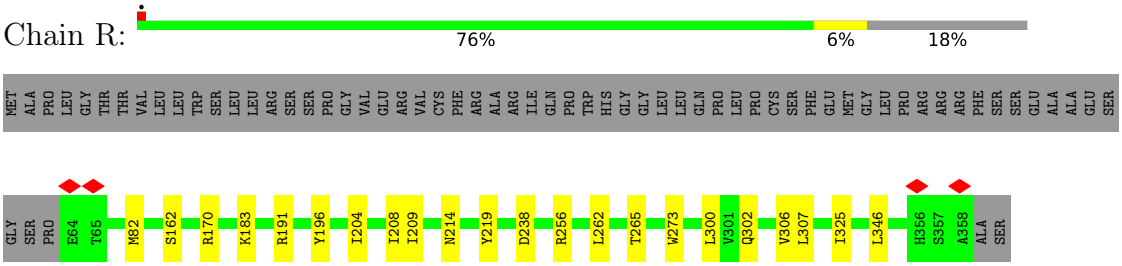






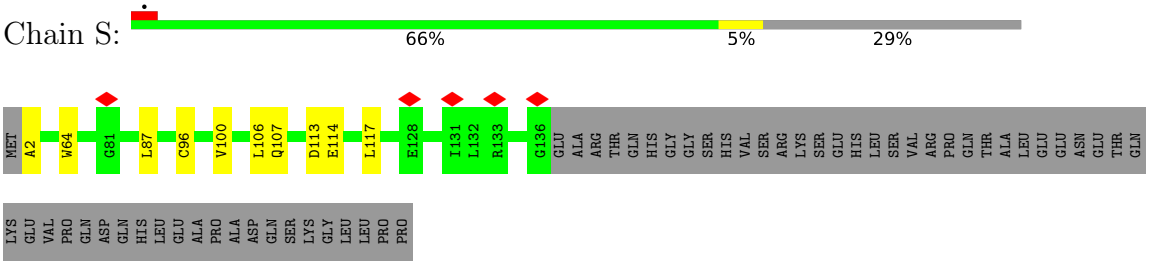
• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:



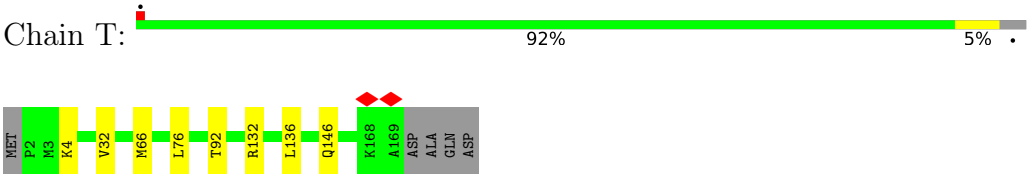
• Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S:



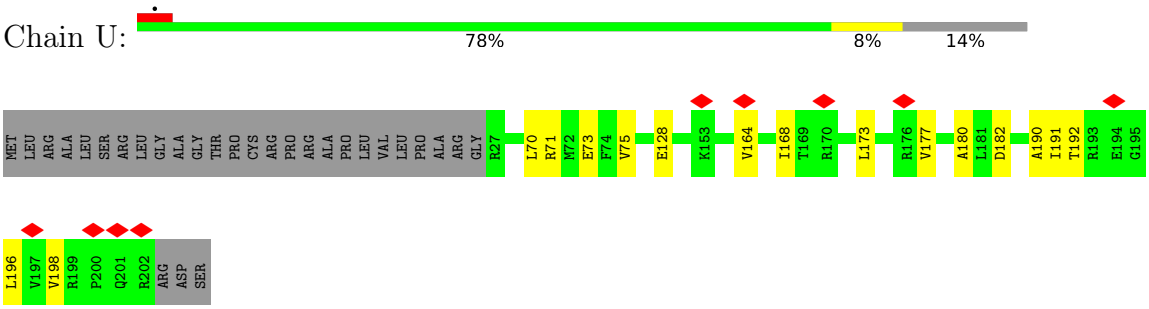
• Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T:



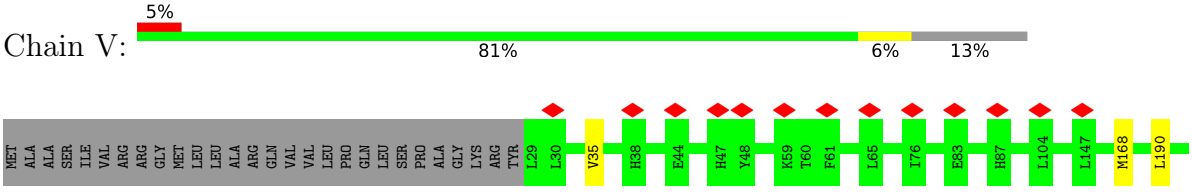
• Molecule 21: 28S ribosomal protein S26, mitochondrial

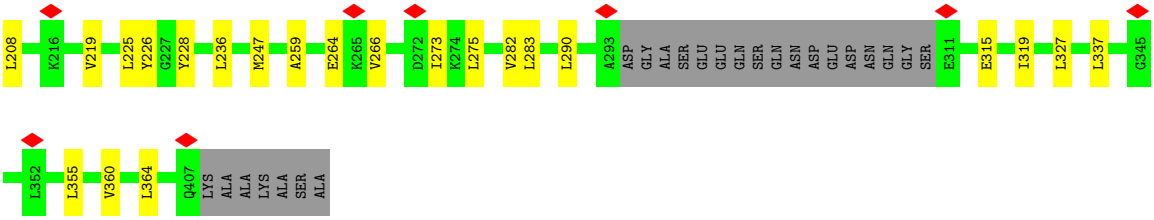
Chain U:



• Molecule 22: 28S ribosomal protein S27, mitochondrial

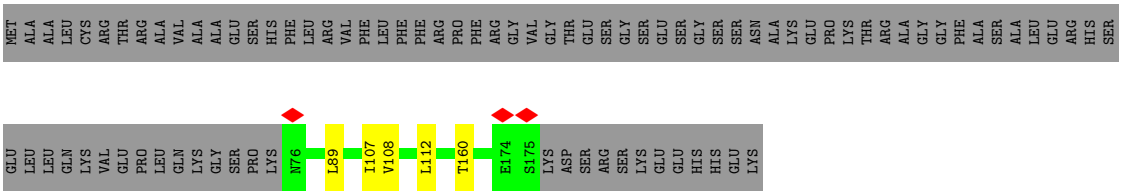
Chain V:



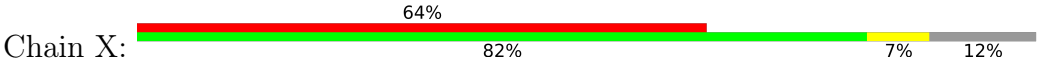


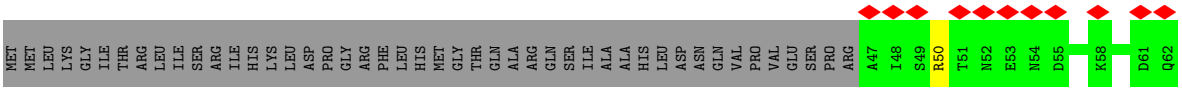
• Molecule 23: 28S ribosomal protein S28, mitochondrial

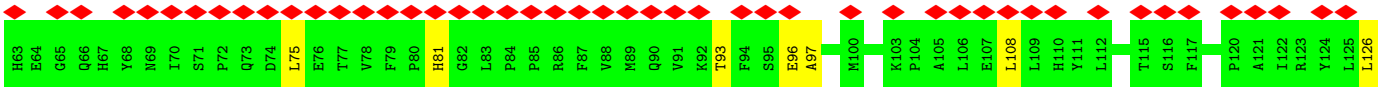


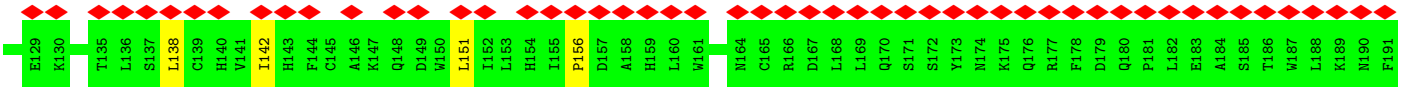


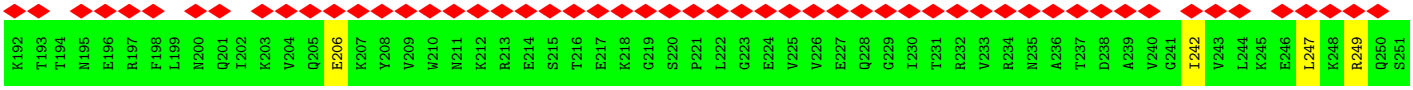
• Molecule 24: 28S ribosomal protein S29, mitochondrial

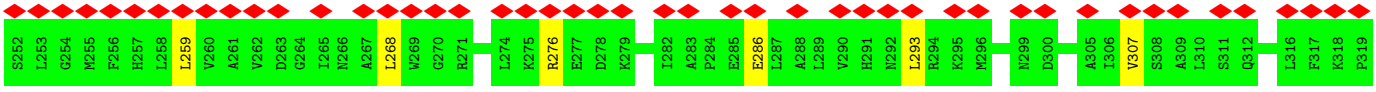


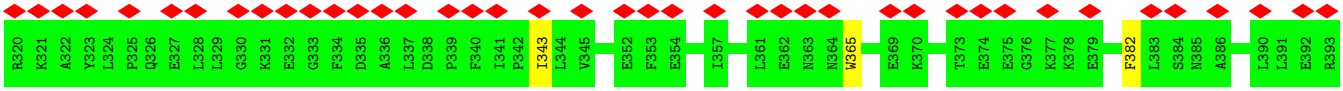


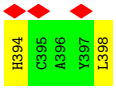






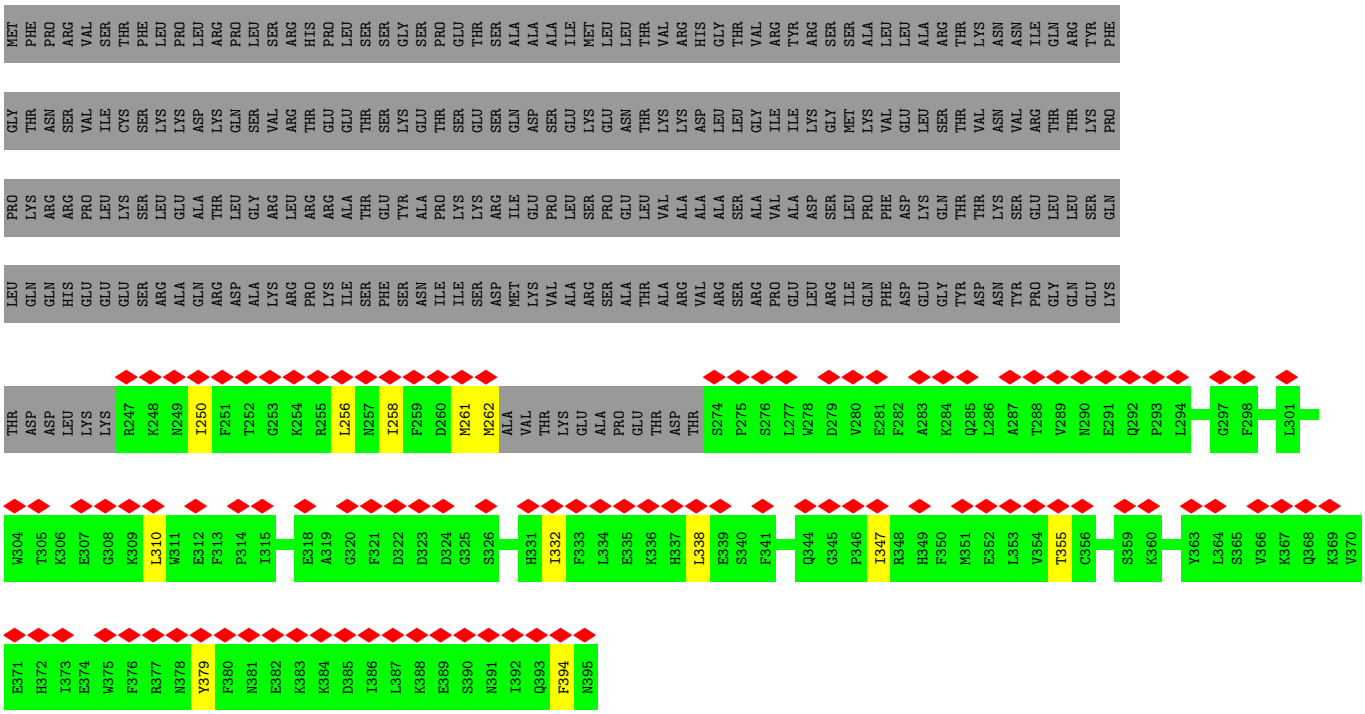






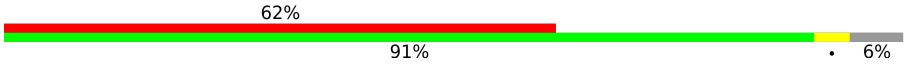
• Molecule 25: 28S ribosomal protein S31, mitochondrial

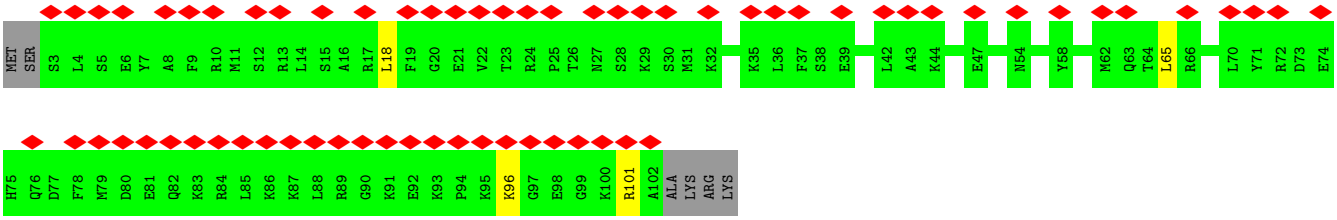




• Molecule 26: 28S ribosomal protein S33, mitochondrial

Chain Z:

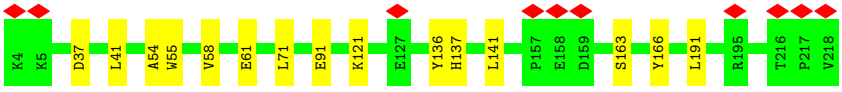




• Molecule 27: Small ribosomal subunit protein mS34

Chain 0:

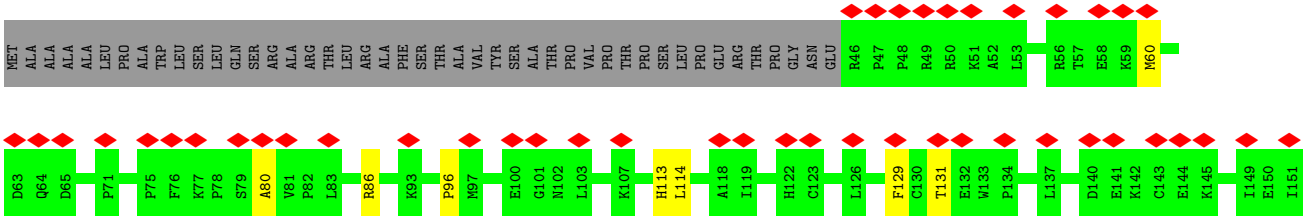


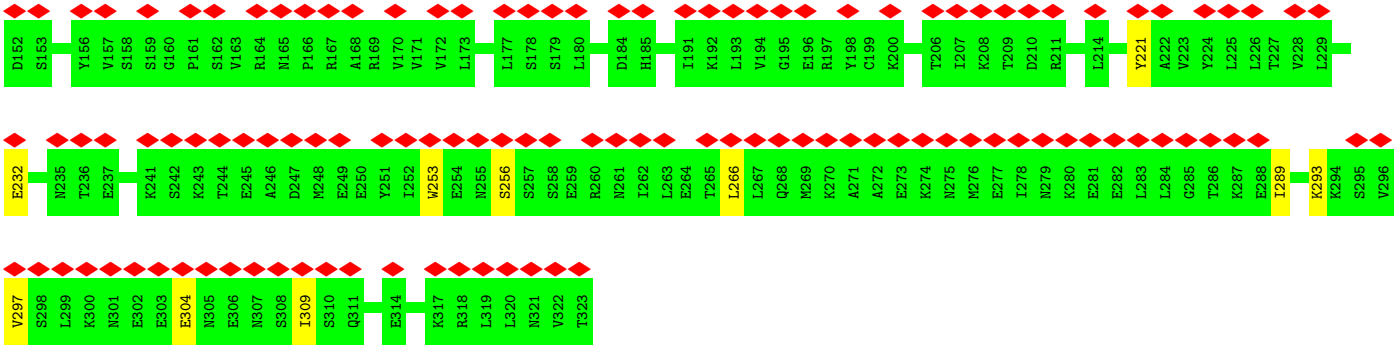


• Molecule 28: 28S ribosomal protein S35, mitochondrial

Chain 1:





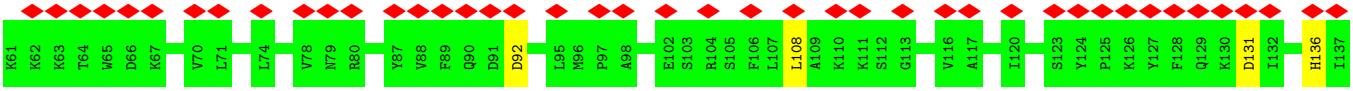


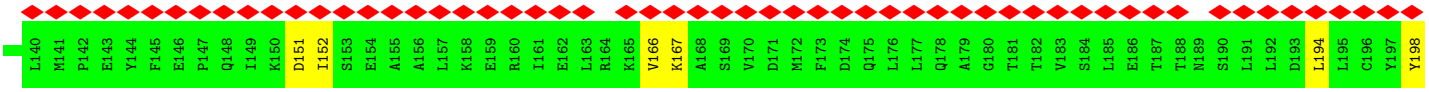
• Molecule 29: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

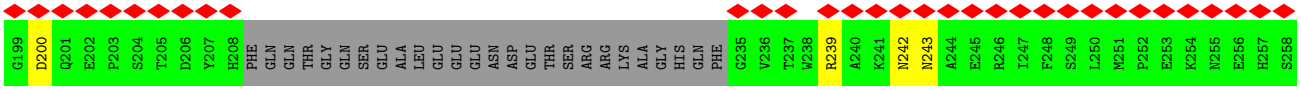
Chain 4:

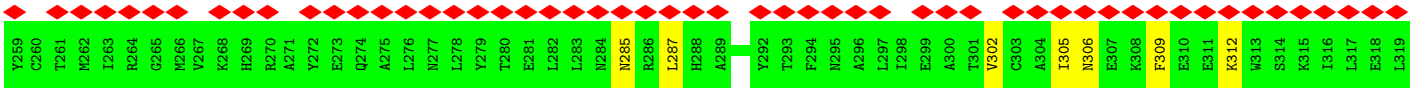


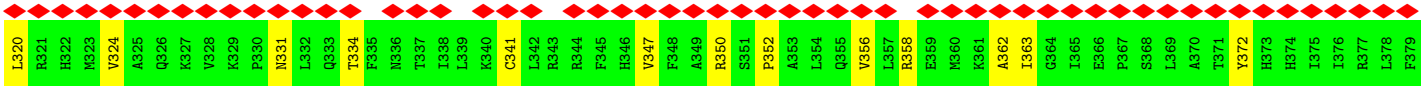


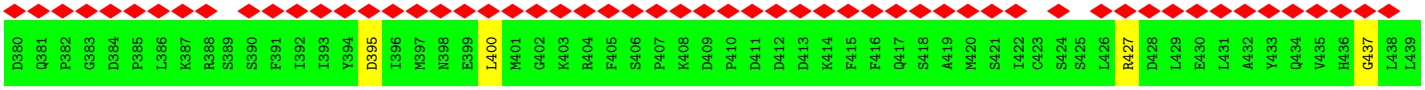


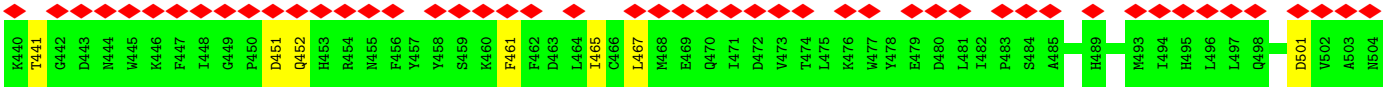


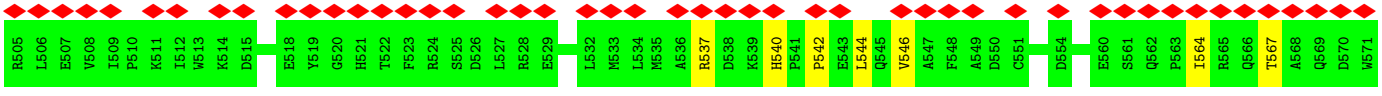


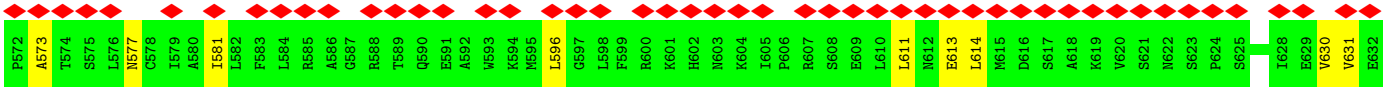


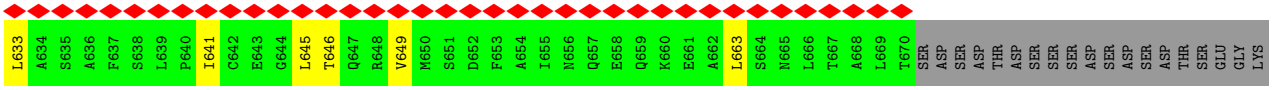








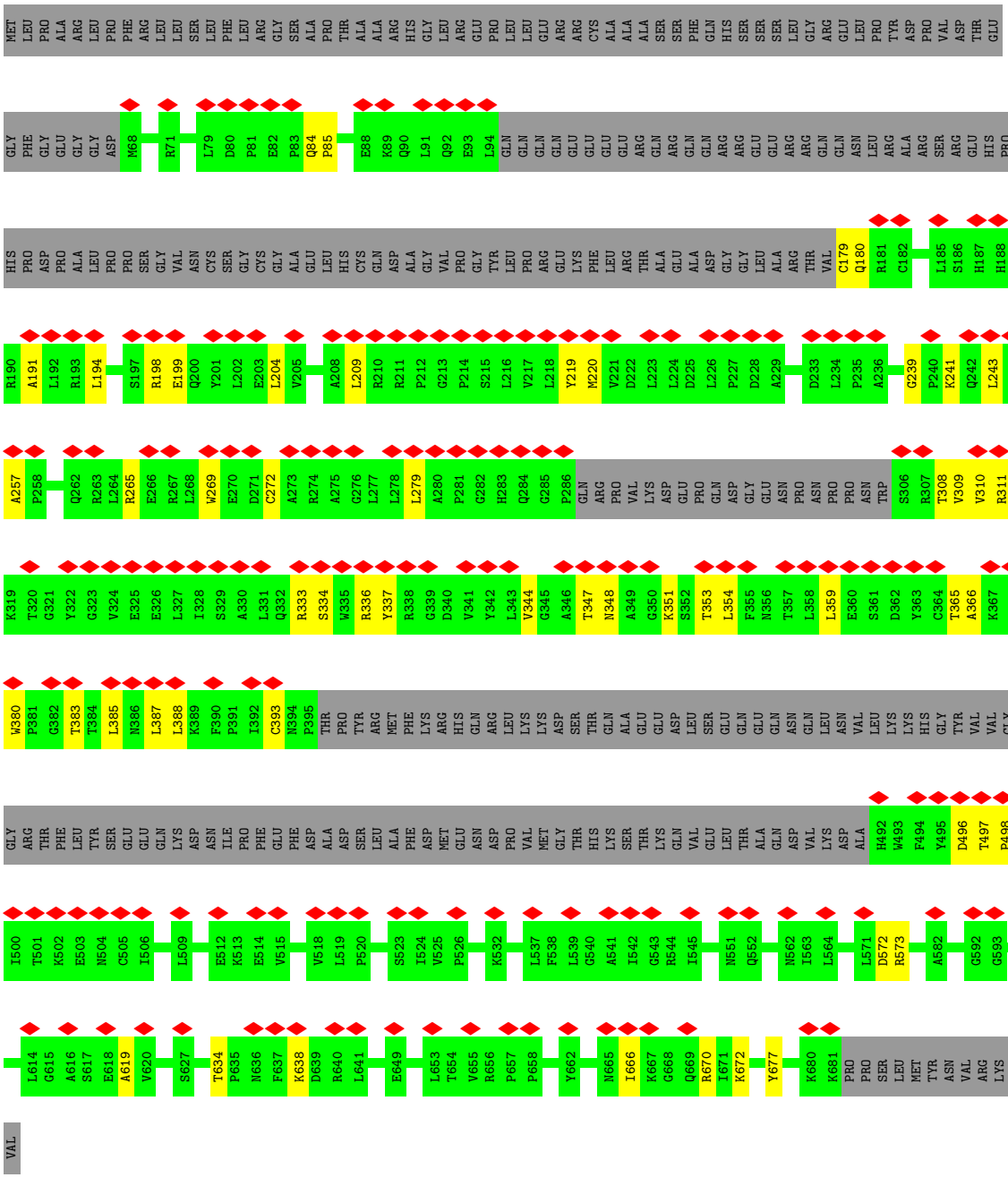




• Molecule 30: Nitric oxide-associated protein 1

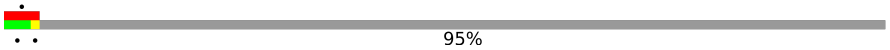
Chain 9:

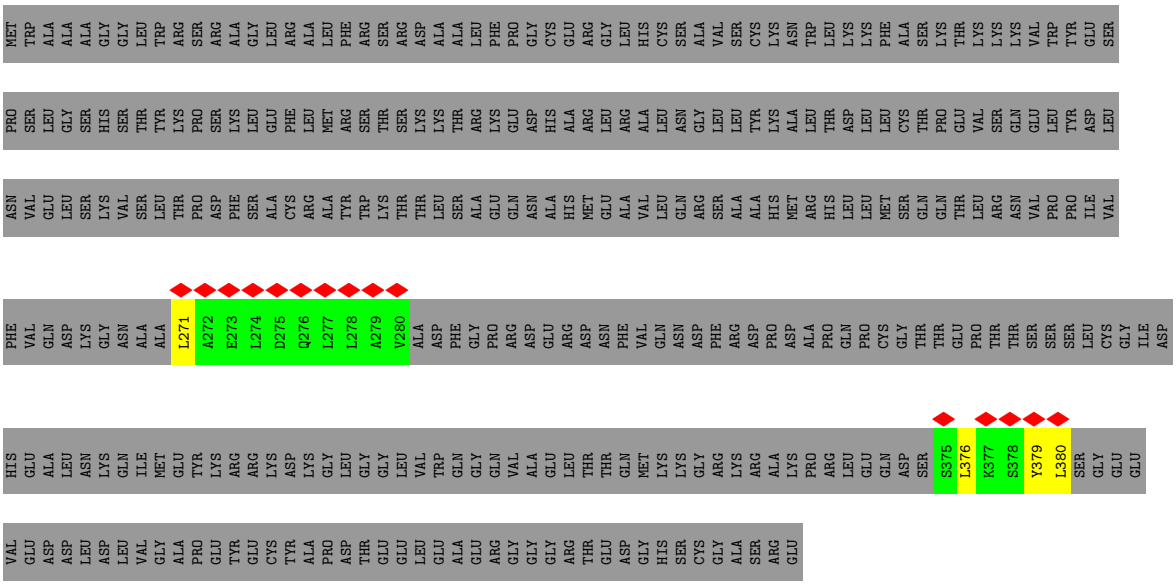




• Molecule 31: Putative ribosome-binding factor A, mitochondrial

Chain a:




MET TRP ALA ALA ALA GLY GLY LEU TRP ARG SER ARG ALA GLY LEU ARG ALA LEU PHE ARG SER ARG ASP ALA ALA LEU PHE PRO GLY CYS GLU ARG GLY LEU HIS CYS SER ALA VAL SER CYS LYS ASN TRP LEU LYS LYS PHE ALA SER LYS THR LYS LYS LYS VAL TRP TYR GLU SER
PRO SER LEU GLY SER HIS SER THR TYR LYS PRO SER LYS LEU GLU PHE LEU MET ARG SER THR SER LYS LYS THR ARG LYS GLU ASP HIS ALA ARG LEU ARG ALA LEU ASN GLY LEU LEU TYR LYS ALA LEU THR ASP LEU LEU CYS THR PRO GLU VAL SER GLN GLU LEU TYR ASP LEU
ASN VAL GLU LEU SER LYS VAL SER LEU THR PRO ASP PHE SER ALA CYS ARG ALA TYR TRP LYS THR THR LEU SER ALA GLU GLN ASN ALA HIS MET GLU ALA VAL LEU GLN ARG SER ALA ALA HIS MET ARG HIS LEU LEU MET SER GLN GLN THR LEU ARG ASN VAL PRO PRO ILE VAL
PHE VAL GLN ASP LYS GLY ASN ALA ALA L271 A272 E273 L274 D275 Q276 L277 L278 A279 V280 ALA ASP PHE GLY PRO ARG ASP GLU ARG ASP ASN PHE VAL GLN ASN ASP PHE ARG ASP PRO ASP ALA PRO GLN PRO CYS GLY THR THR GLU PRO THR THR SER SER SER LEU CYS GLY ILE ASP
HIS GLU ALA LEU ASN LYS GLN ILE MET GLU TYR LYS ARG ARG LYS ASP LYS GLY LEU GLY GLY LEU VAL TRP GLN GLY GLN VAL ALA GLU LEU THR THR GLN MET LYS LYS GLY ARG LYS ARG ALA LYS PRO ARG LEU GLU GLN ASP SER S375 L376 K377 S378 Y379 L380 SER GLY GLU GLU
VAL GLU ASP ASP LEU ASP LEU VAL GLY ALA PRO GLU TYR GLU CYS TYR ALA PRO ASP THR GLU GLU LEU GLU ALA GLU ARG GLY GLY GLY ARG THR GLU ASP GLY HIS SER CYS GLY ALA SER ARG GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33988	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	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: ACE, ZN, GDP, 5F0, FES, MG, ATP, 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	A	0.13	0/19025	0.22	0/29610
2	B	0.12	0/1871	0.25	0/2531
3	C	0.11	0/1076	0.25	0/1454
4	D	0.12	0/2755	0.25	0/3688
5	E	0.09	0/880	0.25	0/1189
6	F	0.08	0/1653	0.21	0/2218
7	G	0.10	0/2632	0.22	0/3527
8	H	0.11	0/1178	0.25	0/1598
9	I	0.10	0/976	0.27	0/1318
10	J	0.11	0/855	0.24	0/1148
11	K	0.09	0/880	0.21	0/1182
12	L	0.09	0/1408	0.22	0/1882
13	M	0.14	0/963	0.27	0/1295
14	N	0.12	0/886	0.26	0/1199
15	O	0.12	0/1648	0.25	0/2243
16	P	0.10	0/798	0.28	0/1070
17	Q	0.14	0/709	0.26	0/940
18	R	0.13	0/2456	0.25	0/3317
19	S	0.11	0/1138	0.22	0/1533
20	T	0.12	0/1402	0.25	0/1883
21	U	0.11	0/1510	0.23	0/2025
22	V	0.11	0/3030	0.24	0/4093
23	W	0.09	0/801	0.23	0/1079
24	X	0.09	0/2921	0.24	0/3954
25	Y	0.10	0/1198	0.22	0/1610
26	Z	0.09	0/857	0.20	0/1141
27	0	0.12	0/1834	0.27	0/2484
28	1	0.09	0/2304	0.22	0/3117
29	4	0.08	0/4883	0.22	0/6608
30	9	0.11	0/3347	0.29	0/4548
31	a	0.08	0/123	0.20	0/164
All	All	0.11	0/67997	0.24	0/95648

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	184	5F0	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17011	8633	8642	64	0
2	B	1828	1826	1815	8	0
3	C	1047	1052	1043	15	0
4	D	2704	2775	2764	25	0
5	E	865	882	878	19	0
6	F	1619	1677	1666	4	0
7	G	2577	2570	2560	12	0
8	H	1152	1191	1183	9	0
9	I	966	998	985	17	0
10	J	839	892	887	8	0
11	K	862	889	885	7	0
12	L	1384	1467	1462	12	0
13	M	942	972	965	4	0
14	N	868	933	928	7	0
15	O	1592	1566	1557	5	0
16	P	781	809	806	22	0
17	Q	702	723	721	9	0
18	R	2409	2436	2428	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	1111	1117	1115	7	0
20	T	1371	1396	1393	6	0
21	U	1488	1505	1499	24	0
22	V	2969	2972	2961	16	0
23	W	789	806	802	4	0
24	X	2849	2858	2843	16	0
25	Y	1166	1127	1120	14	0
26	Z	839	862	858	5	0
27	0	1787	1802	1796	11	0
28	1	2256	2294	2288	13	0
29	4	4775	4797	4779	49	0
30	9	3273	3374	3366	46	0
31	a	124	58	133	7	0
32	A	40	0	0	0	0
32	B	1	0	0	0	0
32	X	1	0	0	0	0
33	A	11	0	0	0	0
34	O	1	0	0	0	0
35	P	4	0	0	2	0
35	T	4	0	0	0	0
36	X	31	11	12	0	0
37	9	28	10	12	1	0
37	X	28	10	12	2	0
All	All	65094	57290	57164	396	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 (396) 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)
1:A:1152:A:O2'	1:A:1153:C:O4'	1.96	0.82
1:A:1230:C:O3'	11:K:98:ARG:NH1	2.16	0.78
1:A:1272:A:N1	1:A:1303:G:O2'	2.16	0.78
2:B:180:ARG:NH2	4:D:211:CYS:SG	2.58	0.77
12:L:112:MET:O	12:L:116:VAL:HG22	1.85	0.76
1:A:1265:C:OP2	3:C:39:ALA:N	2.18	0.76
31:a:376:LEU:HB3	31:a:380:LEU:HG	1.67	0.75
1:A:1032:C:OP1	16:P:109:LYS:NZ	2.20	0.74
29:4:200:ASP:OD2	29:4:243:ASN:N	2.21	0.73
30:9:209:LEU:O	30:9:241:LYS:NZ	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:596:LEU:HD21	29:4:614:LEU:HD11	1.72	0.71
31:a:376:LEU:HD22	31:a:379:TYR:CD2	2.27	0.70
16:P:70:LYS:O	16:P:103:LYS:NZ	2.25	0.70
17:Q:30:LEU:HD22	17:Q:35:LEU:HD22	1.72	0.69
9:I:111:SER:OG	9:I:114:THR:HG23	1.92	0.69
11:K:58:ARG:NE	11:K:72:ASP:OD1	2.26	0.69
31:a:376:LEU:O	31:a:380:LEU:N	2.15	0.68
16:P:133:PRO:HG2	21:U:198:VAL:HG21	1.76	0.68
1:A:899:G:O2'	1:A:907:A:N1	2.26	0.67
9:I:97:ILE:HG21	9:I:165:LEU:HD21	1.74	0.67
6:F:176:ASP:OD1	6:F:179:ARG:NH2	2.29	0.65
1:A:977:A:OP2	17:Q:2:ALA:HB2	1.96	0.65
13:M:55:ASP:OD2	20:T:146:GLN:NE2	2.30	0.65
16:P:65:CYS:SG	35:P:201:FES:S1	2.94	0.65
7:G:320:VAL:HG21	7:G:352:LEU:HD21	1.79	0.65
1:A:1005:U:O4'	9:I:98:GLN:NE2	2.30	0.64
16:P:80:LEU:HD22	16:P:111:ILE:HG13	1.80	0.64
1:A:974:U:O2'	1:A:975:A:N7	2.32	0.62
3:C:118:GLU:OE2	3:C:152:ARG:NH2	2.31	0.62
1:A:760:A:N1	1:A:780:C:O2'	2.29	0.62
18:R:325:ILE:HG23	18:R:346:LEU:HD21	1.83	0.61
20:T:32:VAL:HG22	20:T:76:LEU:HD22	1.82	0.61
4:D:196:ASN:HA	31:a:376:LEU:HD12	1.83	0.61
1:A:1267:U:O4	3:C:36:LYS:N	2.34	0.60
21:U:192:THR:CG2	21:U:198:VAL:HG23	2.31	0.60
16:P:54:MET:HE2	19:S:64:TRP:HB3	1.82	0.60
29:4:564:ILE:HG22	29:4:567:THR:HB	1.81	0.60
29:4:501:ASP:OD2	29:4:537:ARG:NH1	2.34	0.60
1:A:843:G:N2	1:A:846:A:OP2	2.34	0.60
30:9:572:ASP:OD1	30:9:573:ARG:N	2.35	0.60
1:A:1164:U:OP1	10:J:122:LYS:NZ	2.31	0.60
9:I:110:ALA:HB3	9:I:135:ALA:HB2	1.83	0.60
3:C:131:LYS:NZ	4:D:144:LEU:O	2.35	0.60
30:9:256:ASP:OD1	30:9:257:ALA:N	2.34	0.60
1:A:769:G:OP2	14:N:73:ARG:NH2	2.35	0.60
1:A:749:G:O3'	14:N:78:LYS:NZ	2.35	0.59
30:9:220:MET:HE2	30:9:354:LEU:HD23	1.83	0.59
1:A:986:G:HO2'	1:A:987:A:P	2.24	0.59
1:A:1340:C:O2'	26:Z:101:ARG:NH2	2.35	0.59
1:A:986:G:O2'	1:A:987:A:OP1	2.14	0.59
18:R:162:SER:O	18:R:170:ARG:NH2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:OP1	1:A:1153:C:N4	2.36	0.59
29:4:631:VAL:CG2	29:4:649:VAL:HG21	2.32	0.59
12:L:86:ASP:OD1	12:L:87:ASP:N	2.35	0.59
16:P:133:PRO:CG	21:U:198:VAL:HG21	2.32	0.59
4:D:196:ASN:C	31:a:376:LEU:HD12	2.28	0.59
4:D:217:ASP:OD2	4:D:251:LYS:NZ	2.34	0.58
11:K:120:LEU:HB3	11:K:123:ILE:HD12	1.85	0.58
29:4:151:ASP:OD1	29:4:152:ILE:N	2.37	0.58
30:9:194:LEU:HD21	30:9:385:LEU:HB3	1.86	0.58
20:T:132:ARG:NH1	20:T:136:LEU:O	2.37	0.58
25:Y:258:ILE:HG21	29:4:320:LEU:CB	2.33	0.58
1:A:1344:U:OP1	26:Z:101:ARG:NH1	2.36	0.57
4:D:417:MET:O	4:D:419:ARG:NH1	2.37	0.57
5:E:94:VAL:HG11	16:P:117:MET:HE1	1.86	0.57
19:S:106:LEU:HB2	19:S:117:LEU:HD11	1.87	0.57
1:A:700:A:N1	1:A:709:G:O2'	2.32	0.57
3:C:58:ALA:HB1	3:C:59:PRO:CD	2.35	0.57
1:A:1008:A:OP2	5:E:50:ARG:NH2	2.38	0.57
5:E:47:LEU:HD12	5:E:59:ASN:HA	1.87	0.57
5:E:50:ARG:NH1	5:E:57:GLN:OE1	2.38	0.56
7:G:209:LEU:HD12	7:G:213:LEU:HD11	1.87	0.56
13:M:67:ALA:HB2	18:R:196:TYR:CE1	2.40	0.56
25:Y:258:ILE:HG21	29:4:320:LEU:HB3	1.86	0.56
28:1:266:LEU:HD11	28:1:289:ILE:HD11	1.86	0.56
18:R:302:GLN:O	18:R:306:VAL:HG23	2.05	0.56
28:1:60:MET:HE1	28:1:80:ALA:O	2.06	0.56
29:4:302:VAL:HG21	29:4:341:CYS:HB3	1.86	0.55
1:A:1033:U:O3'	5:E:94:VAL:HG12	2.07	0.55
1:A:702:C:OP1	1:A:848:U:O2'	2.24	0.55
5:E:54:HIS:O	5:E:55:SER:OG	2.22	0.55
4:D:245:VAL:HG22	4:D:271:ALA:HB1	1.89	0.55
30:9:198:ARG:NH2	30:9:199:GLU:OE2	2.40	0.55
1:A:1272:A:N6	1:A:1320:G:O2'	2.37	0.55
3:C:51:VAL:HG11	3:C:167:LEU:HD12	1.89	0.55
1:A:761:A:O2'	1:A:784:A:N1	2.32	0.54
4:D:273:ASN:O	4:D:276:VAL:HG12	2.07	0.54
21:U:173:LEU:O	21:U:177:VAL:HG23	2.07	0.54
22:V:190:LEU:HD11	22:V:208:LEU:HD11	1.88	0.54
1:A:941:G:O2'	1:A:1109:A:OP2	2.25	0.54
7:G:166:TYR:CE1	7:G:170:LEU:HD11	2.43	0.54
24:X:268:LEU:HD21	24:X:293:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:LEU:HD21	4:D:222:ILE:HD11	1.89	0.53
5:E:8:LEU:HD11	5:E:82:LEU:HD22	1.89	0.53
7:G:315:PHE:CD2	7:G:369:LEU:HD21	2.42	0.53
16:P:63:LYS:O	16:P:64:LYS:HB2	2.08	0.53
24:X:206:GLU:OE2	24:X:249:ARG:NH2	2.41	0.53
1:A:986:G:O2'	1:A:987:A:P	2.66	0.53
10:J:115:THR:HG21	10:J:118:LEU:HD12	1.90	0.53
22:V:35:VAL:HG12	22:V:35:VAL:O	2.07	0.53
16:P:73:ASP:OD1	16:P:74:TYR:N	2.42	0.53
1:A:1248:C:O2	11:K:28:HIS:N	2.42	0.53
7:G:70:THR:HG23	7:G:73:PHE:H	1.73	0.53
29:4:573:ALA:O	29:4:577:ASN:ND2	2.42	0.53
12:L:85:VAL:HG23	12:L:90:LYS:HG3	1.91	0.52
21:U:192:THR:HG23	21:U:198:VAL:HG23	1.90	0.52
7:G:210:VAL:HG12	7:G:210:VAL:O	2.09	0.52
3:C:100:PHE:HB3	3:C:103:CYS:SG	2.50	0.52
1:A:1247:G:N7	26:Z:96:LYS:NZ	2.54	0.52
9:I:97:ILE:HD11	9:I:161:ALA:HB1	1.90	0.52
5:E:90:ARG:NH1	16:P:116:ILE:O	2.43	0.52
18:R:208:ILE:O	18:R:214:ASN:ND2	2.39	0.52
29:4:645:LEU:O	29:4:649:VAL:HG23	2.10	0.52
29:4:451:ASP:OD1	29:4:452:GLN:N	2.43	0.51
29:4:611:LEU:HD21	29:4:633:LEU:HD23	1.91	0.51
5:E:28:ALA:HB3	5:E:78:MET:HE1	1.91	0.51
16:P:82:GLN:NE2	21:U:190:ALA:HB1	2.25	0.51
25:Y:332:ILE:HD13	28:1:221:TYR:CD1	2.44	0.51
1:A:871:A:N1	1:A:918:A:O2'	2.41	0.51
11:K:34:MET:O	11:K:38:VAL:HG23	2.09	0.51
29:4:372:TYR:CE2	29:4:400:LEU:HD21	2.46	0.51
5:E:80:GLU:OE1	5:E:84:ARG:NE	2.44	0.51
21:U:192:THR:HG23	21:U:196:LEU:O	2.10	0.51
29:4:166:VAL:HG12	29:4:194:LEU:HG	1.91	0.51
21:U:73:GLU:OE2	27:0:166:TYR:OH	2.26	0.51
24:X:242:ILE:HD11	37:X:502:GDP:N3	2.26	0.51
29:4:239:ARG:O	29:4:242:ASN:ND2	2.38	0.51
10:J:31:ALA:O	20:T:4:LYS:NZ	2.38	0.51
1:A:662:U:OP2	4:D:339:SER:OG	2.29	0.50
1:A:1186:A:N6	1:A:1465:C:O2	2.44	0.50
29:4:630:VAL:HG12	29:4:645:LEU:HD21	1.92	0.50
31:a:271:LEU:C	31:a:271:LEU:HD23	2.36	0.50
1:A:967:A:O4'	1:A:1023:C:O2'	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:83:ILE:O	9:I:148:ARG:NH2	2.41	0.50
12:L:120:GLU:N	12:L:120:GLU:OE1	2.44	0.50
17:Q:12:VAL:HG23	17:Q:26:LEU:HD13	1.94	0.50
30:9:194:LEU:HD23	30:9:387:LEU:HG	1.94	0.50
1:A:934:G:O2'	1:A:940:A:N1	2.30	0.50
1:A:1001:C:H5"	1:A:1002:C:H5"	1.93	0.50
17:Q:75:LEU:HD21	23:W:160:THR:HG21	1.93	0.50
22:V:225:LEU:HD11	22:V:283:LEU:HD22	1.93	0.50
27:0:54:ALA:O	27:0:58:VAL:HG23	2.12	0.50
28:1:86:ARG:NH1	28:1:96:PRO:O	2.43	0.50
5:E:7:ALA:HA	5:E:65:LEU:HD23	1.93	0.50
30:9:309:VAL:HG21	30:9:311:ARG:HH21	1.76	0.50
4:D:243:VAL:HG11	4:D:268:PHE:CD1	2.46	0.49
1:A:1257:U:O2'	1:A:1260:A:OP2	2.21	0.49
1:A:1095:U:O4	1:A:1096:A:N6	2.45	0.49
30:9:220:MET:CE	30:9:354:LEU:HD23	2.42	0.49
1:A:812:A:O2'	1:A:814:A:N1	2.45	0.49
9:I:158:ARG:NH2	9:I:177:ASP:OD2	2.45	0.49
10:J:55:ARG:HD3	10:J:58:LEU:HD21	1.94	0.49
21:U:70:LEU:CD2	27:0:191:LEU:HD11	2.42	0.49
25:Y:250:ILE:O	29:4:358:ARG:NH2	2.46	0.49
4:D:103:LEU:HD11	4:D:123:ARG:HB2	1.95	0.49
1:A:705:C:H2'	27:0:136:TYR:CE1	2.47	0.49
18:R:82:MET:HE1	18:R:300:LEU:HD13	1.94	0.49
25:Y:262:MET:HE2	29:4:363:ILE:CG2	2.42	0.49
1:A:1053:A:N6	1:A:1100:C:O2'	2.45	0.49
1:A:1150:C:H2'	1:A:1152:A:N7	2.27	0.49
3:C:138:TYR:OH	26:Z:65:LEU:HD22	2.12	0.49
24:X:242:ILE:HD11	37:X:502:GDP:C2	2.47	0.49
25:Y:338:LEU:HD11	25:Y:355:THR:HG21	1.95	0.48
1:A:1229:U:O2'	1:A:1442:G:O4'	2.31	0.48
16:P:78:GLN:HE21	21:U:190:ALA:HB2	1.77	0.48
27:0:71:LEU:HD11	27:0:141:LEU:HD22	1.94	0.48
25:Y:256:LEU:HD11	29:4:356:VAL:HG22	1.94	0.48
28:1:304:GLU:OE2	28:1:309:ILE:HD11	2.13	0.48
29:4:437:GLY:O	29:4:441:THR:HG23	2.13	0.48
30:9:317:SER:OG	30:9:354:LEU:HD22	2.13	0.48
12:L:115:ILE:HG21	12:L:181:ILE:HD13	1.95	0.48
2:B:93:HIS:CD2	2:B:224:ASP:OD2	2.66	0.48
3:C:132:TYR:O	3:C:136:VAL:HG23	2.13	0.48
4:D:132:ILE:HG22	4:D:144:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:62:ILE:HG23	16:P:141:ARG:NH2	2.28	0.48
30:9:619:ALA:HA	30:9:634:THR:HG22	1.95	0.48
19:S:87:LEU:HD13	23:W:89:LEU:HD13	1.94	0.48
29:4:540:HIS:HB3	29:4:544:LEU:HD23	1.96	0.48
12:L:143:LEU:HD11	12:L:153:LYS:HA	1.96	0.48
30:9:366:ALA:HB1	30:9:374:ARG:NE	2.29	0.48
1:A:1145:A:H2'	1:A:1146:C:O4'	2.13	0.48
3:C:77:ASP:O	8:H:81:LYS:NZ	2.40	0.48
12:L:76:TYR:O	12:L:79:VAL:HG22	2.14	0.48
12:L:112:MET:HE3	12:L:116:VAL:HG21	1.96	0.48
29:4:461:PHE:CZ	29:4:465:ILE:HD11	2.49	0.48
12:L:89:VAL:HG22	21:U:164:VAL:HG21	1.95	0.48
29:4:305:ILE:O	29:4:312:LYS:NZ	2.43	0.48
30:9:666:ILE:HG23	30:9:666:ILE:O	2.13	0.47
4:D:148:LEU:HD23	4:D:149:MET:HE2	1.95	0.47
9:I:91:SER:N	9:I:94:ASN:O	2.47	0.47
24:X:108:LEU:HD21	24:X:307:VAL:CG1	2.44	0.47
25:Y:262:MET:HE2	29:4:363:ILE:HG23	1.96	0.47
5:E:36:VAL:HG12	21:U:168:ILE:HD12	1.95	0.47
30:9:239:GLY:O	30:9:308:THR:OG1	2.24	0.47
1:A:1294:A:OP1	2:B:201:ASN:ND2	2.46	0.47
4:D:196:ASN:CA	31:a:376:LEU:HD12	2.43	0.47
30:9:387:LEU:HD11	30:9:498:PRO:HG3	1.97	0.47
29:4:581:ILE:HG23	29:4:613:GLU:OE2	2.15	0.47
30:9:351:LYS:NZ	30:9:497:THR:O	2.45	0.47
21:U:70:LEU:HD21	27:0:191:LEU:HD11	1.96	0.47
10:J:96:PRO:O	10:J:127:ARG:NH1	2.43	0.47
22:V:266:VAL:HG13	22:V:273:ILE:HG22	1.96	0.47
22:V:315:GLU:O	22:V:315:GLU:HG2	2.14	0.47
5:E:26:ILE:HG21	21:U:173:LEU:HD13	1.98	0.46
8:H:125:HIS:CD2	8:H:126:ILE:HG23	2.50	0.46
2:B:179:ALA:CB	2:B:189:LEU:HD21	2.45	0.46
4:D:213:GLU:OE2	19:S:2:ALA:N	2.48	0.46
14:N:31:THR:HG22	14:N:46:ARG:HB3	1.97	0.46
16:P:103:LYS:HG2	35:P:201:FES:S1	2.56	0.46
30:9:670:ARG:HA	30:9:677:TYR:HA	1.98	0.46
1:A:738:A:H2'	1:A:740:G:C5	2.50	0.46
9:I:179:THR:O	17:Q:10:ARG:NH1	2.48	0.46
18:R:273:TRP:CZ3	18:R:307:LEU:HD11	2.50	0.46
14:N:69:LEU:HD21	14:N:80:GLU:HB3	1.97	0.46
18:R:162:SER:O	18:R:170:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:U:O2'	1:A:1445:G:N7	2.34	0.46
2:B:220:VAL:HG22	2:B:234:TYR:HB2	1.98	0.46
30:9:220:MET:SD	30:9:248:ASN:ND2	2.87	0.46
9:I:147:ILE:HD13	9:I:170:LEU:HD13	1.98	0.46
29:4:611:LEU:HA	29:4:614:LEU:HD12	1.96	0.46
23:W:107:ILE:HG23	23:W:112:LEU:HD23	1.98	0.45
30:9:334:SER:HB3	30:9:337:TYR:CD2	2.52	0.45
30:9:366:ALA:HB1	30:9:374:ARG:HE	1.81	0.45
30:9:84:GLN:N	30:9:85:PRO:HD3	2.30	0.45
21:U:190:ALA:HB3	21:U:198:VAL:HB	1.98	0.45
16:P:141:ARG:O	16:P:142:GLU:C	2.59	0.45
9:I:121:LYS:O	9:I:124:THR:OG1	2.24	0.45
22:V:228:TYR:HB3	22:V:259:ALA:HB2	1.97	0.45
29:4:631:VAL:HG23	29:4:649:VAL:HG21	1.97	0.45
15:O:208:PRO:HG2	15:O:213:LEU:HD21	1.99	0.45
29:4:347:VAL:HG22	29:4:350:ARG:NH1	2.31	0.45
18:R:325:ILE:CG2	18:R:346:LEU:HD21	2.47	0.45
27:0:41:LEU:HD13	27:0:55:TRP:CG	2.52	0.45
29:4:305:ILE:HG22	29:4:306:ASN:N	2.32	0.45
30:9:607:ASP:OD1	30:9:608:ILE:N	2.49	0.45
4:D:243:VAL:HG11	4:D:268:PHE:HD1	1.81	0.45
19:S:107:GLN:HB2	19:S:117:LEU:HD21	1.98	0.45
8:H:149:THR:OG1	28:1:131:THR:OG1	1.99	0.44
29:4:58:VAL:HG23	29:4:58:VAL:O	2.15	0.44
30:9:191:ALA:HB3	30:9:388:LEU:HD21	1.99	0.44
1:A:1034:U:O2'	5:E:75:VAL:HG11	2.17	0.44
30:9:243:LEU:O	30:9:311:ARG:N	2.48	0.44
30:9:638:LYS:O	30:9:638:LYS:HG3	2.17	0.44
8:H:94:PHE:CD1	28:1:114:LEU:HD13	2.52	0.44
17:Q:10:ARG:HB3	17:Q:30:LEU:HD21	2.00	0.44
24:X:50:ARG:NH2	24:X:96:GLU:OE2	2.47	0.44
30:9:265:ARG:O	30:9:269:TRP:CD1	2.71	0.44
6:F:155:MET:N	6:F:155:MET:HE2	2.31	0.44
24:X:276:ARG:NH2	24:X:286:GLU:OE1	2.51	0.44
25:Y:258:ILE:O	29:4:324:VAL:HG21	2.17	0.44
22:V:264:GLU:HG3	22:V:337:LEU:HD21	1.99	0.44
30:9:219:TYR:O	30:9:246:LEU:N	2.43	0.44
30:9:359:LEU:HD11	30:9:375:ALA:HB2	1.99	0.44
1:A:1429:C:OP1	7:G:388:ARG:NH1	2.50	0.44
3:C:157:THR:OG1	29:4:92:ASP:OD2	2.11	0.44
5:E:26:ILE:HG21	21:U:173:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:193:ASP:OD1	6:F:194:LYS:N	2.51	0.44
29:4:331:ASN:OD1	29:4:334:THR:OG1	2.35	0.44
30:9:336:ARG:NH1	30:9:337:TYR:CE1	2.86	0.44
11:K:67:LEU:HD11	25:Y:379:TYR:HE2	1.83	0.44
27:0:163:SER:HA	27:0:191:LEU:O	2.18	0.44
29:4:285:ASN:HB2	29:4:287:LEU:HD12	1.99	0.44
29:4:646:THR:HG23	29:4:663:LEU:HD22	1.99	0.44
1:A:1366:C:O2'	1:A:1419:G:N3	2.46	0.44
2:B:159:ALA:CB	2:B:166:ALA:HB2	2.48	0.44
7:G:346:LEU:HD11	7:G:350:LYS:HE3	2.00	0.44
28:1:293:LYS:O	28:1:297:VAL:HG23	2.17	0.44
9:I:153:GLY:O	9:I:158:ARG:NH1	2.43	0.43
24:X:93:THR:HG21	24:X:365:TRP:CZ3	2.53	0.43
13:M:19:ILE:HB	13:M:83:LEU:HD23	2.00	0.43
24:X:151:LEU:CD2	24:X:247:LEU:HD22	2.48	0.43
29:4:131:ASP:OD2	29:4:136:HIS:ND1	2.50	0.43
10:J:78:ARG:CB	10:J:118:LEU:HD11	2.48	0.43
29:4:320:LEU:O	29:4:324:VAL:HG23	2.18	0.43
14:N:58:CYS:SG	14:N:81:LEU:HD22	2.57	0.43
30:9:191:ALA:HB3	30:9:388:LEU:CD2	2.49	0.43
7:G:300:TYR:OH	24:X:382:PHE:O	2.24	0.43
20:T:92:THR:O	20:T:92:THR:HG22	2.19	0.43
3:C:96:MET:HB2	3:C:108:LEU:HD11	2.00	0.43
5:E:15:ARG:NH2	21:U:182:ASP:OD1	2.52	0.43
5:E:17:GLU:OE1	5:E:17:GLU:N	2.48	0.43
11:K:79:PRO:O	11:K:82:SER:OG	2.32	0.43
15:O:185:SER:O	18:R:183:LYS:NZ	2.52	0.43
22:V:208:LEU:HD13	22:V:226:TYR:CD1	2.54	0.43
1:A:1017:A:O3'	16:P:104:GLN:NE2	2.52	0.43
3:C:116:GLN:HE21	25:Y:310:LEU:HD11	1.82	0.43
9:I:151:VAL:HG22	9:I:158:ARG:NH1	2.33	0.43
18:R:262:LEU:O	18:R:265:THR:OG1	2.29	0.43
9:I:99:VAL:HG12	9:I:107:LEU:HD12	2.01	0.42
22:V:360:VAL:HG13	22:V:364:LEU:HD22	2.01	0.42
30:9:194:LEU:HD23	30:9:387:LEU:CD2	2.49	0.42
4:D:243:VAL:HG12	4:D:245:VAL:HG13	2.01	0.42
9:I:172:VAL:O	17:Q:14:VAL:HG21	2.18	0.42
15:O:182:GLY:O	18:R:183:LYS:NZ	2.41	0.42
21:U:71:ARG:O	21:U:75:VAL:HG23	2.20	0.42
24:X:126:LEU:HD23	24:X:343:ILE:HB	2.00	0.42
1:A:691:A:N7	1:A:716:U:O2'	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:135:VAL:HG11	21:U:191:ILE:O	2.18	0.42
27:0:61:GLU:HB2	27:0:137:HIS:O	2.20	0.42
28:1:253:TRP:O	28:1:256:SER:OG	2.35	0.42
1:A:769:G:N2	1:A:772:A:OP2	2.50	0.42
18:R:209:ILE:HD12	18:R:214:ASN:HB3	2.01	0.42
30:9:380:TRP:HB2	30:9:387:LEU:HD12	2.01	0.42
30:9:365:THR:HG22	30:9:393:CYS:SG	2.59	0.42
8:H:155:VAL:HG21	28:1:129:PHE:CB	2.49	0.42
15:O:137:ALA:HB3	15:O:138:PRO:HD3	2.01	0.42
21:U:190:ALA:O	21:U:198:VAL:N	2.53	0.42
30:9:315:LEU:N	30:9:315:LEU:HD12	2.35	0.42
12:L:82:ILE:O	12:L:85:VAL:HG22	2.19	0.42
30:9:204:LEU:HB3	30:9:383:THR:HG21	2.02	0.42
13:M:29:ARG:CD	13:M:57:LEU:HD12	2.49	0.42
19:S:96:CYS:O	19:S:100:VAL:HG23	2.19	0.42
22:V:236:LEU:CD1	22:V:327:LEU:HD21	2.49	0.42
27:0:37:ASP:O	27:0:41:LEU:N	2.48	0.42
29:4:427:ARG:NE	29:4:467:LEU:HD21	2.34	0.42
29:4:542:PRO:O	29:4:546:VAL:HG23	2.20	0.42
1:A:1421:G:H5"	1:A:1422:G:OP1	2.19	0.42
3:C:51:VAL:HG22	3:C:165:LYS:O	2.20	0.42
3:C:58:ALA:HB1	3:C:59:PRO:HD2	2.00	0.42
8:H:172:VAL:HG13	8:H:172:VAL:O	2.20	0.42
24:X:75:LEU:HD11	24:X:97:ALA:HB3	2.02	0.42
29:4:461:PHE:CE2	29:4:465:ILE:HD11	2.54	0.42
4:D:323:ILE:HG21	4:D:349:LEU:HD23	2.02	0.41
9:I:136:ALA:HB2	9:I:165:LEU:HA	2.02	0.41
10:J:78:ARG:HB2	10:J:118:LEU:HD11	2.02	0.41
22:V:226:TYR:CE2	22:V:282:VAL:HG21	2.55	0.41
24:X:138:LEU:O	24:X:142:ILE:HG12	2.20	0.41
26:Z:18:LEU:HD21	28:1:232:GLU:HG3	2.02	0.41
8:H:184:ILE:O	8:H:184:ILE:HG22	2.19	0.41
19:S:113:ASP:OD1	19:S:114:GLU:N	2.54	0.41
22:V:266:VAL:HG11	22:V:275:LEU:HG	2.02	0.41
29:4:166:VAL:HG23	29:4:167:LYS:N	2.34	0.41
30:9:250:VAL:HG23	30:9:315:LEU:HD23	2.02	0.41
30:9:347:THR:O	30:9:348:ASN:CB	2.68	0.41
1:A:692:C:H4'	30:9:672:LYS:HB2	2.02	0.41
6:F:154:PRO:C	6:F:155:MET:HE2	2.45	0.41
7:G:353:CYS:SG	7:G:370:LEU:HD21	2.60	0.41
8:H:104:ILE:HG21	8:H:145:LEU:HD23	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:193:PRO:HG2	12:L:196:TYR:CE1	2.55	0.41
16:P:54:MET:HE3	16:P:57:PRO:HG3	2.00	0.41
22:V:219:VAL:HG22	22:V:355:LEU:HD23	2.02	0.41
30:9:248:ASN:OD1	30:9:249:LYS:N	2.53	0.41
30:9:387:LEU:HD13	30:9:496:ASP:O	2.20	0.41
1:A:1132:U:H2'	1:A:1133:C:C6	2.55	0.41
16:P:123:THR:HG23	17:Q:4:HIS:CE1	2.55	0.41
29:4:631:VAL:HG21	29:4:649:VAL:HG21	2.02	0.41
1:A:1035:U:OP1	5:E:4:TYR:OH	2.24	0.41
1:A:1206:G:O2'	1:A:1224:C:O2'	2.38	0.41
18:R:191:ARG:HG3	18:R:204:ILE:HG23	2.01	0.41
4:D:209:GLY:HA3	4:D:213:GLU:HB2	2.03	0.41
24:X:142:ILE:HD13	24:X:259:LEU:HD21	2.03	0.41
24:X:394:HIS:CE1	24:X:398:LEU:HD11	2.56	0.41
1:A:986:G:H2'	1:A:987:A:C8	2.56	0.41
7:G:356:VAL:HG23	7:G:361:VAL:HG23	2.01	0.41
16:P:78:GLN:NE2	21:U:190:ALA:HB2	2.35	0.41
21:U:192:THR:HG22	21:U:198:VAL:HG23	1.99	0.41
28:1:113:HIS:CD2	28:1:114:LEU:HG	2.55	0.41
1:A:1271:C:N4	1:A:1320:G:O2'	2.54	0.41
2:B:159:ALA:HB2	2:B:166:ALA:HB2	2.02	0.41
2:B:179:ALA:HB2	2:B:189:LEU:HD21	2.03	0.41
4:D:154:VAL:HG21	29:4:108:LEU:HD22	2.03	0.41
5:E:41:ASN:HB3	21:U:180:ALA:O	2.20	0.41
14:N:110:LEU:HD12	21:U:128:GLU:CD	2.45	0.41
16:P:67:LEU:HD12	16:P:99:LEU:CD1	2.51	0.41
29:4:641:ILE:O	29:4:645:LEU:N	2.44	0.41
30:9:333:ARG:O	30:9:333:ARG:HG2	2.21	0.41
30:9:353:THR:OG1	37:9:801:GDP:H5"	2.21	0.41
1:A:1208:U:H2'	1:A:1209:C:O4'	2.20	0.41
12:L:213:VAL:O	12:L:217:THR:HG23	2.21	0.41
27:0:91:GLU:HB2	27:0:121:LYS:HA	2.02	0.41
29:4:309:PHE:CZ	29:4:352:PRO:HG2	2.56	0.41
4:D:290:ILE:HD12	4:D:292:HIS:O	2.20	0.41
18:R:238:ASP:OD1	18:R:238:ASP:N	2.47	0.41
25:Y:347:ILE:HD13	25:Y:394:PHE:HD2	1.85	0.41
30:9:219:TYR:HA	30:9:344:VAL:O	2.21	0.41
1:A:1356:A:H2'	1:A:1357:A:O5'	2.20	0.40
4:D:258:ILE:HD11	4:D:343:LEU:CD1	2.51	0.40
10:J:81:CYS:HB3	10:J:95:ILE:HD11	2.02	0.40
14:N:33:LEU:HD11	20:T:66:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:168:MET:HE1	22:V:247:MET:HE1	2.03	0.40
4:D:132:ILE:CG2	4:D:144:LEU:HD11	2.52	0.40
18:R:219:TYR:O	18:R:256:ARG:NH2	2.53	0.40
25:Y:261:MET:HE2	29:4:362:ALA:O	2.22	0.40
30:9:272:CYS:CB	30:9:279:LEU:HD21	2.51	0.40
1:A:1053:A:N1	1:A:1100:C:O2'	2.42	0.40
1:A:1454:G:OP2	7:G:377:ARG:NH1	2.54	0.40
4:D:203:LEU:HD11	4:D:222:ILE:HG12	2.04	0.40
15:O:214:SER:OG	22:V:319:ILE:HG23	2.20	0.40
22:V:236:LEU:HD12	22:V:290:LEU:HD13	2.02	0.40
25:Y:250:ILE:HG23	29:4:395:ASP:OD2	2.21	0.40
30:9:179:CYS:SG	30:9:180:GLN:N	2.92	0.40
30:9:309:VAL:HG22	30:9:310:VAL:N	2.37	0.40
17:Q:83:PRO:HA	23:W:108:VAL:HG21	2.03	0.40
24:X:81:HIS:CD2	24:X:156:PRO:HD3	2.57	0.40
29:4:194:LEU:HD12	29:4:198:TYR:CD2	2.56	0.40
8:H:155:VAL:HG21	28:1:129:PHE:HB2	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	
2	B	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
3	C	124/167 (74%)	122 (98%)	2 (2%)	0	100	100
4	D	336/430 (78%)	330 (98%)	6 (2%)	0	100	100
5	E	107/125 (86%)	106 (99%)	1 (1%)	0	100	100
6	F	193/242 (80%)	191 (99%)	2 (1%)	0	100	100
7	G	309/396 (78%)	306 (99%)	3 (1%)	0	100	100
8	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	128/194 (66%)	123 (96%)	5 (4%)	0	100	100
10	J	106/138 (77%)	105 (99%)	1 (1%)	0	100	100
11	K	99/128 (77%)	99 (100%)	0	0	100	100
12	L	162/257 (63%)	160 (99%)	2 (1%)	0	100	100
13	M	117/137 (85%)	117 (100%)	0	0	100	100
14	N	108/130 (83%)	108 (100%)	0	0	100	100
15	O	191/258 (74%)	190 (100%)	1 (0%)	0	100	100
16	P	95/142 (67%)	92 (97%)	2 (2%)	1 (1%)	11	43
17	Q	79/87 (91%)	77 (98%)	2 (2%)	0	100	100
18	R	293/360 (81%)	289 (99%)	4 (1%)	0	100	100
19	S	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
20	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
21	U	174/205 (85%)	174 (100%)	0	0	100	100
22	V	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
23	W	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
24	X	350/398 (88%)	348 (99%)	2 (1%)	0	100	100
25	Y	134/395 (34%)	133 (99%)	1 (1%)	0	100	100
26	Z	98/106 (92%)	98 (100%)	0	0	100	100
27	0	213/215 (99%)	212 (100%)	1 (0%)	0	100	100
28	1	276/323 (85%)	274 (99%)	2 (1%)	0	100	100
29	4	586/689 (85%)	581 (99%)	5 (1%)	0	100	100
30	9	407/698 (58%)	399 (98%)	8 (2%)	0	100	100
31	a	12/343 (4%)	12 (100%)	0	0	100	100
All	All	5813/8024 (72%)	5752 (99%)	59 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	126	ILE
16	P	64	LYS

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	
2	B	198/249 (80%)	198 (100%)	0	100	100
3	C	111/143 (78%)	111 (100%)	0	100	100
4	D	283/357 (79%)	283 (100%)	0	100	100
5	E	92/107 (86%)	92 (100%)	0	100	100
6	F	176/209 (84%)	176 (100%)	0	100	100
7	G	272/342 (80%)	272 (100%)	0	100	100
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	99/146 (68%)	99 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	153/226 (68%)	153 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	174/230 (76%)	174 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100
17	Q	74/78 (95%)	74 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100
19	S	116/164 (71%)	116 (100%)	0	100	100
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	V	325/364 (89%)	325 (100%)	0	100	100
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	311 (100%)	0	100	100
25	Y	128/357 (36%)	128 (100%)	0	100	100
26	Z	90/95 (95%)	90 (100%)	0	100	100
27	0	188/188 (100%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	1	256/291 (88%)	256 (100%)	0	100	100
29	4	527/609 (86%)	527 (100%)	0	100	100
30	9	357/600 (60%)	357 (100%)	0	100	100
31	a	14/288 (5%)	14 (100%)	0	100	100
All	All	5195/6963 (75%)	5195 (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 (47) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	64	ASN
2	B	201	ASN
2	B	216	ASN
3	C	116	GLN
3	C	154	HIS
4	D	127	ASN
4	D	361	GLN
4	D	415	GLN
6	F	113	GLN
6	F	147	GLN
6	F	196	HIS
6	F	207	HIS
7	G	77	GLN
7	G	288	HIS
8	H	83	HIS
8	H	109	HIS
9	I	141	GLN
10	J	105	HIS
15	O	160	HIS
16	P	71	HIS
16	P	78	GLN
17	Q	4	HIS
18	R	347	GLN
19	S	66	HIS
20	T	56	GLN
20	T	101	HIS
22	V	78	ASN
24	X	67	HIS
24	X	69	ASN

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Mol	Chain	Res	Type
24	X	110	HIS
24	X	154	HIS
24	X	235	ASN
24	X	302	HIS
25	Y	257	ASN
25	Y	349	HIS
27	0	26	ASN
27	0	192	ASN
28	1	185	HIS
28	1	235	ASN
29	4	288	HIS
29	4	504	ASN
30	9	262	GLN
30	9	348	ASN
30	9	492	HIS
30	9	551	ASN
30	9	636	ASN
30	9	669	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	795/955 (83%)	89 (11%)	3 (0%)

All (89) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	651	A
1	A	680	U
1	A	688	A
1	A	704	U
1	A	721	U
1	A	737	C
1	A	738	A
1	A	739	C
1	A	740	G
1	A	753	A
1	A	761	A
1	A	766	G
1	A	777	G
1	A	791	G

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Mol	Chain	Res	Type
1	A	796	G
1	A	830	U
1	A	832	U
1	A	835	C
1	A	836	A
1	A	860	A
1	A	868	C
1	A	871	A
1	A	890	C
1	A	892	A
1	A	893	G
1	A	919	A
1	A	938	A
1	A	939	A
1	A	942	A
1	A	956	C
1	A	958	C
1	A	967	A
1	A	987	A
1	A	988	G
1	A	993	A
1	A	1001	C
1	A	1002	C
1	A	1015	A
1	A	1019	A
1	A	1020	C
1	A	1042	U
1	A	1046	A
1	A	1047	A
1	A	1049	A
1	A	1098	C
1	A	1105	C
1	A	1106	C
1	A	1107	U
1	A	1116	A
1	A	1118	A
1	A	1119	U
1	A	1121	A
1	A	1126	A
1	A	1151	C
1	A	1152	A
1	A	1154	A

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Mol	Chain	Res	Type
1	A	1167	A
1	A	1187	U
1	A	1188	A
1	A	1189	U
1	A	1190	C
1	A	1223	C
1	A	1225	C
1	A	1229	U
1	A	1247	G
1	A	1248	C
1	A	1251	A
1	A	1271	C
1	A	1273	G
1	A	1284	U
1	A	1285	G
1	A	1290	C
1	A	1291	U
1	A	1293	C
1	A	1326	A
1	A	1327	G
1	A	1343	A
1	A	1356	A
1	A	1357	A
1	A	1367	A
1	A	1376	C
1	A	1378	C
1	A	1390	A
1	A	1405	C
1	A	1421	G
1	A	1422	G
1	A	1447	G
1	A	1462	G
1	A	1481	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	986	G
1	A	1046	A
1	A	1152	A

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	$\#\|Z\| > 2$
9	5F0	I	184	9	8,8,9	0.58	0	7,9,11	1.13	1 (14%)

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
9	5F0	I	184	9	-	1/9/9/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	184	5F0	O-C-CB	-2.70	117.55	125.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	184	5F0	OD1-C1-CA-CB

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 59 ligands modelled in this entry, 54 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
36	ATP	X	501	32	29,33,33	0.49	0	44,52,52	0.54	0
37	GDP	9	801	-	28,30,30	0.44	0	44,47,47	0.52	0
37	GDP	X	502	-	28,30,30	0.43	0	44,47,47	0.41	0
35	FES	P	201	16,5	0,4,4	-	-	-		
35	FES	T	201	20,13	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
36	ATP	X	501	32	-	0/22/38/38	0/3/3/3
37	GDP	9	801	-	-	4/16/32/32	0/3/3/3
37	GDP	X	502	-	-	1/16/32/32	0/3/3/3
35	FES	P	201	16,5	-	-	0/1/1/1
35	FES	T	201	20,13	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	9	801	GDP	C5'-O5'-PA-O1A
37	9	801	GDP	C4'-C5'-O5'-PA
37	9	801	GDP	C3'-C4'-C5'-O5'
37	9	801	GDP	O4'-C4'-C5'-O5'
37	X	502	GDP	C4'-C5'-O5'-PA

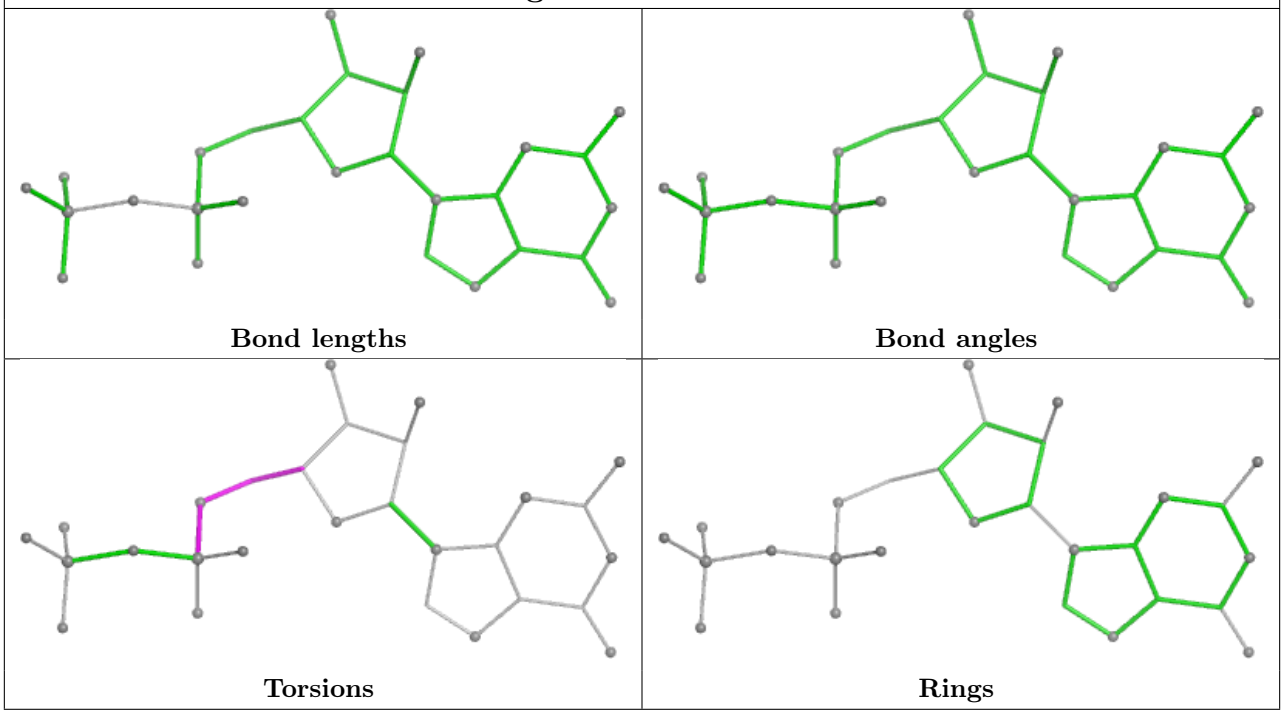
There are no ring outliers.

3 monomers are involved in 5 short contacts:

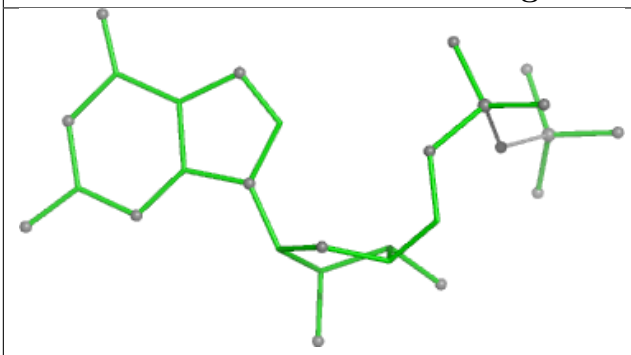
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	9	801	GDP	1	0
37	X	502	GDP	2	0
35	P	201	FES	2	0

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.

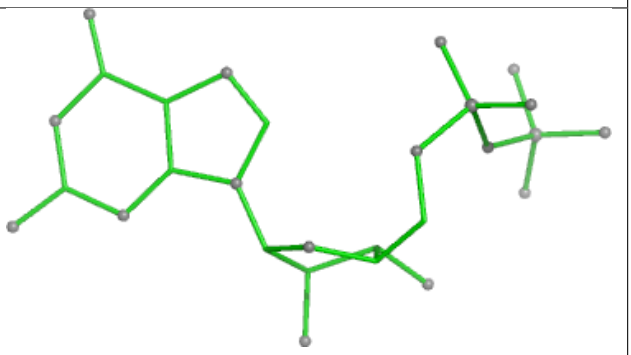
Ligand GDP 9 801



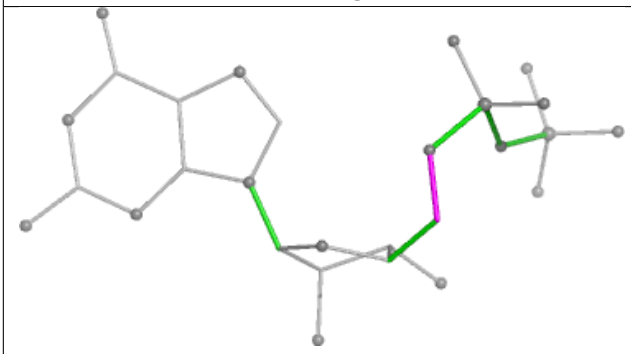
Ligand GDP X 502



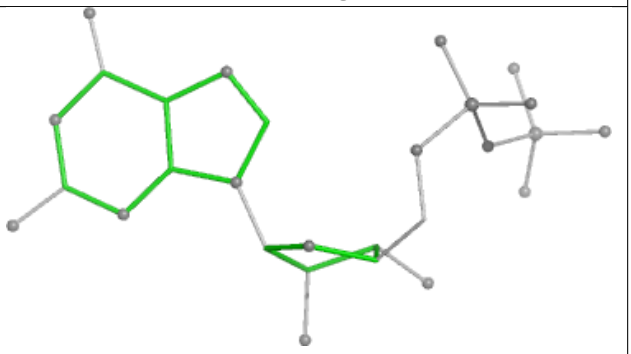
Bond lengths



Bond angles



Torsions



Rings

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.

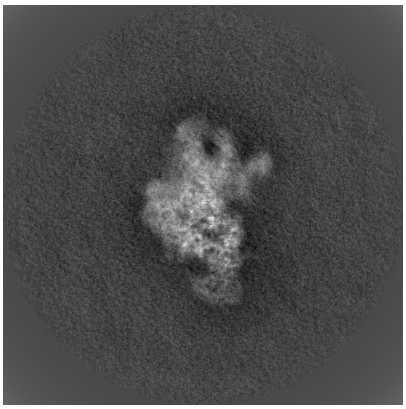
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51876. These allow visual inspection of the internal detail of the map and identification of artifacts.

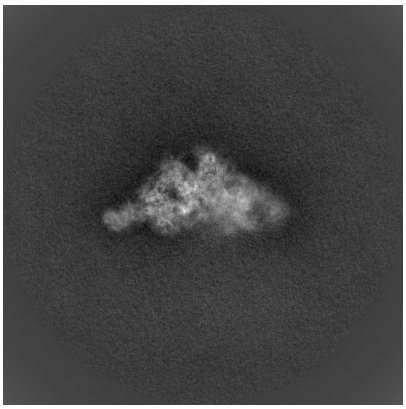
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

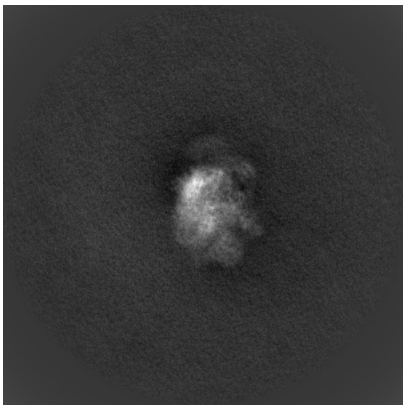
6.1.1 Primary map



X

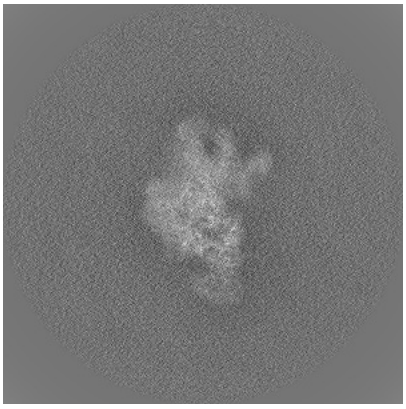


Y

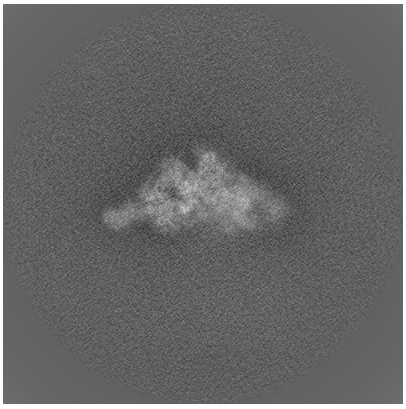


Z

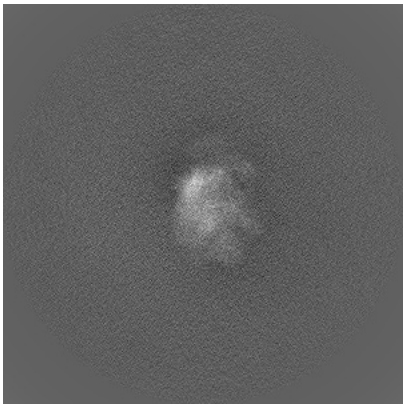
6.1.2 Raw map



X



Y

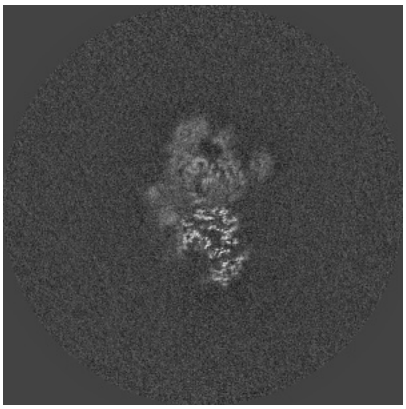


Z

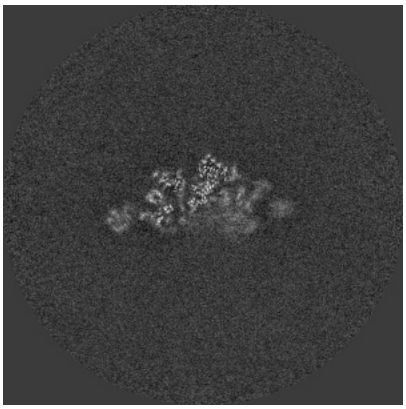
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

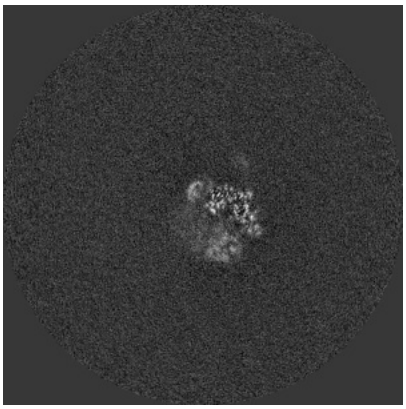
6.2.1 Primary map



X Index: 300

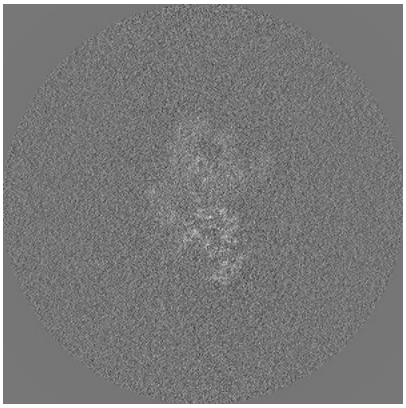


Y Index: 300

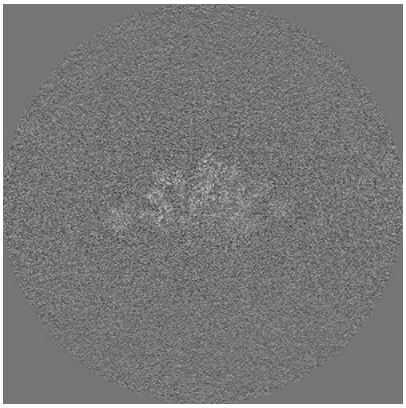


Z Index: 300

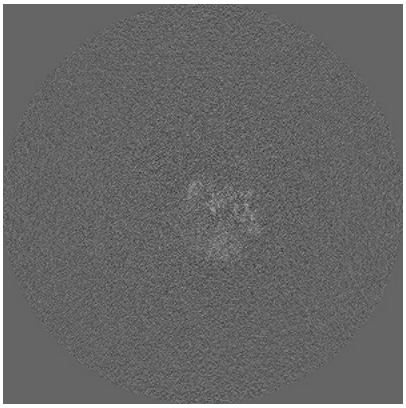
6.2.2 Raw map



X Index: 300



Y Index: 300

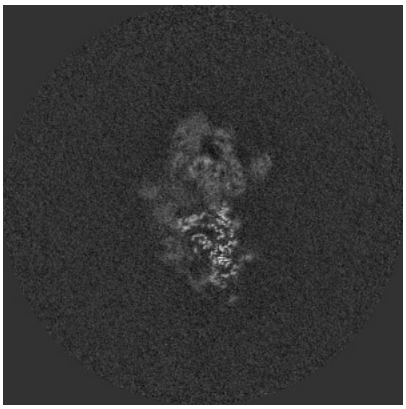


Z Index: 300

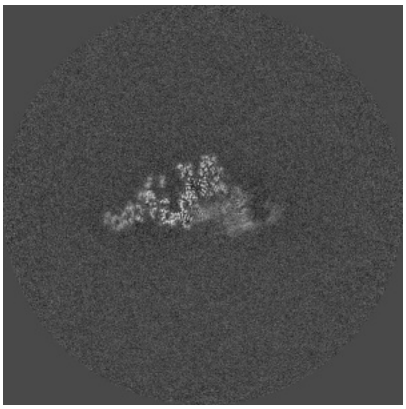
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

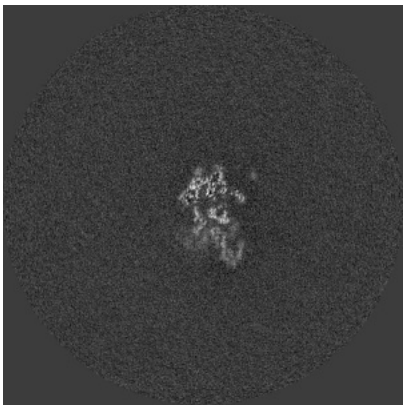
6.3.1 Primary map



X Index: 294

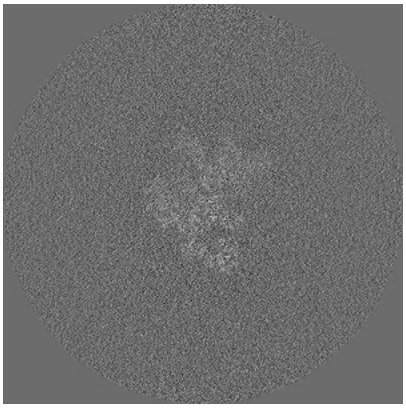


Y Index: 313

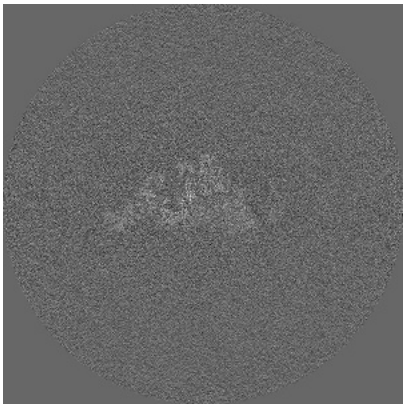


Z Index: 273

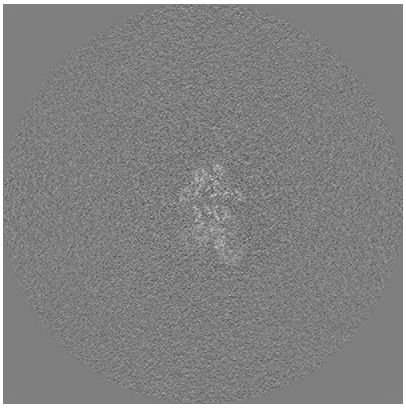
6.3.2 Raw map



X Index: 319



Y Index: 312

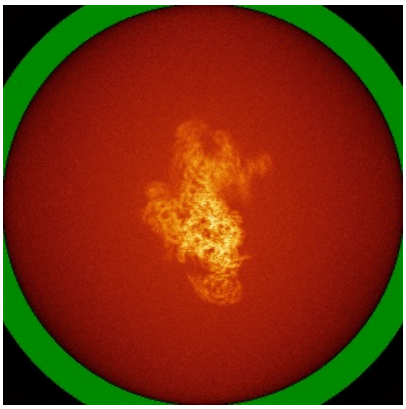


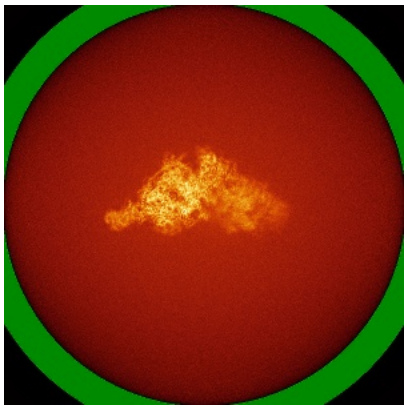
Z Index: 276

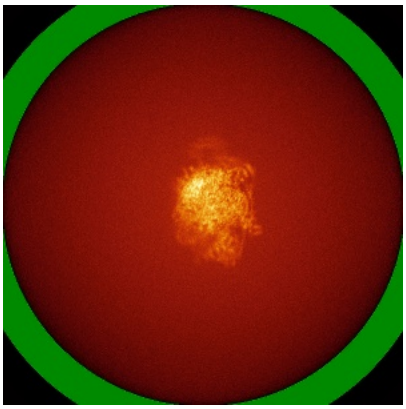
The images above show the largest variance slices of the map in three orthogonal directions.

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

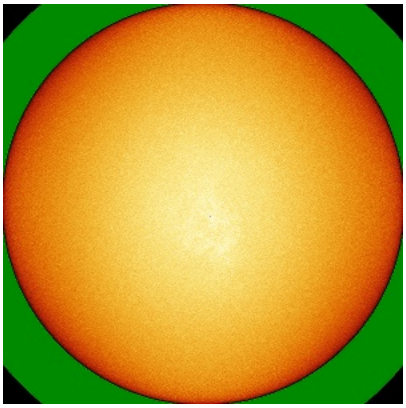
6.4.1 Primary map

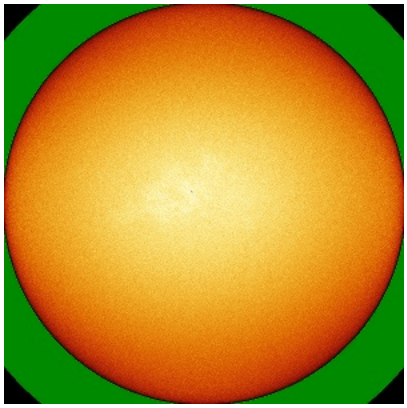

X

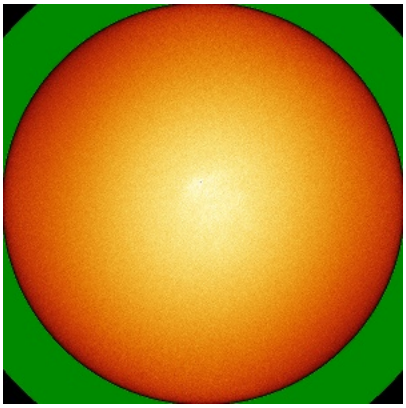

Y


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)

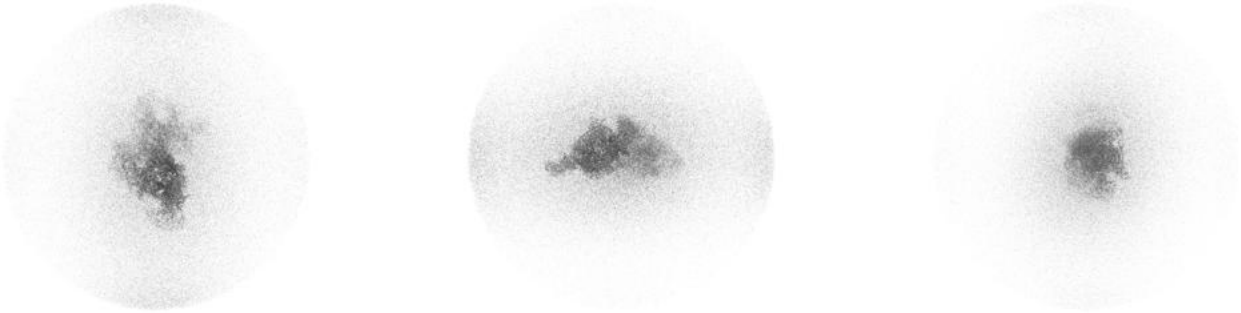
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

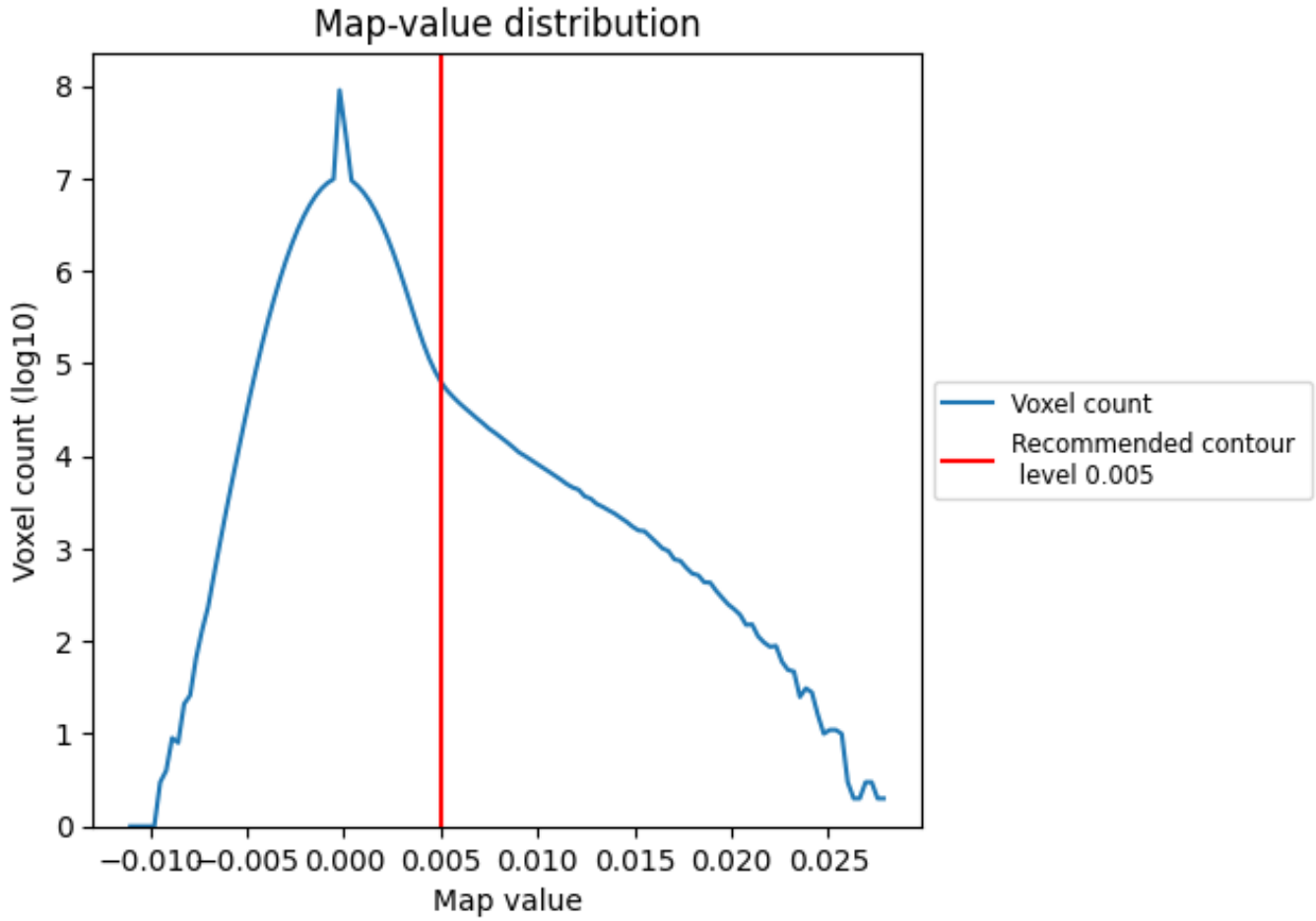
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

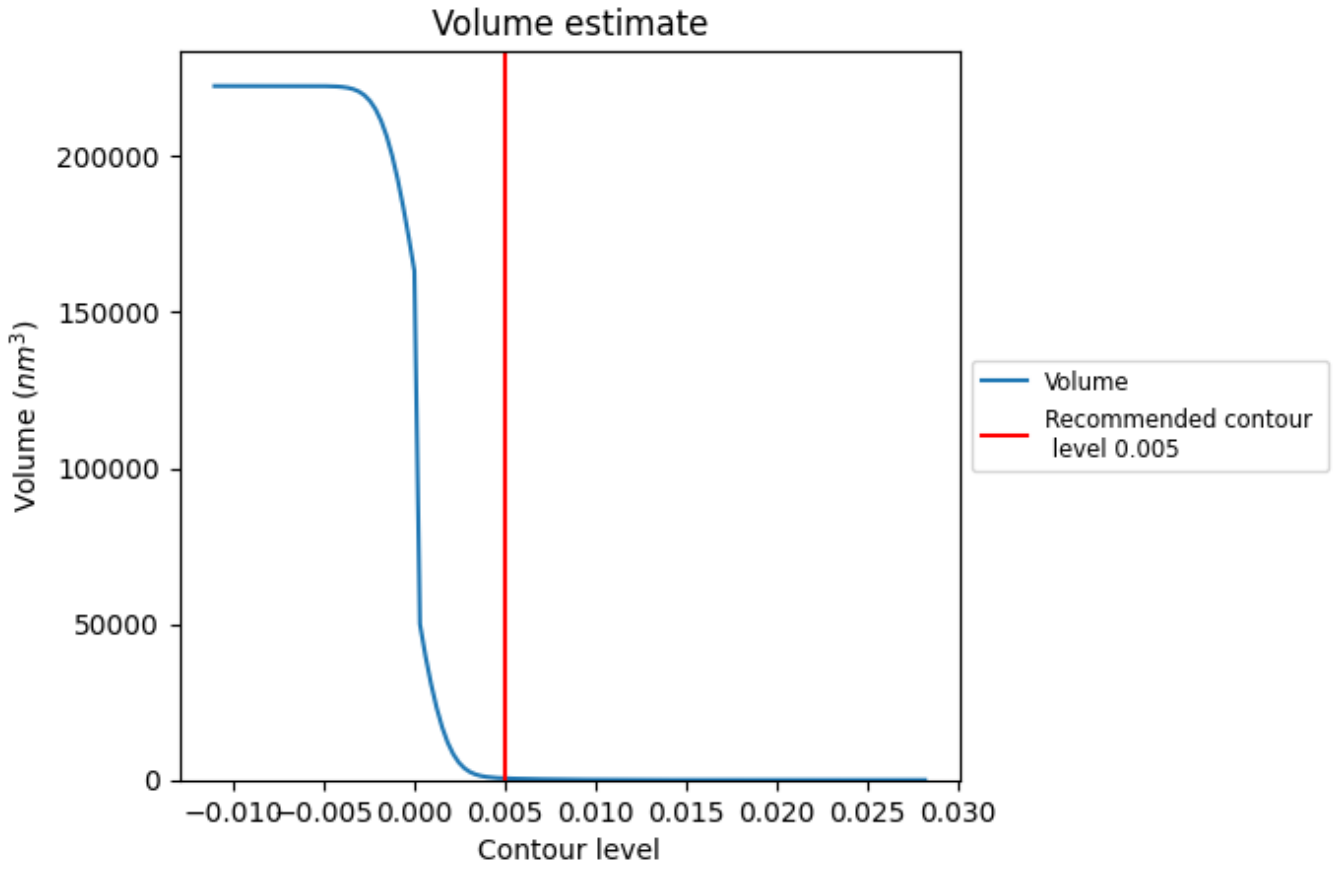
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

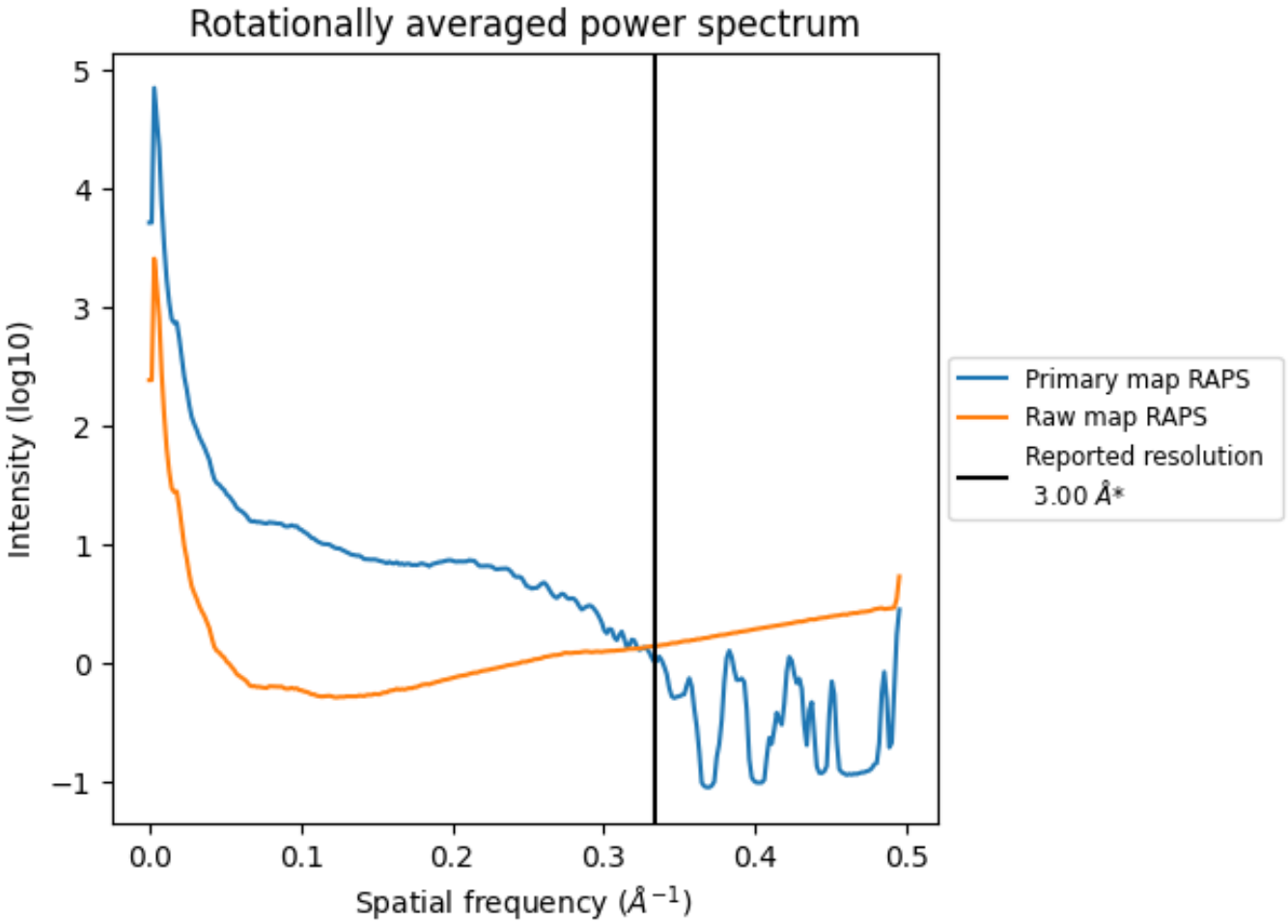
7.2 Volume estimate



The volume at the recommended contour level is 524 nm^3; this corresponds to an approximate mass of 473 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)

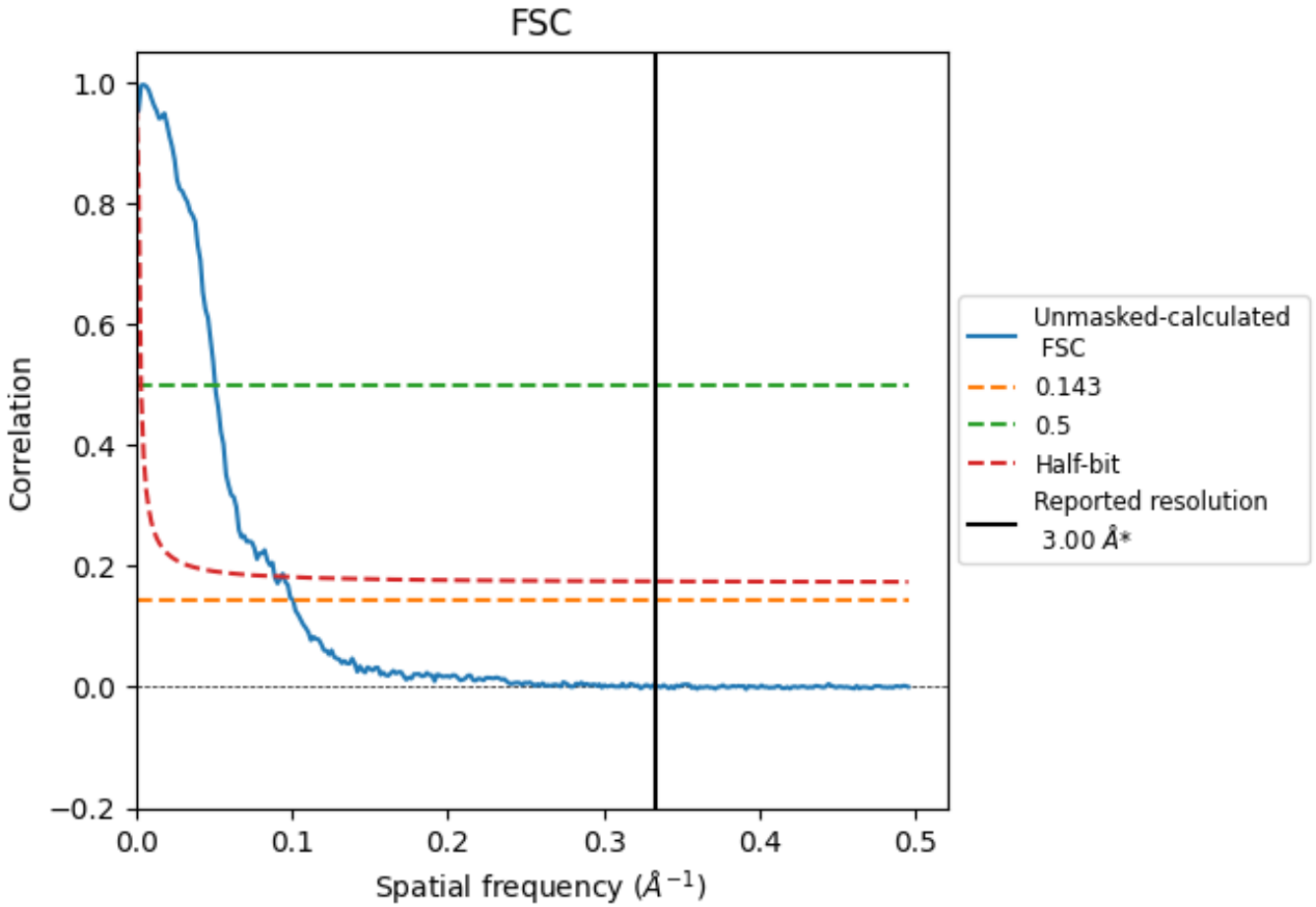


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

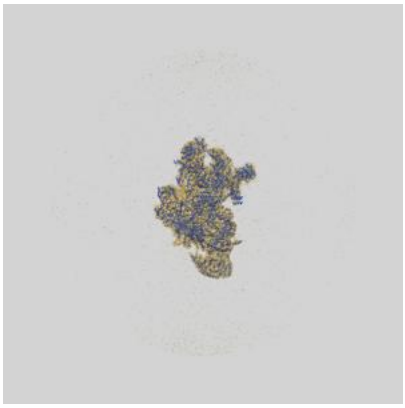
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.93	19.72	11.24

*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 9.93 differs from the reported value 3.0 by more than 10 %

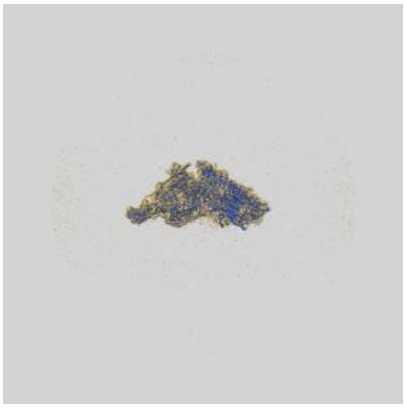
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51876 and PDB model 9H54. Per-residue inclusion information can be found in section 3 on page 12.

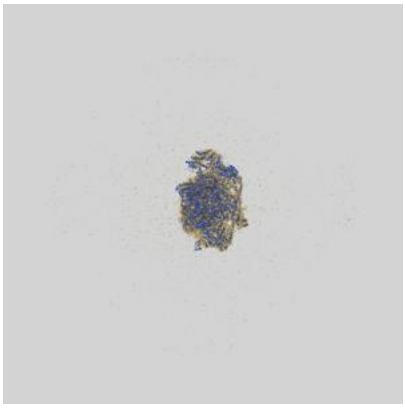
9.1 Map-model overlay



X



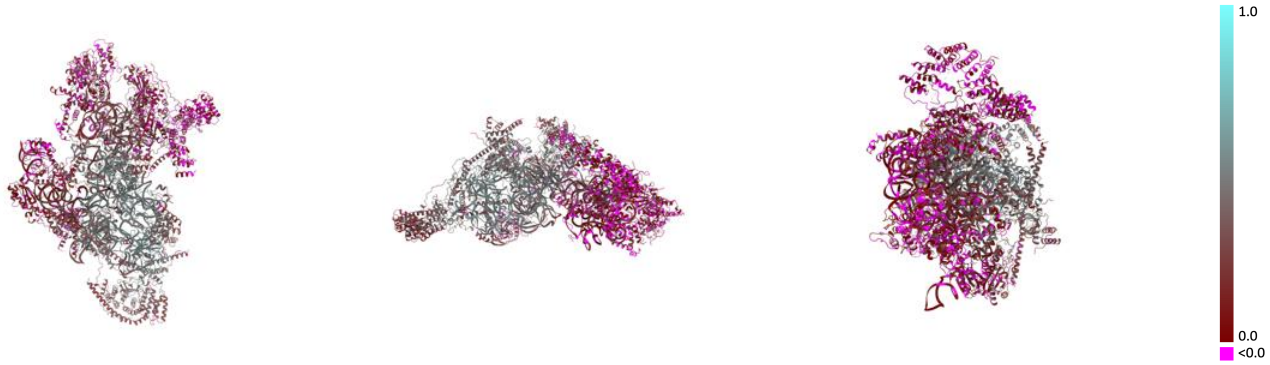
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

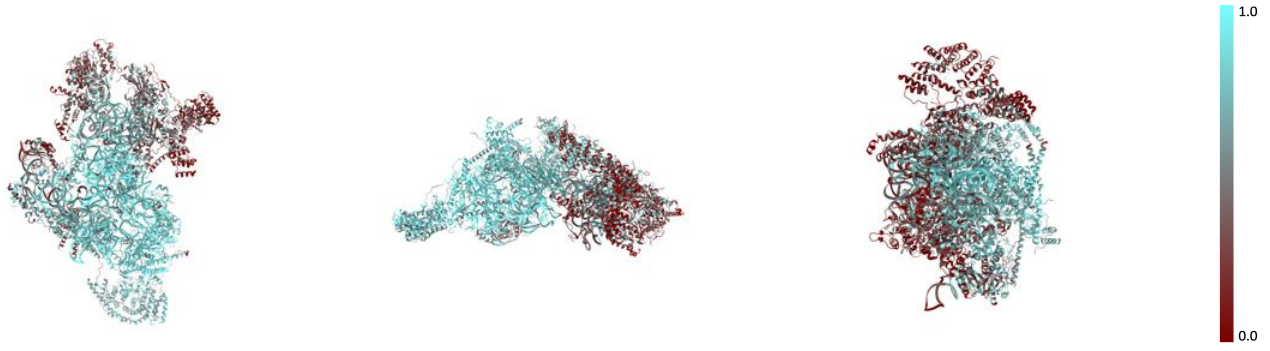
9.2 Q-score mapped to coordinate model (i)



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.

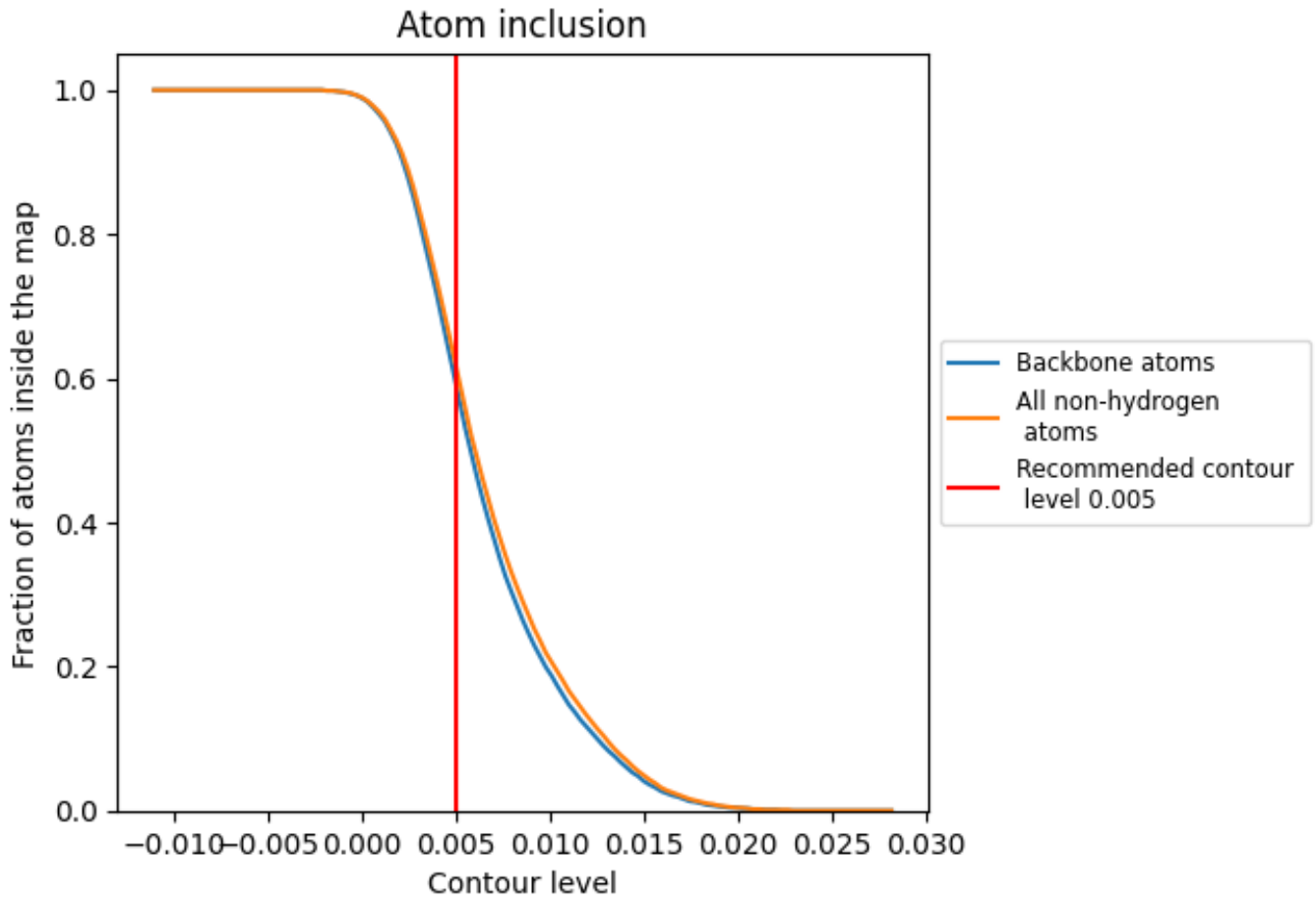
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6190	0.2570
0	0.8020	0.4130
1	0.3710	0.0920
4	0.2030	0.0480
9	0.3870	0.1340
A	0.7740	0.3100
B	0.8330	0.4570
C	0.4890	0.1950
D	0.6430	0.3690
E	0.5620	0.1470
F	0.3420	0.1070
G	0.5900	0.2190
H	0.4320	0.1430
I	0.3470	0.0650
J	0.7680	0.4050
K	0.4980	0.1520
L	0.6420	0.2710
M	0.8740	0.4970
N	0.8270	0.4510
O	0.8700	0.4720
P	0.5660	0.1690
Q	0.4230	0.1520
R	0.8380	0.4430
S	0.7680	0.3680
T	0.8330	0.4600
U	0.7290	0.3000
V	0.6920	0.2570
W	0.7560	0.3800
X	0.2770	0.0850
Y	0.2430	0.0890
Z	0.3300	0.0690
a	0.1300	-0.0010

