Full wwPDB EM Validation Report

Aug 26, 2026 – 05:30 pm BST

PDB ID	:	9G5E / pdb_00009g5e
EMDB ID	:	EMD-51086
Title	:	Translation-initiation state of human mitochondrial ribosome small subunit (State F)
Authors	:	Finke, A.F.; Heinrichs, M.; Aibara, S.; Richter-Dennerlein, R.; Hillen, H.S.
Deposited on	:	2024-07-16
Resolution	:	3.20 Å(reported)
Based on initial models	:	7PO2, 7PO1

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 (1)) were used in the production of this report:

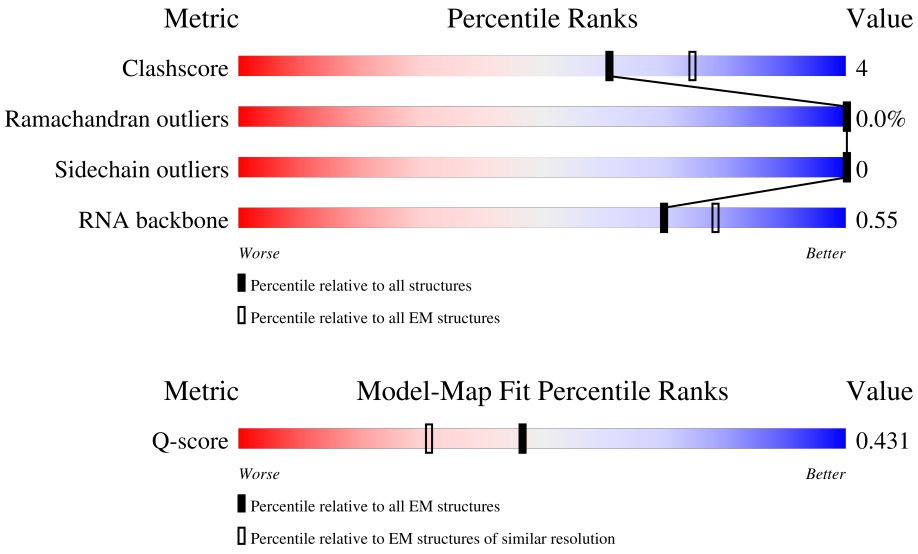
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

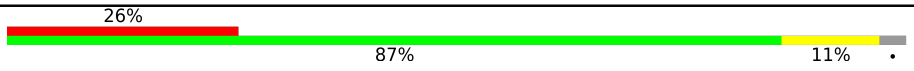
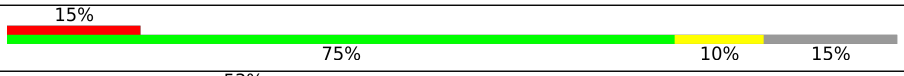
The reported resolution of this entry is 3.20 Å.

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.



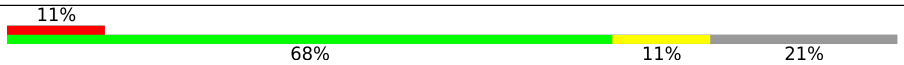
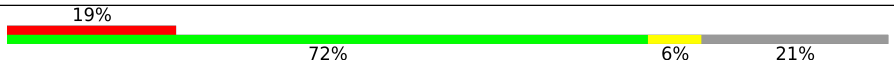
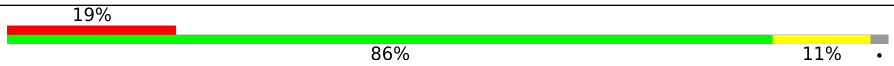
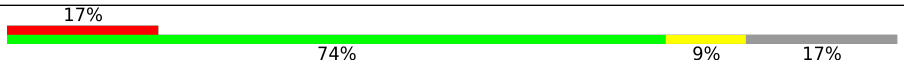
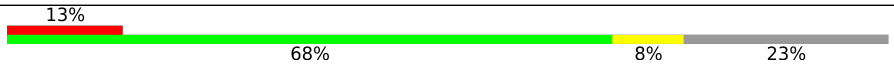
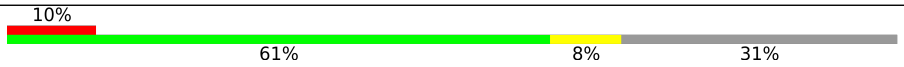
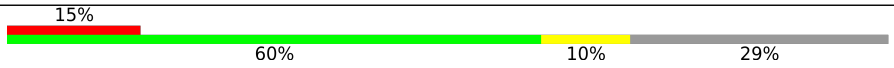
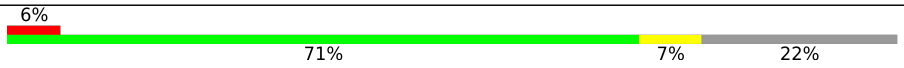
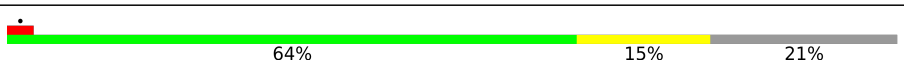
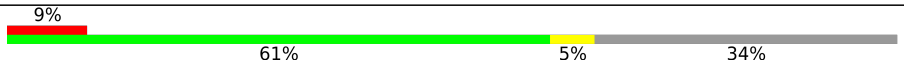
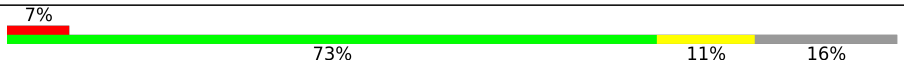
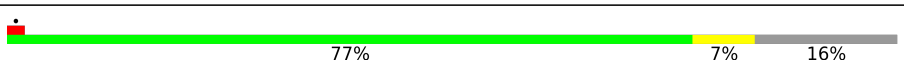
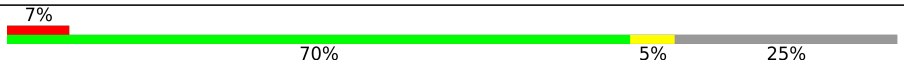
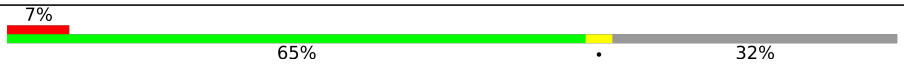
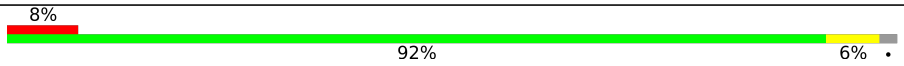
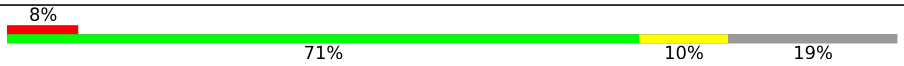
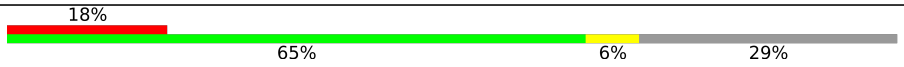
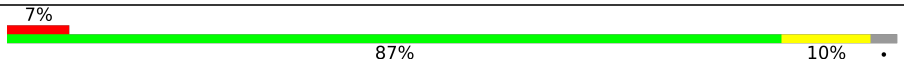
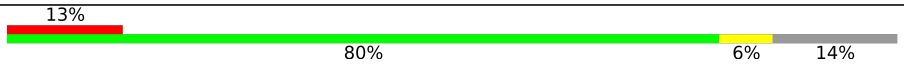
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	
2	1	323	
3	2	118	

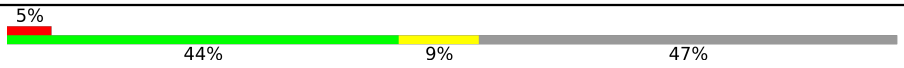
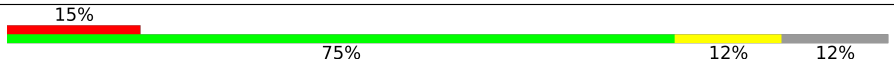
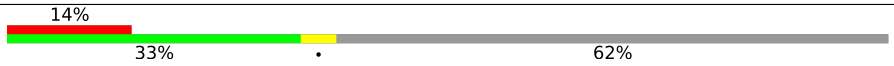
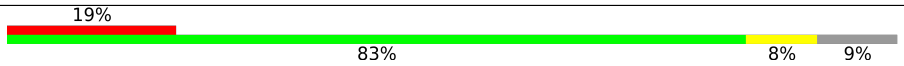
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Mol	Chain	Length	Quality of chain
4	3	199	
5	4	689	
6	7	727	
7	A	955	
8	B	296	
9	C	167	
10	D	430	
11	E	125	
12	F	242	
13	G	396	
14	H	201	
15	I	194	
16	J	138	
17	K	128	
18	L	257	
19	M	137	
20	N	130	
21	O	258	
22	P	142	
23	Q	87	
24	R	360	
25	S	190	
26	T	173	
27	U	205	
28	V	414	

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

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 68648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	212	Total	C	N	O	S	0	0
			1765	1116	336	308	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	276	Total	C	N	O	S	0	0
			2238	1419	381	427	11		

- Molecule 3 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	108	Total	C	N	O	S	0	0
			867	540	171	148	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 4 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	71	Total	C	N	O	S	0	0
			629	403	135	90	1		

- Molecule 5 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	592	Total	C	N	O	S	0	0
			4795	3070	812	885	28		

- Molecule 6 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	435	Total	C	N	O	S	0	0
			3334	2088	584	651	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	896	Total	C	N	O	P	0	0
			19041	8535	3441	6169	896		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	338	Total	C	N	O	S	0	0
			2691	1689	508	481	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	201	Total	C	N	O	S	0	0
			1666	1064	301	290	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	303	Total	C	N	O	S	0	0
			2491	1584	442	451	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	139	Total	C	N	O	S	0	0
			1138	734	192	209	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	170	Total	C	N	O	S	0	0
			1421	906	263	245	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	96	Total	C	N	O	S	0	0
			771	496	133	134	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	85	Total	C	N	O	S	0	0
			736	455	149	124	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 24 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	293	Total	C	N	O	S	0	0
			2393	1524	411	450	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	99	Total	C	N	O	S	0	0
			783	495	140	144	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	349	Total	C	N	O	S	0	0
			2830	1810	496	513	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	149	Total	C	N	O	S	0	0
			1246	801	207	234	4		

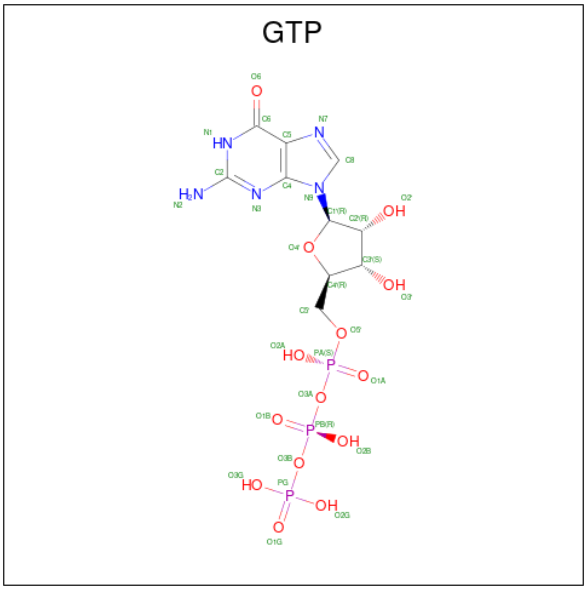
- Molecule 32 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	96	Total	C	N	O	S	0	0
			810	517	145	144	4		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
33	3	1	Total Mg 1 1	0
33	7	1	Total Mg 1 1	0
33	A	41	Total Mg 41 41	0
33	B	1	Total Mg 1 1	0
33	X	1	Total Mg 1 1	0

- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	AltConf
34	7	1	Total C N O P 32 10 5 14 3	0

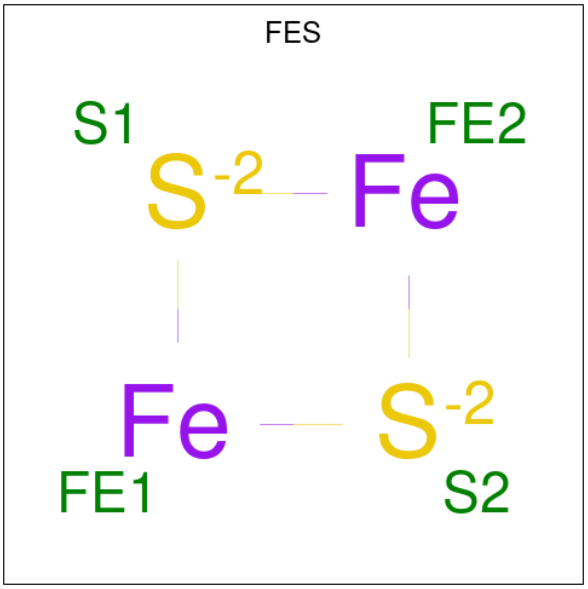
- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total K 1 1	0

- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

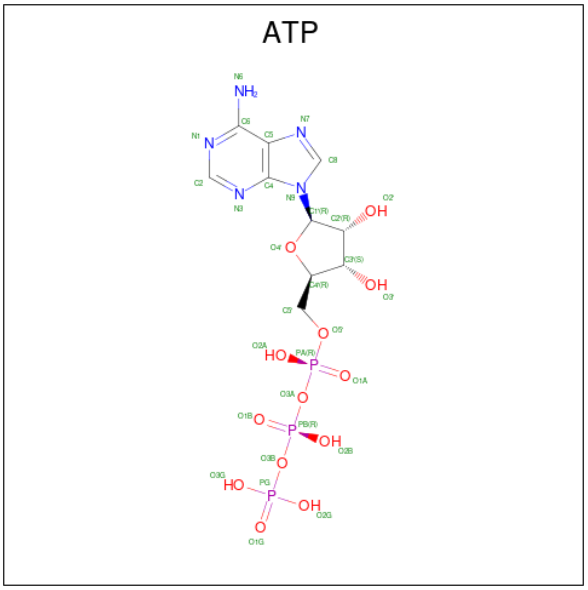
Mol	Chain	Residues	Atoms	AltConf
36	O	1	Total Zn 1 1	0

- Molecule 37 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



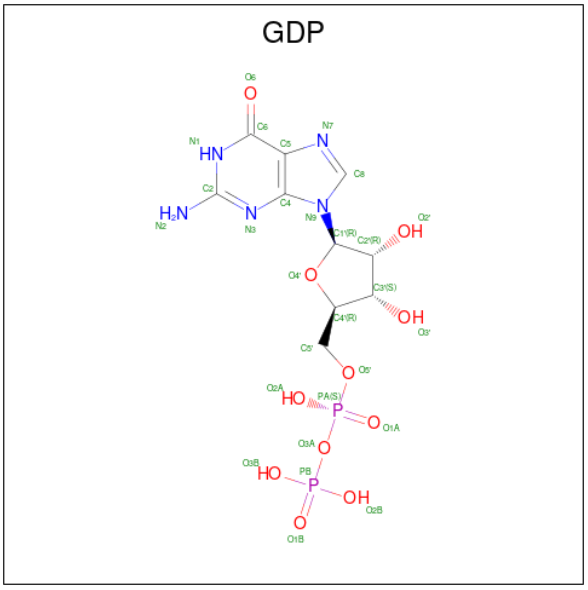
Mol	Chain	Residues	Atoms	AltConf
37	P	1	Total Fe S 4 2 2	0
37	T	1	Total Fe S 4 2 2	0

- Molecule 38 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 39 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



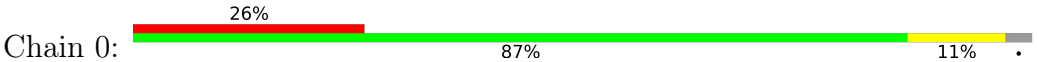
Mol	Chain	Residues	Atoms					AltConf
39	X	1	Total	C	N	O	P	0
			28	10	5	11	2	

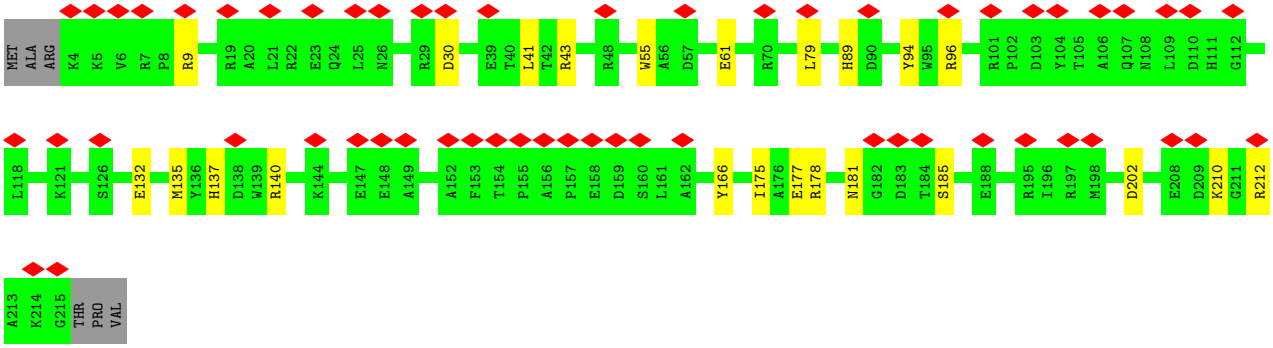
3 Residue-property plots (i)

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: 28S ribosomal protein S34, mitochondrial

Chain 0:

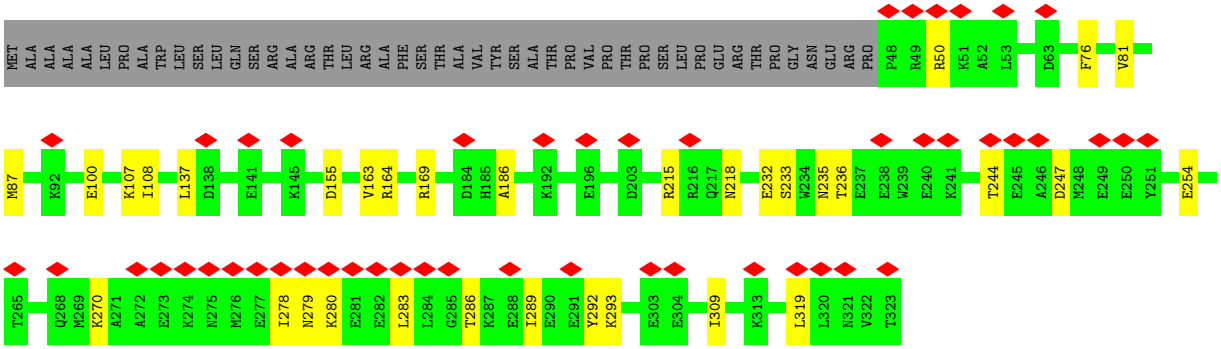




• Molecule 2: 28S ribosomal protein S35, mitochondrial

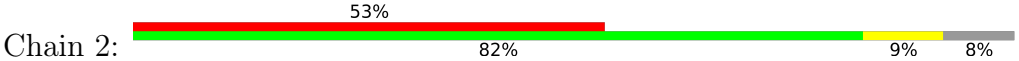
Chain 1:

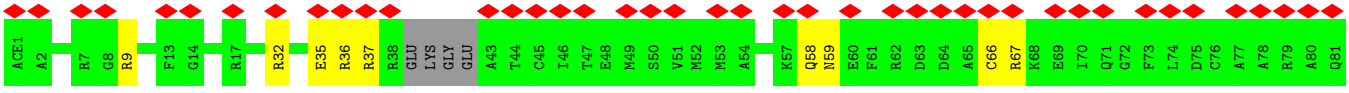


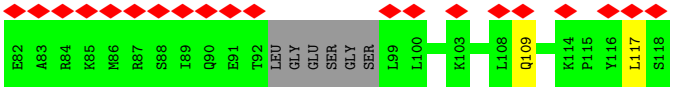


• Molecule 3: Small ribosomal subunit protein mS37

Chain 2:



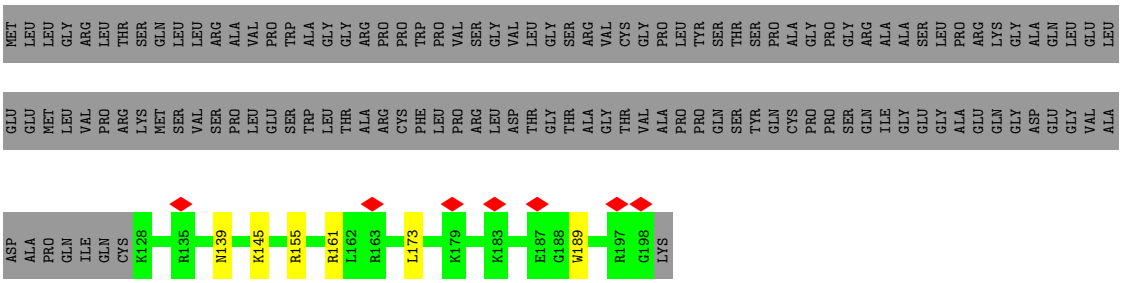




• Molecule 4: Aurora kinase A-interacting protein

Chain 3:

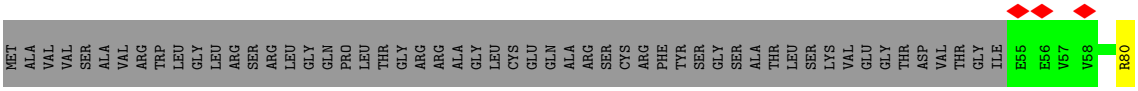


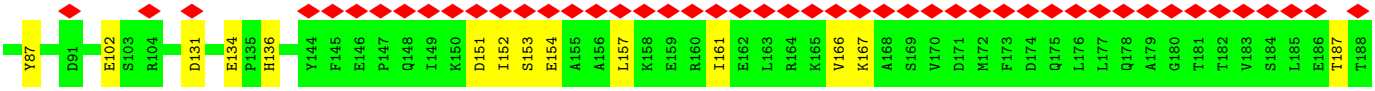


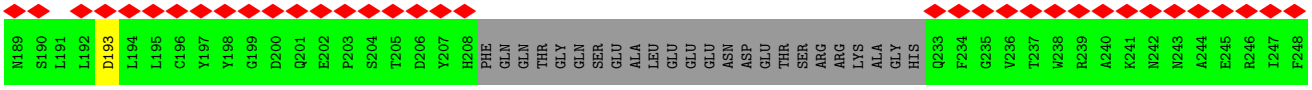
• Molecule 5: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

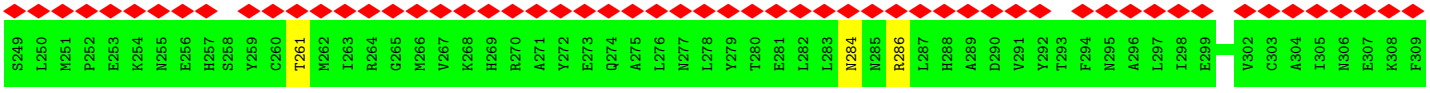
Chain 4:

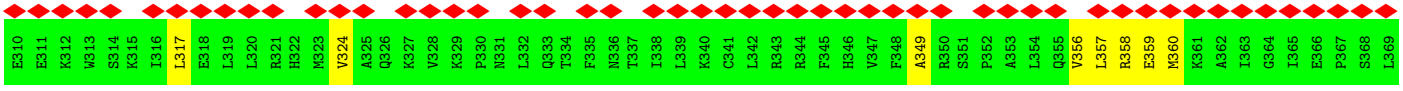


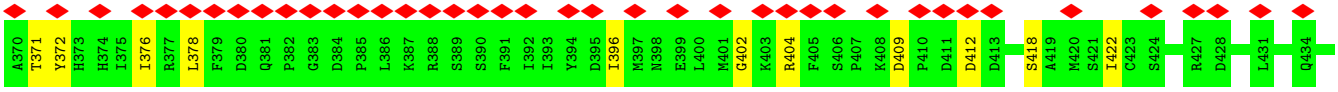


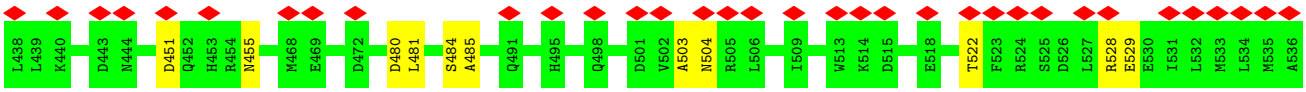




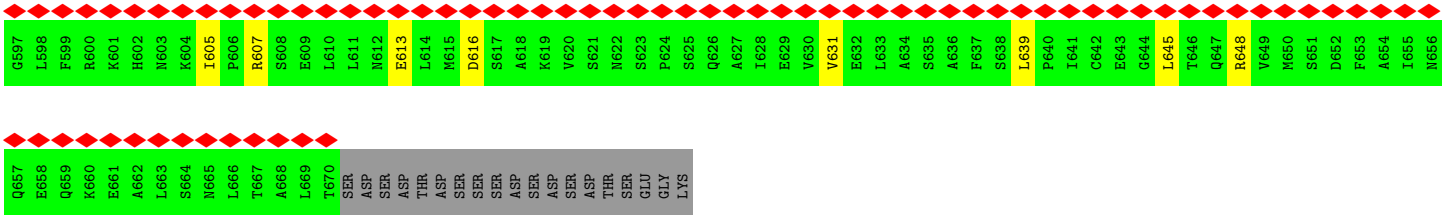




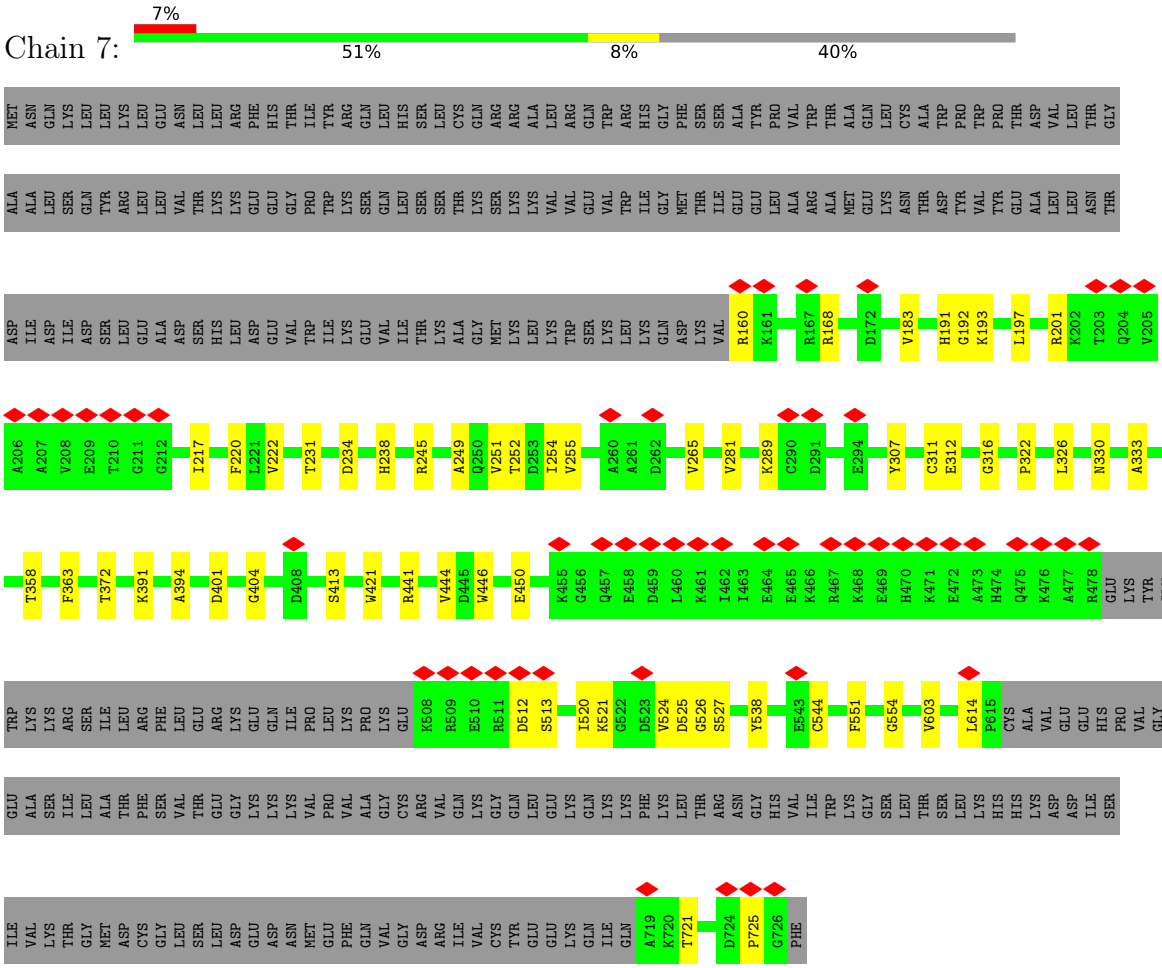




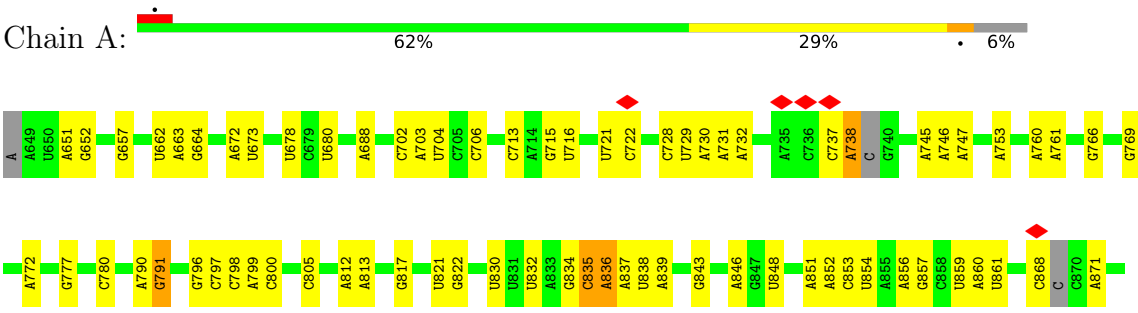


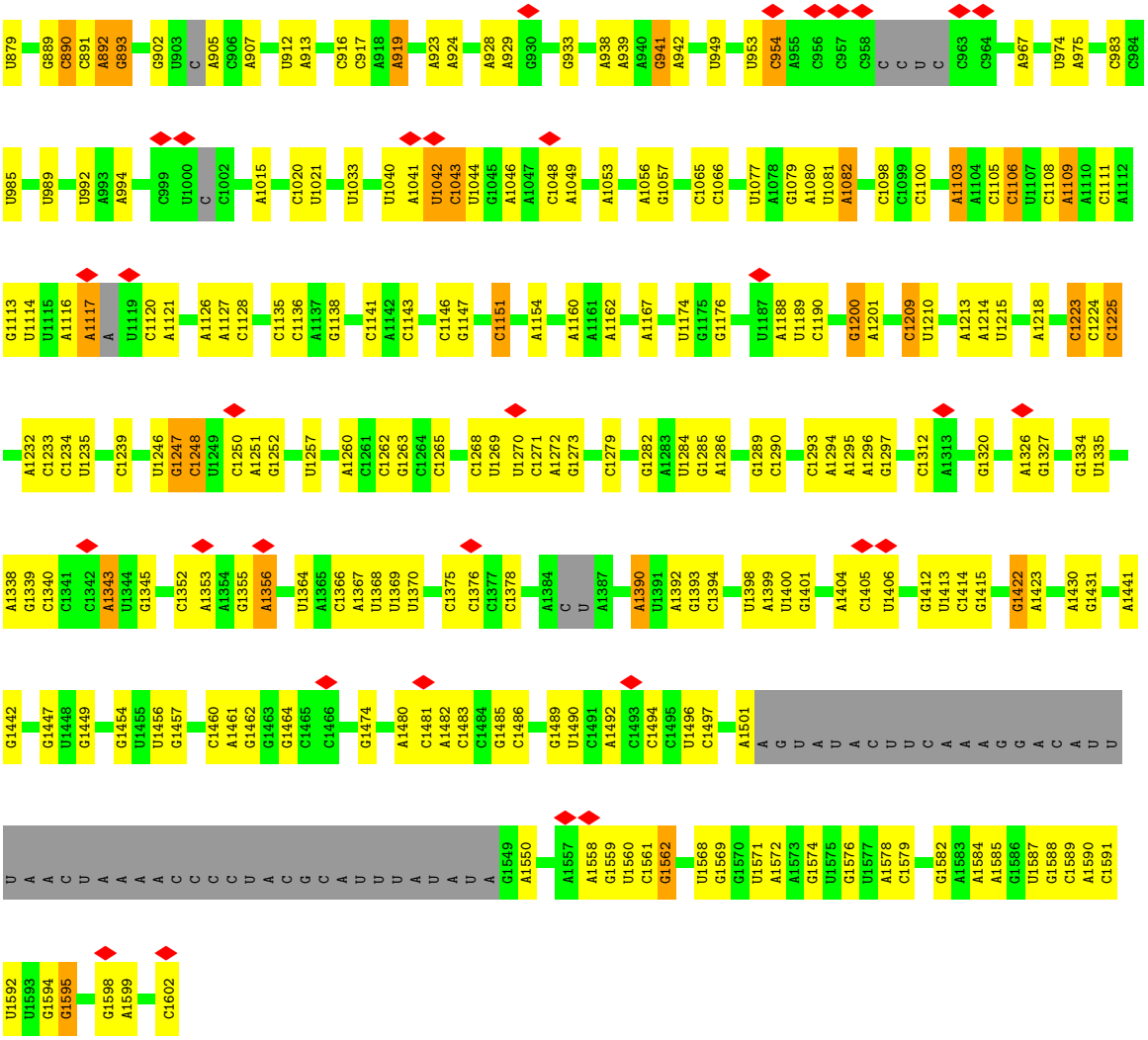


• Molecule 6: Translation initiation factor IF-2, mitochondrial



• Molecule 7: 12S mitochondrial rRNA

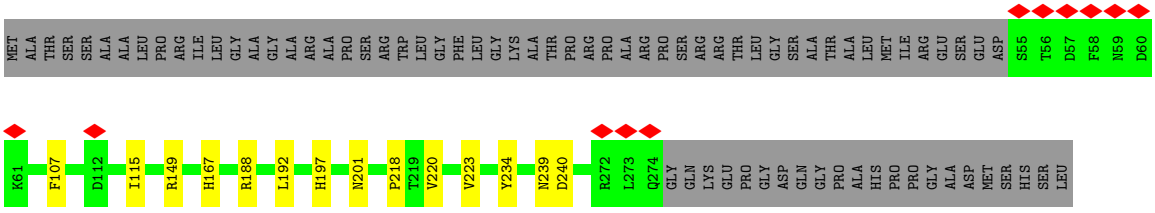




• Molecule 8: 28S ribosomal protein S2, mitochondrial

Chain B:

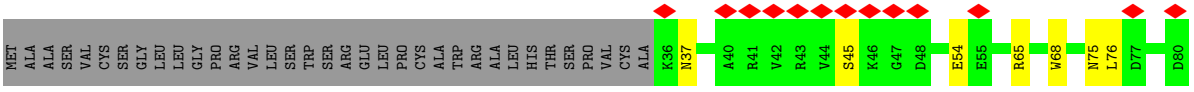


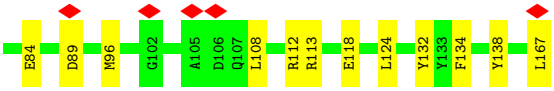


• Molecule 9: 28S ribosomal protein S24, mitochondrial

Chain C:



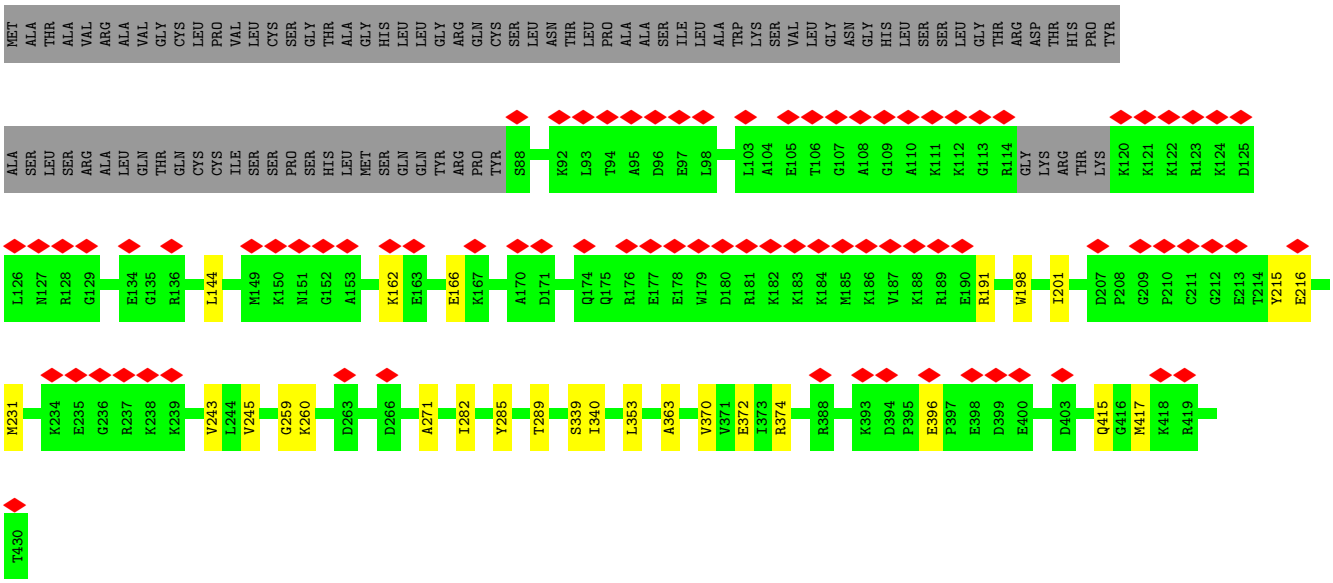




• Molecule 10: 28S ribosomal protein S5, mitochondrial

Chain D:

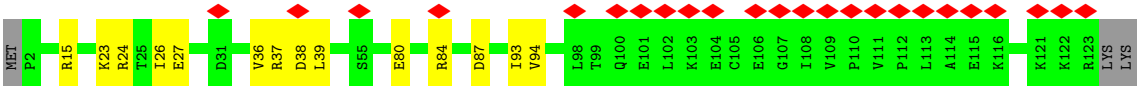




• Molecule 11: 28S ribosomal protein S6, mitochondrial

Chain E:

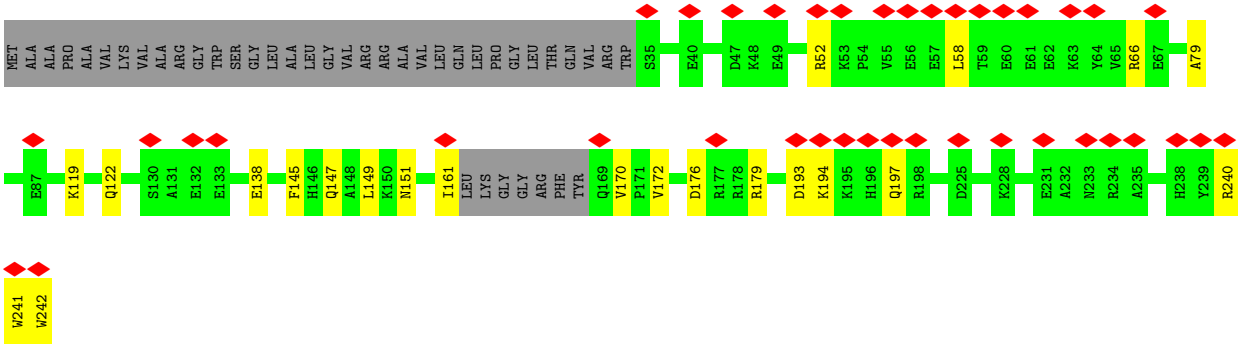




• Molecule 12: 28S ribosomal protein S7, mitochondrial

Chain F:

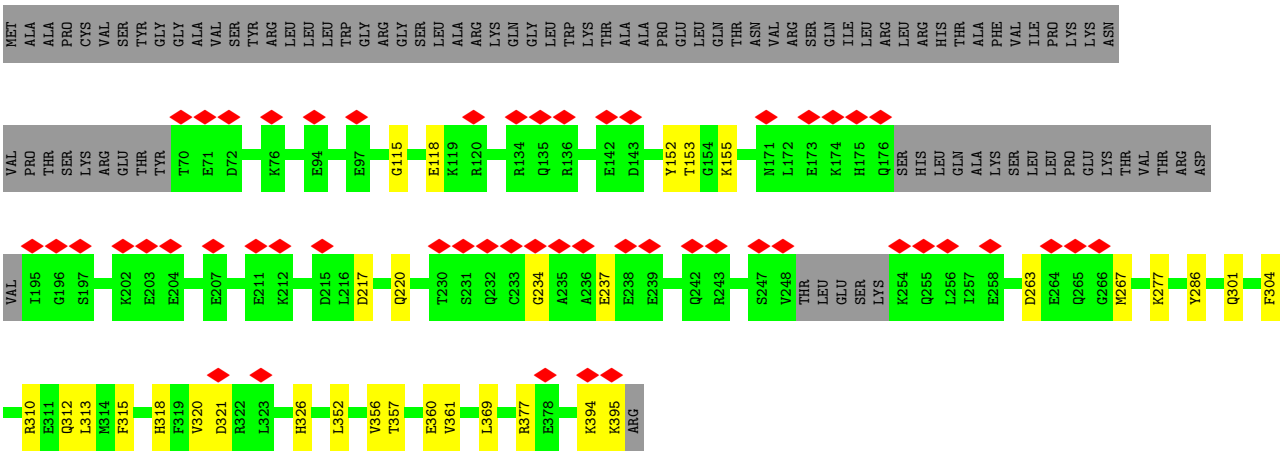




• Molecule 13: 28S ribosomal protein S9, mitochondrial

Chain G:

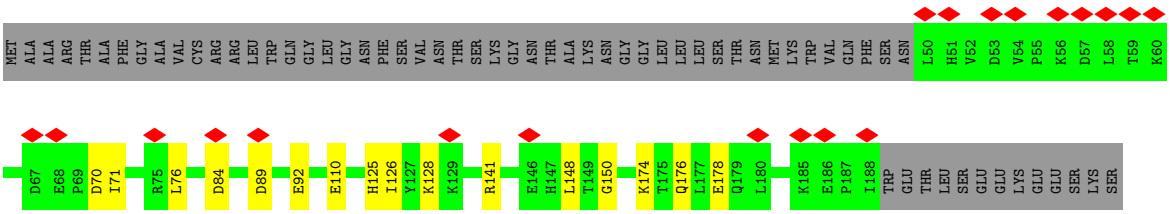




• Molecule 14: 28S ribosomal protein S10, mitochondrial

Chain H:

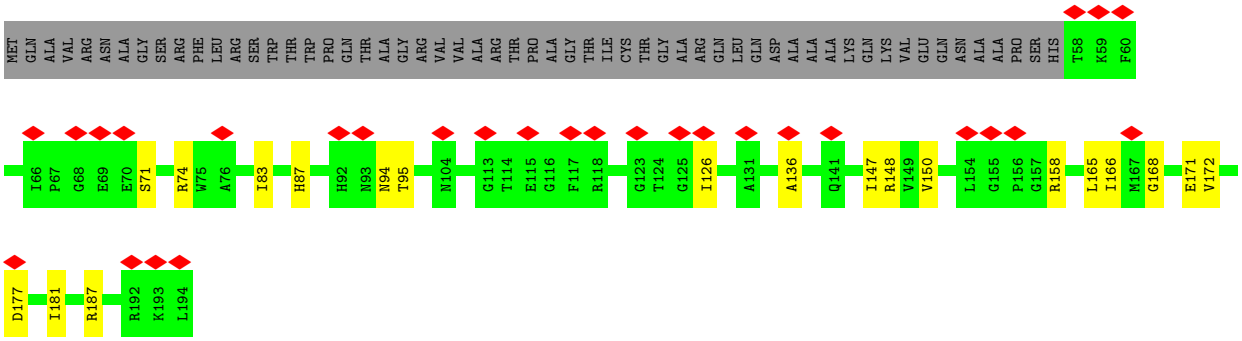




• Molecule 15: 28S ribosomal protein S11, mitochondrial

Chain I:

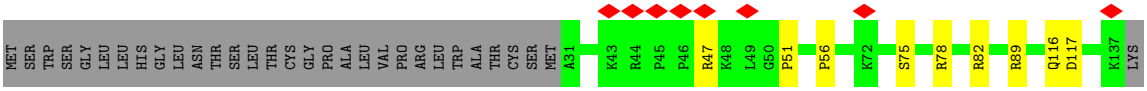




• Molecule 16: 28S ribosomal protein S12, mitochondrial

Chain J:

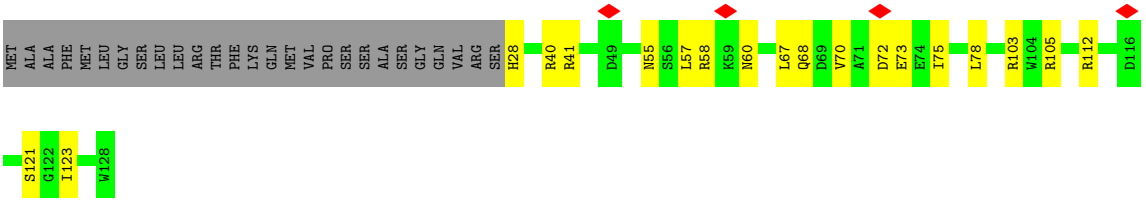




• Molecule 17: 28S ribosomal protein S14, mitochondrial

Chain K:

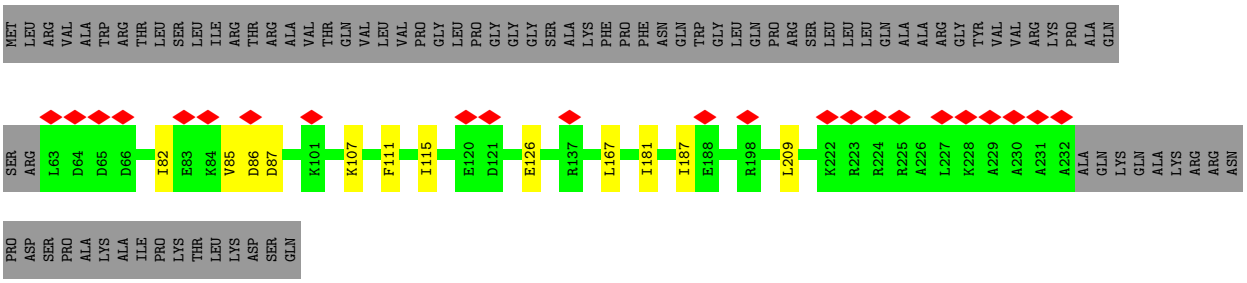




• Molecule 18: 28S ribosomal protein S15, mitochondrial

Chain L:

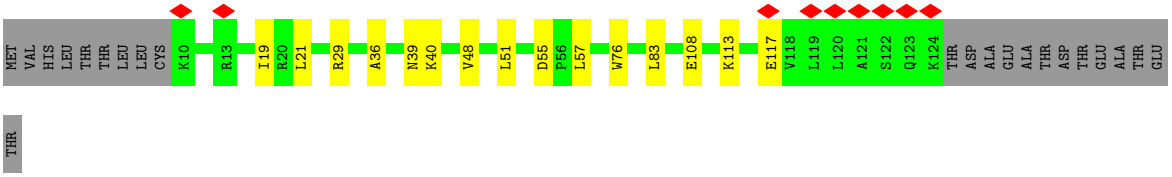




• Molecule 19: 28S ribosomal protein S16, mitochondrial

Chain M:

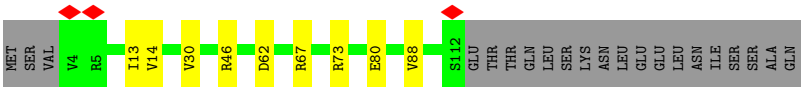




• Molecule 20: 28S ribosomal protein S17, mitochondrial

Chain N:

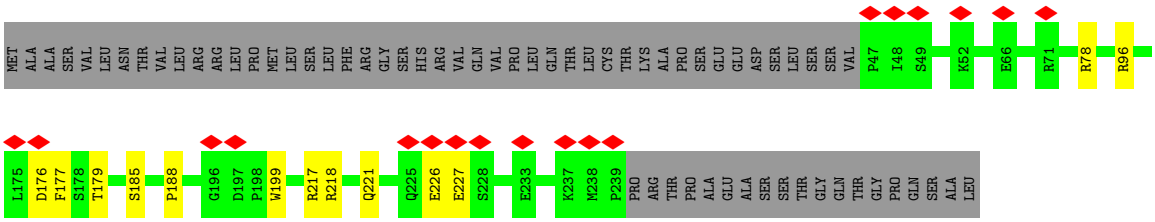




• Molecule 21: 28S ribosomal protein S18b, mitochondrial

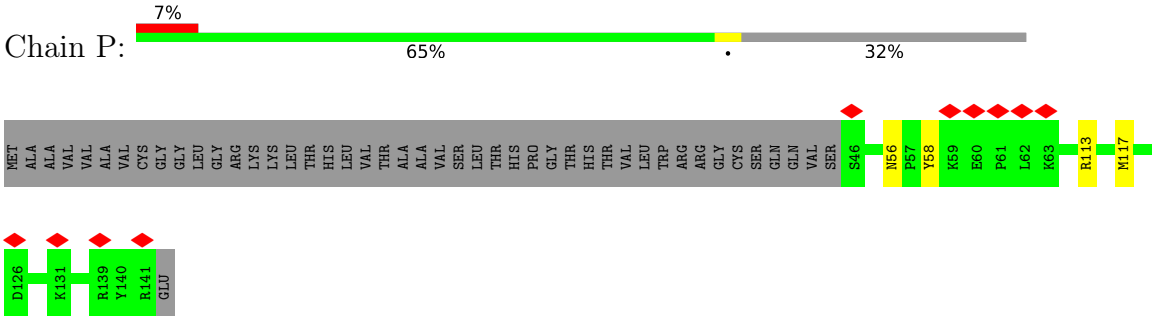
Chain O:





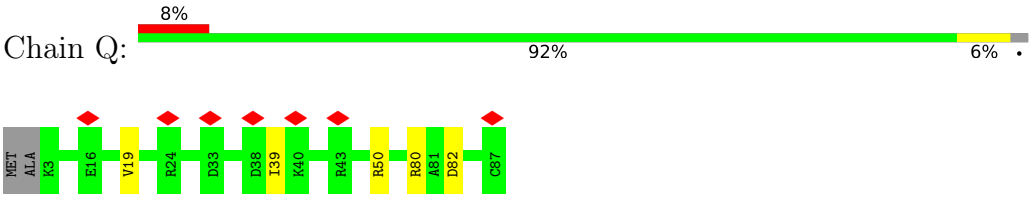
• Molecule 22: 28S ribosomal protein S18c, mitochondrial

Chain P:



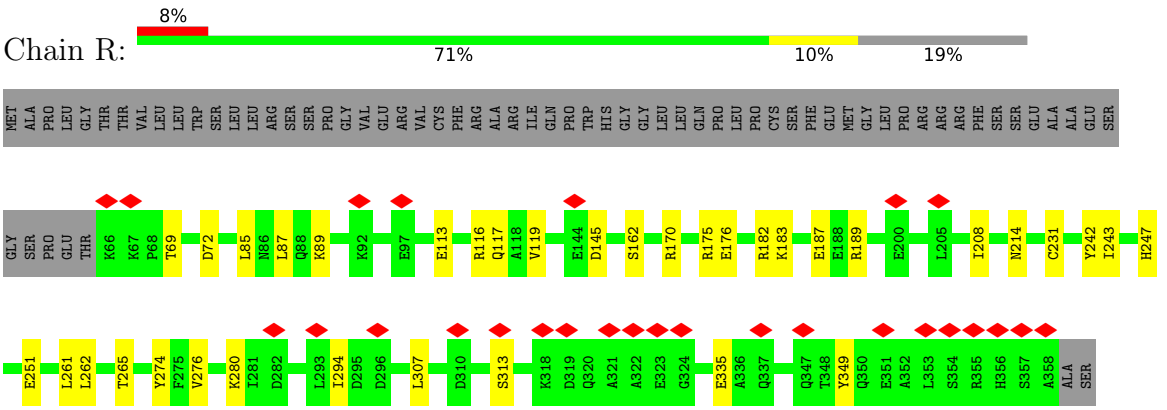
• Molecule 23: 28S ribosomal protein S21, mitochondrial

Chain Q:



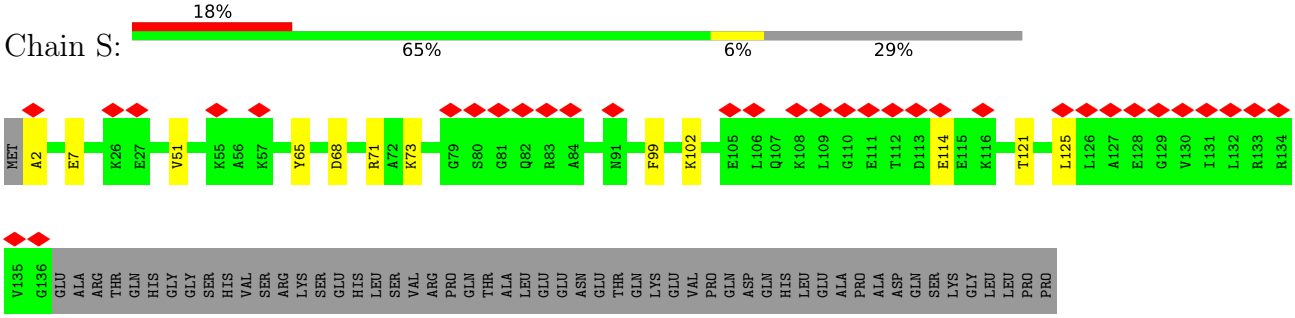
• Molecule 24: 28S ribosomal protein S22, mitochondrial

Chain R:



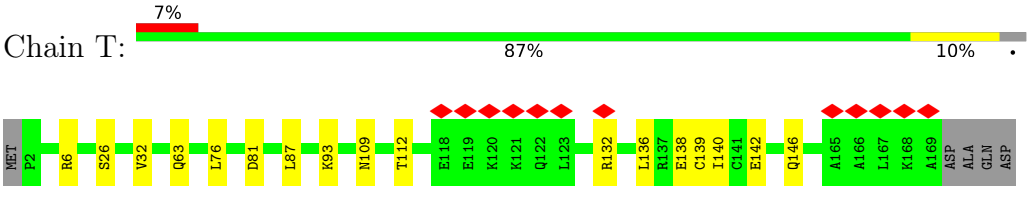
• Molecule 25: 28S ribosomal protein S23, mitochondrial

Chain S:

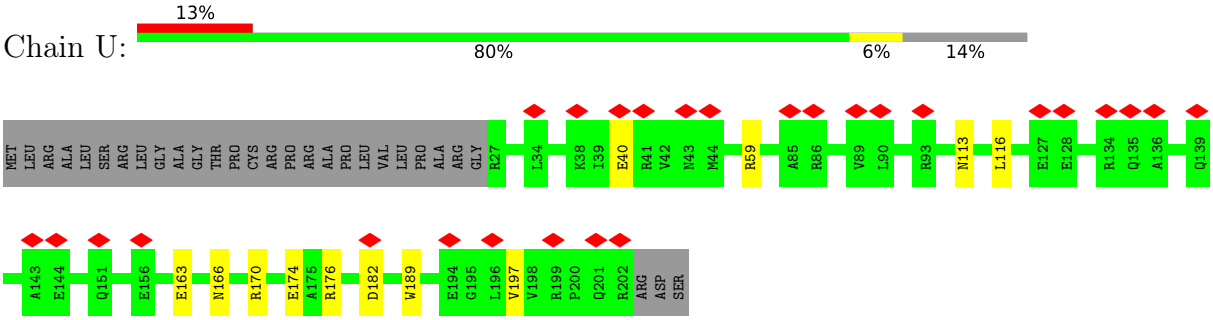


• Molecule 26: 28S ribosomal protein S25, mitochondrial

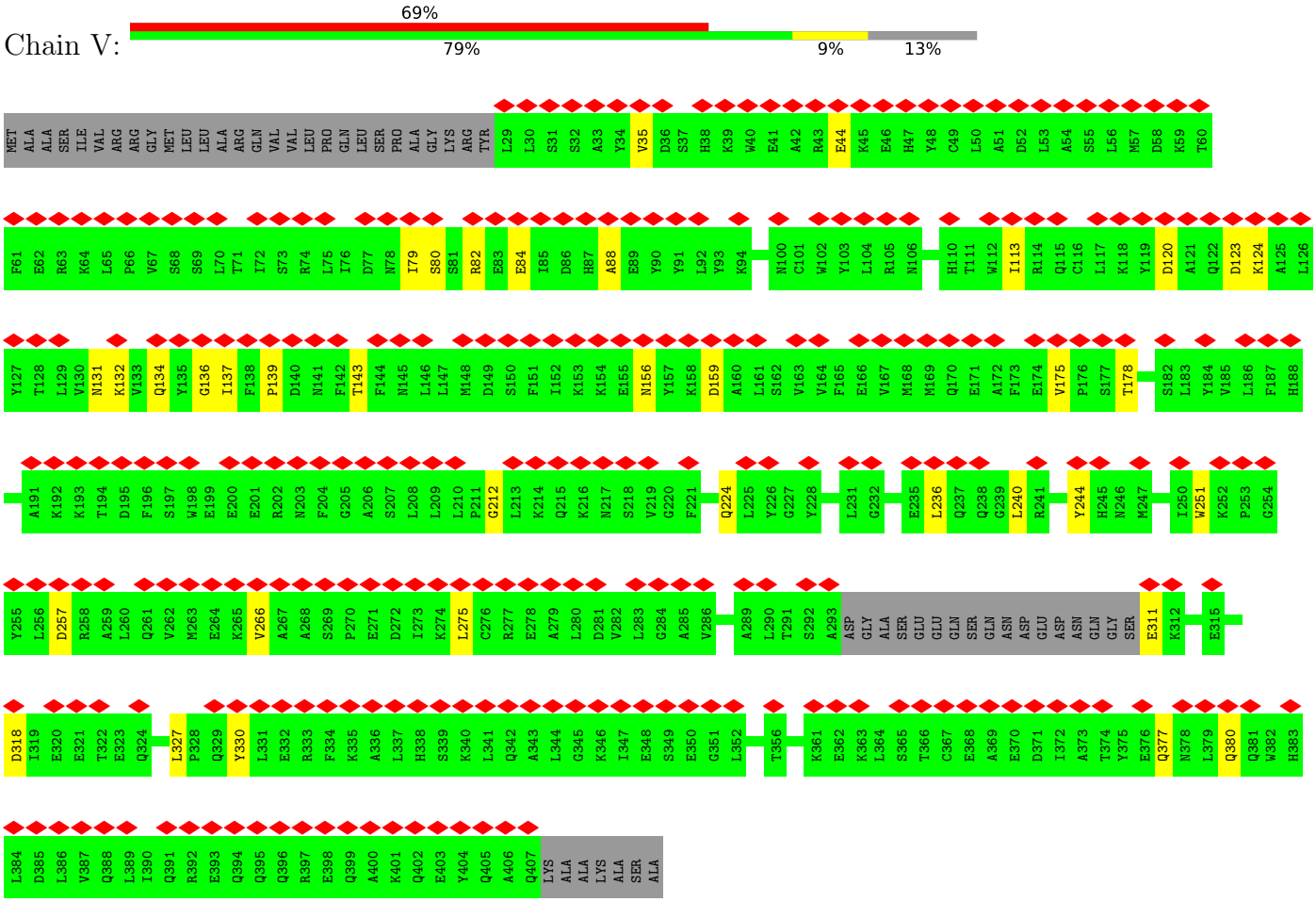
Chain T:



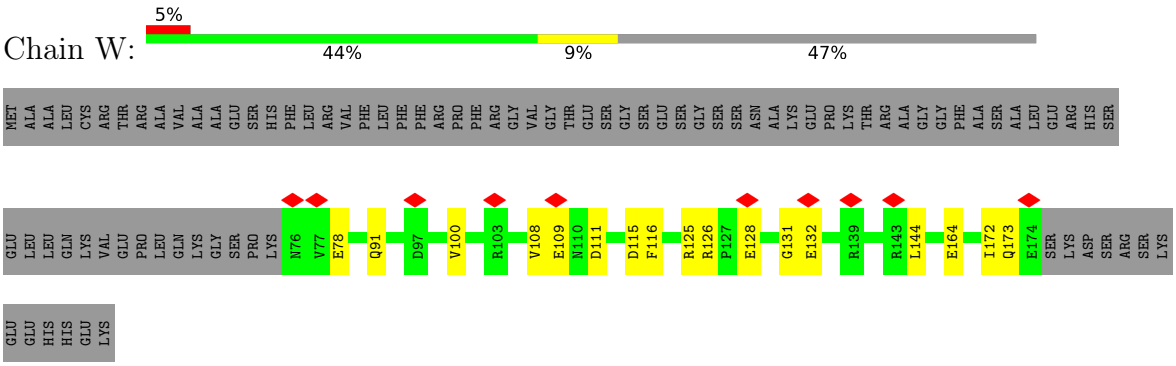
• Molecule 27: 28S ribosomal protein S26, mitochondrial



• Molecule 28: 28S ribosomal protein S27, mitochondrial

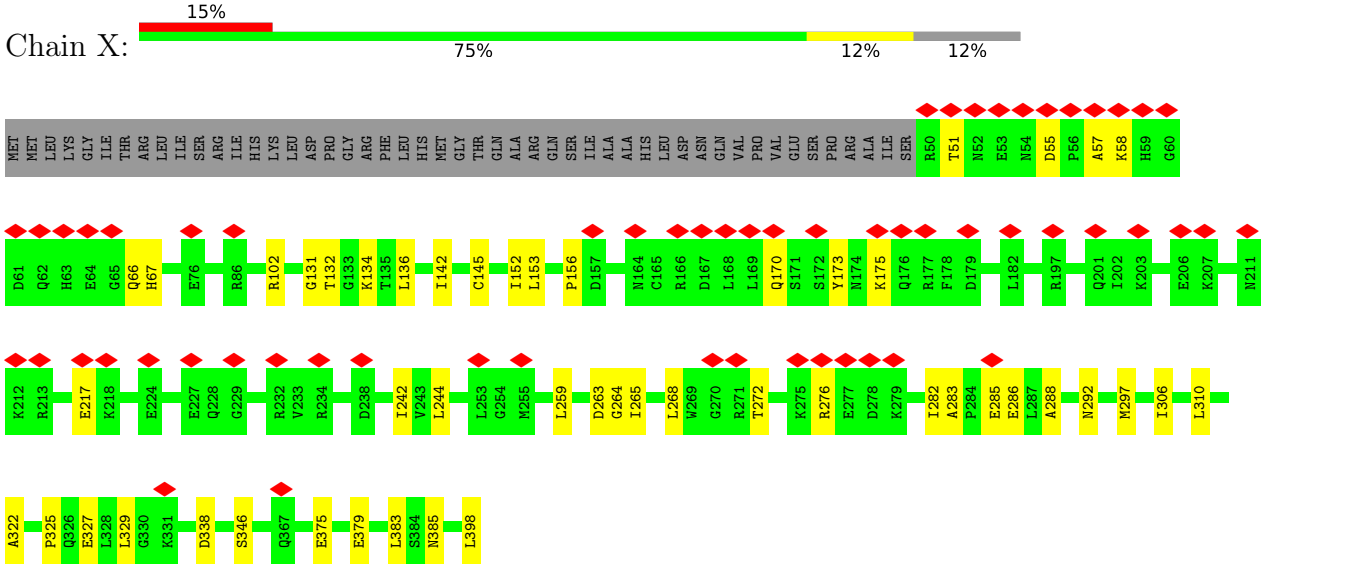


• Molecule 29: 28S ribosomal protein S28, mitochondrial



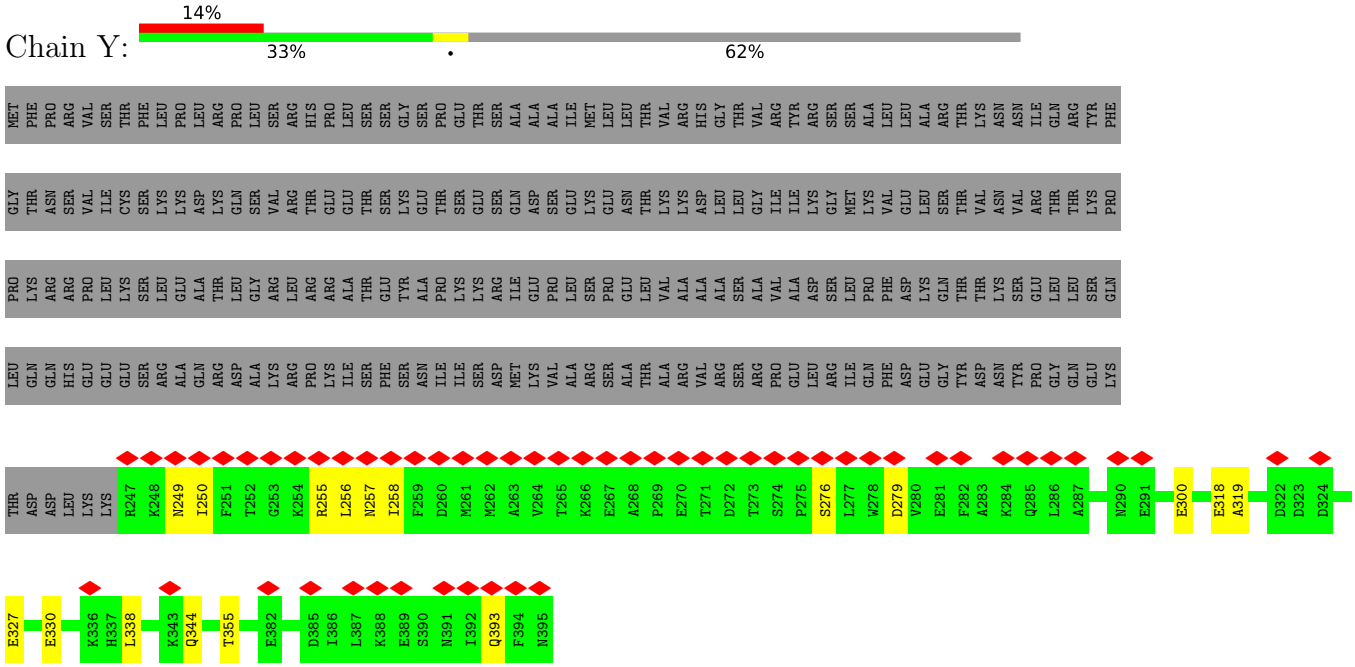
• Molecule 30: 28S ribosomal protein S29, mitochondrial

Chain X:



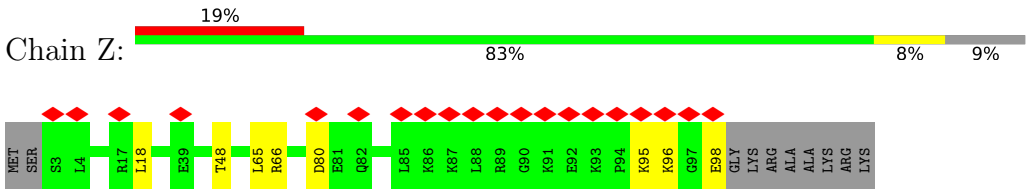
• Molecule 31: 28S ribosomal protein S31, mitochondrial

Chain Y:



• Molecule 32: 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	27943	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.463	Depositor
Minimum map value	-0.301	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.485	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: ZN, FES, GDP, ATP, GTP, K, ACE, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.10	0/1811	0.26	0/2452
2	1	0.10	0/2285	0.24	0/3090
3	2	0.10	0/877	0.23	0/1171
4	3	0.12	0/640	0.29	0/844
5	4	0.10	0/4904	0.23	0/6636
6	7	0.13	0/3382	0.27	0/4573
7	A	0.12	0/21295	0.25	0/33141
8	B	0.11	0/1832	0.25	0/2480
9	C	0.11	0/1113	0.26	0/1505
10	D	0.11	0/2742	0.24	0/3670
11	E	0.10	0/989	0.25	0/1335
12	F	0.10	0/1705	0.24	0/2290
13	G	0.10	0/2544	0.23	0/3408
14	H	0.10	0/1162	0.28	0/1575
15	I	0.10	0/1039	0.28	0/1400
16	J	0.14	0/845	0.27	0/1137
17	K	0.11	0/880	0.24	0/1182
18	L	0.11	0/1445	0.24	0/1932
19	M	0.13	0/934	0.28	0/1255
20	N	0.12	0/877	0.26	0/1187
21	O	0.10	0/1648	0.24	0/2243
22	P	0.11	0/788	0.25	0/1058
23	Q	0.10	0/748	0.24	0/994
24	R	0.10	0/2440	0.23	0/3295
25	S	0.10	0/1138	0.23	0/1533
26	T	0.12	0/1402	0.26	0/1883
27	U	0.11	0/1510	0.24	0/2025
28	V	0.10	0/3030	0.26	0/4093
29	W	0.12	0/795	0.25	0/1071
30	X	0.11	0/2902	0.27	0/3928
31	Y	0.11	0/1280	0.23	0/1725
32	Z	0.10	0/828	0.23	0/1104

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.11	0/71810	0.25	0/101215

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1765	0	1773	16	0
2	1	2238	0	2269	25	0
3	2	867	0	910	7	0
4	3	629	0	702	7	0
5	4	4795	0	4796	46	0
6	7	3334	0	3367	43	0
7	A	19041	0	9676	163	0
8	B	1789	0	1781	10	0
9	C	1083	0	1088	15	0
10	D	2691	0	2754	17	0
11	E	972	0	1000	12	0
12	F	1666	0	1707	14	0
13	G	2491	0	2473	24	0
14	H	1138	0	1173	16	0
15	I	1019	0	1059	16	0
16	J	829	0	874	8	0
17	K	862	0	885	16	0
18	L	1421	0	1506	10	0
19	M	913	0	943	9	0
20	N	859	0	922	8	0
21	O	1592	0	1557	11	0
22	P	771	0	800	4	0
23	Q	736	0	749	7	0
24	R	2393	0	2415	24	0
25	S	1111	0	1115	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	T	1371	0	1393	13	0
27	U	1488	0	1499	10	0
28	V	2969	0	2961	22	0
29	W	783	0	797	14	0
30	X	2830	0	2823	35	0
31	Y	1246	0	1197	16	0
32	Z	810	0	824	6	0
33	3	1	0	0	0	0
33	7	1	0	0	0	0
33	A	41	0	0	0	0
33	B	1	0	0	0	0
33	X	1	0	0	0	0
34	7	32	0	12	6	0
35	A	1	0	0	0	0
36	O	1	0	0	0	0
37	P	4	0	0	0	0
37	T	4	0	0	0	0
38	X	31	0	12	5	0
39	X	28	0	12	2	0
All	All	68648	0	59824	544	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 4.

All (544) 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)
6:7:538:TYR:OH	6:7:544:CYS:O	1.88	0.90
7:A:992:U:O2'	7:A:994:A:OP2	1.92	0.85
30:X:51:THR:OG1	30:X:67:HIS:O	1.92	0.85
5:4:616:ASP:OD1	5:4:648:ARG:NH2	2.12	0.83
7:A:769:G:OP2	20:N:73:ARG:NH2	2.12	0.82
7:A:1106:C:O2'	7:A:1108:C:OP2	1.98	0.80
28:V:377:GLN:OE1	28:V:380:GLN:NE2	2.14	0.80
5:4:376:ILE:HG23	5:4:422:ILE:HD11	1.63	0.80
26:T:138:GLU:N	26:T:142:GLU:OE2	2.14	0.80
28:V:311:GLU:N	28:V:311:GLU:OE1	2.15	0.79
6:7:168:ARG:NH2	6:7:354:PRO:O	2.15	0.79
7:A:1162:A:N3	7:A:1497:C:O2'	2.14	0.79
3:2:36:ARG:NH1	3:2:37:ARG:O	2.15	0.79
5:4:529:GLU:OE2	5:4:559:TYR:OH	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:409:ASP:N	5:4:412:ASP:OD2	2.18	0.76
7:A:1294:A:OP1	8:B:201:ASN:ND2	2.19	0.76
7:A:1268:C:OP2	7:A:1269:U:O2'	2.04	0.76
1:0:177:GLU:OE2	1:0:181:ASN:ND2	2.20	0.75
14:H:125:HIS:CE1	14:H:126:ILE:HG23	2.22	0.74
4:3:139:ASN:ND2	7:A:1141:C:OP1	2.19	0.74
7:A:1098:C:O2'	7:A:1151:C:O2'	2.05	0.74
1:0:140:ARG:NH2	28:V:244:TYR:OH	2.21	0.73
3:2:58:GLN:NE2	3:2:59:ASN:OD1	2.21	0.73
7:A:702:C:OP1	7:A:848:U:O2'	2.05	0.73
6:7:322:PRO:O	6:7:330:ASN:ND2	2.23	0.72
14:H:92:GLU:OE1	14:H:141:ARG:NH1	2.23	0.72
24:R:187:GLU:N	24:R:187:GLU:OE1	2.23	0.71
7:A:1053:A:N1	7:A:1100:C:O2'	2.21	0.71
26:T:132:ARG:NH1	26:T:136:LEU:O	2.22	0.71
6:7:446:TRP:NE1	6:7:450:GLU:OE1	2.23	0.71
17:K:58:ARG:NE	17:K:72:ASP:OD1	2.23	0.71
7:A:1431:G:O2'	7:A:1457:G:O6	2.08	0.70
5:4:151:ASP:OD1	5:4:152:ILE:N	2.25	0.70
16:J:116:GLN:N	16:J:116:GLN:OE1	2.24	0.69
17:K:75:ILE:HD12	17:K:78:LEU:HD12	1.74	0.69
29:W:111:ASP:OD1	29:W:125:ARG:NH1	2.24	0.69
3:2:32:ARG:NH2	3:2:35:GLU:OE2	2.25	0.69
5:4:528:ARG:NH2	5:4:562:GLN:OE1	2.25	0.69
13:G:263:ASP:OD1	13:G:267:MET:N	2.25	0.69
24:R:176:GLU:OE2	24:R:182:ARG:NE	2.24	0.69
24:R:262:LEU:O	24:R:265:THR:OG1	2.10	0.69
12:F:79:ALA:O	13:G:312:GLN:NE2	2.26	0.69
31:Y:276:SER:N	31:Y:279:ASP:OD2	2.26	0.69
31:Y:344:GLN:N	31:Y:344:GLN:OE1	2.25	0.69
10:D:162:LYS:NZ	10:D:166:GLU:OE2	2.26	0.68
7:A:760:A:N1	7:A:780:C:O2'	2.24	0.68
14:H:176:GLN:NE2	14:H:178:GLU:OE2	2.27	0.68
1:0:166:TYR:O	21:O:199:TRP:NE1	2.26	0.68
3:2:9:ARG:NH2	7:A:1021:U:OP2	2.26	0.67
5:4:157:LEU:O	5:4:161:ILE:HD12	1.94	0.67
15:I:166:ILE:CD1	23:Q:19:VAL:HG21	2.24	0.67
28:V:123:ASP:OD1	28:V:124:LYS:N	2.27	0.67
7:A:1355:G:O2'	7:A:1356:A:OP2	2.11	0.67
5:4:522:THR:O	5:4:528:ARG:NH1	2.28	0.66
6:7:330:ASN:OD1	6:7:333:ALA:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:155:LYS:NZ	13:G:217:ASP:OD2	2.27	0.66
7:A:1343:A:O2'	7:A:1345:G:N7	2.26	0.66
30:X:131:GLY:N	38:X:402:ATP:O1B	2.28	0.66
5:4:349:ALA:HB1	5:4:378:LEU:HD11	1.78	0.66
19:M:39:ASN:OD1	19:M:40:LYS:N	2.30	0.65
7:A:1218:A:O2'	14:H:126:ILE:HD13	1.95	0.65
11:E:80:GLU:OE2	11:E:84:ARG:NE	2.27	0.65
15:I:94:ASN:OD1	15:I:95:THR:N	2.29	0.65
7:A:1454:G:OP2	13:G:377:ARG:NH1	2.29	0.65
18:L:86:ASP:OD1	18:L:87:ASP:N	2.31	0.65
30:X:131:GLY:CA	38:X:402:ATP:O1B	2.46	0.64
7:A:1066:C:O2'	15:I:187:ARG:O	2.15	0.64
6:7:197:LEU:HD22	6:7:234:ASP:HB2	1.80	0.64
24:R:85:LEU:HD21	24:R:119:VAL:HG13	1.78	0.64
6:7:363:PHE:HB3	6:7:524:VAL:HG12	1.80	0.63
16:J:51:PRO:O	16:J:89:ARG:NH2	2.31	0.63
5:4:402:GLY:O	5:4:404:ARG:NH1	2.31	0.63
7:A:713:C:HO2'	7:A:852:A:HO2'	1.41	0.63
7:A:890:C:O3'	16:J:75:SER:OG	2.18	0.62
6:7:401:ASP:OD1	6:7:404:GLY:N	2.33	0.62
7:A:890:C:O2'	7:A:902:G:N2	2.31	0.62
17:K:57:LEU:O	17:K:60:ASN:ND2	2.33	0.62
13:G:301:GLN:OE1	30:X:385:ASN:ND2	2.31	0.61
30:X:283:ALA:N	30:X:286:GLU:OE1	2.33	0.61
2:1:169:ARG:O	2:1:218:ASN:ND2	2.33	0.61
28:V:132:LYS:O	28:V:136:GLY:N	2.32	0.61
28:V:236:LEU:CD2	28:V:327:LEU:HD21	2.29	0.61
27:U:40:GLU:OE1	27:U:40:GLU:N	2.31	0.61
12:F:122:GLN:NE2	12:F:138:GLU:O	2.34	0.61
13:G:318:HIS:NE2	30:X:379:GLU:OE2	2.34	0.60
19:M:55:ASP:OD2	26:T:146:GLN:NE2	2.33	0.60
7:A:1415:G:OP2	7:A:1415:G:N2	2.20	0.60
5:4:87:TYR:OH	31:Y:300:GLU:OE1	2.16	0.60
13:G:315:PHE:CD2	13:G:369:LEU:HD21	2.36	0.60
2:1:107:LYS:NZ	9:C:54:GLU:OE2	2.35	0.60
7:A:928:A:OP2	16:J:47:ARG:NH2	2.34	0.60
7:A:1352:C:O2'	7:A:1353:A:O4'	2.20	0.60
4:3:161:ARG:NH2	7:A:1146:C:OP1	2.36	0.59
7:A:1285:G:O2'	7:A:1286:A:O4'	2.19	0.59
7:A:1289:G:O2'	7:A:1297:G:OP2	2.20	0.59
24:R:162:SER:O	24:R:170:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:135:MET:SD	1:0:135:MET:N	2.75	0.59
7:A:1234:C:O2'	17:K:40:ARG:NH1	2.36	0.59
7:A:1033:U:OP1	22:P:113:ARG:NH2	2.35	0.59
7:A:1213:A:O2'	7:A:1239:C:O2'	2.04	0.59
14:H:126:ILE:O	14:H:128:LYS:N	2.36	0.59
29:W:78:GLU:N	29:W:78:GLU:OE1	2.32	0.59
13:G:115:GLY:N	14:H:84:ASP:OD2	2.35	0.59
24:R:69:THR:N	24:R:72:ASP:OD2	2.36	0.59
5:4:356:VAL:HG12	5:4:360:MET:HE2	1.85	0.58
6:7:372:THR:OG1	6:7:421:TRP:NE1	2.32	0.58
1:0:43:ARG:NE	7:A:706:C:OP1	2.35	0.58
17:K:60:ASN:O	17:K:68:GLN:NE2	2.35	0.58
20:N:67:ARG:NH1	20:N:80:GLU:OE2	2.36	0.58
17:K:55:ASN:OD1	17:K:58:ARG:NH1	2.36	0.58
6:7:441:ARG:NH2	7:A:859:U:OP1	2.36	0.58
2:1:186:ALA:O	2:1:233:SER:OG	2.22	0.58
19:M:108:GLU:OE2	27:U:59:ARG:NH2	2.33	0.58
2:1:244:THR:N	2:1:247:ASP:OD2	2.35	0.58
7:A:1282:G:N2	7:A:1286:A:OP2	2.34	0.58
11:E:94:VAL:CG1	22:P:117:MET:HE1	2.34	0.58
2:1:254:GLU:OE2	2:1:293:LYS:NZ	2.28	0.58
7:A:838:U:O2'	19:M:21:LEU:O	2.22	0.58
16:J:78:ARG:NE	16:J:117:ASP:OD2	2.30	0.58
28:V:212:GLY:O	28:V:224:GLN:NE2	2.37	0.58
6:7:525:ASP:OD1	6:7:526:GLY:N	2.37	0.57
10:D:415:GLN:NE2	10:D:417:MET:SD	2.77	0.57
1:0:9:ARG:NE	7:A:805:C:O2	2.37	0.57
7:A:893:G:N7	16:J:78:ARG:NH1	2.51	0.57
7:A:1339:G:C2	7:A:1340:C:C5	2.93	0.57
30:X:102:ARG:NH2	30:X:346:SER:O	2.34	0.57
30:X:132:THR:N	38:X:402:ATP:O1B	2.37	0.57
30:X:217:GLU:N	30:X:217:GLU:OE1	2.37	0.57
5:4:359:GLU:OE2	31:Y:255:ARG:NH1	2.37	0.57
6:7:238:HIS:O	6:7:245:ARG:NH1	2.35	0.57
7:A:1176:G:O2'	7:A:1483:C:OP2	2.23	0.57
10:D:285:TYR:N	10:D:289:THR:O	2.37	0.57
6:7:512:ASP:OD1	6:7:513:SER:N	2.38	0.57
9:C:138:TYR:OH	32:Z:65:LEU:HD22	2.05	0.57
28:V:175:VAL:HG13	28:V:178:THR:H	1.70	0.56
1:0:89:HIS:NE2	1:0:202:ASP:OD2	2.36	0.56
25:S:102:LYS:HB3	25:S:121:THR:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1033:U:O2'	11:E:93:ILE:O	2.24	0.56
19:M:19:ILE:HB	19:M:83:LEU:HD23	1.88	0.56
1:0:30:ASP:OD1	1:0:212:ARG:NH1	2.38	0.56
5:4:605:ILE:HG23	5:4:639:LEU:HD11	1.88	0.56
31:Y:249:ASN:OD1	31:Y:250:ILE:N	2.39	0.56
13:G:320:VAL:HG21	13:G:352:LEU:HD21	1.86	0.56
25:S:73:LYS:NZ	25:S:114:GLU:OE1	2.39	0.56
6:7:252:THR:OG1	6:7:254:ILE:O	2.23	0.56
15:I:147:ILE:CD1	15:I:165:LEU:HD21	2.37	0.55
2:1:137:LEU:HD12	2:1:137:LEU:O	2.06	0.55
28:V:44:GLU:OE1	28:V:44:GLU:N	2.39	0.55
5:4:80:ARG:NH2	5:4:480:ASP:O	2.39	0.55
9:C:75:ASN:ND2	17:K:121:SER:O	2.38	0.55
31:Y:327:GLU:N	31:Y:330:GLU:OE1	2.36	0.55
15:I:150:VAL:O	15:I:150:VAL:HG13	2.07	0.55
6:7:197:LEU:HD21	6:7:220:PHE:CD2	2.42	0.55
7:A:652:G:HO2'	7:A:879:U:HO2'	1.54	0.55
15:I:171:GLU:OE1	15:I:172:VAL:N	2.38	0.54
5:4:376:ILE:HG21	5:4:418:SER:HB3	1.89	0.54
7:A:919:A:OP2	21:O:96:ARG:NH1	2.40	0.54
7:A:843:G:N1	7:A:846:A:OP2	2.41	0.54
6:7:217:ILE:O	6:7:217:ILE:HG23	2.07	0.54
2:1:232:GLU:HG3	32:Z:18:LEU:HD21	1.90	0.54
7:A:1286:A:OP1	10:D:260:LYS:NZ	2.37	0.54
18:L:82:ILE:O	18:L:85:VAL:HG22	2.07	0.54
6:7:394:ALA:HB2	6:7:421:TRP:HA	1.89	0.54
7:A:1578:A:H2'	7:A:1579:C:C6	2.43	0.53
6:7:193:LYS:HZ3	34:7:802:GTP:PB	2.31	0.53
7:A:1103:A:N7	7:A:1574:G:O2'	2.38	0.53
7:A:1257:U:O2'	7:A:1260:A:OP2	2.14	0.53
10:D:245:VAL:HG22	10:D:271:ALA:HB1	1.90	0.53
2:1:292:TYR:OH	30:X:338:ASP:OD2	2.26	0.53
14:H:70:ASP:OD1	14:H:71:ILE:N	2.41	0.53
6:7:311:CYS:O	6:7:316:GLY:N	2.41	0.53
7:A:954:C:O2	7:A:1111:C:O2'	2.23	0.53
5:4:131:ASP:OD2	5:4:136:HIS:ND1	2.42	0.52
7:A:1265:C:OP1	17:K:112:ARG:NH2	2.40	0.52
26:T:109:ASN:OD1	26:T:112:THR:N	2.37	0.52
29:W:128:GLU:OE1	29:W:128:GLU:N	2.40	0.52
30:X:153:LEU:HD21	30:X:244:LEU:CD2	2.40	0.52
4:3:189:TRP:CE2	18:L:209:LEU:HD12	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:160:ARG:NH2	7:A:678:U:OP1	2.43	0.52
24:R:243:ILE:HG23	24:R:247:HIS:CE1	2.45	0.52
5:4:284:ASN:O	5:4:286:ARG:NH1	2.42	0.52
12:F:147:GLN:NE2	12:F:151:ASN:OD1	2.43	0.52
19:M:29:ARG:HD3	19:M:57:LEU:HD12	1.91	0.52
2:1:279:ASN:OD1	2:1:280:LYS:N	2.43	0.52
4:3:155:ARG:NH1	7:A:1154:A:OP2	2.40	0.52
20:N:13:ILE:HD12	20:N:30:VAL:HG21	1.92	0.52
6:7:192:GLY:N	34:7:802:GTP:O1B	2.42	0.52
10:D:340:ILE:O	10:D:340:ILE:HG22	2.09	0.52
5:4:451:ASP:O	5:4:455:ASN:ND2	2.40	0.52
9:C:96:MET:HB2	9:C:108:LEU:HD11	1.92	0.52
28:V:240:LEU:HD21	28:V:251:TRP:O	2.10	0.52
7:A:1252:G:HO2'	7:A:1345:G:HO2'	1.53	0.51
13:G:234:GLY:N	13:G:237:GLU:OE1	2.37	0.51
1:0:79:LEU:HD21	1:0:96:ARG:CZ	2.40	0.51
2:1:286:THR:HG23	2:1:289:ILE:H	1.76	0.51
21:O:176:ASP:OD1	21:O:177:PHE:N	2.43	0.51
2:1:50:ARG:NH1	5:4:102:GLU:OE2	2.43	0.51
6:7:249:ALA:O	6:7:252:THR:HG22	2.10	0.51
7:A:836:A:C2	7:A:837:A:C8	2.98	0.51
7:A:1375:C:H2'	7:A:1376:C:O4'	2.11	0.51
29:W:108:VAL:HG12	29:W:109:GLU:H	1.75	0.51
29:W:126:ARG:NH1	29:W:131:GLY:O	2.43	0.51
11:E:15:ARG:NH1	27:U:182:ASP:OD1	2.44	0.51
21:O:218:ARG:O	21:O:221:GLN:NE2	2.41	0.51
7:A:949:U:O2'	20:N:46:ARG:NH1	2.44	0.51
7:A:1591:C:C2	7:A:1592:U:C5	2.99	0.51
7:A:1056:A:H4'	7:A:1588:G:H22	1.76	0.51
6:7:265:VAL:HG11	6:7:307:TYR:CE2	2.45	0.50
2:1:235:ASN:OD1	2:1:236:THR:N	2.44	0.50
7:A:941:G:O2'	7:A:1109:A:OP2	2.26	0.50
15:I:147:ILE:HD12	15:I:165:LEU:HD21	1.93	0.50
1:0:79:LEU:HD22	1:0:94:TYR:CD1	2.47	0.50
8:B:220:VAL:HG22	8:B:234:TYR:HB2	1.93	0.50
6:7:191:HIS:N	34:7:802:GTP:O1B	2.44	0.50
1:0:178:ARG:NH2	1:0:185:SER:O	2.43	0.50
7:A:856:A:C2	7:A:857:G:C8	3.00	0.50
7:A:1225:C:OP1	13:G:394:LYS:NZ	2.45	0.50
7:A:1355:G:N2	7:A:1356:A:N7	2.55	0.50
5:4:372:TYR:CD1	5:4:396:ILE:HG23	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:577:ASN:OD1	5:4:607:ARG:N	2.43	0.49
28:V:80:SER:OG	28:V:84:GLU:OE1	2.27	0.49
1:0:132:GLU:OE1	1:0:210:LYS:NZ	2.41	0.49
7:A:1456:U:OP2	13:G:277:LYS:NZ	2.39	0.49
7:A:657:G:O4'	7:A:1480:A:O2'	2.30	0.49
8:B:239:ASN:OD1	8:B:240:ASP:N	2.45	0.49
23:Q:80:ARG:NH2	29:W:164:GLU:OE1	2.41	0.49
2:1:164:ARG:NH2	31:Y:319:ALA:O	2.41	0.49
6:7:252:THR:HG21	6:7:255:VAL:CG2	2.42	0.49
7:A:974:U:O2'	7:A:975:A:N7	2.35	0.49
11:E:94:VAL:HG11	22:P:117:MET:HE1	1.94	0.49
12:F:52:ARG:NH2	13:G:321:ASP:OD2	2.42	0.49
31:Y:393:GLN:OE1	31:Y:393:GLN:N	2.38	0.49
1:0:79:LEU:HD23	1:0:96:ARG:HA	1.95	0.49
7:A:1218:A:H1'	14:H:126:ILE:HG21	1.93	0.49
30:X:142:ILE:HG23	30:X:152:ILE:HG21	1.94	0.49
7:A:1056:A:H4'	7:A:1588:G:N2	2.28	0.49
6:7:521:LYS:NZ	6:7:554:GLY:O	2.43	0.49
9:C:84:GLU:OE2	17:K:105:ARG:NH1	2.44	0.49
14:H:71:ILE:O	14:H:150:GLY:N	2.45	0.49
8:B:107:PHE:N	8:B:115:ILE:O	2.42	0.49
7:A:1040:U:H2'	7:A:1041:A:O4'	2.13	0.48
10:D:191:ARG:O	21:O:78:ARG:NH1	2.46	0.48
10:D:372:GLU:OE2	10:D:374:ARG:NE	2.41	0.48
2:1:215:ARG:N	31:Y:318:GLU:OE2	2.46	0.48
7:A:1247:G:N7	32:Z:96:LYS:NZ	2.59	0.48
22:P:56:ASN:OD1	22:P:58:TYR:N	2.46	0.48
24:R:294:ILE:HD11	24:R:349:TYR:CE1	2.48	0.48
30:X:134:LYS:HZ3	38:X:402:ATP:PB	2.36	0.48
30:X:173:TYR:CE2	39:X:403:GDP:H3'	2.48	0.48
7:A:1232:A:C2	7:A:1404:A:N3	2.81	0.48
10:D:282:ILE:HG23	10:D:353:LEU:HB3	1.95	0.48
30:X:55:ASP:OD1	30:X:58:LYS:N	2.45	0.48
30:X:170:GLN:NE2	30:X:175:LYS:O	2.40	0.48
2:1:87:MET:SD	2:1:108:ILE:HD11	2.54	0.48
7:A:715:G:H2'	7:A:716:U:C6	2.49	0.48
7:A:745:A:C4	7:A:746:A:C8	3.02	0.48
7:A:812:A:O2'	7:A:813:A:O4'	2.25	0.48
14:H:125:HIS:ND1	14:H:126:ILE:HG23	2.28	0.48
1:0:61:GLU:HB2	1:0:137:HIS:O	2.13	0.48
5:4:376:ILE:HG23	5:4:422:ILE:CD1	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:255:VAL:HG23	6:7:281:VAL:HG21	1.96	0.48
10:D:198:TRP:HA	10:D:201:ILE:HD12	1.96	0.48
19:M:113:LYS:NZ	19:M:117:GLU:OE2	2.38	0.48
25:S:71:ARG:NH2	29:W:91:GLN:OE1	2.43	0.48
28:V:137:ILE:HG22	28:V:139:PRO:HD3	1.96	0.48
11:E:27:GLU:OE2	27:U:170:ARG:NH1	2.47	0.47
17:K:72:ASP:O	17:K:75:ILE:HG22	2.14	0.47
24:R:208:ILE:O	24:R:214:ASN:ND2	2.38	0.47
5:4:193:ASP:OD1	5:4:261:THR:HG21	2.14	0.47
30:X:272:THR:OG1	30:X:282:ILE:O	2.31	0.47
20:N:88:VAL:O	20:N:88:VAL:HG13	2.13	0.47
7:A:821:U:H2'	7:A:822:G:H8	1.79	0.47
7:A:1248:C:O2	17:K:28:HIS:N	2.47	0.47
7:A:1320:G:OP2	9:C:37:ASN:ND2	2.43	0.47
21:O:179:THR:HG22	21:O:179:THR:O	2.13	0.47
3:2:117:LEU:HD11	25:S:51:VAL:HG13	1.96	0.47
7:A:790:A:H2'	7:A:791:G:H4'	1.95	0.47
5:4:481:LEU:O	5:4:485:ALA:N	2.41	0.47
26:T:93:LYS:HE3	27:U:116:LEU:HD11	1.95	0.47
6:7:252:THR:HG21	6:7:255:VAL:HG23	1.97	0.47
7:A:663:A:H2'	7:A:664:G:C8	2.49	0.47
7:A:852:A:H3'	7:A:853:C:H6	1.79	0.47
7:A:1272:A:N6	7:A:1320:G:O2'	2.41	0.47
7:A:1392:A:C2	7:A:1393:G:C8	3.02	0.47
8:B:197:HIS:NE2	8:B:240:ASP:O	2.48	0.47
7:A:1460:C:H2'	7:A:1461:A:O4'	2.15	0.47
5:4:357:LEU:HA	5:4:360:MET:HE3	1.97	0.47
29:W:108:VAL:HG12	29:W:109:GLU:N	2.29	0.47
30:X:263:ASP:OD1	30:X:264:GLY:N	2.48	0.47
7:A:1279:C:O2'	7:A:1296:A:N1	2.38	0.47
7:A:1368:U:O4'	7:A:1370:U:C6	2.68	0.47
30:X:285:GLU:OE1	30:X:285:GLU:N	2.38	0.47
7:A:1496:U:OP1	16:J:82:ARG:NH1	2.47	0.46
25:S:65:TYR:N	25:S:68:ASP:OD2	2.40	0.46
29:W:108:VAL:O	29:W:109:GLU:C	2.58	0.46
12:F:119:LYS:NZ	30:X:398:LEU:OXT	2.45	0.46
7:A:664:G:H4'	7:A:1138:G:C8	2.50	0.46
18:L:126:GLU:HB3	18:L:181:ILE:HD11	1.97	0.46
7:A:889:G:N2	7:A:902:G:OP1	2.47	0.46
9:C:89:ASP:OD1	9:C:112:ARG:NH2	2.43	0.46
12:F:176:ASP:OD2	12:F:179:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:139:CYS:SG	26:T:140:ILE:N	2.88	0.46
14:H:89:ASP:OD1	14:H:141:ARG:NH1	2.45	0.46
5:4:359:GLU:OE1	31:Y:257:ASN:N	2.35	0.46
7:A:662:U:OP2	10:D:339:SER:OG	2.28	0.46
7:A:1461:A:H4'	7:A:1462:G:C8	2.51	0.46
7:A:1560:U:H2'	7:A:1561:C:C6	2.51	0.46
24:R:251:GLU:OE2	24:R:280:LYS:NZ	2.47	0.46
7:A:730:A:C4	7:A:731:A:C8	3.04	0.46
7:A:769:G:N2	7:A:772:A:OP2	2.47	0.46
7:A:1293:C:OP2	13:G:220:GLN:NE2	2.48	0.46
9:C:45:SER:OG	9:C:167:LEU:OXT	2.34	0.46
13:G:357:THR:N	13:G:360:GLU:OE1	2.43	0.46
30:X:322:ALA:HB1	30:X:327:GLU:HG3	1.98	0.46
12:F:161:ILE:HG23	12:F:241:TRP:CZ3	2.51	0.46
6:7:197:LEU:HD21	6:7:220:PHE:CE2	2.50	0.45
7:A:1224:C:N4	13:G:395:LYS:O	2.49	0.45
15:I:158:ARG:NH2	15:I:177:ASP:OD2	2.46	0.45
2:1:155:ASP:OD2	14:H:174:LYS:NZ	2.46	0.45
7:A:1355:G:HO2'	7:A:1356:A:P	2.37	0.45
7:A:672:A:H2'	7:A:673:U:C6	2.52	0.45
7:A:746:A:C4	7:A:747:A:C8	3.04	0.45
7:A:843:G:N2	7:A:846:A:OP2	2.50	0.45
17:K:70:VAL:HA	17:K:73:GLU:HG2	1.99	0.45
21:O:217:ARG:NH1	21:O:227:GLU:OE1	2.50	0.45
7:A:905:A:O2'	7:A:907:A:OP2	2.17	0.45
7:A:1127:A:H2'	7:A:1128:C:O4'	2.17	0.45
7:A:1200:G:C2	7:A:1201:A:C8	3.05	0.45
28:V:266:VAL:HG11	28:V:275:LEU:HG	1.97	0.45
30:X:288:ALA:O	30:X:292:ASN:ND2	2.45	0.45
5:4:80:ARG:NE	5:4:484:SER:OG	2.47	0.45
6:7:524:VAL:HG23	6:7:527:SER:H	1.80	0.45
25:S:99:PHE:HA	25:S:125:LEU:HD11	1.99	0.45
2:1:164:ARG:NH1	31:Y:319:ALA:O	2.49	0.45
5:4:317:LEU:HD22	31:Y:258:ILE:HD11	1.98	0.45
5:4:567:THR:HG22	5:4:568:ALA:H	1.81	0.45
8:B:149:ARG:NH2	23:Q:82:ASP:OD2	2.43	0.45
9:C:68:TRP:NE1	17:K:123:ILE:O	2.45	0.45
14:H:110:GLU:OE2	14:H:141:ARG:NH2	2.50	0.45
28:V:82:ARG:NH2	28:V:120:ASP:O	2.47	0.45
30:X:145:CYS:SG	30:X:259:LEU:HD22	2.56	0.45
32:Z:95:LYS:N	32:Z:98:GLU:OE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1080:A:H1'	7:A:1082:A:N7	2.32	0.45
7:A:1398:U:H2'	7:A:1399:A:H8	1.82	0.45
30:X:310:LEU:HD21	30:X:329:LEU:HD21	1.98	0.45
15:I:83:ILE:O	15:I:148:ARG:NH2	2.50	0.44
18:L:115:ILE:HG21	18:L:181:ILE:HD13	1.98	0.44
20:N:30:VAL:HG13	26:T:63:GLN:NE2	2.32	0.44
28:V:257:ASP:OD1	28:V:330:TYR:CE1	2.70	0.44
30:X:55:ASP:OD1	30:X:57:ALA:N	2.49	0.44
8:B:188:ARG:O	13:G:152:TYR:OH	2.32	0.44
7:A:728:C:H2'	7:A:729:U:O4'	2.17	0.44
18:L:167:LEU:HD11	18:L:187:ILE:HG21	1.98	0.44
31:Y:338:LEU:HD11	31:Y:355:THR:HG21	1.99	0.44
5:4:584:LEU:HD13	5:4:613:GLU:HG3	2.00	0.44
7:A:1077:U:O2'	7:A:1079:G:N7	2.47	0.44
10:D:363:ALA:HB2	10:D:370:VAL:HG23	2.00	0.44
13:G:304:PHE:CD2	13:G:313:LEU:HD11	2.53	0.44
7:A:1422:G:O2'	7:A:1423:A:O4'	2.20	0.44
12:F:161:ILE:HD12	12:F:170:VAL:HB	1.99	0.44
24:R:89:LYS:NZ	24:R:261:LEU:O	2.41	0.44
24:R:170:ARG:O	24:R:189:ARG:NH2	2.48	0.44
26:T:26:SER:O	26:T:81:ASP:N	2.50	0.44
5:4:567:THR:HG22	5:4:568:ALA:N	2.33	0.44
7:A:953:U:OP1	26:T:6:ARG:NH2	2.43	0.44
9:C:65:ARG:NE	13:G:118:GLU:OE2	2.32	0.44
10:D:243:VAL:O	10:D:259:GLY:N	2.46	0.44
25:S:7:GLU:OE1	25:S:7:GLU:N	2.42	0.44
2:1:309:ILE:HD12	30:X:325:PRO:HG2	1.99	0.44
5:4:153:SER:O	5:4:157:LEU:HD23	2.17	0.44
7:A:1364:U:O2'	7:A:1390:A:OP1	2.32	0.44
7:A:1400:U:H2'	7:A:1401:G:O4'	2.17	0.44
10:D:216:GLU:OE1	10:D:216:GLU:N	2.40	0.44
5:4:166:VAL:HG23	5:4:167:LYS:N	2.33	0.44
7:A:837:A:C4	7:A:838:U:C5	3.06	0.44
5:4:324:VAL:HG21	31:Y:258:ILE:HG22	2.00	0.44
5:4:360:MET:HE1	5:4:371:THR:CG2	2.48	0.44
7:A:1057:G:H4'	7:A:1578:A:H4'	2.00	0.44
7:A:1366:C:H3'	7:A:1367:A:H5'	2.00	0.44
18:L:167:LEU:CD1	18:L:187:ILE:HG21	2.47	0.44
29:W:100:VAL:HG11	29:W:144:LEU:HD11	1.99	0.44
29:W:172:ILE:HG22	29:W:173:GLN:N	2.33	0.44
3:2:66:CYS:O	3:2:67:ARG:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:37:ARG:NH1	27:U:163:GLU:OE1	2.47	0.43
24:R:85:LEU:O	24:R:87:LEU:HD12	2.18	0.43
29:W:132:GLU:OE1	29:W:132:GLU:N	2.40	0.43
7:A:1589:C:H2'	7:A:1590:A:C8	2.54	0.43
9:C:45:SER:N	9:C:167:LEU:O	2.41	0.43
14:H:148:LEU:HD23	14:H:148:LEU:H	1.84	0.43
20:N:14:VAL:O	26:T:63:GLN:NE2	2.41	0.43
21:O:217:ARG:NE	28:V:318:ASP:OD2	2.39	0.43
19:M:36:ALA:HB2	19:M:51:LEU:HD11	2.00	0.43
24:R:145:ASP:OD2	24:R:175:ARG:NH1	2.47	0.43
7:A:1393:G:C6	7:A:1394:C:C4	3.06	0.43
7:A:1561:C:C4	7:A:1562:G:N7	2.87	0.43
13:G:286:TYR:O	13:G:326:HIS:ND1	2.47	0.43
13:G:356:VAL:HG23	13:G:361:VAL:HG23	2.00	0.43
27:U:166:ASN:O	27:U:176:ARG:NH1	2.48	0.43
5:4:359:GLU:OE1	31:Y:256:LEU:N	2.52	0.43
7:A:702:C:H2'	7:A:703:A:O4'	2.17	0.43
7:A:1412:G:C5	7:A:1413:U:C5	3.07	0.43
12:F:172:VAL:HG12	12:F:240:ARG:HD3	2.01	0.43
30:X:276:ARG:NH2	30:X:286:GLU:OE2	2.38	0.43
2:1:76:PHE:CE1	2:1:81:VAL:HG21	2.54	0.43
6:7:201:ARG:HG2	6:7:222:VAL:HG12	2.00	0.43
7:A:1334:G:H2'	7:A:1335:U:O4'	2.19	0.43
7:A:1461:A:O3'	7:A:1462:G:H8	2.02	0.43
9:C:76:LEU:O	17:K:103:ARG:NH2	2.51	0.43
27:U:189:TRP:CE3	27:U:197:VAL:HG13	2.53	0.43
2:1:155:ASP:OD1	2:1:215:ARG:NH2	2.45	0.43
7:A:1233:C:O2	7:A:1233:C:H2'	2.19	0.43
7:A:1338:A:C4	7:A:1339:G:C8	3.06	0.43
4:3:145:LYS:NZ	7:A:1584:A:OP2	2.52	0.43
8:B:167:HIS:CD2	13:G:153:THR:HA	2.54	0.43
15:I:71:SER:O	15:I:74:ARG:NH1	2.42	0.43
15:I:166:ILE:HD11	23:Q:19:VAL:HG11	2.01	0.43
2:1:100:GLU:OE1	2:1:100:GLU:N	2.48	0.43
5:4:358:ARG:NH2	31:Y:250:ILE:O	2.42	0.43
7:A:1485:G:H2'	7:A:1486:C:O4'	2.19	0.43
11:E:24:ARG:NH2	11:E:87:ASP:OD2	2.46	0.43
12:F:197:GLN:OE1	12:F:197:GLN:N	2.52	0.43
24:R:162:SER:O	24:R:170:ARG:NH2	2.52	0.43
5:4:360:MET:HE1	5:4:371:THR:HG21	2.01	0.42
7:A:853:C:C2	7:A:854:U:C5	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1368:U:H4'	7:A:1369:U:O5'	2.19	0.42
24:R:113:GLU:OE1	24:R:116:ARG:NH1	2.52	0.42
28:V:79:ILE:HD11	28:V:88:ALA:CB	2.49	0.42
30:X:51:THR:HG23	30:X:66:GLN:HB3	1.99	0.42
6:7:289:LYS:HA	34:7:802:GTP:N1	2.34	0.42
7:A:891:C:C2'	7:A:892:A:O5'	2.67	0.42
7:A:1413:U:N3	7:A:1414:C:C5	2.88	0.42
7:A:1562:G:H21	7:A:1584:A:H8	1.67	0.42
21:O:185:SER:O	24:R:183:LYS:NZ	2.41	0.42
6:7:311:CYS:SG	6:7:312:GLU:N	2.91	0.42
7:A:797:C:C2	7:A:798:C:C5	3.07	0.42
7:A:1595:G:O6	23:Q:50:ARG:NH2	2.49	0.42
10:D:215:TYR:OH	25:S:2:ALA:HB2	2.19	0.42
14:H:76:LEU:HD13	14:H:148:LEU:HD21	2.01	0.42
20:N:62:ASP:OD1	20:N:88:VAL:N	2.41	0.42
21:O:226:GLU:OE1	21:O:226:GLU:N	2.44	0.42
26:T:32:VAL:HG22	26:T:76:LEU:HD22	2.01	0.42
28:V:131:ASN:O	28:V:134:GLN:N	2.50	0.42
2:1:289:ILE:HD13	2:1:319:LEU:HD21	2.00	0.42
7:A:834:G:H2'	7:A:835:C:O4'	2.20	0.42
7:A:1262:C:C4	7:A:1263:G:C5	3.07	0.42
8:B:192:LEU:HD12	8:B:218:PRO:O	2.20	0.42
13:G:318:HIS:NE2	30:X:375:GLU:OE2	2.52	0.42
7:A:799:A:H2'	7:A:800:C:C6	2.54	0.42
24:R:69:THR:OG1	24:R:72:ASP:OD1	2.37	0.42
2:1:278:ILE:HD12	2:1:283:LEU:HD11	2.01	0.42
9:C:134:PHE:CE1	10:D:144:LEU:HD22	2.54	0.42
11:E:38:ASP:OD1	11:E:39:LEU:N	2.52	0.42
5:4:573:ALA:O	5:4:577:ASN:ND2	2.52	0.42
5:4:504:ASN:OD1	5:4:504:ASN:C	2.61	0.42
6:7:251:VAL:CG1	6:7:358:THR:HG21	2.50	0.42
6:7:183:VAL:HG22	6:7:254:ILE:HB	2.02	0.42
7:A:731:A:C4	7:A:732:A:C8	3.08	0.42
7:A:853:C:H2'	7:A:854:U:H6	1.85	0.42
28:V:113:ILE:HG21	28:V:143:THR:CG2	2.50	0.42
2:1:270:LYS:HG3	2:1:278:ILE:HG21	2.02	0.42
5:4:631:VAL:HA	5:4:645:LEU:HD23	2.02	0.42
6:7:614:LEU:HD11	6:7:721:THR:HA	2.01	0.42
7:A:1569:G:OP2	7:A:1572:A:O2'	2.31	0.42
12:F:58:LEU:HD13	12:F:66:ARG:HD2	2.01	0.42
12:F:240:ARG:NH1	12:F:242:TRP:OXT	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:242:ILE:HG13	39:X:403:GDP:H1'	2.02	0.42
7:A:837:A:C6	7:A:838:U:C4	3.08	0.41
7:A:1213:A:H2'	7:A:1214:A:C4	2.55	0.41
15:I:87:HIS:HA	15:I:150:VAL:HG13	2.02	0.41
15:I:136:ALA:HB3	15:I:168:GLY:HA3	2.01	0.41
32:Z:66:ARG:NH2	32:Z:80:ASP:OD2	2.43	0.41
6:7:231:THR:OG1	6:7:413:SER:O	2.35	0.41
7:A:737:C:H3'	7:A:738:A:C8	2.55	0.41
7:A:838:U:C2	7:A:839:A:C8	3.08	0.41
7:A:1116:A:H2'	7:A:1117:A:O4'	2.20	0.41
7:A:1174:U:O2'	10:D:231:MET:O	2.34	0.41
17:K:67:LEU:O	17:K:70:VAL:HG12	2.20	0.41
7:A:1143:C:N4	7:A:1576:G:OP1	2.54	0.41
7:A:1146:C:C2	7:A:1147:G:C8	3.08	0.41
26:T:32:VAL:HG22	26:T:76:LEU:CD2	2.51	0.41
30:X:136:LEU:HD12	38:X:402:ATP:H5'2	2.02	0.41
1:0:175:ILE:HG21	21:O:188:PRO:HD2	2.02	0.41
7:A:1223:C:OP1	14:H:126:ILE:HD12	2.20	0.41
7:A:1352:C:HO2'	7:A:1353:A:C1'	2.32	0.41
18:L:107:LYS:O	18:L:111:PHE:CD2	2.73	0.41
24:R:231:CYS:SG	24:R:242:TYR:HA	2.61	0.41
5:4:154:GLU:OE2	5:4:187:THR:OG1	2.25	0.41
6:7:238:HIS:O	6:7:245:ARG:NH2	2.53	0.41
7:A:989:U:OP1	15:I:94:ASN:ND2	2.45	0.41
11:E:23:LYS:NZ	27:U:174:GLU:OE2	2.47	0.41
17:K:41:ARG:NH1	32:Z:48:THR:O	2.48	0.41
1:0:41:LEU:HD13	1:0:55:TRP:CG	2.55	0.41
5:4:503:ALA:O	5:4:504:ASN:OD1	2.38	0.41
6:7:326:LEU:HB2	34:7:802:GTP:C5	2.55	0.41
6:7:391:LYS:O	6:7:444:VAL:HG13	2.21	0.41
7:A:1108:C:H4'	7:A:1109:A:OP2	2.21	0.41
15:I:126:ILE:H	15:I:126:ILE:HD12	1.85	0.41
28:V:236:LEU:HD21	28:V:327:LEU:HD21	2.02	0.41
30:X:297:MET:HE1	30:X:306:ILE:HG23	2.02	0.41
7:A:924:A:C2	16:J:56:PRO:HB3	2.56	0.41
7:A:1020:C:C5	7:A:1021:U:C4	3.08	0.41
7:A:1209:C:C2	7:A:1210:U:C5	3.08	0.41
8:B:223:VAL:HG23	8:B:223:VAL:O	2.21	0.41
24:R:243:ILE:HG23	24:R:247:HIS:HE1	1.83	0.41
7:A:1033:U:H4'	11:E:94:VAL:HG12	2.03	0.41
7:A:1441:A:H2'	7:A:1442:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:115:ASP:OD1	29:W:116:PHE:N	2.54	0.41
30:X:156:PRO:O	30:X:263:ASP:HB3	2.21	0.41
2:1:163:VAL:HG12	5:4:134:GLU:O	2.20	0.41
4:3:173:LEU:HB3	18:L:209:LEU:HD13	2.02	0.41
7:A:662:U:H2'	7:A:663:A:O4'	2.21	0.41
7:A:916:C:H2'	7:A:917:C:C6	2.55	0.41
7:A:1041:A:H2'	7:A:1042:U:H4'	2.03	0.41
7:A:1441:A:H2	7:A:1449:G:H22	1.69	0.41
9:C:124:LEU:O	9:C:132:TYR:OH	2.26	0.41
12:F:193:ASP:OD1	12:F:194:LYS:N	2.54	0.41
13:G:310:ARG:NE	30:X:383:LEU:O	2.48	0.41
19:M:48:VAL:HG11	19:M:76:TRP:CH2	2.55	0.41
26:T:87:LEU:O	27:U:113:ASN:ND2	2.44	0.41
28:V:35:VAL:O	28:V:35:VAL:HG12	2.19	0.41
29:W:100:VAL:HG11	29:W:144:LEU:CD1	2.51	0.41
7:A:1587:U:H2'	7:A:1588:G:H8	1.86	0.41
15:I:181:ILE:HD11	23:Q:39:ILE:HD11	2.03	0.41
24:R:313:SER:N	24:R:335:GLU:OE2	2.43	0.41
6:7:603:VAL:HG11	6:7:725:PRO:HG3	2.03	0.40
3:2:109:GLN:O	7:A:1295:A:N6	2.54	0.40
6:7:520:ILE:O	6:7:551:PHE:HA	2.21	0.40
7:A:912:U:H2'	7:A:913:A:O4'	2.21	0.40
7:A:1135:C:C2	7:A:1136:C:C5	3.09	0.40
7:A:1595:G:O6	23:Q:50:ARG:NH1	2.50	0.40
4:3:189:TRP:NE1	18:L:209:LEU:HD12	2.35	0.40
7:A:1489:G:H2'	7:A:1490:U:H6	1.86	0.40
24:R:113:GLU:OE2	24:R:117:GLN:NE2	2.48	0.40
5:4:565:ARG:HA	5:4:569:GLN:HG3	2.03	0.40
7:A:1043:C:N4	7:A:1044:U:O4	2.55	0.40
12:F:145:PHE:CZ	12:F:149:LEU:HD11	2.56	0.40
24:R:247:HIS:HD2	24:R:274:TYR:CE1	2.39	0.40
28:V:156:ASN:ND2	28:V:159:ASP:OD2	2.50	0.40
6:7:193:LYS:NZ	34:7:802:GTP:PB	2.95	0.40
7:A:1113:G:O2'	7:A:1114:U:H5'	2.22	0.40
9:C:113:ARG:NH2	9:C:118:GLU:OE2	2.54	0.40
11:E:26:ILE:HG23	11:E:36:VAL:HG21	2.02	0.40
24:R:276:VAL:HG11	24:R:307:LEU:HD12	2.03	0.40
30:X:265:ILE:HD11	30:X:268:LEU:HD12	2.04	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	210/218 (96%)	203 (97%)	7 (3%)	0	100	100
2	1	274/323 (85%)	269 (98%)	5 (2%)	0	100	100
3	2	102/118 (86%)	101 (99%)	1 (1%)	0	100	100
4	3	69/199 (35%)	65 (94%)	4 (6%)	0	100	100
5	4	588/689 (85%)	568 (97%)	20 (3%)	0	100	100
6	7	429/727 (59%)	419 (98%)	10 (2%)	0	100	100
8	B	218/296 (74%)	214 (98%)	4 (2%)	0	100	100
9	C	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
10	D	334/430 (78%)	320 (96%)	13 (4%)	1 (0%)	36	68
11	E	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
12	F	197/242 (81%)	193 (98%)	4 (2%)	0	100	100
13	G	297/396 (75%)	289 (97%)	8 (3%)	0	100	100
14	H	137/201 (68%)	132 (96%)	5 (4%)	0	100	100
15	I	135/194 (70%)	130 (96%)	5 (4%)	0	100	100
16	J	105/138 (76%)	96 (91%)	9 (9%)	0	100	100
17	K	99/128 (77%)	99 (100%)	0	0	100	100
18	L	168/257 (65%)	165 (98%)	3 (2%)	0	100	100
19	M	113/137 (82%)	112 (99%)	1 (1%)	0	100	100
20	N	107/130 (82%)	104 (97%)	3 (3%)	0	100	100
21	O	191/258 (74%)	189 (99%)	2 (1%)	0	100	100
22	P	94/142 (66%)	92 (98%)	2 (2%)	0	100	100
23	Q	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
24	R	291/360 (81%)	279 (96%)	12 (4%)	0	100	100
25	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
26	T	166/173 (96%)	166 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
28	V	358/414 (86%)	350 (98%)	8 (2%)	0	100	100
29	W	97/187 (52%)	88 (91%)	9 (9%)	0	100	100
30	X	347/398 (87%)	340 (98%)	7 (2%)	0	100	100
31	Y	147/395 (37%)	142 (97%)	5 (3%)	0	100	100
32	Z	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
All	All	6007/8030 (75%)	5845 (97%)	161 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	D	396	GLU

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	185/190 (97%)	185 (100%)	0	100	100
2	1	254/291 (87%)	254 (100%)	0	100	100
3	2	93/100 (93%)	93 (100%)	0	100	100
4	3	65/166 (39%)	65 (100%)	0	100	100
5	4	529/609 (87%)	529 (100%)	0	100	100
6	7	359/621 (58%)	359 (100%)	0	100	100
8	B	194/249 (78%)	194 (100%)	0	100	100
9	C	115/143 (80%)	115 (100%)	0	100	100
10	D	282/357 (79%)	282 (100%)	0	100	100
11	E	104/107 (97%)	104 (100%)	0	100	100
12	F	180/209 (86%)	180 (100%)	0	100	100
13	G	262/342 (77%)	262 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	H	129/180 (72%)	129 (100%)	0	100	100
15	I	105/147 (71%)	105 (100%)	0	100	100
16	J	92/118 (78%)	92 (100%)	0	100	100
17	K	91/113 (80%)	91 (100%)	0	100	100
18	L	155/226 (69%)	155 (100%)	0	100	100
19	M	94/113 (83%)	94 (100%)	0	100	100
20	N	95/115 (83%)	95 (100%)	0	100	100
21	O	174/230 (76%)	174 (100%)	0	100	100
22	P	87/123 (71%)	87 (100%)	0	100	100
23	Q	78/79 (99%)	78 (100%)	0	100	100
24	R	262/318 (82%)	262 (100%)	0	100	100
25	S	116/164 (71%)	116 (100%)	0	100	100
26	T	153/157 (98%)	153 (100%)	0	100	100
27	U	152/174 (87%)	152 (100%)	0	100	100
28	V	325/364 (89%)	325 (100%)	0	100	100
29	W	86/158 (54%)	86 (100%)	0	100	100
30	X	309/351 (88%)	309 (100%)	0	100	100
31	Y	137/357 (38%)	137 (100%)	0	100	100
32	Z	88/95 (93%)	88 (100%)	0	100	100
All	All	5350/6966 (77%)	5350 (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 (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	321	ASN
3	2	109	GLN
4	3	140	HIS
5	4	540	HIS
5	4	603	ASN
6	7	268	GLN
6	7	550	HIS
8	B	167	HIS
10	D	341	ASN

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Mol	Chain	Res	Type
10	D	415	GLN
13	G	77	GLN
13	G	255	GLN
13	G	261	GLN
15	I	93	ASN
15	I	146	HIS
16	J	35	GLN
16	J	136	GLN
17	K	113	HIS
17	K	117	HIS
17	K	119	GLN
19	M	38	HIS
24	R	139	ASN
28	V	245	HIS
28	V	246	ASN
29	W	86	HIS
30	X	73	GLN
30	X	114	ASN
30	X	159	HIS
30	X	235	ASN
30	X	302	HIS
30	X	368	HIS
31	Y	391	ASN
32	Z	63	GLN
32	Z	76	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	887/955 (92%)	109 (12%)	0

All (109) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	651	A
7	A	680	U
7	A	688	A
7	A	704	U
7	A	721	U
7	A	722	C
7	A	738	A

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Mol	Chain	Res	Type
7	A	753	A
7	A	761	A
7	A	766	G
7	A	777	G
7	A	791	G
7	A	796	G
7	A	817	G
7	A	830	U
7	A	832	U
7	A	835	C
7	A	836	A
7	A	851	A
7	A	860	A
7	A	861	U
7	A	868	C
7	A	871	A
7	A	890	C
7	A	892	A
7	A	893	G
7	A	919	A
7	A	923	A
7	A	929	A
7	A	933	G
7	A	938	A
7	A	939	A
7	A	941	G
7	A	942	A
7	A	954	C
7	A	967	A
7	A	983	C
7	A	985	U
7	A	1015	A
7	A	1042	U
7	A	1043	C
7	A	1046	A
7	A	1048	C
7	A	1049	A
7	A	1065	C
7	A	1081	U
7	A	1082	A
7	A	1103	A
7	A	1105	C

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Mol	Chain	Res	Type
7	A	1106	C
7	A	1109	A
7	A	1117	A
7	A	1120	C
7	A	1121	A
7	A	1126	A
7	A	1151	C
7	A	1160	A
7	A	1167	A
7	A	1188	A
7	A	1189	U
7	A	1190	C
7	A	1200	G
7	A	1209	C
7	A	1215	U
7	A	1223	C
7	A	1225	C
7	A	1235	U
7	A	1246	U
7	A	1247	G
7	A	1248	C
7	A	1250	C
7	A	1251	A
7	A	1270	U
7	A	1271	C
7	A	1273	G
7	A	1284	U
7	A	1290	C
7	A	1312	C
7	A	1326	A
7	A	1327	G
7	A	1343	A
7	A	1356	A
7	A	1378	C
7	A	1390	A
7	A	1405	C
7	A	1406	U
7	A	1422	G
7	A	1430	A
7	A	1447	G
7	A	1464	G
7	A	1474	G

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Mol	Chain	Res	Type
7	A	1481	C
7	A	1482	A
7	A	1492	A
7	A	1494	C
7	A	1501	A
7	A	1550	A
7	A	1558	A
7	A	1559	G
7	A	1562	G
7	A	1568	U
7	A	1571	U
7	A	1582	G
7	A	1585	A
7	A	1594	G
7	A	1595	G
7	A	1598	G
7	A	1599	A
7	A	1602	C

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 47 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	$\#\|Z\|>2$
37	FES	P	201	11,22	0,4,4	-	-	-		
34	GTP	7	802	33	30,34,34	0.64	0	46,54,54	0.57	0
39	GDP	X	403	-	28,30,30	0.49	0	44,47,47	0.49	0
37	FES	T	201	26,19	0,4,4	-	-	-		
38	ATP	X	402	33	29,33,33	1.00	1 (3%)	44,52,52	0.69	0

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
37	FES	P	201	11,22	-	-	0/1/1/1
34	GTP	7	802	33	-	5/22/38/38	0/3/3/3
39	GDP	X	403	-	-	1/16/32/32	0/3/3/3
37	FES	T	201	26,19	-	-	0/1/1/1
38	ATP	X	402	33	-	5/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	402	ATP	PB-O1B	-4.46	1.35	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

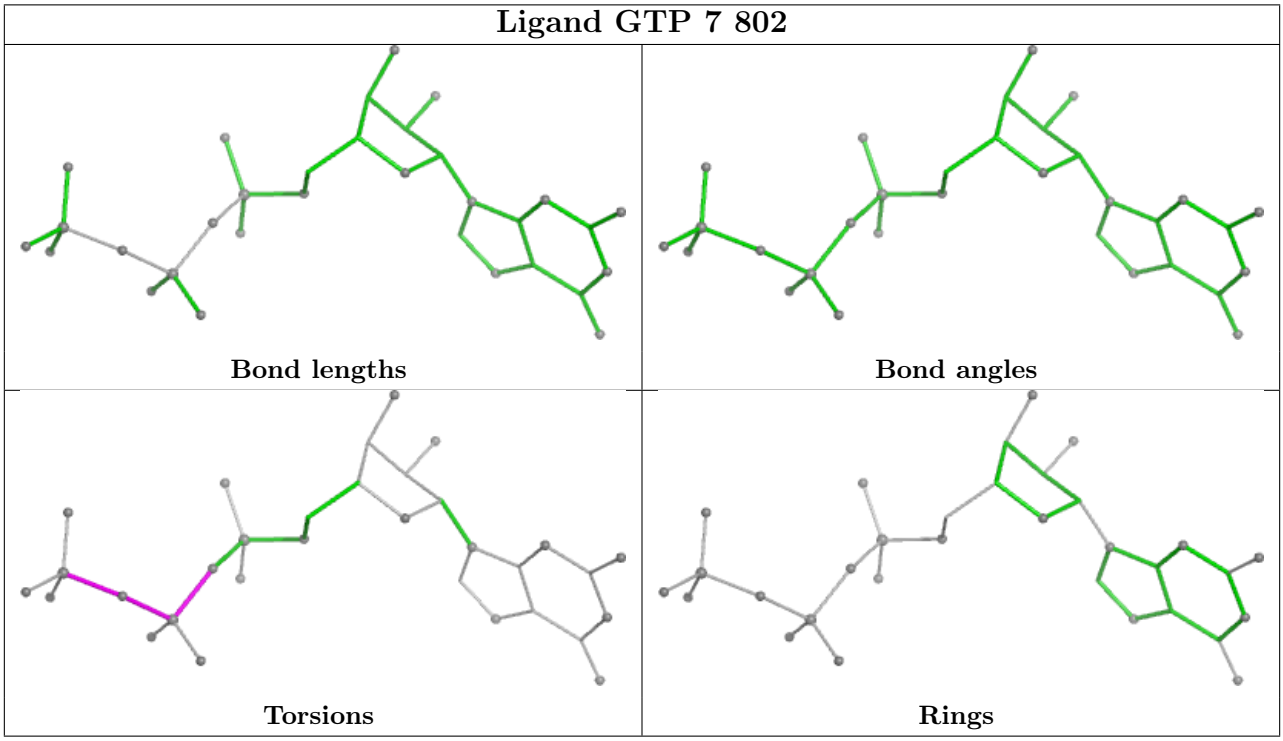
Mol	Chain	Res	Type	Atoms
38	X	402	ATP	PA-O3A-PB-O1B
39	X	403	GDP	PB-O3A-PA-O5'
38	X	402	ATP	PB-O3B-PG-O1G
38	X	402	ATP	PA-O3A-PB-O2B
34	7	802	GTP	PG-O3B-PB-O1B
34	7	802	GTP	PA-O3A-PB-O2B
34	7	802	GTP	PB-O3B-PG-O2G
38	X	402	ATP	PB-O3B-PG-O2G
38	X	402	ATP	PB-O3B-PG-O3G
34	7	802	GTP	PG-O3B-PB-O2B
34	7	802	GTP	PA-O3A-PB-O1B

There are no ring outliers.

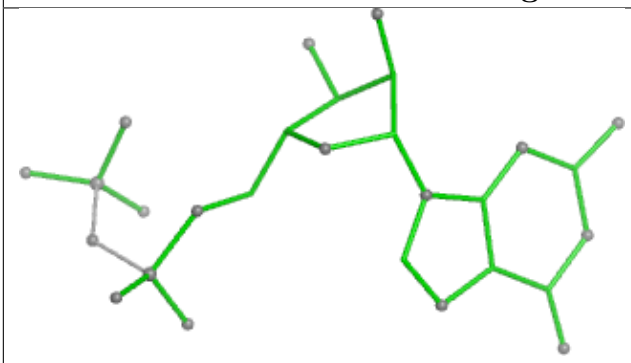
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	7	802	GTP	6	0
39	X	403	GDP	2	0
38	X	402	ATP	5	0

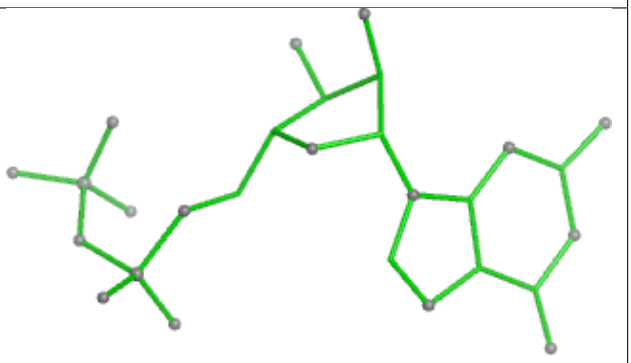
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



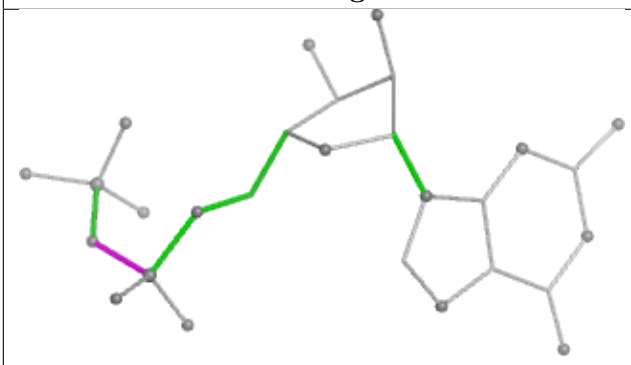
Ligand GDP X 403



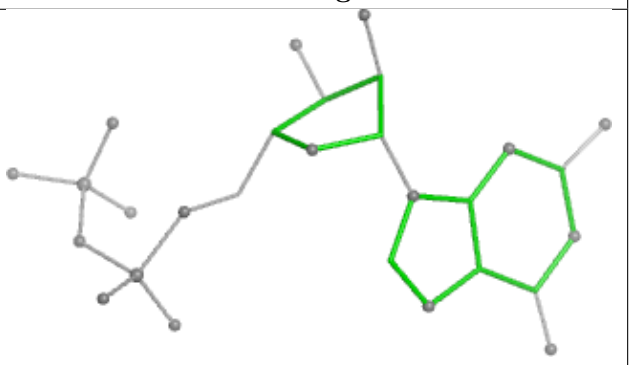
Bond lengths



Bond angles

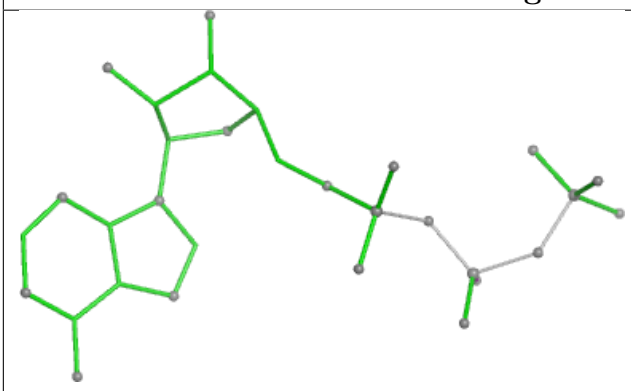


Torsions

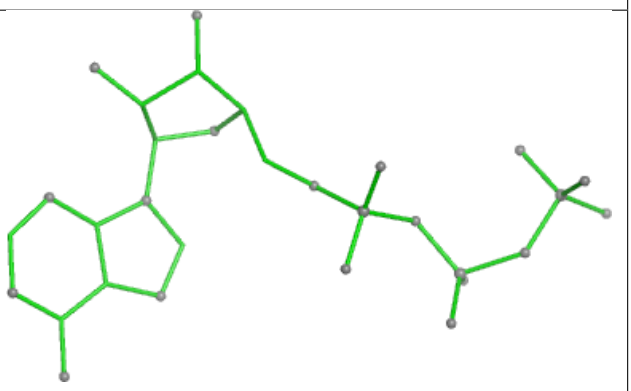


Rings

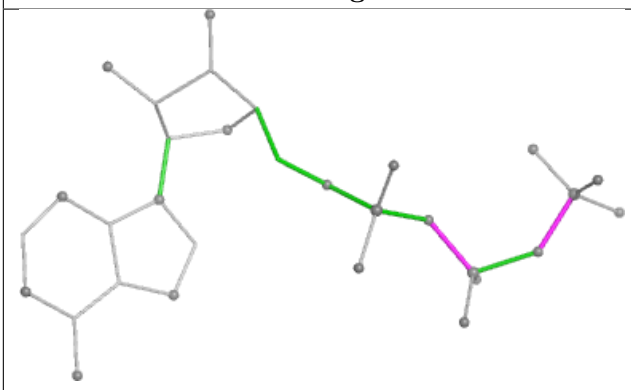
Ligand ATP X 402



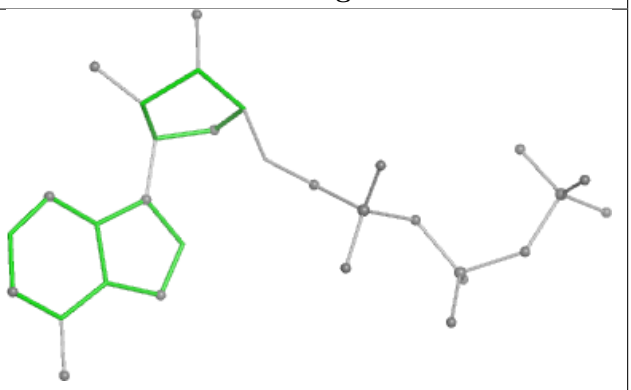
Bond lengths



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.

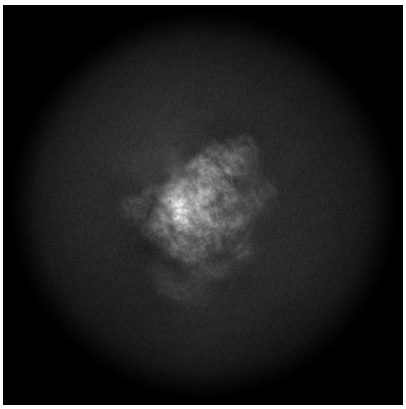
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51086. These allow visual inspection of the internal detail of the map and identification of artifacts.

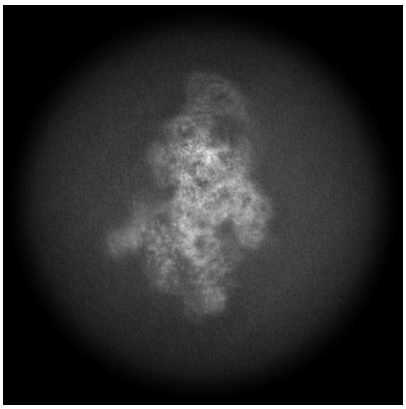
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

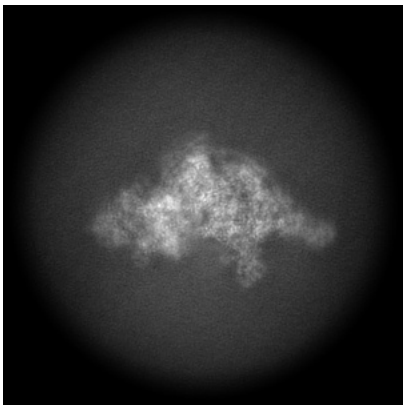
6.1.1 Primary map



X

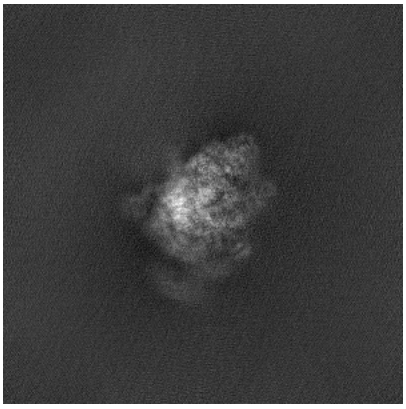


Y

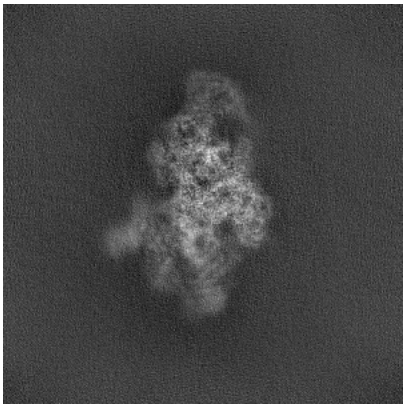


Z

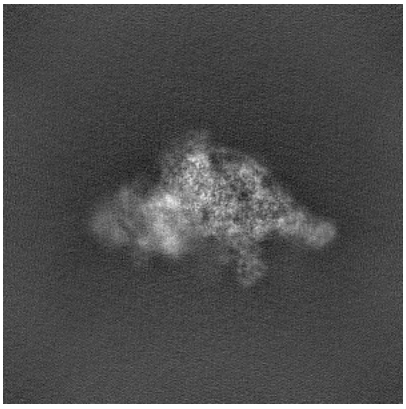
6.1.2 Raw map



X



Y

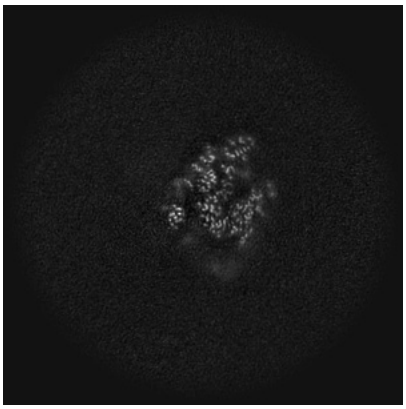


Z

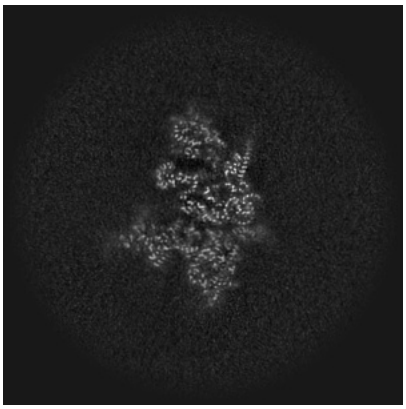
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

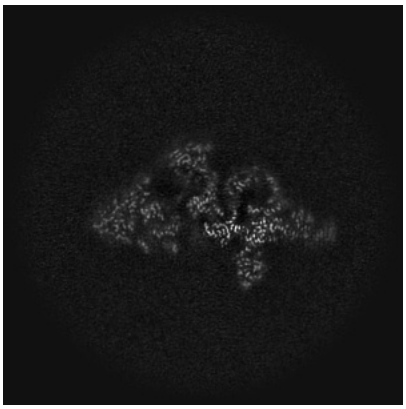
6.2.1 Primary map



X Index: 220

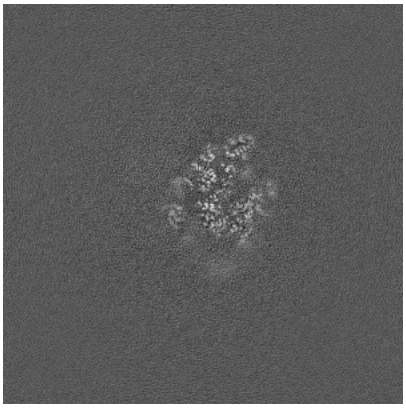


Y Index: 220

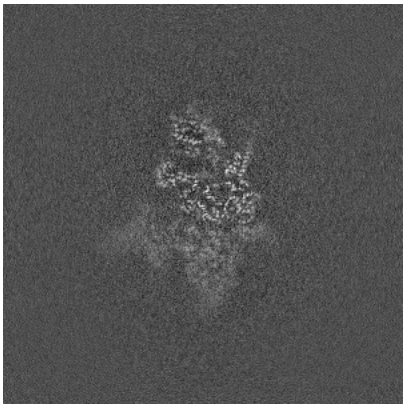


Z Index: 220

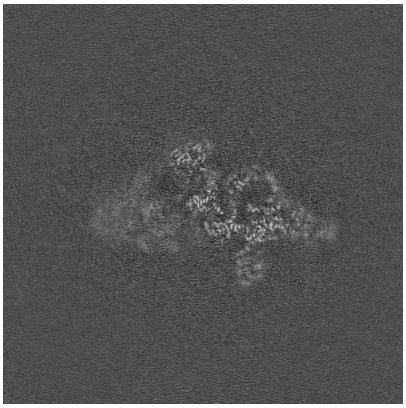
6.2.2 Raw map



X Index: 220



Y Index: 220

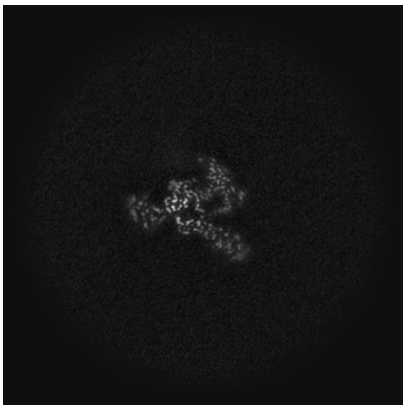


Z Index: 220

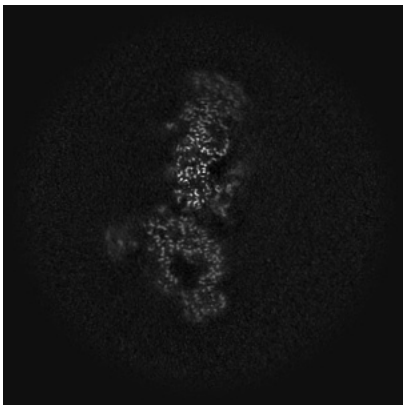
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

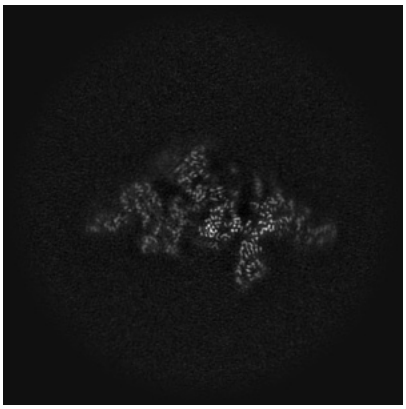
6.3.1 Primary map



X Index: 279

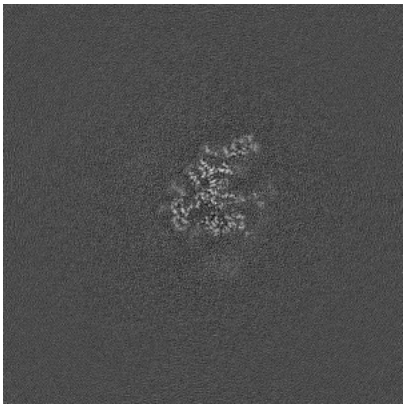


Y Index: 195

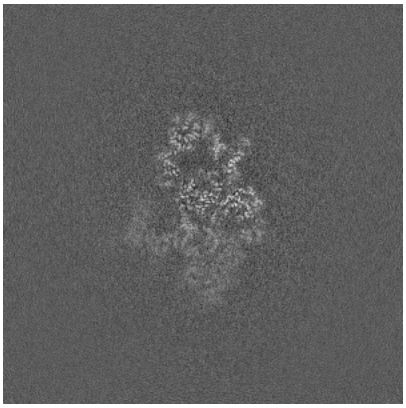


Z Index: 213

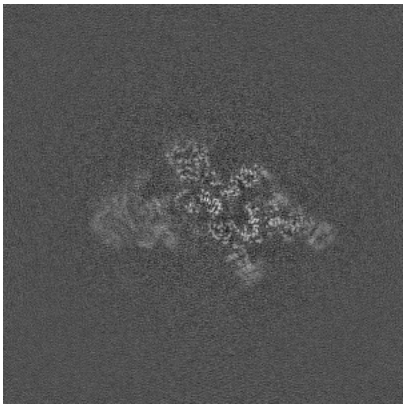
6.3.2 Raw map



X Index: 226



Y Index: 226

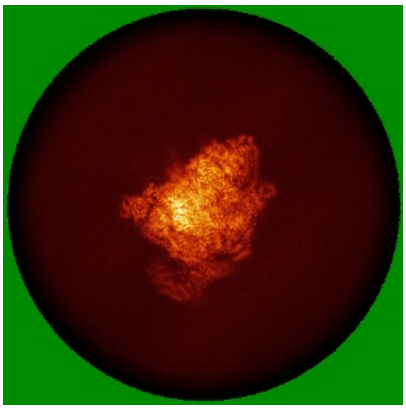


Z Index: 225

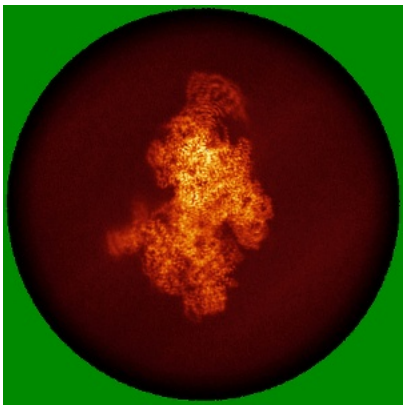
The images above show the largest variance slices of the map in three orthogonal directions.

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

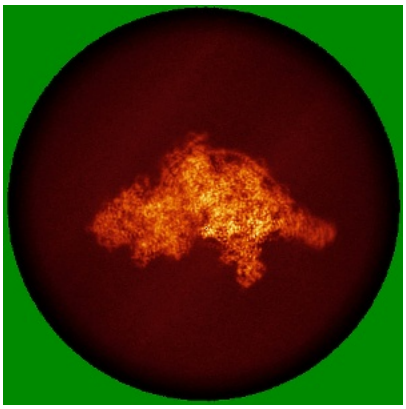
6.4.1 Primary map



X

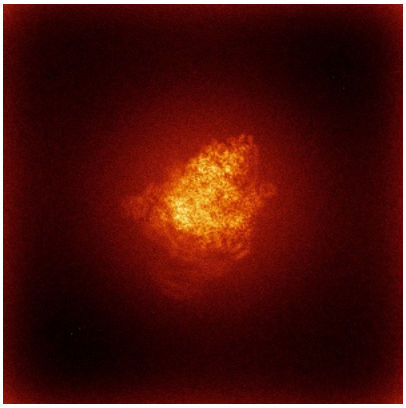


Y

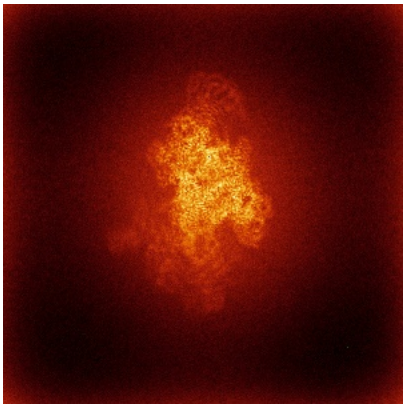


Z

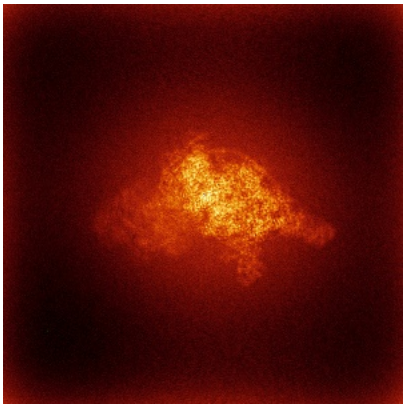
6.4.2 Raw map



X



Y

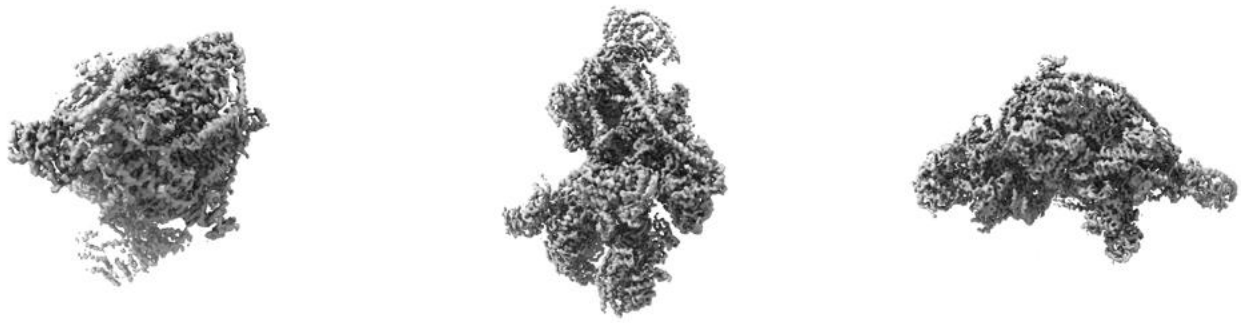


Z

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)

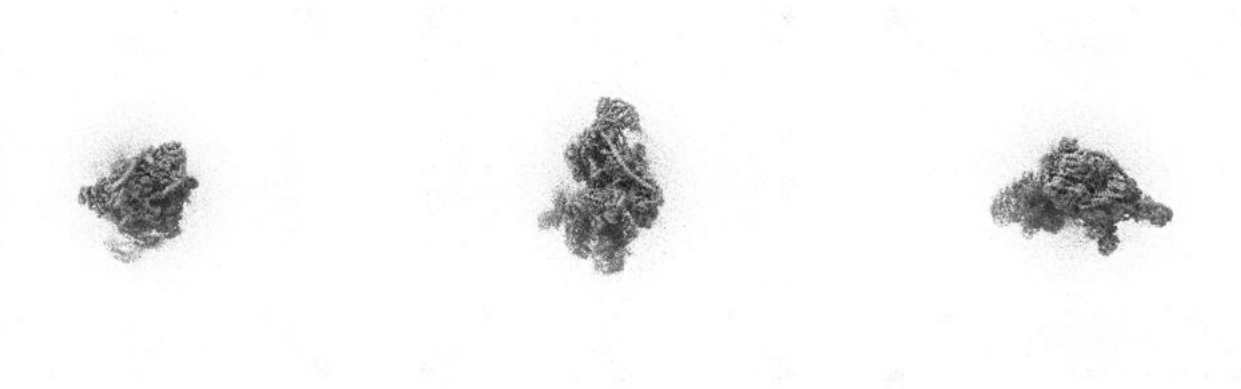
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.485. 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.

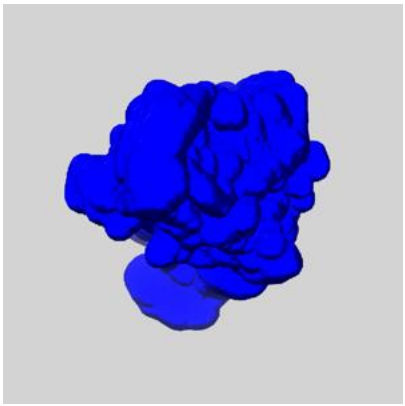
6.6 Mask visualisation

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

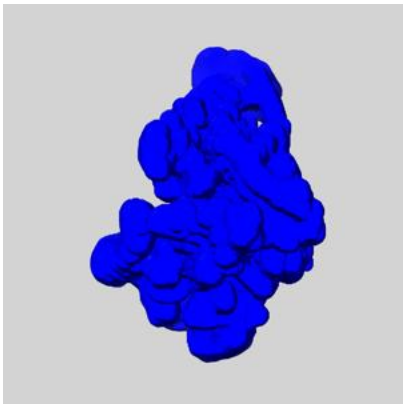
A mask typically either:

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

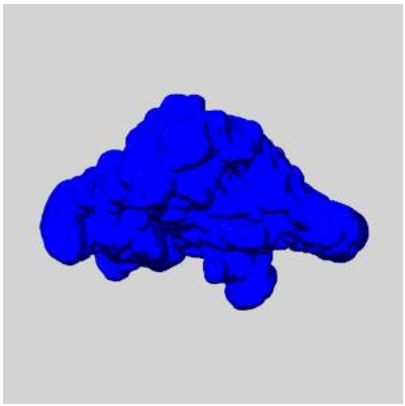
6.6.1 emd_51086_msk_1.map



X



Y

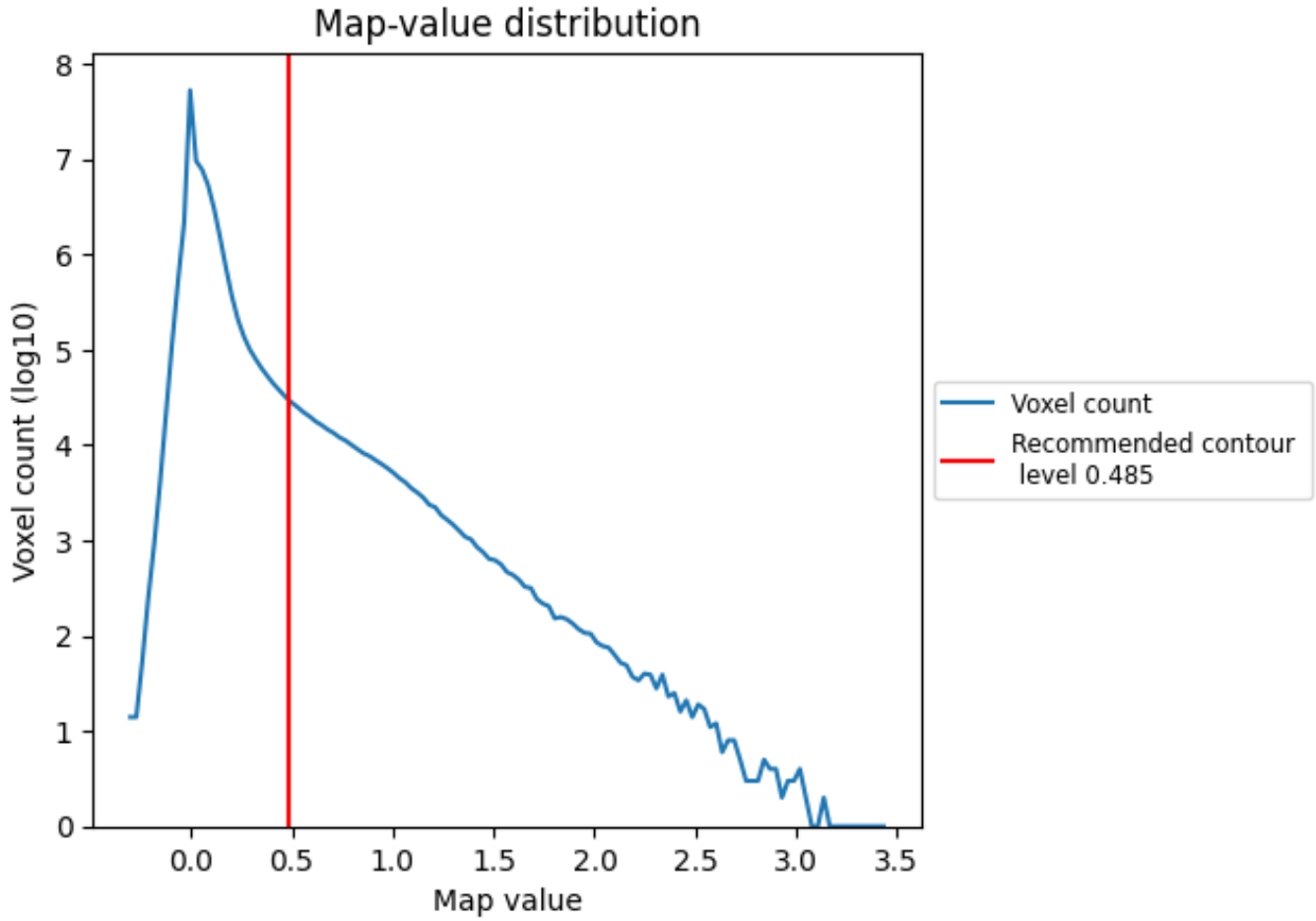


Z

7 Map analysis

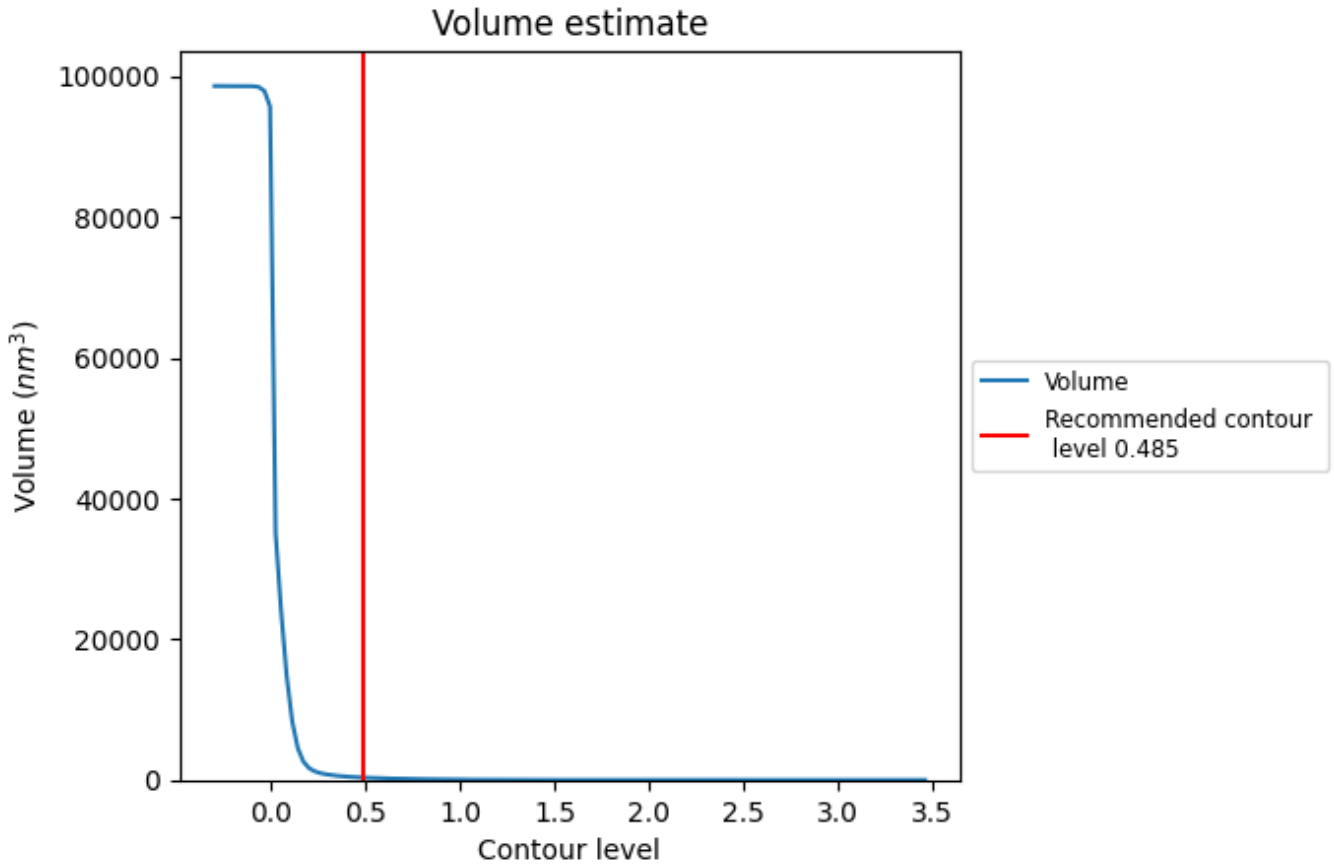
This section contains the results of statistical analysis of the map.

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.

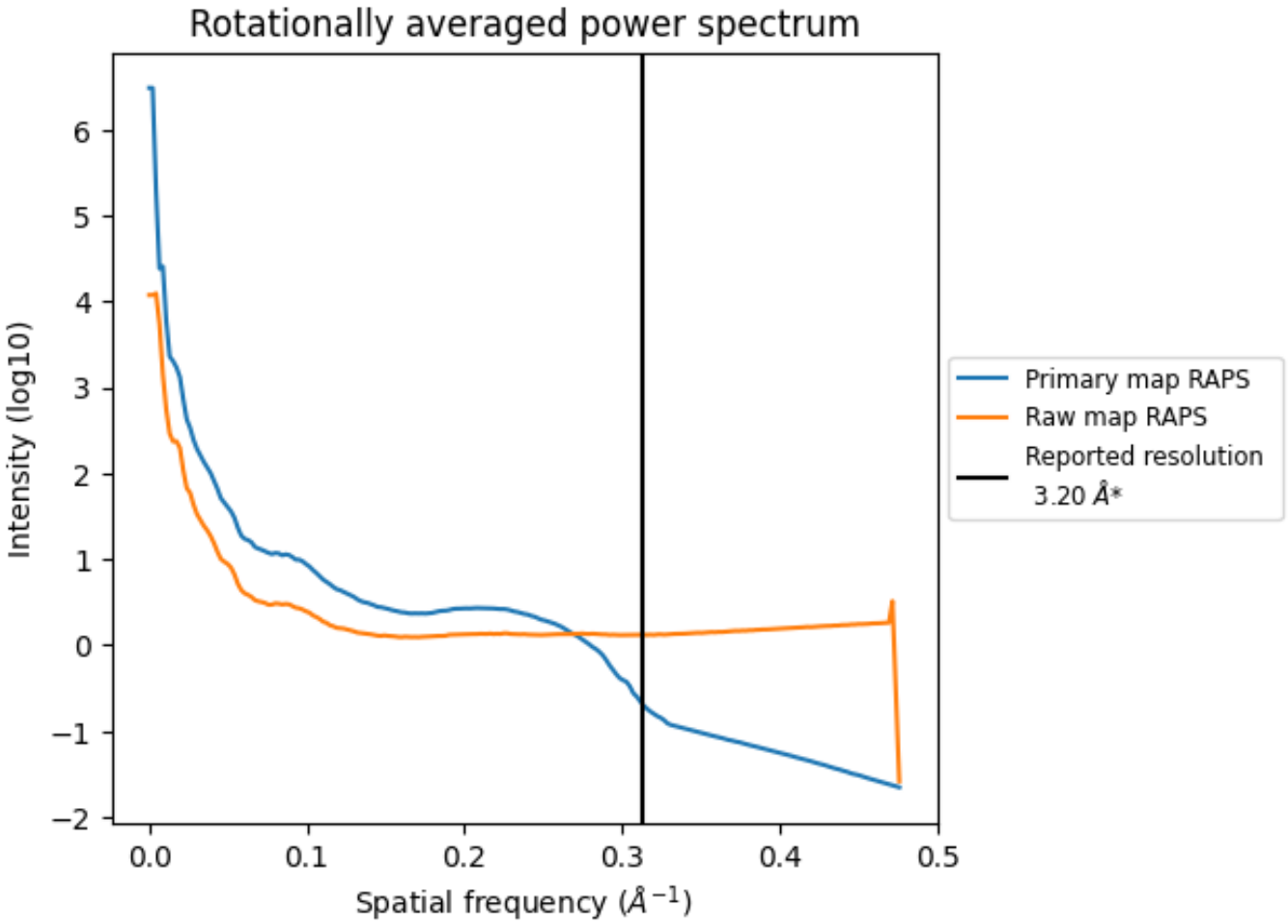
7.2 Volume estimate



The volume at the recommended contour level is 339 nm^3; this corresponds to an approximate mass of 307 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)

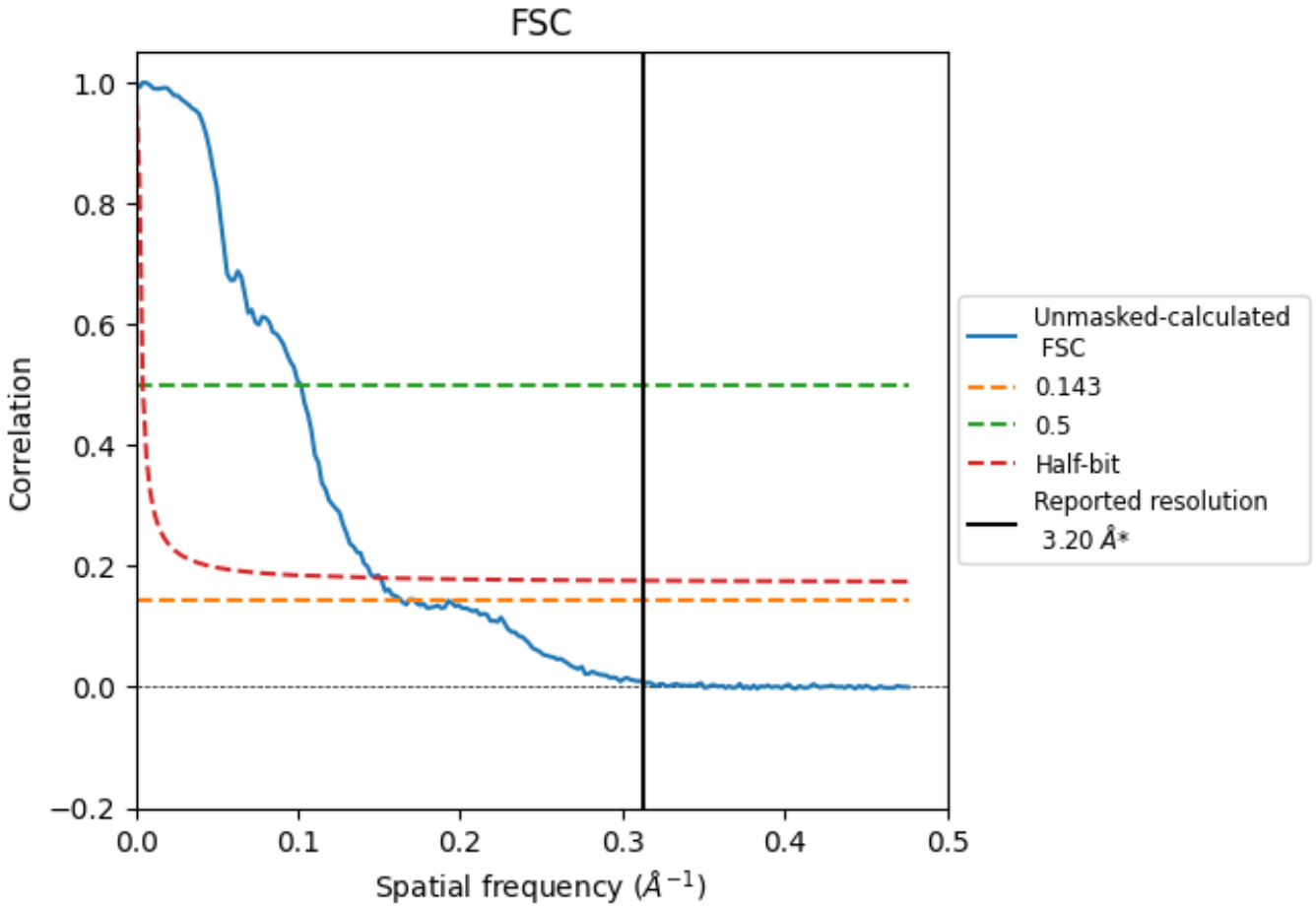


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

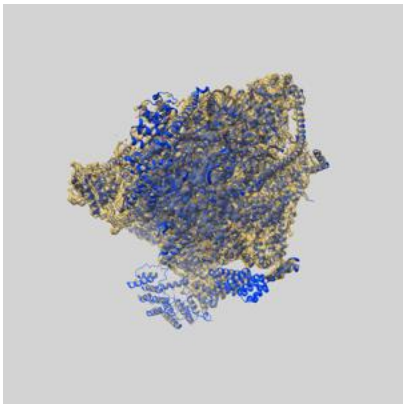
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.12	9.84	6.64

*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 6.12 differs from the reported value 3.2 by more than 10 %

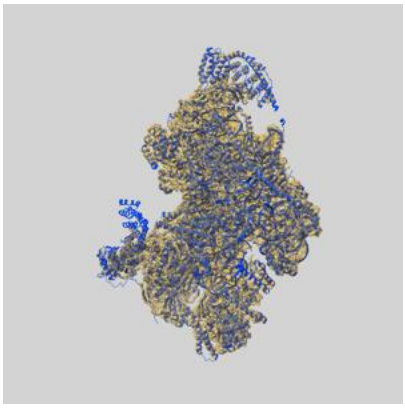
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51086 and PDB model 9G5E. Per-residue inclusion information can be found in section 3 on page 13.

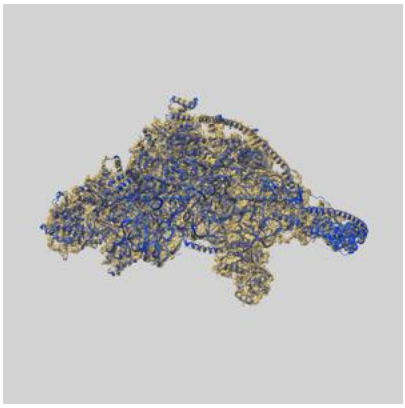
9.1 Map-model overlay



X



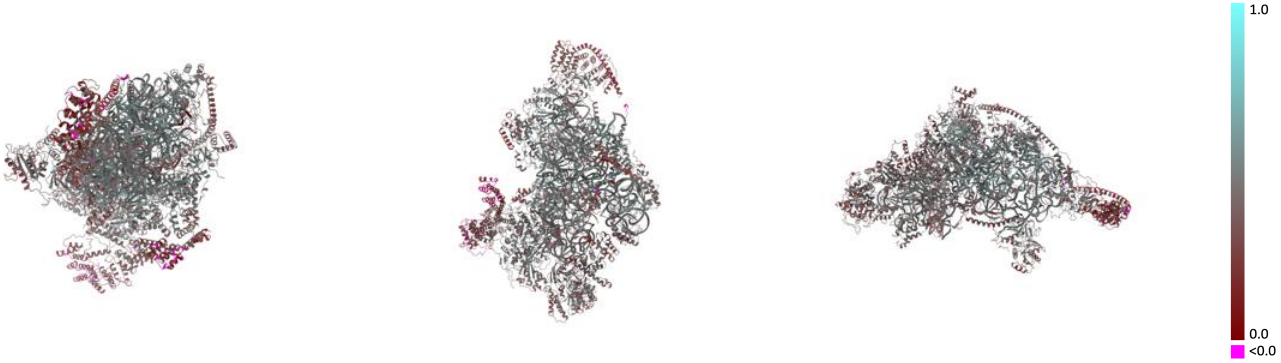
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.485 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.

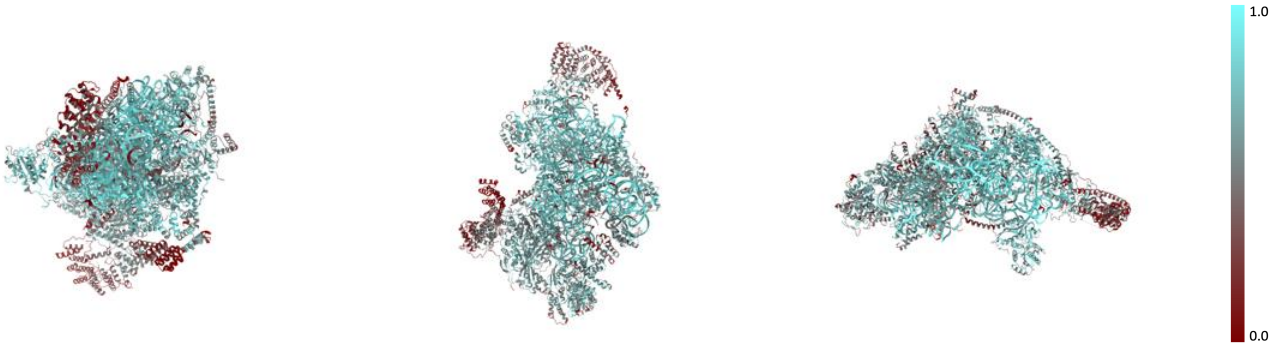
9.2 Q-score mapped to coordinate model (i)



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.

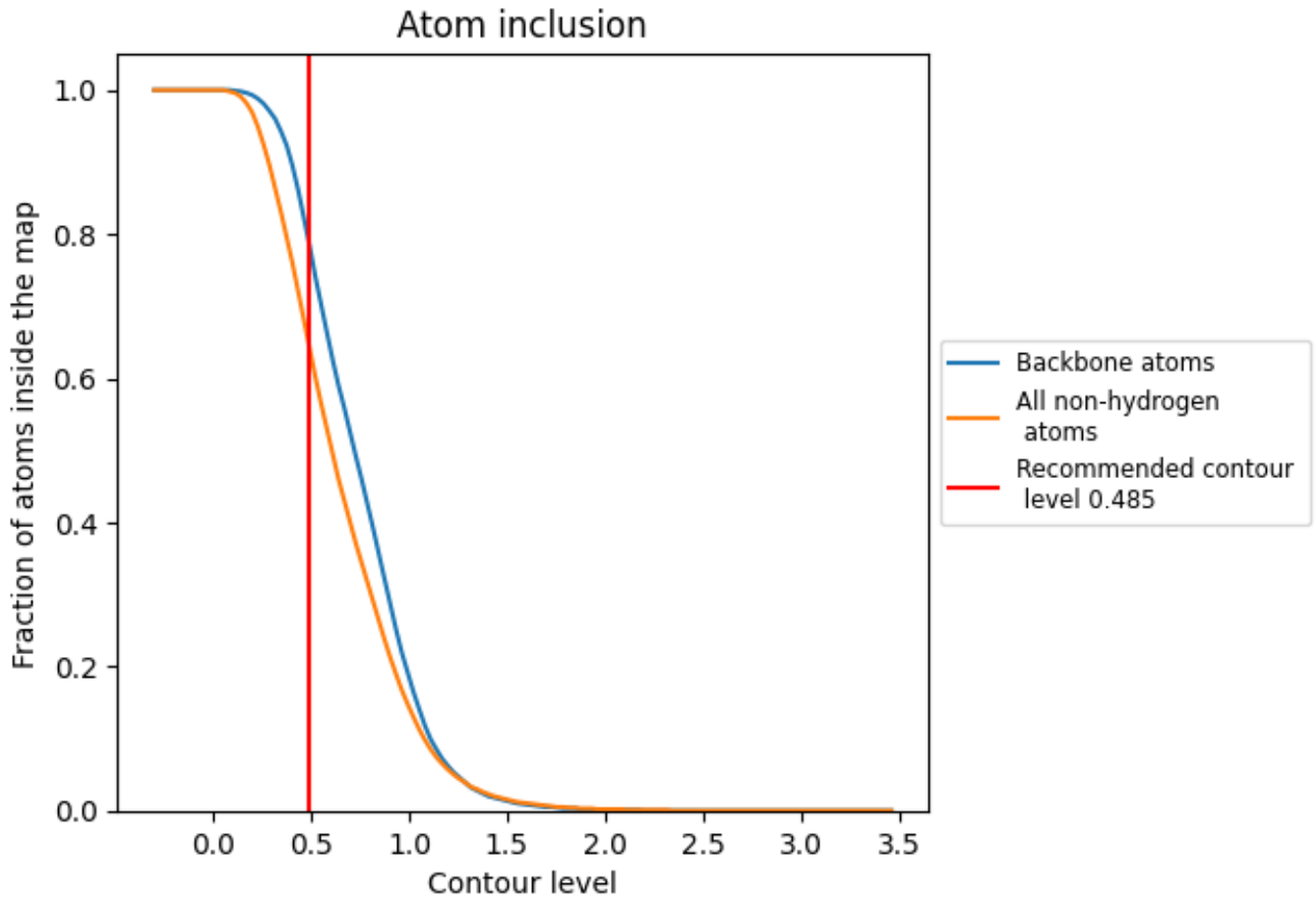
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.485).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 65% 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 (0.485) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6520	0.4310
0	0.5470	0.4280
1	0.5870	0.4050
2	0.3650	0.3810
3	0.6580	0.4800
4	0.2750	0.2590
7	0.6780	0.4100
A	0.8470	0.4800
B	0.7550	0.4840
C	0.6410	0.4710
D	0.5950	0.4560
E	0.5910	0.4490
F	0.5500	0.4100
G	0.6110	0.4260
H	0.6060	0.4550
I	0.5770	0.4280
J	0.7640	0.5170
K	0.7200	0.4700
L	0.6720	0.4590
M	0.7680	0.5010
N	0.7790	0.5220
O	0.7300	0.4900
P	0.6990	0.4770
Q	0.6640	0.4560
R	0.6800	0.4410
S	0.5810	0.4330
T	0.7320	0.4850
U	0.6180	0.4110
V	0.2570	0.2700
W	0.6420	0.4620
X	0.5850	0.4050
Y	0.4680	0.3590
Z	0.5570	0.4040

