



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:50 AM UTC

PDB ID : 9HFM / pdb_00009hfm
EMDB ID : EMD-52117
Title : Translation-initiation state of human mitochondrial ribosome small subunit (State D)
Authors : Finke, A.F.; Heinrichs, M.; Aibara, S.; Richter-Dennerlein, R.; Hillen, H.S.
Deposited on : 2024-11-18
Resolution : 3.00 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

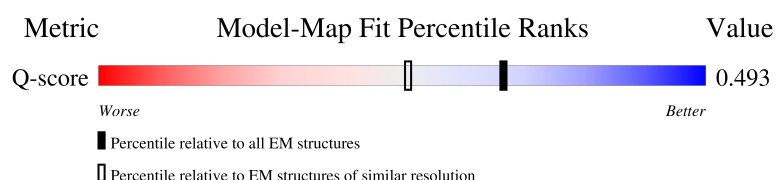
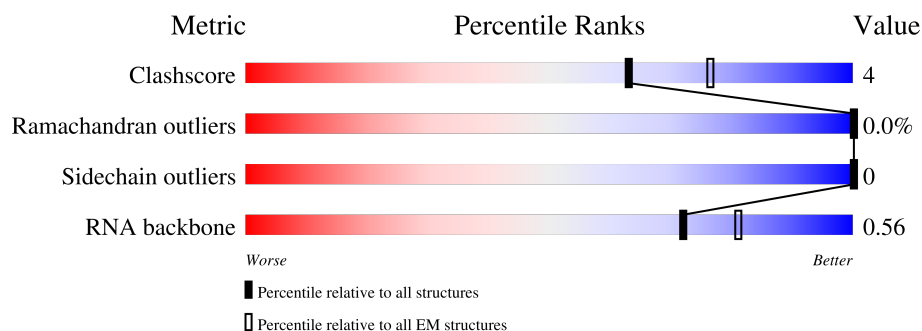
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



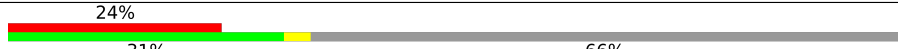
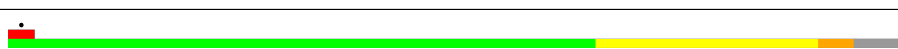
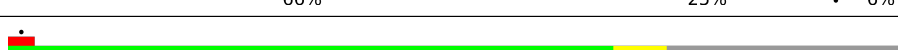
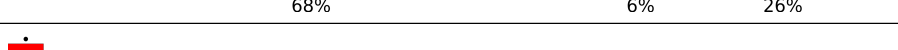
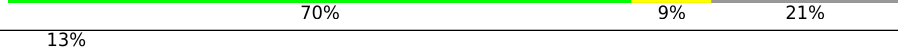
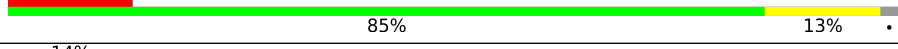
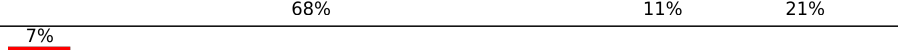
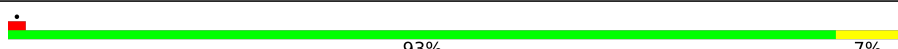
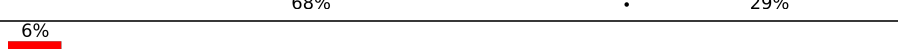
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	218	
2	1	323	
3	2	118	

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Mol	Chain	Length	Quality of chain
4	3	199	
5	4	689	
6	8	278	
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	51% 47%
30	X	398	9% 76% 12% 12%
31	Y	395	12% 34% 62%
32	Z	106	14% 82% 8% 9%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 66106 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	2	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-3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	95	Total	C	N	O	S	0	0
			758	478	135	141	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	243	LEU	PHE	variant	UNP Q9H2K0

- 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	208	Total	C	N	O	S	0	0
			1725	1104	312	298	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 Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	87	Total	C	N	O	S	0	0
			744	460	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	2	ACE	-	acetylation	UNP P82921
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	0
			1	1	
33	A	41	Total	Mg	0
			41	41	
33	B	1	Total	Mg	0
			1	1	
33	X	1	Total	Mg	0
			1	1	

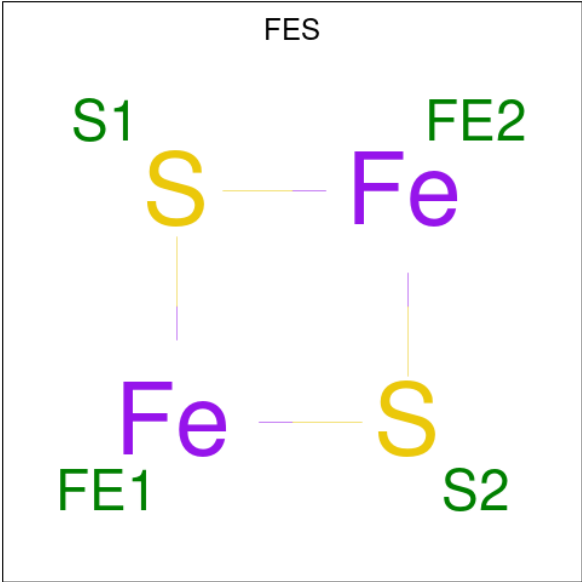
- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

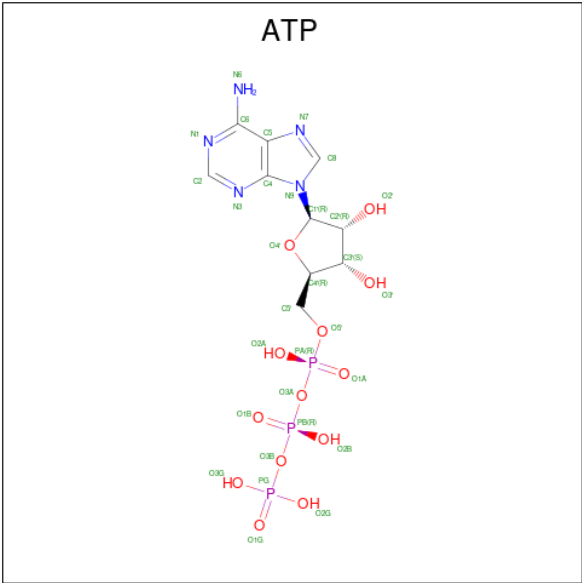
Mol	Chain	Residues	Atoms		AltConf
35	O	1	Total	Zn	0
			1	1	

- Molecule 36 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



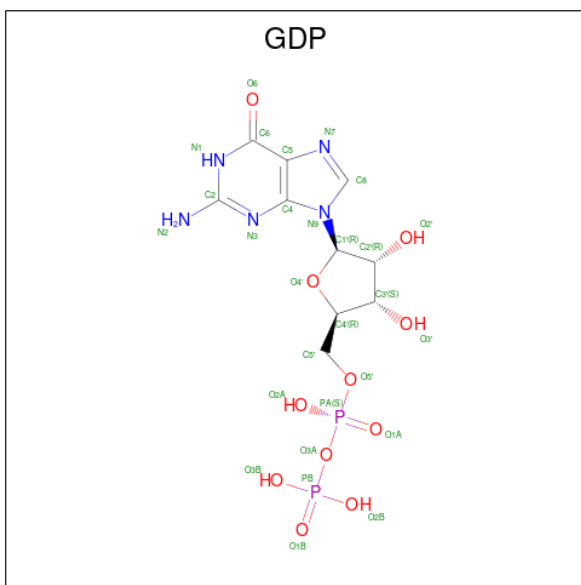
Mol	Chain	Residues	Atoms			AltConf
36	P	1	Total	Fe	S	0
			4	2	2	
36	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 38 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

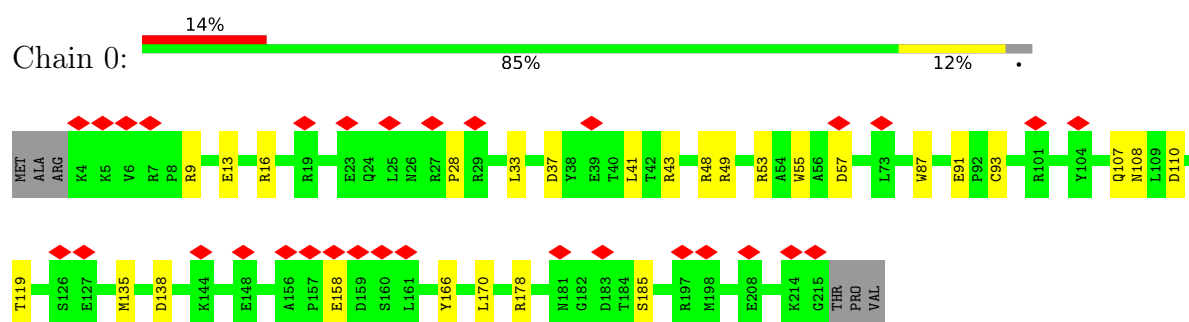


Mol	Chain	Residues	Atoms					AltConf
38	X	1	Total	C	N	O	P	0
			28	10	5	11	2	

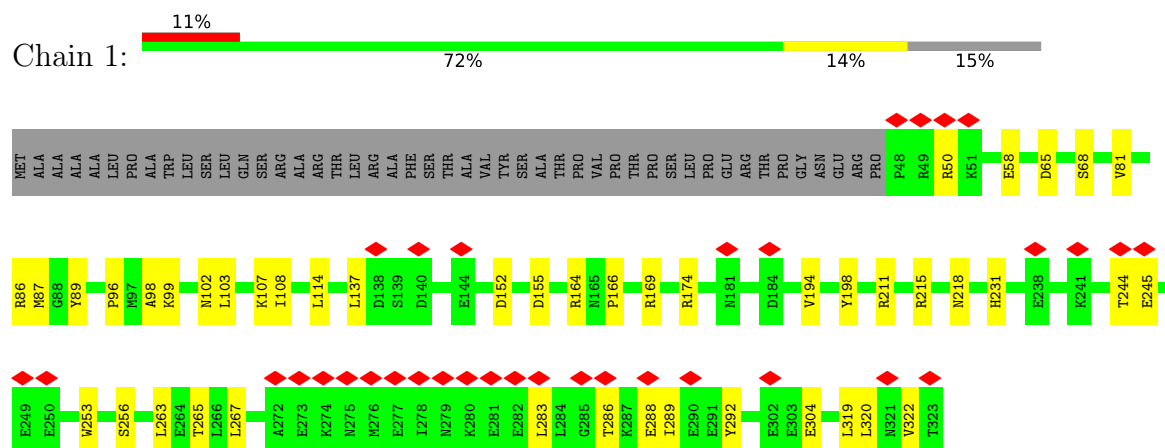
3 Residue-property plots [i](#)

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.

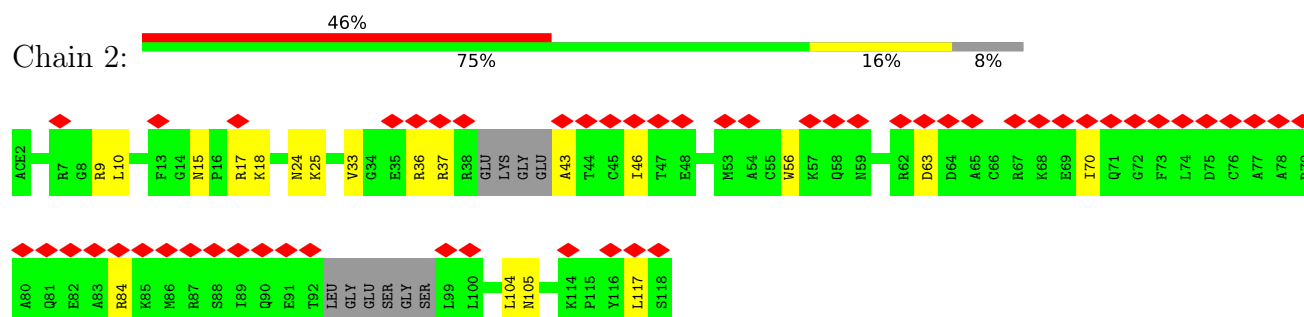
- Molecule 1: 28S ribosomal protein S34, mitochondrial



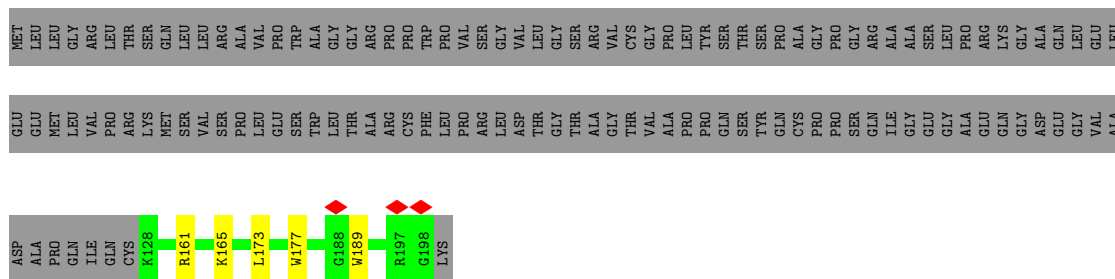
- Molecule 2: 28S ribosomal protein S35, mitochondrial



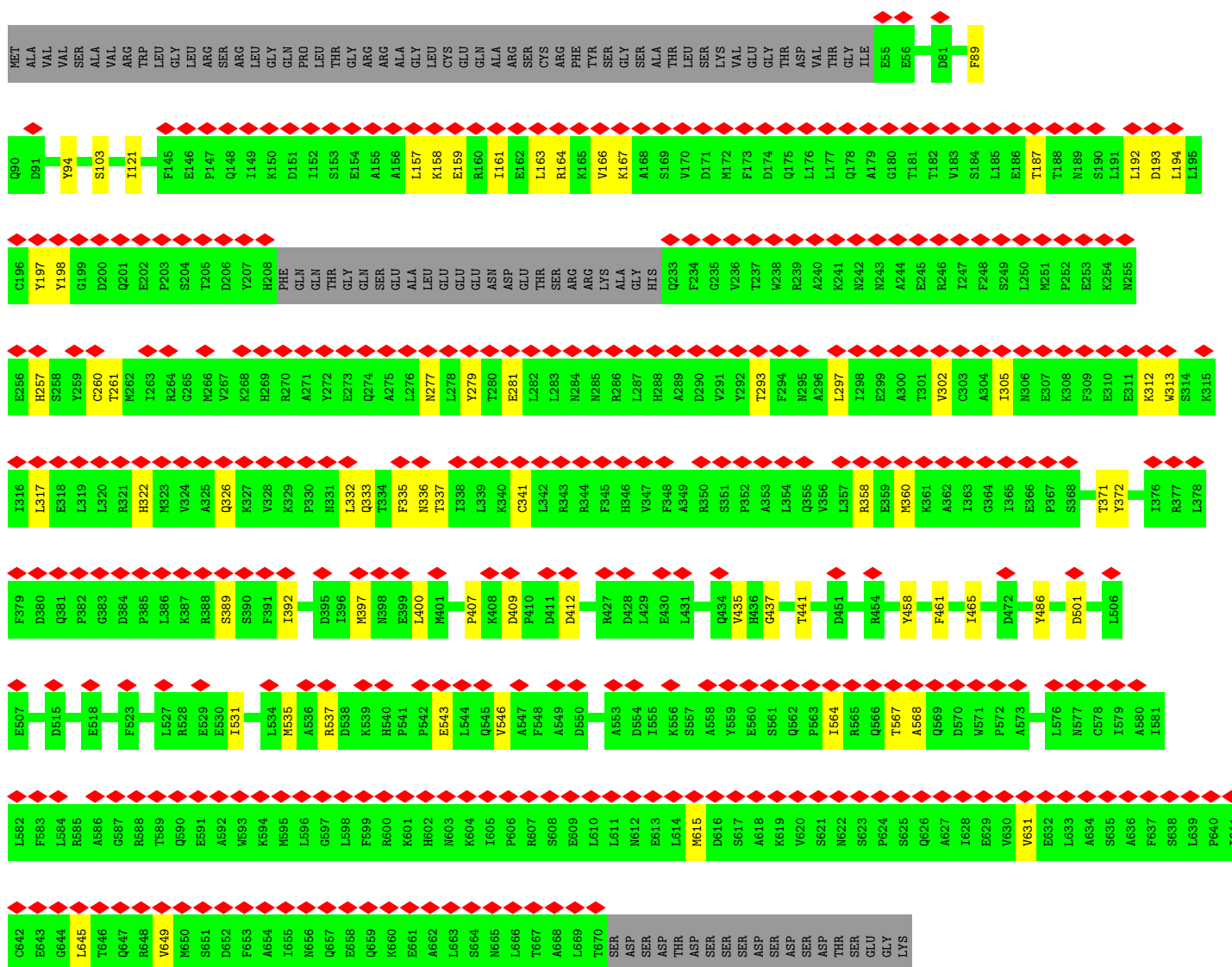
- Molecule 3: Small ribosomal subunit protein mS37



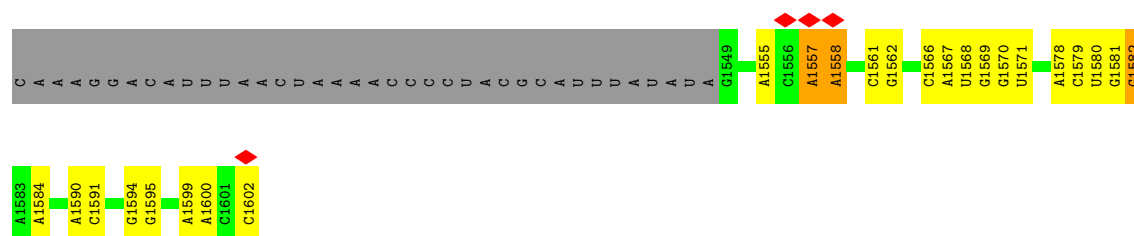
Chain 3: 33% 64%



Chain 4: 52% 76% 10% 14%

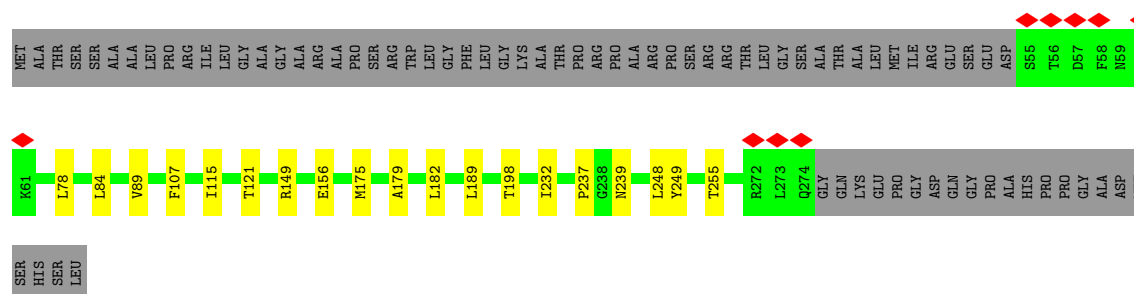






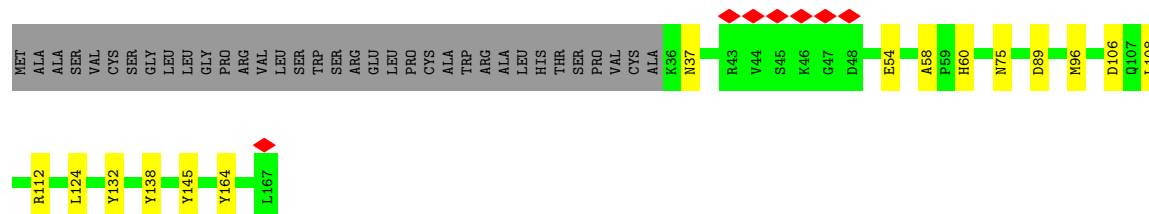
- Molecule 8: 28S ribosomal protein S2, mitochondrial

Chain B: 68% 6% 26%



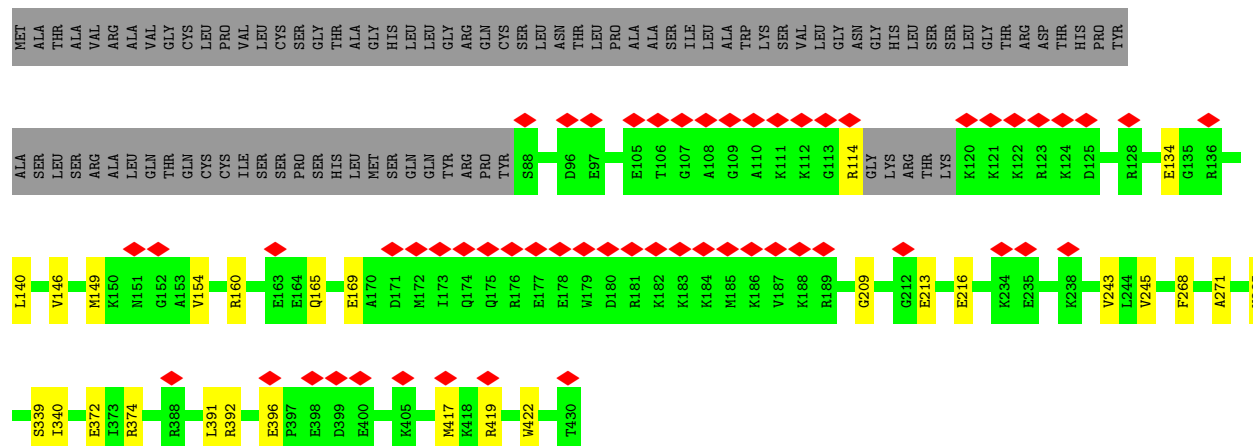
- Molecule 9: 28S ribosomal protein S24, mitochondrial

Chain C: 70% 9% 21%

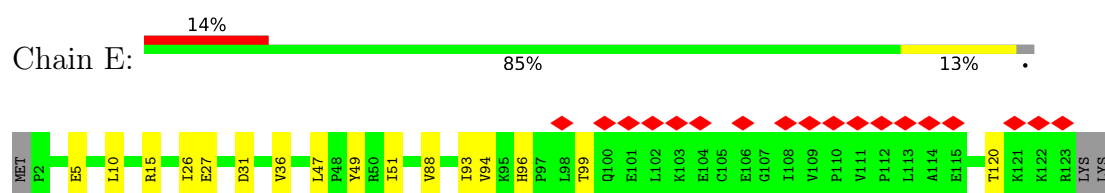


- Molecule 10: 28S ribosomal protein S5, mitochondrial

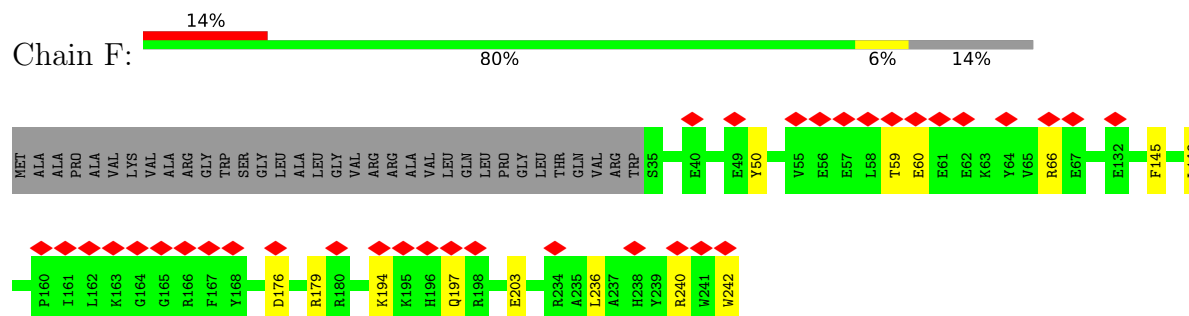
Chain D: 13% 72% 6% 21%



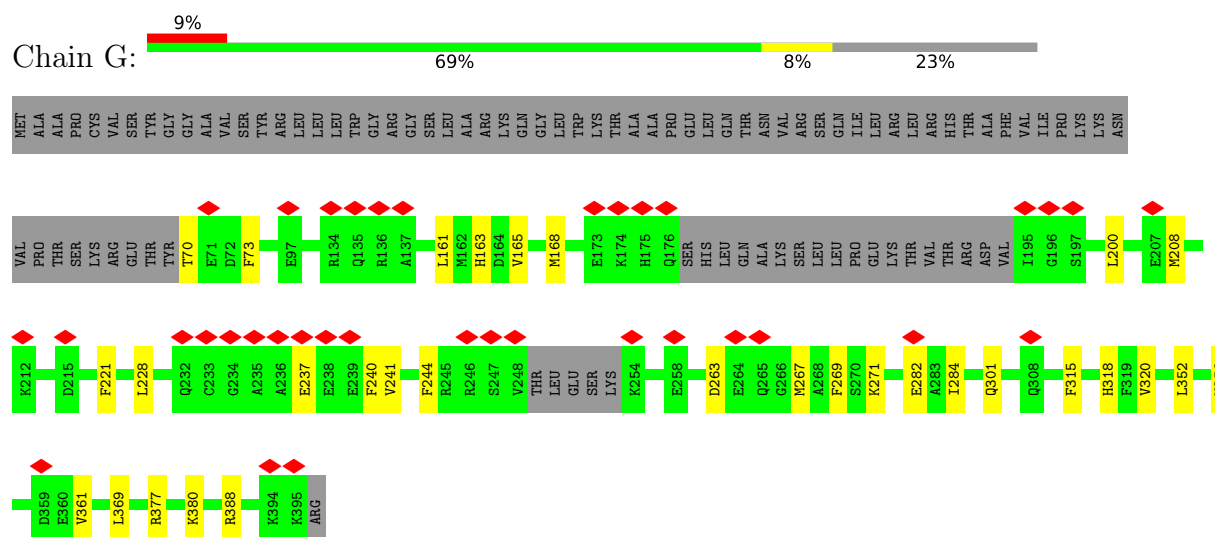
- Molecule 11: 28S ribosomal protein S6, mitochondrial



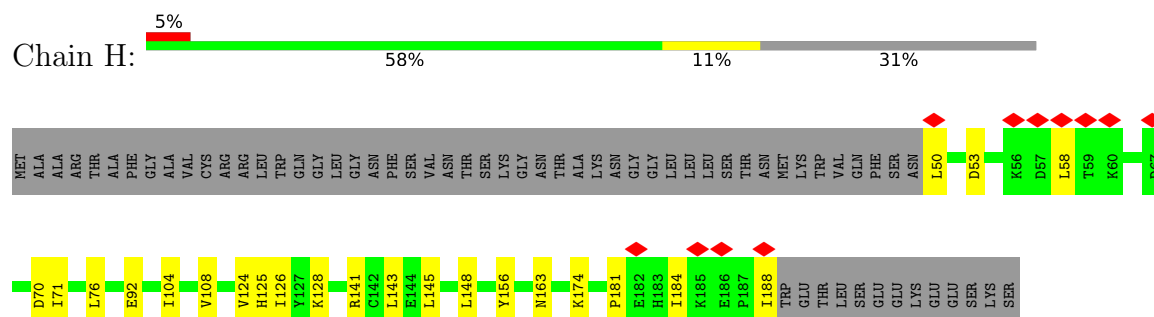
- Molecule 12: 28S ribosomal protein S7, mitochondrial



- Molecule 13: 28S ribosomal protein S9, mitochondrial



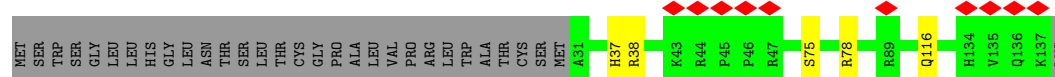
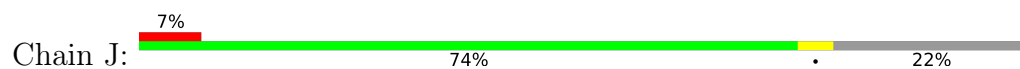
- Molecule 14: 28S ribosomal protein S10, mitochondrial



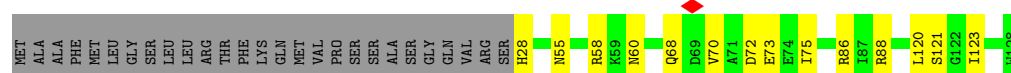
- Molecule 15: 28S ribosomal protein S11, mitochondrial



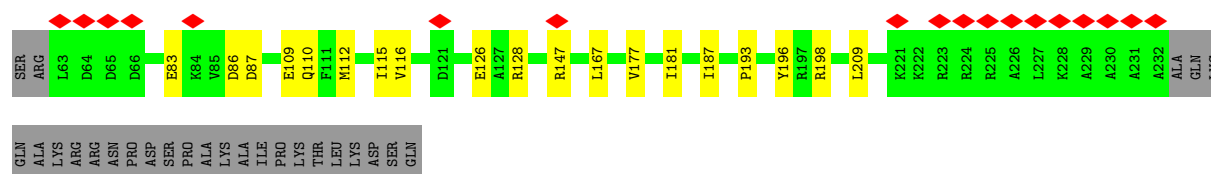
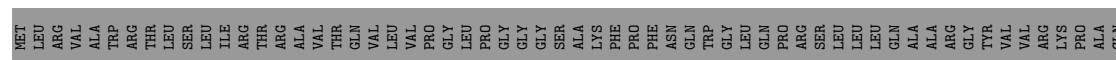
- Molecule 16: 28S ribosomal protein S12, mitochondrial



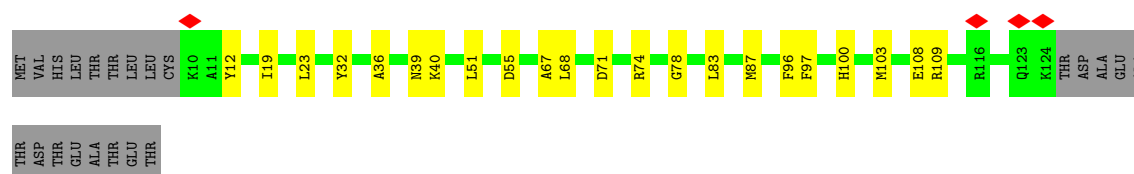
- Molecule 17: 28S ribosomal protein S14, mitochondrial



- Molecule 18: 28S ribosomal protein S15, mitochondrial

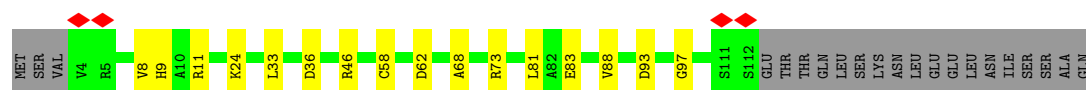


- Molecule 19: 28S ribosomal protein S16, mitochondrial

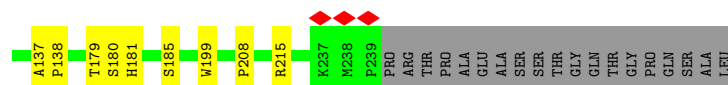
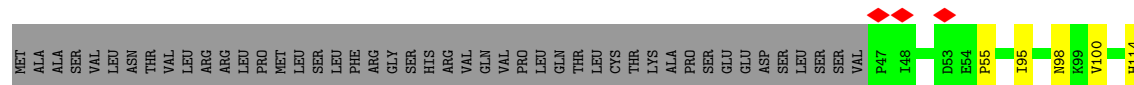


- Molecule 20: 28S ribosomal protein S17, mitochondrial

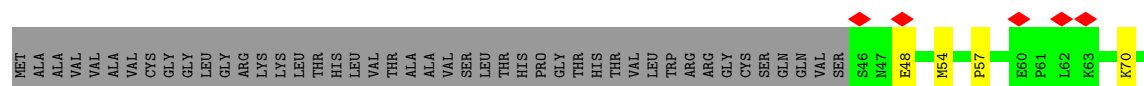




- Molecule 21: 28S ribosomal protein S18b, mitochondrial



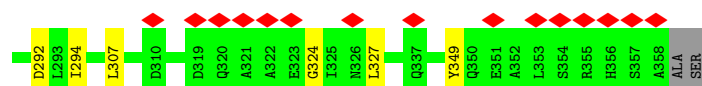
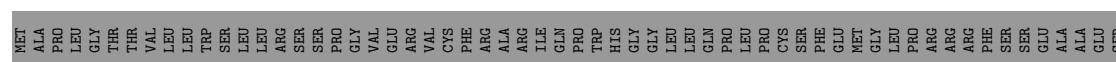
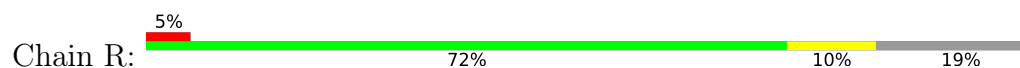
- Molecule 22: 28S ribosomal protein S18c, mitochondrial



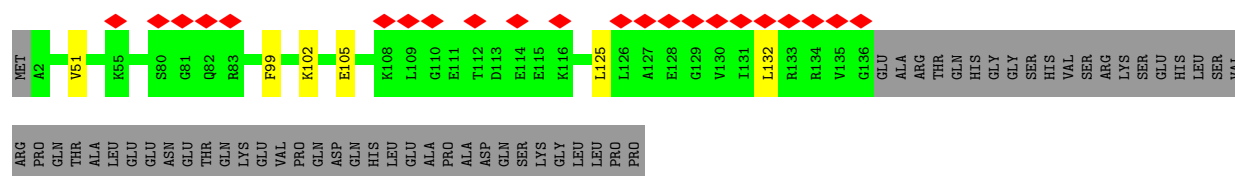
- Molecule 23: Small ribosomal subunit protein bS21m



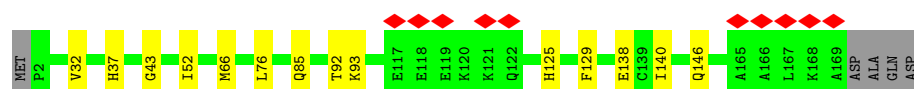
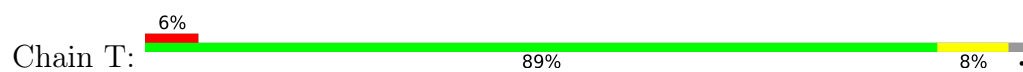
- Molecule 24: 28S ribosomal protein S22, mitochondrial



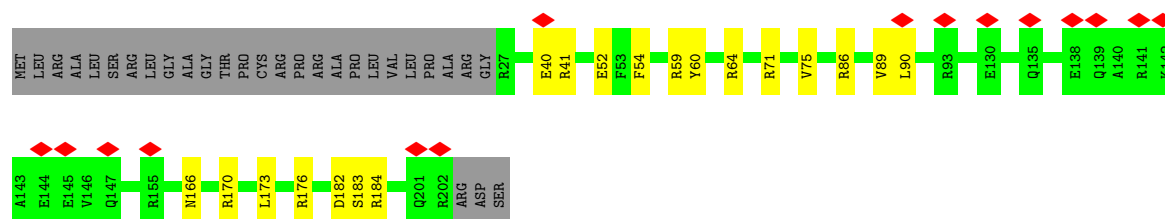
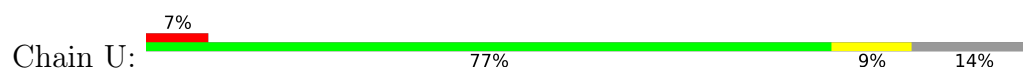
- Molecule 25: 28S ribosomal protein S23, mitochondrial



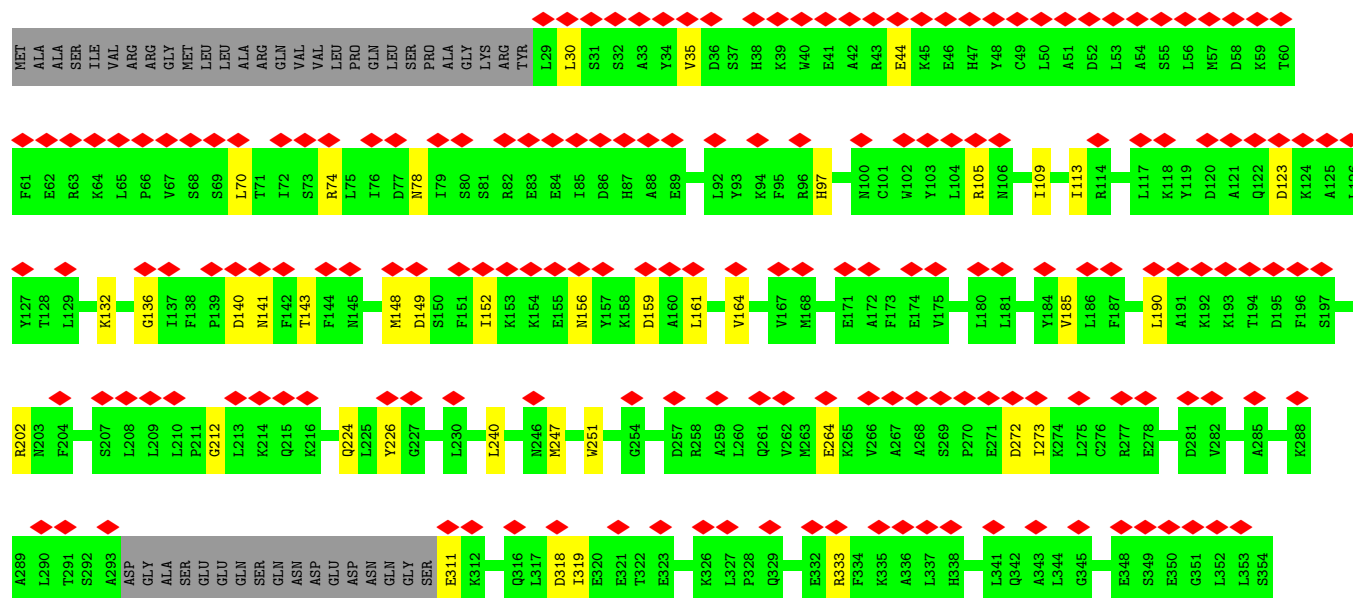
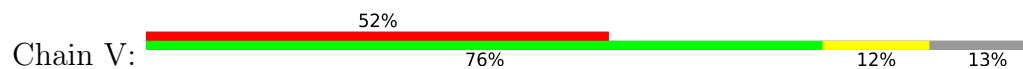
- Molecule 26: 28S ribosomal protein S25, mitochondrial

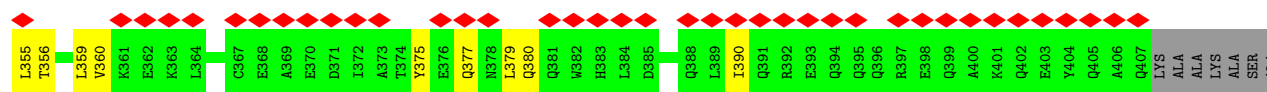


- Molecule 27: 28S ribosomal protein S26, mitochondrial



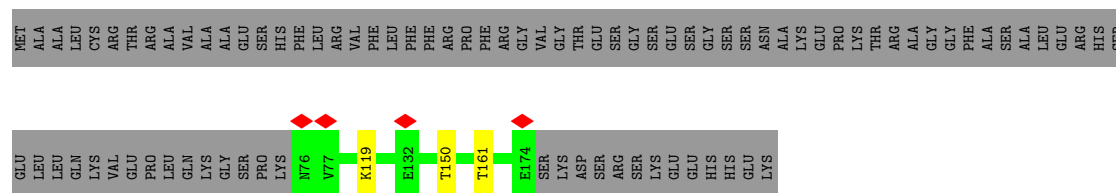
- Molecule 28: 28S ribosomal protein S27, mitochondrial





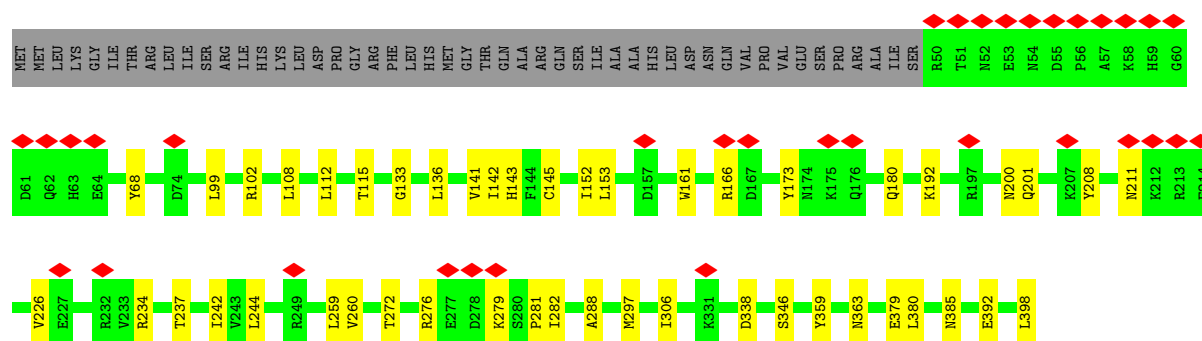
- Molecule 29: 28S ribosomal protein S28, mitochondrial

Chain W: 51% 47%



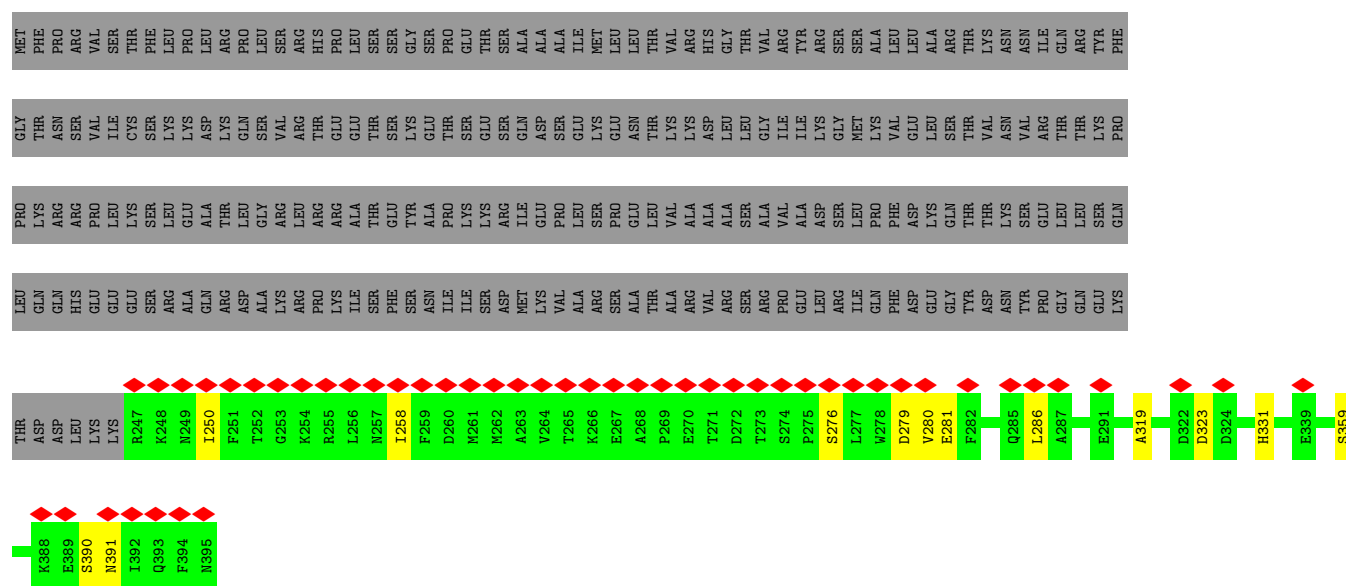
- Molecule 30: 28S ribosomal protein S29, mitochondrial

Chain X: 9% 76% 12% 12%

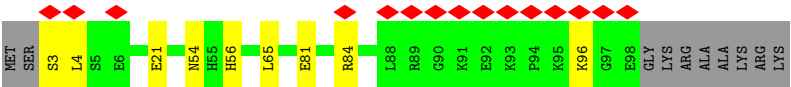
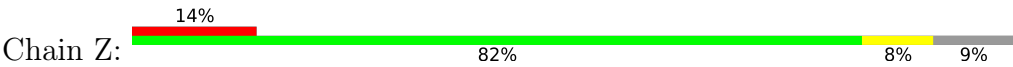


- Molecule 31: 28S ribosomal protein S31, mitochondrial

Chain Y: 12% 34% 62%



- Molecule 32: 28S ribosomal protein S33, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80262	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 ($e^-/\text{\AA}^2$)	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	3.984	Depositor
Minimum map value	-0.422	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.51	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.17	0/1811	0.26	0/2452
2	1	0.17	0/2285	0.24	0/3090
3	2	0.16	0/877	0.27	0/1171
4	3	0.22	0/640	0.35	0/844
5	4	0.13	0/4904	0.24	0/6636
6	8	0.10	0/766	0.21	0/1023
7	A	0.27	0/21295	0.28	3/33141 (0.0%)
8	B	0.25	0/1832	0.27	0/2480
9	C	0.22	0/1113	0.24	0/1505
10	D	0.23	0/2742	0.27	0/3670
11	E	0.20	0/989	0.25	0/1335
12	F	0.15	0/1767	0.23	0/2373
13	G	0.18	0/2544	0.23	0/3408
14	H	0.22	0/1162	0.31	0/1575
15	I	0.17	0/1039	0.28	0/1400
16	J	0.22	0/845	0.26	0/1137
17	K	0.23	0/880	0.26	0/1182
18	L	0.22	0/1445	0.24	0/1932
19	M	0.29	0/934	0.29	0/1255
20	N	0.24	0/877	0.26	0/1187
21	O	0.24	0/1648	0.26	0/2243
22	P	0.22	0/788	0.24	0/1058
23	Q	0.22	0/754	0.25	0/1003
24	R	0.22	0/2440	0.25	0/3295
25	S	0.19	0/1138	0.23	0/1533
26	T	0.24	0/1402	0.27	0/1883
27	U	0.18	0/1510	0.26	0/2025
28	V	0.11	0/3030	0.23	0/4093
29	W	0.21	0/795	0.25	0/1071
30	X	0.16	0/2902	0.25	0/3928
31	Y	0.16	0/1280	0.24	0/1725
32	Z	0.18	0/828	0.24	0/1104

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.22	0/69262	0.26	3/97757 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1582	G	P-O3'-C3'	-7.96	108.26	120.20
7	A	1581	G	P-O3'-C3'	-6.80	110.00	120.20
7	A	1580	U	P-O3'-C3'	-6.24	110.84	120.20

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	22	0
2	1	2238	0	2269	32	0
3	2	867	0	908	19	0
4	3	629	0	702	7	0
5	4	4795	0	4796	46	0
6	8	758	0	796	5	0
7	A	19041	0	9676	139	0
8	B	1789	0	1781	12	0
9	C	1083	0	1088	11	0
10	D	2691	0	2754	17	0
11	E	972	0	1000	14	0
12	F	1725	0	1769	10	0
13	G	2491	0	2473	22	0
14	H	1138	0	1173	18	0
15	I	1019	0	1059	12	0
16	J	829	0	874	5	0
17	K	862	0	885	10	0
18	L	1421	0	1506	19	0
19	M	913	0	943	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	859	0	922	12	0
21	O	1592	0	1557	11	0
22	P	771	0	800	13	0
23	Q	744	0	758	8	0
24	R	2393	0	2415	22	0
25	S	1111	0	1115	5	0
26	T	1371	0	1393	11	0
27	U	1488	0	1499	17	0
28	V	2969	0	2961	31	0
29	W	783	0	797	2	0
30	X	2830	0	2822	37	0
31	Y	1246	0	1197	11	0
32	Z	810	0	824	6	0
33	3	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	A	1	0	0	0	0
35	O	1	0	0	0	0
36	P	4	0	0	0	0
36	T	4	0	0	0	0
37	X	31	0	12	4	0
38	X	28	0	12	7	0
All	All	66106	0	57309	509	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 (509) 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)
30:X:108:LEU:HD23	30:X:141:VAL:HG21	1.51	0.93
7:A:1382:A:OP1	30:X:166:ARG:NH2	2.06	0.87
7:A:1050:C:OP2	18:L:198:ARG:NH1	2.09	0.85
7:A:955:A:OP1	7:A:957:C:N4	2.09	0.84
28:V:156:ASN:ND2	28:V:159:ASP:OD2	2.10	0.84
5:4:260:CYS:SG	5:4:293:THR:OG1	2.36	0.84
6:8:160:GLU:O	7:A:1078:A:O2'	1.95	0.82
24:R:69:THR:OG1	24:R:72:ASP:OD1	1.98	0.81
7:A:1248:C:O2	17:K:28:HIS:N	2.14	0.80
7:A:1096:A:OP1	18:L:147:ARG:NH2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:702:C:OP1	7:A:848:U:O2'	1.98	0.80
7:A:1412:G:OP1	30:X:279:LYS:NZ	2.14	0.80
12:F:176:ASP:OD1	12:F:179:ARG:NH2	2.16	0.78
6:8:159:LYS:NZ	7:A:1077:U:O4	2.17	0.77
7:A:1134:G:OP2	16:J:38:ARG:NH2	2.18	0.77
30:X:68:TYR:HH	30:X:143:HIS:HD1	1.30	0.77
2:1:155:ASP:OD1	2:1:215:ARG:NH2	2.18	0.77
7:A:769:G:OP2	20:N:73:ARG:NH2	2.18	0.76
30:X:272:THR:OG1	30:X:282:ILE:O	2.03	0.76
12:F:194:LYS:O	12:F:197:GLN:NE2	2.18	0.76
2:1:286:THR:OG1	2:1:288:GLU:OE1	2.03	0.76
7:A:1272:A:N1	7:A:1303:G:O2'	2.19	0.75
1:0:49:ARG:NH2	27:U:41:ARG:O	2.19	0.75
2:1:169:ARG:O	2:1:218:ASN:ND2	2.19	0.75
21:O:95:ILE:CD1	21:O:100:VAL:HG22	2.18	0.74
9:C:124:LEU:O	9:C:132:TYR:OH	2.03	0.74
24:R:212:GLU:OE1	24:R:216:ARG:NH2	2.22	0.73
3:2:36:ARG:NH1	3:2:37:ARG:O	2.21	0.73
28:V:202:ARG:NH1	28:V:247:MET:SD	2.62	0.72
7:A:1494:C:H42	7:A:1555:A:H61	1.36	0.72
17:K:60:ASN:O	17:K:68:GLN:NE2	2.22	0.71
28:V:377:GLN:OE1	28:V:380:GLN:NE2	2.23	0.71
2:1:304:GLU:OE1	2:1:304:GLU:N	2.23	0.71
19:M:108:GLU:OE2	27:U:59:ARG:NH2	2.22	0.71
19:M:55:ASP:OD2	26:T:146:GLN:NE2	2.23	0.70
5:4:322:HIS:ND1	5:4:326:GLN:OE1	2.24	0.70
7:A:1104:A:OP1	7:A:1591:C:O2'	2.09	0.70
5:4:335:PHE:HB3	5:4:360:MET:HE2	1.72	0.70
15:I:166:ILE:CD1	23:Q:19:VAL:HG21	2.22	0.69
17:K:58:ARG:NE	17:K:72:ASP:OD1	2.26	0.69
18:L:115:ILE:HG21	18:L:181:ILE:HD13	1.73	0.69
7:A:1162:A:N3	7:A:1497:C:O2'	2.25	0.69
7:A:941:G:O2'	7:A:1109:A:OP2	2.07	0.69
10:D:372:GLU:OE2	10:D:374:ARG:NE	2.25	0.69
30:X:359:TYR:O	30:X:363:ASN:ND2	2.26	0.69
13:G:263:ASP:OD1	13:G:267:MET:N	2.26	0.69
2:1:107:LYS:NZ	9:C:54:GLU:OE2	2.25	0.68
7:A:1098:C:O2'	7:A:1151:C:O2'	2.08	0.68
30:X:211:ASN:OD1	30:X:234:ARG:NH2	2.27	0.67
15:I:166:ILE:HD13	23:Q:19:VAL:HG21	1.75	0.67
11:E:31:ASP:OD1	27:U:170:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:137:LEU:HD12	2:1:137:LEU:O	1.95	0.66
2:1:292:TYR:OH	30:X:338:ASP:OD1	2.12	0.66
22:P:54:MET:HE2	22:P:57:PRO:HD3	1.78	0.66
24:R:85:LEU:O	24:R:85:LEU:HD23	1.95	0.66
30:X:102:ARG:NH2	30:X:346:SER:O	2.29	0.66
7:A:1106:C:O2'	7:A:1108:C:OP2	2.10	0.65
30:X:208:TYR:HA	38:X:403:GDP:O6	1.95	0.65
27:U:40:GLU:N	27:U:40:GLU:OE1	2.30	0.65
15:I:183:HIS:O	15:I:184:ASN:HB2	1.96	0.65
7:A:867:C:O2'	7:A:870:C:N4	2.30	0.65
7:A:991:G:O6	15:I:122:LYS:NZ	2.30	0.65
16:J:116:GLN:N	16:J:116:GLN:OE1	2.29	0.65
13:G:318:HIS:NE2	30:X:379:GLU:OE2	2.30	0.64
30:X:68:TYR:OH	30:X:143:HIS:ND1	2.26	0.64
5:4:358:ARG:NE	31:Y:250:ILE:O	2.29	0.64
19:M:19:ILE:HB	19:M:83:LEU:HD23	1.78	0.64
5:4:335:PHE:CB	5:4:360:MET:HE2	2.27	0.64
7:A:890:C:O3'	16:J:75:SER:OG	2.16	0.64
5:4:461:PHE:CZ	5:4:465:ILE:HD11	2.33	0.64
5:4:531:ILE:HG22	5:4:535:MET:HE2	1.79	0.64
18:L:86:ASP:OD1	18:L:87:ASP:N	2.31	0.63
8:B:239:ASN:OD1	29:W:119:LYS:NZ	2.30	0.63
8:B:175:MET:HE2	8:B:182:LEU:HD13	1.81	0.63
7:A:1431:G:O2'	7:A:1457:G:O6	2.14	0.63
7:A:890:C:O2'	7:A:902:G:N2	2.32	0.62
7:A:1355:G:N2	7:A:1356:A:N7	2.46	0.62
11:E:27:GLU:OE2	27:U:170:ARG:NH1	2.31	0.62
13:G:237:GLU:O	13:G:241:VAL:HG23	1.99	0.62
3:2:43:ALA:HB1	3:2:46:ILE:HD11	1.81	0.62
5:4:372:TYR:CE2	5:4:400:LEU:HD21	2.35	0.62
18:L:112:MET:O	18:L:116:VAL:HG22	1.99	0.61
6:8:241:ARG:NH2	6:8:247:GLU:OE2	2.34	0.61
21:O:179:THR:HG22	21:O:179:THR:O	1.99	0.61
7:A:893:G:N7	16:J:78:ARG:NH1	2.49	0.61
26:T:138:GLU:OE1	26:T:138:GLU:N	2.33	0.61
7:A:1233:C:O2	17:K:86:ARG:NH1	2.34	0.61
16:J:37:HIS:ND1	20:N:36:ASP:OD2	2.34	0.60
30:X:136:LEU:HD11	37:X:402:ATP:H2'	1.83	0.60
7:A:860:A:N7	7:A:919:A:O2'	2.31	0.60
11:E:94:VAL:CG1	22:P:117:MET:HE1	2.32	0.60
28:V:311:GLU:N	28:V:311:GLU:OE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:41:LEU:HD13	1:0:55:TRP:CG	2.36	0.60
1:0:107:GLN:NE2	1:0:108:ASN:OD1	2.33	0.60
11:E:94:VAL:HG11	22:P:117:MET:HE1	1.84	0.60
28:V:74:ARG:O	28:V:78:ASN:ND2	2.34	0.60
10:D:285:TYR:OH	10:D:372:GLU:OE1	2.20	0.60
18:L:167:LEU:HD11	18:L:187:ILE:HG21	1.84	0.59
21:O:95:ILE:HD12	21:O:100:VAL:HG22	1.82	0.59
2:1:253:TRP:O	2:1:256:SER:OG	2.20	0.59
30:X:153:LEU:HD21	30:X:244:LEU:CD2	2.32	0.59
4:3:161:ARG:NH1	7:A:1146:C:OP1	2.35	0.59
10:D:417:MET:O	10:D:419:ARG:NH1	2.35	0.59
13:G:228:LEU:HD23	13:G:241:VAL:HG22	1.85	0.59
1:0:53:ARG:NH1	7:A:704:U:OP1	2.36	0.59
4:3:177:TRP:CE3	18:L:209:LEU:HD11	2.38	0.59
8:B:156:GLU:OE1	13:G:163:HIS:ND1	2.35	0.59
15:I:118:ARG:NH1	15:I:119:ASN:OD1	2.35	0.59
14:H:145:LEU:HD21	14:H:156:TYR:CE2	2.38	0.59
2:1:58:GLU:N	2:1:58:GLU:OE1	2.36	0.58
28:V:105:ARG:O	28:V:109:ILE:HD12	2.03	0.58
5:4:302:VAL:HG11	5:4:341:CYS:HB3	1.83	0.58
14:H:92:GLU:OE1	14:H:141:ARG:NH1	2.33	0.58
30:X:99:LEU:HD21	30:X:136:LEU:HD22	1.85	0.58
6:8:251:TYR:O	6:8:254:THR:OG1	2.21	0.58
32:Z:81:GLU:OE2	32:Z:84:ARG:NH2	2.37	0.58
7:A:976:A:H5''	23:Q:2:ACE:H1	1.86	0.57
3:2:9:ARG:NH2	7:A:1021:U:OP2	2.35	0.57
13:G:208:MET:HE1	13:G:244:PHE:CD1	2.39	0.57
7:A:917:C:O2'	7:A:921:U:OP1	2.23	0.57
7:A:1066:C:O2'	15:I:187:ARG:O	2.22	0.57
2:1:164:ARG:NH2	31:Y:319:ALA:O	2.34	0.57
5:4:313:TRP:NE1	5:4:317:LEU:HD11	2.20	0.57
9:C:138:TYR:OH	32:Z:65:LEU:HD22	2.05	0.57
7:A:949:U:O2'	20:N:46:ARG:NH1	2.37	0.56
1:0:166:TYR:O	21:O:199:TRP:NE1	2.37	0.56
7:A:768:A:O2'	20:N:24:LYS:NZ	2.38	0.56
7:A:992:U:O2'	7:A:994:A:OP2	2.18	0.56
14:H:181:PRO:O	14:H:184:ILE:HG22	2.04	0.56
31:Y:279:ASP:OD1	31:Y:280:VAL:N	2.39	0.56
1:0:48:ARG:NH2	7:A:701:G:O6	2.35	0.56
8:B:107:PHE:N	8:B:115:ILE:O	2.38	0.56
21:O:181:HIS:O	21:O:185:SER:OG	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:162:SER:O	24:R:170:ARG:NH1	2.29	0.56
5:4:193:ASP:OD1	5:4:261:THR:HG21	2.05	0.56
3:2:117:LEU:HD11	25:S:51:VAL:HG13	1.87	0.56
30:X:133:GLY:HA2	37:X:402:ATP:O2A	2.05	0.56
30:X:108:LEU:CD2	30:X:141:VAL:HG21	2.31	0.56
11:E:96:HIS:O	11:E:99:THR:OG1	2.24	0.56
7:A:738:A:H2'	7:A:740:G:C4	2.40	0.55
18:L:126:GLU:OE2	18:L:177:VAL:HG11	2.06	0.55
31:Y:323:ASP:OD2	31:Y:331:HIS:NE2	2.38	0.55
28:V:355:LEU:O	28:V:359:LEU:HD23	2.07	0.55
30:X:142:ILE:HG23	30:X:152:ILE:HG21	1.89	0.55
2:1:86:ARG:NH1	2:1:96:PRO:O	2.39	0.55
28:V:148:MET:HE1	28:V:164:VAL:HB	1.87	0.55
7:A:662:U:OP2	10:D:339:SER:OG	2.22	0.55
9:C:75:ASN:ND2	17:K:121:SER:O	2.39	0.55
1:0:135:MET:SD	1:0:135:MET:N	2.79	0.55
8:B:179:ALA:CB	8:B:189:LEU:HD21	2.38	0.54
7:A:889:G:N2	7:A:902:G:OP1	2.41	0.54
9:C:89:ASP:OD1	9:C:112:ARG:NH2	2.40	0.54
7:A:1578:A:H2'	7:A:1579:C:C6	2.43	0.54
24:R:161:ILE:O	26:T:125:HIS:NE2	2.40	0.54
24:R:251:GLU:OE2	24:R:280:LYS:NZ	2.41	0.53
1:0:13:GLU:OE1	1:0:16:ARG:NH2	2.41	0.53
10:D:216:GLU:N	10:D:216:GLU:OE1	2.36	0.53
28:V:152:ILE:HD11	28:V:185:VAL:HG22	1.90	0.53
18:L:126:GLU:HB3	18:L:181:ILE:HD11	1.89	0.53
3:2:15:ASN:OD1	3:2:17:ARG:NH1	2.42	0.53
7:A:1227:G:OP1	14:H:128:LYS:NZ	2.30	0.53
9:C:96:MET:HB2	9:C:108:LEU:HD11	1.90	0.53
18:L:83:GLU:N	18:L:83:GLU:OE1	2.40	0.53
1:0:170:LEU:HD21	19:M:96:PHE:CE1	2.43	0.53
5:4:161:ILE:HD12	5:4:194:LEU:HD22	1.90	0.53
7:A:1108:C:H4'	7:A:1109:A:OP2	2.08	0.53
10:D:243:VAL:HG11	10:D:268:PHE:CD1	2.44	0.53
4:3:177:TRP:CZ3	18:L:209:LEU:HD11	2.44	0.52
4:3:189:TRP:NE1	18:L:209:LEU:HD12	2.24	0.52
5:4:257:HIS:O	5:4:261:THR:HG23	2.09	0.52
7:A:1590:A:OP2	23:Q:47:LYS:NZ	2.42	0.52
26:T:92:THR:O	26:T:92:THR:HG22	2.08	0.52
7:A:1339:G:C2	7:A:1340:C:C5	2.97	0.52
13:G:271:LYS:NZ	13:G:282:GLU:OE1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:9:HIS:O	20:N:11:ARG:NH1	2.42	0.52
30:X:392:GLU:HG3	37:X:402:ATP:O3'	2.09	0.52
11:E:120:THR:HG21	25:S:51:VAL:HG11	1.92	0.52
13:G:161:LEU:HD21	13:G:221:PHE:CZ	2.45	0.52
14:H:104:ILE:HG21	14:H:145:LEU:HD23	1.91	0.52
19:M:23:LEU:HD13	19:M:32:TYR:CE1	2.44	0.51
19:M:109:ARG:NE	27:U:52:GLU:OE2	2.42	0.51
28:V:272:ASP:OD1	28:V:273:ILE:N	2.43	0.51
7:A:834:G:H2'	7:A:835:C:O4'	2.10	0.51
5:4:615:MET:HE1	5:4:631:VAL:HG23	1.93	0.51
22:P:78:GLN:NE2	22:P:132:ASP:OD2	2.44	0.51
25:S:125:LEU:HD12	25:S:132:LEU:HD11	1.92	0.51
5:4:277:ASN:O	5:4:281:GLU:OE1	2.29	0.51
22:P:88:THR:OG1	23:Q:33:ASP:OD2	2.20	0.51
2:1:65:ASP:OD2	2:1:68:SER:OG	2.19	0.51
28:V:132:LYS:O	28:V:136:GLY:N	2.38	0.51
24:R:292:ASP:OD1	24:R:292:ASP:C	2.54	0.51
27:U:89:VAL:HG23	27:U:90:LEU:HD12	1.92	0.51
19:M:71:ASP:OD1	19:M:74:ARG:NH2	2.43	0.51
5:4:409:ASP:N	5:4:412:ASP:OD2	2.38	0.51
21:O:180:SER:O	21:O:185:SER:OG	2.28	0.51
30:X:237:THR:HG21	30:X:288:ALA:HB3	1.92	0.50
1:0:57:ASP:OD2	7:A:704:U:N3	2.39	0.50
2:1:166:PRO:O	2:1:169:ARG:NH1	2.42	0.50
4:3:189:TRP:CE2	18:L:209:LEU:HD12	2.46	0.50
11:E:26:ILE:HG23	11:E:36:VAL:HG21	1.93	0.50
13:G:356:VAL:HG23	13:G:361:VAL:HG23	1.94	0.50
3:2:33:VAL:HG21	3:2:104:LEU:HD23	1.93	0.50
14:H:58:LEU:HD23	14:H:58:LEU:H	1.77	0.50
27:U:71:ARG:O	27:U:75:VAL:HG23	2.11	0.50
5:4:192:LEU:O	5:4:193:ASP:C	2.55	0.50
7:A:1352:C:H2'	7:A:1353:A:O4'	2.11	0.50
10:D:134:GLU:OE1	10:D:160:ARG:NH2	2.43	0.50
10:D:340:ILE:O	10:D:340:ILE:HG22	2.11	0.50
22:P:70:LYS:O	22:P:103:LYS:NZ	2.45	0.50
28:V:240:LEU:HD21	28:V:251:TRP:O	2.11	0.50
3:2:104:LEU:HD11	23:Q:72:ILE:HG12	1.93	0.49
7:A:942:A:N6	7:A:1047:A:OP2	2.44	0.49
30:X:136:LEU:CD1	37:X:402:ATP:H2'	2.41	0.49
1:0:178:ARG:NH2	1:0:185:SER:O	2.45	0.49
3:2:17:ARG:NE	7:A:1022:A:OP2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:149:MET:SD	10:D:154:VAL:HG22	2.52	0.49
10:D:245:VAL:HG22	10:D:271:ALA:HB1	1.93	0.49
13:G:200:LEU:CD1	13:G:208:MET:HE2	2.41	0.49
24:R:75:VAL:HG11	24:R:273:TRP:CZ3	2.47	0.49
30:X:173:TYR:CG	38:X:403:GDP:H3'	2.48	0.49
21:O:137:ALA:HB3	21:O:138:PRO:HD3	1.95	0.49
7:A:1043:C:C2'	7:A:1044:U:H5'	2.42	0.49
7:A:867:C:O2'	7:A:870:C:N3	2.46	0.49
26:T:129:PHE:CZ	26:T:140:ILE:HD12	2.48	0.49
2:1:152:ASP:OD2	2:1:174:ARG:NH1	2.43	0.49
10:D:209:GLY:N	10:D:213:GLU:O	2.44	0.49
28:V:264:GLU:OE2	28:V:333:ARG:NH2	2.40	0.49
13:G:315:PHE:CD2	13:G:369:LEU:HD21	2.48	0.48
1:0:9:ARG:NE	7:A:805:C:O2	2.44	0.48
7:A:834:G:H21	7:A:836:A:N6	2.10	0.48
32:Z:3:SER:OG	32:Z:4:LEU:N	2.45	0.48
5:4:336:ASN:ND2	5:4:371:THR:OG1	2.46	0.48
7:A:988:G:O5'	15:I:114:THR:HG22	2.13	0.48
7:A:672:A:H2'	7:A:673:U:C6	2.48	0.48
7:A:1057:G:H4'	7:A:1578:A:H4'	1.95	0.48
12:F:50:TYR:O	12:F:66:ARG:NH2	2.47	0.48
10:D:391:LEU:HD23	10:D:392:ARG:O	2.13	0.48
1:0:107:GLN:O	28:V:97:HIS:NE2	2.43	0.48
7:A:934:G:O2'	7:A:940:A:N1	2.41	0.48
7:A:845:A:H4'	27:U:60:TYR:CE2	2.49	0.48
3:2:56:TRP:NE1	3:2:63:ASP:OD1	2.47	0.48
7:A:853:C:H2'	7:A:854:U:C6	2.48	0.48
20:N:93:ASP:O	20:N:97:GLY:N	2.41	0.48
30:X:112:LEU:O	30:X:115:THR:HG22	2.14	0.48
24:R:69:THR:N	24:R:72:ASP:OD1	2.47	0.47
24:R:239:SER:OG	24:R:241:GLU:OE1	2.32	0.47
28:V:212:GLY:O	28:V:224:GLN:NE2	2.47	0.47
7:A:1557:A:H2	7:A:1558:A:H62	1.62	0.47
27:U:166:ASN:O	27:U:176:ARG:NH1	2.45	0.47
12:F:59:THR:HG22	12:F:60:GLU:N	2.29	0.47
5:4:121:ILE:HD13	9:C:145:TYR:CG	2.49	0.47
5:4:501:ASP:OD2	5:4:537:ARG:NH1	2.47	0.47
7:A:947:U:C4	7:A:948:U:C5	3.02	0.47
30:X:380:LEU:HD21	30:X:398:LEU:HD13	1.96	0.47
24:R:82:MET:HE2	24:R:272:VAL:HG21	1.97	0.47
1:0:87:TRP:O	21:O:215:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:84:ARG:NH2	12:F:242:TRP:O	2.48	0.47
7:A:1025:A:H2'	7:A:1026:A:C8	2.50	0.47
7:A:1326:A:O4'	10:D:114:ARG:NH2	2.48	0.47
7:A:1370:U:C2	7:A:1371:U:C5	3.03	0.47
13:G:320:VAL:HG21	13:G:352:LEU:HD21	1.97	0.47
13:G:168:MET:HE1	13:G:240:PHE:CE1	2.50	0.47
30:X:153:LEU:HD23	30:X:260:VAL:HG13	1.96	0.47
5:4:615:MET:HE3	5:4:645:LEU:HD21	1.97	0.47
2:1:211:ARG:NH2	31:Y:359:SER:OG	2.48	0.47
2:1:98:ALA:O	2:1:102:ASN:ND2	2.47	0.46
7:A:1492:A:N1	7:A:1558:A:N1	2.64	0.46
7:A:1566:C:OP2	7:A:1569:G:O2'	2.26	0.46
11:E:10:LEU:CD2	11:E:88:VAL:HG22	2.45	0.46
20:N:62:ASP:OD1	20:N:88:VAL:N	2.43	0.46
8:B:89:VAL:HG13	8:B:249:TYR:OH	2.15	0.46
24:R:70:PHE:O	24:R:76:GLN:NE2	2.43	0.46
28:V:123:ASP:OD1	28:V:123:ASP:N	2.48	0.46
7:A:663:A:H2'	7:A:664:G:C8	2.50	0.46
7:A:835:C:N4	7:A:851:A:OP2	2.37	0.46
21:O:98:ASN:OD1	21:O:98:ASN:C	2.57	0.46
3:2:33:VAL:HG22	3:2:105:ASN:OD1	2.15	0.46
26:T:32:VAL:HG21	26:T:52:ILE:HD11	1.98	0.46
28:V:140:ASP:OD1	28:V:141:ASN:N	2.44	0.46
30:X:242:ILE:HG13	38:X:403:GDP:H1'	1.97	0.46
1:O:37:ASP:O	1:O:41:LEU:N	2.43	0.46
28:V:30:LEU:HD12	28:V:149:ASP:HB2	1.98	0.46
3:2:104:LEU:HD11	23:Q:72:ILE:HG23	1.96	0.46
5:4:317:LEU:HD22	31:Y:258:ILE:HD11	1.98	0.46
7:A:974:U:O2'	7:A:975:A:N7	2.45	0.46
7:A:1279:C:O2'	7:A:1296:A:N1	2.45	0.46
7:A:1443:U:O2'	7:A:1445:G:N7	2.41	0.46
14:H:70:ASP:OD1	14:H:71:ILE:N	2.48	0.46
3:2:24:ASN:OD1	3:2:25:LYS:N	2.49	0.46
5:4:305:ILE:O	5:4:312:LYS:NZ	2.48	0.46
8:B:121:THR:OG1	8:B:237:PRO:O	2.26	0.46
7:A:845:A:OP1	27:U:64:ARG:NH2	2.47	0.46
7:A:1282:G:N2	7:A:1286:A:OP2	2.43	0.46
7:A:1557:A:H2'	7:A:1558:A:C8	2.50	0.46
2:1:231:HIS:NE2	14:H:188:ILE:HD12	2.31	0.45
7:A:1033:U:OP1	22:P:113:ARG:NH2	2.46	0.45
22:P:48:GLU:OE1	22:P:48:GLU:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:138:ASP:CG	1:0:138:ASP:O	2.59	0.45
7:A:1080:A:H1'	7:A:1082:A:N7	2.31	0.45
7:A:1245:U:O2'	32:Z:96:LYS:NZ	2.44	0.45
7:A:1429:C:OP1	13:G:388:ARG:NH1	2.45	0.45
29:W:150:THR:HG22	29:W:161:THR:CB	2.46	0.45
17:K:70:VAL:O	17:K:73:GLU:HG2	2.16	0.45
32:Z:54:ASN:HD21	32:Z:56:HIS:HB2	1.80	0.45
7:A:1140:A:H2	7:A:1163:C:H42	1.63	0.45
20:N:88:VAL:O	20:N:88:VAL:HG13	2.17	0.45
5:4:389:SER:HA	5:4:392:ILE:HG22	1.99	0.45
7:A:1200:G:C2	7:A:1201:A:C8	3.05	0.45
7:A:1452:U:OP2	13:G:380:LYS:NZ	2.48	0.45
7:A:1020:C:C5	7:A:1021:U:C4	3.05	0.45
7:A:654:U:O2'	7:A:1167:A:OP2	2.30	0.45
8:B:198:THR:HG21	8:B:232:ILE:CD1	2.46	0.45
15:I:103:SER:O	15:I:103:SER:OG	2.33	0.45
2:1:89:TYR:O	9:C:164:TYR:OH	2.27	0.45
3:2:56:TRP:HE1	3:2:70:ILE:HD11	1.80	0.45
7:A:1044:U:H2'	7:A:1045:G:O4'	2.16	0.45
24:R:191:ARG:HG3	24:R:204:ILE:HG23	1.99	0.45
7:A:942:A:H61	7:A:1047:A:P	2.40	0.44
7:A:1406:U:H5'	7:A:1407:U:OP2	2.17	0.44
1:0:28:PRO:CG	1:0:33:LEU:HD21	2.47	0.44
7:A:1400:U:H2'	7:A:1401:G:O4'	2.17	0.44
19:M:39:ASN:OD1	19:M:40:LYS:N	2.50	0.44
28:V:161:LEU:HA	28:V:164:VAL:HG12	1.98	0.44
3:2:18:LYS:NZ	7:A:1028:G:O6	2.40	0.44
4:3:173:LEU:HD13	18:L:209:LEU:HD13	1.99	0.44
7:A:1047:A:H62	7:A:1158:U:H5'	1.82	0.44
7:A:1366:C:H3'	7:A:1367:A:H5'	1.99	0.44
38:X:403:GDP:N3	38:X:403:GDP:H2'	2.33	0.44
7:A:1033:U:O2'	11:E:93:ILE:O	2.35	0.44
7:A:1206:G:C6	7:A:1360:G:C6	3.06	0.44
14:H:50:LEU:HD11	14:H:53:ASP:HB3	1.99	0.44
28:V:356:THR:O	28:V:360:VAL:HG23	2.18	0.44
2:1:263:LEU:O	2:1:267:LEU:HD13	2.18	0.44
3:2:104:LEU:HD22	7:A:1600:A:C6	2.53	0.44
7:A:741:A:OP1	27:U:86:ARG:NH2	2.51	0.44
7:A:760:A:N1	7:A:780:C:O2'	2.40	0.44
7:A:1014:A:H4'	15:I:184:ASN:ND2	2.33	0.44
28:V:377:GLN:O	28:V:380:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:91:GLU:OE1	1:0:91:GLU:N	2.48	0.44
5:4:279:TYR:HB2	5:4:297:LEU:HD21	1.99	0.44
5:4:564:ILE:HG22	5:4:564:ILE:O	2.17	0.44
10:D:140:LEU:HB3	10:D:146:VAL:HG11	2.00	0.44
13:G:70:THR:HG23	13:G:73:PHE:H	1.82	0.44
17:K:55:ASN:OD1	17:K:58:ARG:NH1	2.51	0.44
21:O:208:PRO:HB3	27:U:54:PHE:CD2	2.53	0.44
2:1:87:MET:SD	2:1:108:ILE:HD11	2.58	0.44
7:A:1334:G:H2'	7:A:1335:U:O4'	2.17	0.44
27:U:183:SER:OG	27:U:184:ARG:N	2.50	0.44
28:V:190:LEU:HD13	28:V:226:TYR:CE1	2.53	0.44
30:X:276:ARG:NH1	30:X:281:PRO:O	2.50	0.44
5:4:164:ARG:NH1	5:4:198:TYR:OH	2.50	0.43
15:I:110:ALA:HB3	15:I:135:ALA:HB2	1.99	0.43
18:L:126:GLU:HG2	18:L:177:VAL:CG1	2.48	0.43
19:M:67:ALA:HB2	24:R:196:TYR:CZ	2.53	0.43
20:N:83:GLU:OE1	26:T:85:GLN:NE2	2.47	0.43
7:A:669:U:C6	10:D:422:TRP:CH2	3.06	0.43
7:A:843:G:N2	7:A:846:A:OP2	2.46	0.43
7:A:1454:G:OP2	13:G:377:ARG:NH1	2.45	0.43
28:V:375:TYR:CE2	28:V:379:LEU:HD11	2.53	0.43
30:X:161:TRP:O	30:X:180:GLN:NE2	2.41	0.43
7:A:1264:C:H1'	14:H:124:VAL:HG13	1.99	0.43
12:F:59:THR:HG22	12:F:60:GLU:H	1.83	0.43
13:G:200:LEU:HD13	13:G:208:MET:HE2	2.00	0.43
5:4:166:VAL:HG23	5:4:167:LYS:N	2.34	0.43
5:4:543:GLU:O	5:4:546:VAL:HG12	2.19	0.43
7:A:659:U:O2'	7:A:1285:G:H1'	2.19	0.43
10:D:165:GLN:NE2	10:D:169:GLU:OE2	2.51	0.43
12:F:236:LEU:HD12	12:F:236:LEU:N	2.33	0.43
19:M:83:LEU:CD1	19:M:97:PHE:HE2	2.32	0.43
22:P:73:ASP:OD1	22:P:74:TYR:N	2.52	0.43
14:H:108:VAL:HG13	14:H:143:LEU:HD23	2.00	0.43
14:H:125:HIS:CD2	14:H:126:ILE:HG23	2.53	0.43
30:X:297:MET:HE1	30:X:306:ILE:HG23	2.01	0.43
22:P:139:ARG:NE	22:P:141:ARG:O	2.52	0.43
8:B:198:THR:HG21	8:B:232:ILE:HD11	2.01	0.43
30:X:68:TYR:HH	30:X:143:HIS:CE1	2.35	0.43
5:4:567:THR:HG22	5:4:568:ALA:N	2.33	0.42
7:A:1578:A:H2'	7:A:1579:C:H6	1.82	0.42
19:M:100:HIS:H	19:M:103:MET:HE3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:8:VAL:HB	20:N:68:ALA:HB1	2.00	0.42
5:4:437:GLY:O	5:4:441:THR:OG1	2.33	0.42
5:4:458:TYR:HB3	5:4:486:TYR:CD1	2.54	0.42
7:A:1042:U:C2	7:A:1043:C:C5	3.07	0.42
24:R:231:CYS:SG	24:R:242:TYR:HA	2.59	0.42
26:T:43:GLY:HA3	26:T:93:LYS:O	2.20	0.42
31:Y:276:SER:O	31:Y:279:ASP:OD1	2.37	0.42
7:A:728:C:H2'	7:A:729:U:O4'	2.19	0.42
7:A:730:A:C4	7:A:731:A:C8	3.08	0.42
1:0:110:ASP:OD1	1:0:110:ASP:N	2.48	0.42
2:1:194:VAL:HG21	2:1:198:TYR:HB2	2.01	0.42
7:A:1320:G:OP2	9:C:37:ASN:ND2	2.41	0.42
2:1:114:LEU:HD11	14:H:163:ASN:HB3	2.01	0.42
5:4:332:LEU:HD23	5:4:336:ASN:OD1	2.19	0.42
9:C:58:ALA:HB3	9:C:60:HIS:CE1	2.54	0.42
11:E:49:TYR:OH	22:P:115:GLN:O	2.17	0.42
13:G:168:MET:HE1	13:G:240:PHE:CD1	2.54	0.42
24:R:82:MET:HE3	24:R:288:GLN:HE22	1.85	0.42
7:A:983:C:O2	7:A:983:C:H2'	2.19	0.42
8:B:84:LEU:HD23	8:B:248:LEU:HD21	2.01	0.42
17:K:72:ASP:O	17:K:75:ILE:HG22	2.20	0.42
20:N:33:LEU:HD11	26:T:66:MET:HE1	2.01	0.42
24:R:294:ILE:HG13	24:R:349:TYR:CZ	2.54	0.42
30:X:145:CYS:SG	30:X:259:LEU:HD22	2.60	0.42
30:X:208:TYR:HD1	38:X:403:GDP:C6	2.37	0.42
5:4:158:LYS:O	5:4:161:ILE:HG22	2.19	0.42
5:4:159:GLU:OE2	5:4:163:LEU:HD11	2.19	0.42
7:A:953:U:H4'	7:A:954:C:OP1	2.20	0.42
7:A:955:A:C8	26:T:37:HIS:CE1	3.07	0.42
7:A:1338:A:C4	7:A:1339:G:C8	3.08	0.42
20:N:58:CYS:SG	20:N:81:LEU:HD22	2.60	0.42
2:1:81:VAL:O	2:1:99:LYS:NZ	2.52	0.42
3:2:10:LEU:O	3:2:15:ASN:ND2	2.51	0.42
5:4:197:TYR:OH	31:Y:281:GLU:HG2	2.19	0.42
7:A:1096:A:H2'	7:A:1097:G:O4'	2.20	0.42
11:E:15:ARG:NH2	27:U:182:ASP:OD1	2.53	0.42
11:E:26:ILE:HG21	27:U:173:LEU:HD13	2.01	0.42
15:I:150:VAL:O	15:I:150:VAL:HG13	2.19	0.42
30:X:200:ASN:OD1	30:X:201:GLN:N	2.53	0.42
6:8:214:LEU:HD22	6:8:223:PHE:CE2	2.55	0.42
7:A:1049:A:OP1	18:L:198:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1232:A:C2	7:A:1404:A:N3	2.88	0.42
13:G:165:VAL:HA	13:G:168:MET:HE3	2.02	0.42
13:G:269:PHE:CD1	13:G:284:ILE:HG23	2.55	0.42
19:M:78:GLY:O	27:U:75:VAL:HG22	2.20	0.42
30:X:242:ILE:HD11	38:X:403:GDP:C4	2.55	0.42
7:A:947:U:N3	7:A:948:U:C5	2.88	0.41
14:H:126:ILE:O	14:H:128:LYS:N	2.52	0.41
31:Y:390:SER:O	31:Y:391:ASN:HB2	2.20	0.41
2:1:244:THR:HG22	2:1:245:GLU:N	2.35	0.41
2:1:322:VAL:O	2:1:322:VAL:HG13	2.20	0.41
5:4:360:MET:HE1	5:4:371:THR:HG23	2.02	0.41
1:0:43:ARG:NE	7:A:706:C:OP1	2.47	0.41
5:4:157:LEU:HD22	5:4:187:THR:CG2	2.51	0.41
5:4:397:MET:SD	5:4:435:VAL:HG22	2.60	0.41
7:A:800:C:O2'	7:A:801:A:H5'	2.21	0.41
24:R:268:PHE:O	24:R:272:VAL:HG23	2.21	0.41
28:V:44:GLU:OE1	28:V:44:GLU:N	2.49	0.41
28:V:113:ILE:HG21	28:V:143:THR:CG2	2.50	0.41
1:0:93:CYS:HA	1:0:119:THR:O	2.21	0.41
5:4:407:PRO:C	31:Y:286:LEU:HD11	2.46	0.41
7:A:1013:A:H2'	7:A:1014:A:O4'	2.21	0.41
18:L:193:PRO:HG2	18:L:196:TYR:CE1	2.56	0.41
14:H:76:LEU:CD1	14:H:174:LYS:HG2	2.51	0.41
25:S:99:PHE:HA	25:S:125:LEU:HD11	2.02	0.41
28:V:30:LEU:HD12	28:V:149:ASP:CB	2.49	0.41
7:A:1177:C:O2'	7:A:1567:A:N1	2.50	0.41
7:A:1413:U:N3	7:A:1414:C:C5	2.89	0.41
8:B:149:ARG:NH2	23:Q:82:ASP:OD2	2.51	0.41
11:E:47:LEU:HD13	11:E:51:ILE:HD12	2.02	0.41
15:I:115:GLU:OE2	15:I:134:ALA:HB2	2.21	0.41
28:V:70:LEU:HD21	28:V:390:ILE:HD13	2.01	0.41
28:V:318:ASP:OD1	28:V:319:ILE:N	2.53	0.41
30:X:192:LYS:HB2	30:X:226:VAL:HG11	2.02	0.41
2:1:164:ARG:NH1	31:Y:319:ALA:O	2.53	0.41
7:A:1077:U:O2'	7:A:1079:G:N7	2.44	0.41
7:A:1225:C:H4'	7:A:1226:C:H5'	2.03	0.41
7:A:1406:U:H4'	7:A:1407:U:OP2	2.21	0.41
10:D:243:VAL:HG11	10:D:268:PHE:HD1	1.82	0.41
28:V:35:VAL:HG12	28:V:35:VAL:O	2.20	0.41
2:1:50:ARG:NE	5:4:94:TYR:O	2.52	0.41
2:1:265:THR:HG21	2:1:320:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:158:LYS:HA	5:4:161:ILE:HG22	2.01	0.41
26:T:32:VAL:HG22	26:T:76:LEU:HD22	2.02	0.41
28:V:109:ILE:HD12	28:V:109:ILE:H	1.86	0.41
7:A:871:A:N1	7:A:918:A:O2'	2.45	0.41
7:A:1267:U:H2'	7:A:1268:C:C6	2.56	0.41
8:B:78:LEU:HD22	8:B:255:THR:HG21	2.03	0.41
12:F:203:GLU:OE1	12:F:203:GLU:N	2.50	0.41
14:H:76:LEU:HD22	14:H:148:LEU:HD11	2.02	0.41
1:0:158:GLU:HG3	1:0:158:GLU:O	2.21	0.41
2:1:103:LEU:HD22	9:C:106:ASP:OD2	2.21	0.41
2:1:267:LEU:HD12	2:1:283:LEU:CD1	2.51	0.41
7:A:1227:G:O4'	14:H:125:HIS:O	2.39	0.41
7:A:1561:C:C4	7:A:1562:G:N7	2.89	0.41
25:S:102:LYS:O	25:S:105:GLU:HG3	2.20	0.41
7:A:713:C:OP1	19:M:12:TYR:OH	2.39	0.40
7:A:1244:C:O2'	7:A:1245:U:H5'	2.21	0.40
17:K:120:LEU:HB3	17:K:123:ILE:HD12	2.03	0.40
22:P:113:ARG:HG3	22:P:117:MET:HE3	2.03	0.40
2:1:231:HIS:CE1	14:H:188:ILE:HD12	2.56	0.40
3:2:104:LEU:HD22	7:A:1600:A:N6	2.36	0.40
4:3:165:LYS:NZ	7:A:1149:G:OP2	2.47	0.40
5:4:333:GLN:O	5:4:337:THR:HG23	2.20	0.40
5:4:564:ILE:O	5:4:567:THR:N	2.52	0.40
18:L:109:GLU:HG3	18:L:110:GLN:N	2.36	0.40
19:M:36:ALA:HB2	19:M:51:LEU:HD11	2.02	0.40
24:R:208:ILE:O	24:R:214:ASN:ND2	2.44	0.40
30:X:173:TYR:CD1	38:X:403:GDP:H3'	2.56	0.40
32:Z:21:GLU:OE1	32:Z:21:GLU:N	2.52	0.40
2:1:289:ILE:HD13	2:1:319:LEU:HD21	2.04	0.40
7:A:1041:A:H5''	18:L:128:ARG:NE	2.37	0.40
7:A:1201:A:H2'	7:A:1202:G:C8	2.56	0.40
7:A:1231:A:OP1	17:K:88:ARG:NH1	2.46	0.40
11:E:5:GLU:OE2	22:P:74:TYR:OH	2.30	0.40
19:M:68:LEU:HD22	19:M:87:MET:HE1	2.03	0.40
24:R:276:VAL:HG11	24:R:307:LEU:CD1	2.52	0.40
24:R:324:GLY:O	24:R:327:LEU:N	2.54	0.40
5:4:89:PHE:HZ	5:4:103:SER:HG	1.70	0.40
7:A:1047:A:N6	7:A:1158:U:H5'	2.37	0.40
7:A:1136:C:O2'	7:A:1137:A:H5'	2.20	0.40
7:A:1289:G:O2'	7:A:1297:G:OP2	2.27	0.40
12:F:145:PHE:CZ	12:F:149:LEU:HD11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:301:GLN:OE1	30:X:385:ASN:ND2	2.39	0.40
21:O:55:PRO:HB3	21:O:114:HIS:HB2	2.03	0.40
28:V:202:ARG:HG2	28:V:247:MET:HE2	2.03	0.40
3:2:43:ALA:N	12:F:240:ARG:O	2.54	0.40
5:4:631:VAL:CG2	5:4:649:VAL:HG21	2.51	0.40
7:A:1275:A:C6	7:A:1299:A:C6	3.09	0.40
24:R:191:ARG:O	24:R:195:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	210/218 (96%)	206 (98%)	4 (2%)	0	100	100
2	1	274/323 (85%)	267 (97%)	7 (3%)	0	100	100
3	2	102/118 (86%)	99 (97%)	3 (3%)	0	100	100
4	3	69/199 (35%)	66 (96%)	3 (4%)	0	100	100
5	4	588/689 (85%)	572 (97%)	16 (3%)	0	100	100
6	8	91/278 (33%)	88 (97%)	3 (3%)	0	100	100
8	B	218/296 (74%)	213 (98%)	5 (2%)	0	100	100
9	C	130/167 (78%)	130 (100%)	0	0	100	100
10	D	334/430 (78%)	319 (96%)	14 (4%)	1 (0%)	36	70
11	E	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
12	F	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
13	G	297/396 (75%)	289 (97%)	8 (3%)	0	100	100
14	H	137/201 (68%)	134 (98%)	3 (2%)	0	100	100
15	I	135/194 (70%)	128 (95%)	6 (4%)	1 (1%)	18	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J	105/138 (76%)	99 (94%)	6 (6%)	0	100	100
17	K	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
18	L	168/257 (65%)	160 (95%)	8 (5%)	0	100	100
19	M	113/137 (82%)	110 (97%)	3 (3%)	0	100	100
20	N	107/130 (82%)	103 (96%)	4 (4%)	0	100	100
21	O	191/258 (74%)	188 (98%)	3 (2%)	0	100	100
22	P	94/142 (66%)	92 (98%)	2 (2%)	0	100	100
23	Q	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
24	R	291/360 (81%)	276 (95%)	15 (5%)	0	100	100
25	S	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
26	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
27	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
28	V	358/414 (86%)	349 (98%)	9 (2%)	0	100	100
29	W	97/187 (52%)	91 (94%)	6 (6%)	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%)	92 (98%)	2 (2%)	0	100	100
All	All	5680/7581 (75%)	5525 (97%)	153 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	I	184	ASN
10	D	396	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	185/190 (97%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	8	85/247 (34%)	85 (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	185/209 (88%)	185 (100%)	0	100	100
13	G	262/342 (77%)	262 (100%)	0	100	100
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	78/78 (100%)	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	5081/6591 (77%)	5081 (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 (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	107	GLN
1	0	108	ASN
3	2	113	ASN
5	4	336	ASN
5	4	521	HIS
5	4	545	GLN
5	4	569	GLN
5	4	602	HIS
5	4	659	GLN
6	8	190	GLN
6	8	211	HIS
8	B	93	HIS
9	C	60	HIS
10	D	151	ASN
10	D	273	ASN
11	E	100	GLN
12	F	169	GLN
13	G	366	GLN
14	H	130	HIS
14	H	147	HIS
15	I	94	ASN
15	I	184	ASN
19	M	16	HIS
21	O	65	GLN
24	R	117	GLN
24	R	278	ASN
26	T	33	ASN
28	V	78	ASN
28	V	134	GLN
28	V	377	GLN
28	V	380	GLN
29	W	110	ASN
29	W	135	GLN
30	X	66	GLN
30	X	69	ASN
30	X	235	ASN
30	X	291	HIS
31	Y	303	GLN
32	Z	54	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	887/955 (92%)	114 (12%)	1 (0%)

All (114) 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	735	A
7	A	737	C
7	A	738	A
7	A	753	A
7	A	761	A
7	A	766	G
7	A	773	U
7	A	777	G
7	A	791	G
7	A	796	G
7	A	808	C
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	893	G
7	A	919	A
7	A	923	A
7	A	929	A
7	A	930	G
7	A	938	A
7	A	939	A
7	A	941	G
7	A	942	A

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Mol	Chain	Res	Type
7	A	954	C
7	A	967	A
7	A	983	C
7	A	984	C
7	A	1014	A
7	A	1015	A
7	A	1041	A
7	A	1042	U
7	A	1043	C
7	A	1044	U
7	A	1046	A
7	A	1048	C
7	A	1049	A
7	A	1065	C
7	A	1080	A
7	A	1081	U
7	A	1082	A
7	A	1103	A
7	A	1105	C
7	A	1106	C
7	A	1117	A
7	A	1120	C
7	A	1121	A
7	A	1151	C
7	A	1153	C
7	A	1155	G
7	A	1160	A
7	A	1167	A
7	A	1188	A
7	A	1189	U
7	A	1190	C
7	A	1215	U
7	A	1223	C
7	A	1247	G
7	A	1248	C
7	A	1250	C
7	A	1251	A
7	A	1261	C
7	A	1271	C
7	A	1273	G
7	A	1284	U
7	A	1290	C

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Mol	Chain	Res	Type
7	A	1291	U
7	A	1312	C
7	A	1326	A
7	A	1327	G
7	A	1343	A
7	A	1354	A
7	A	1356	A
7	A	1376	C
7	A	1378	C
7	A	1390	A
7	A	1405	C
7	A	1407	U
7	A	1422	G
7	A	1430	A
7	A	1438	G
7	A	1447	G
7	A	1464	G
7	A	1469	G
7	A	1474	G
7	A	1481	C
7	A	1482	A
7	A	1492	A
7	A	1493	C
7	A	1495	C
7	A	1501	A
7	A	1557	A
7	A	1558	A
7	A	1568	U
7	A	1570	G
7	A	1571	U
7	A	1582	G
7	A	1584	A
7	A	1594	G
7	A	1595	G
7	A	1599	A
7	A	1602	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1406	U

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 50 ligands modelled in this entry, 46 are monoatomic - leaving 4 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	FES	T	201	26,19	0,4,4	-	-	-		
38	GDP	X	403	-	29,30,30	0.52	0	45,47,47	0.45	0
36	FES	P	201	22,11	0,4,4	-	-	-		
37	ATP	X	402	33	32,33,33	0.56	0	48,52,52	0.62	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	ATP	X	402	33	-	2/22/38/38	0/3/3/3
38	GDP	X	403	-	-	0/16/32/32	0/3/3/3
36	FES	T	201	26,19	-	-	0/1/1/1
36	FES	P	201	22,11	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

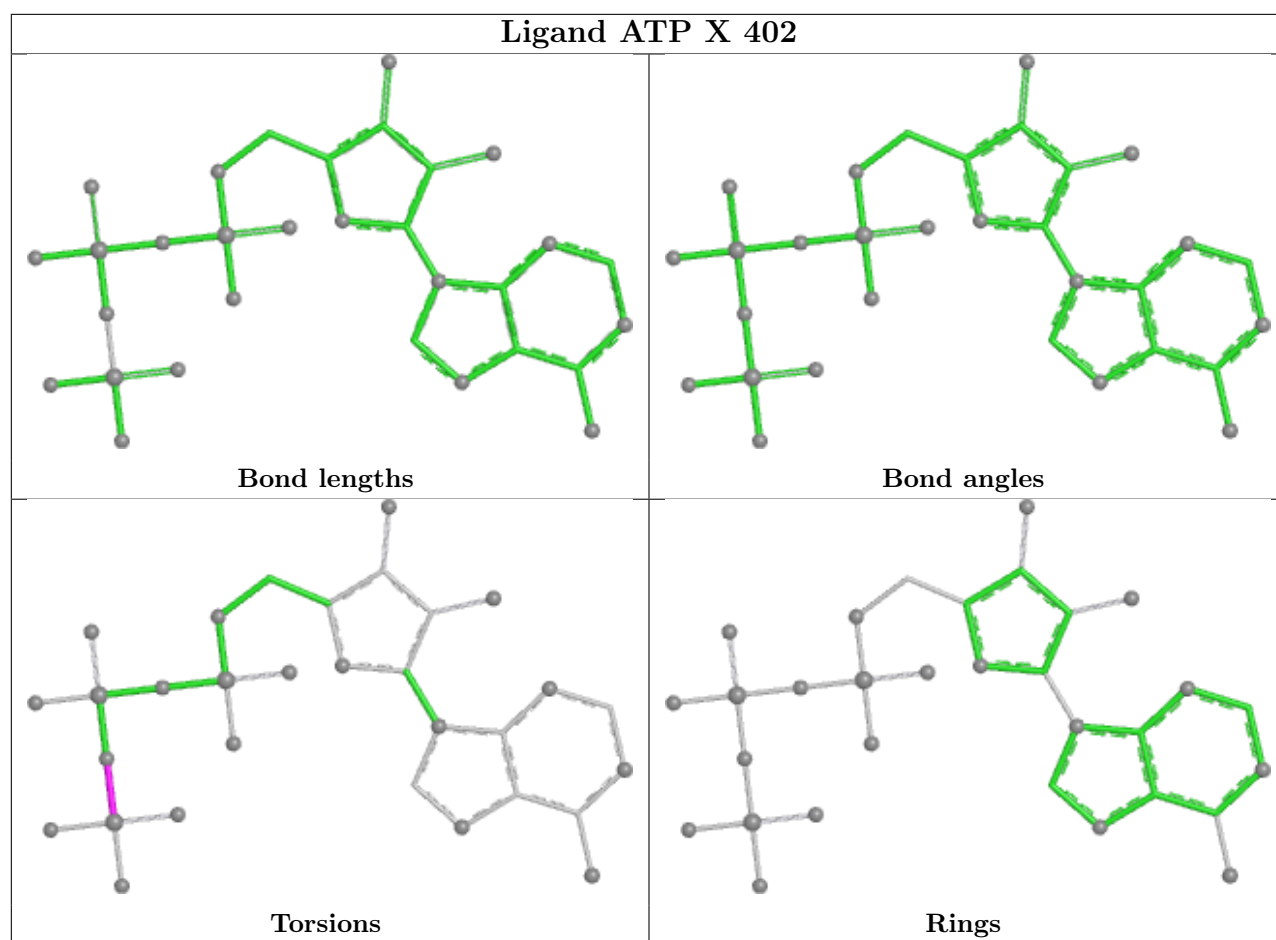
Mol	Chain	Res	Type	Atoms
37	X	402	ATP	PB-O3B-PG-O2G
37	X	402	ATP	PB-O3B-PG-O3G

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	X	403	GDP	7	0
37	X	402	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

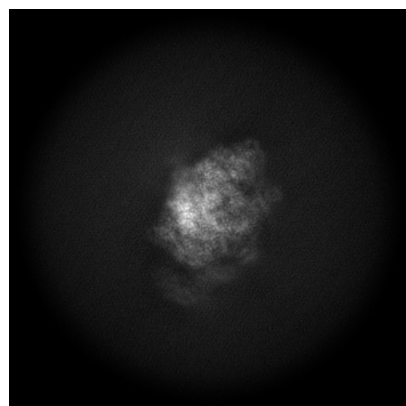
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52117. These allow visual inspection of the internal detail of the map and identification of artifacts.

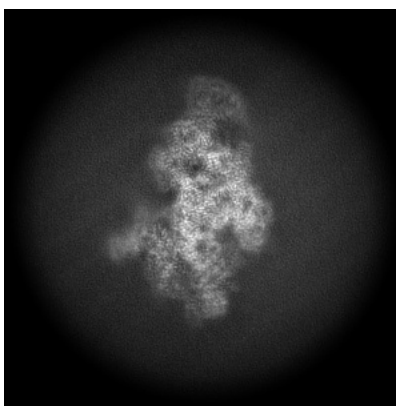
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

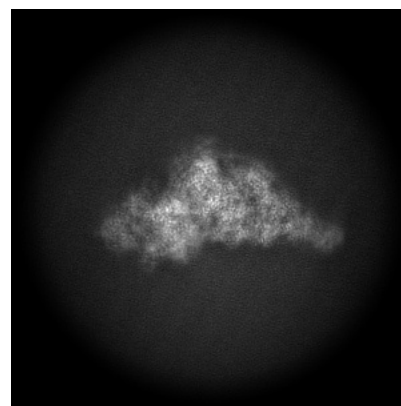
6.1.1 Primary map



X

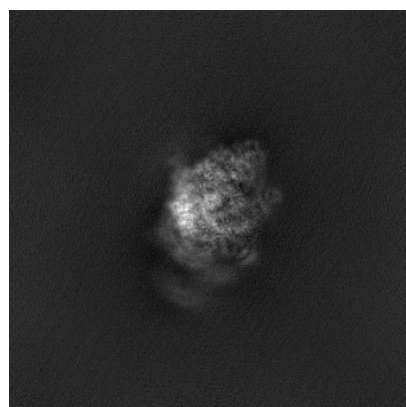


Y

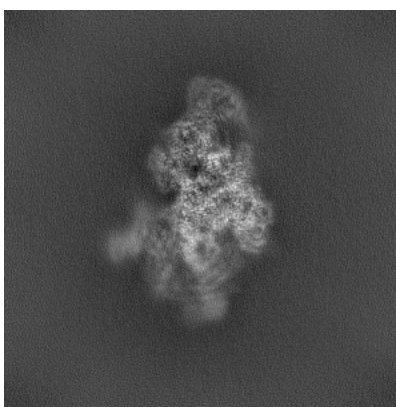


Z

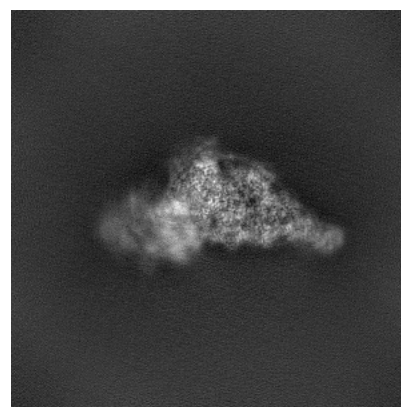
6.1.2 Raw map



X



Y

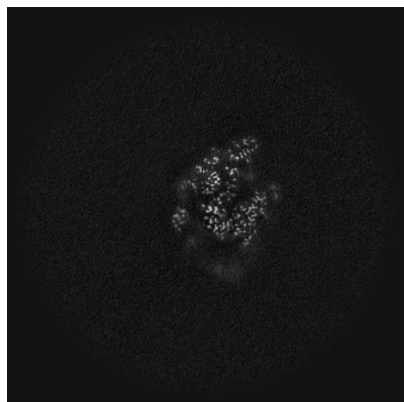


Z

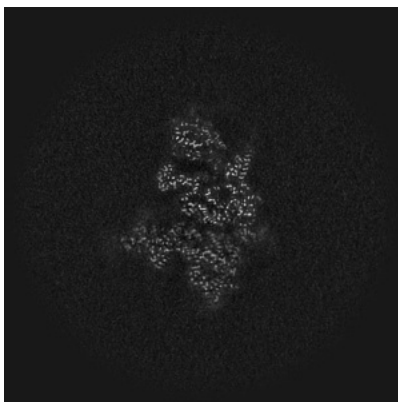
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

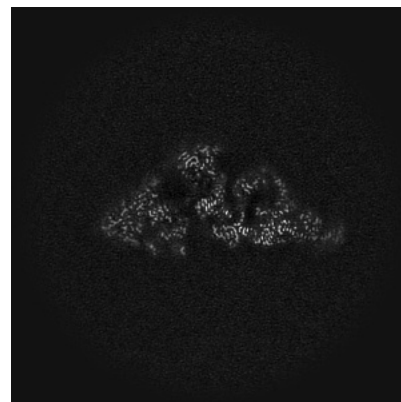
6.2.1 Primary map



X Index: 220

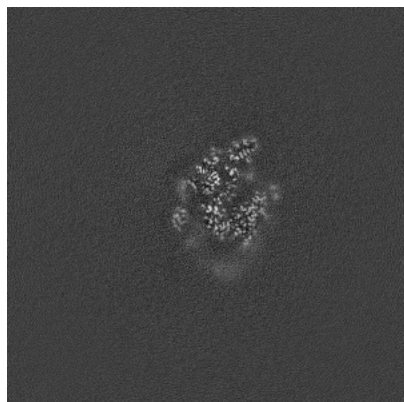


Y Index: 220

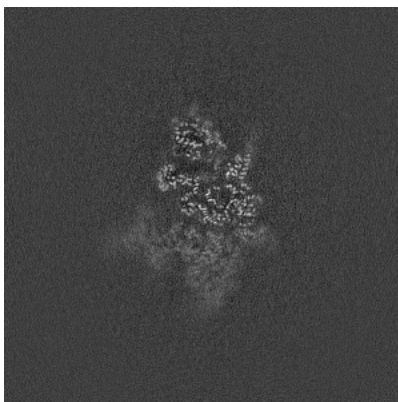


Z Index: 220

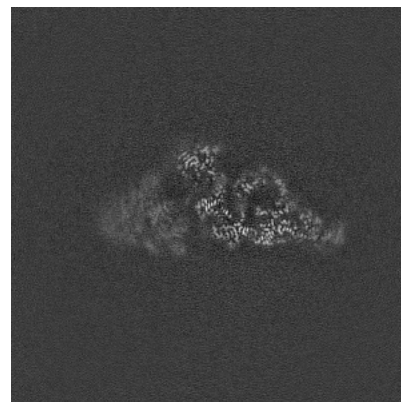
6.2.2 Raw map



X Index: 220



Y Index: 220

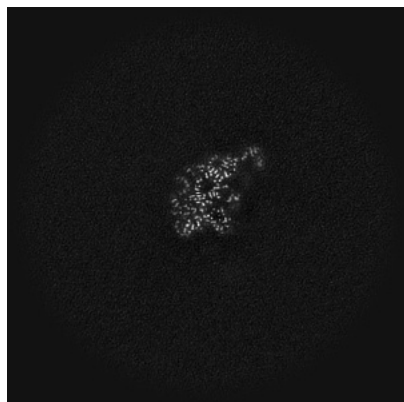


Z Index: 220

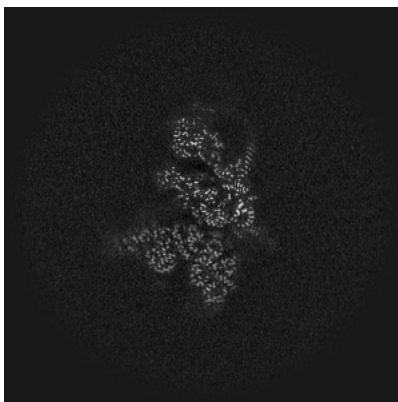
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

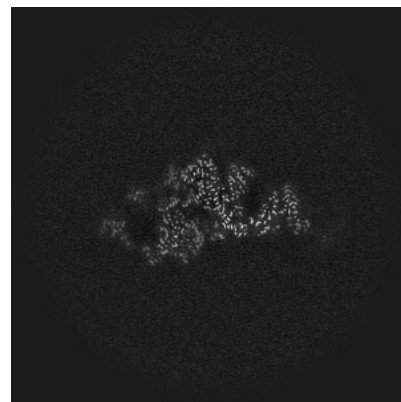
6.3.1 Primary map



X Index: 235

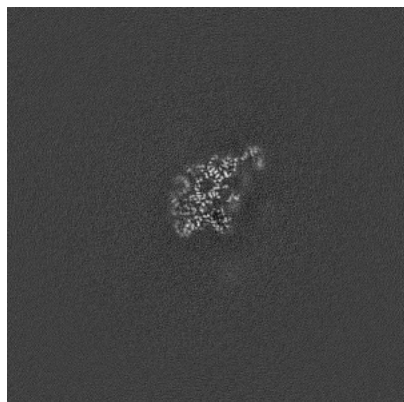


Y Index: 216

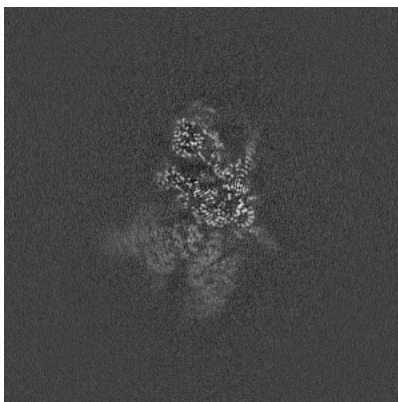


Z Index: 200

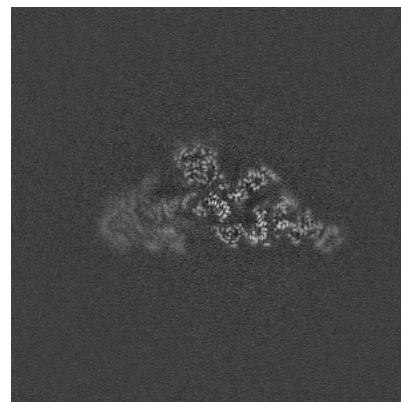
6.3.2 Raw map



X Index: 235



Y Index: 216

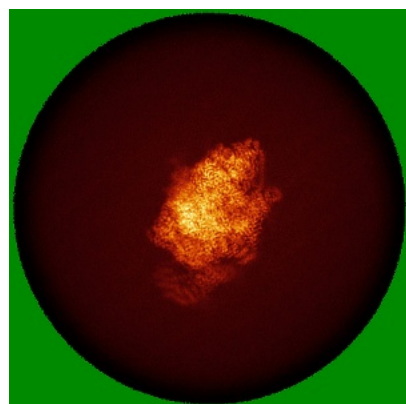


Z Index: 225

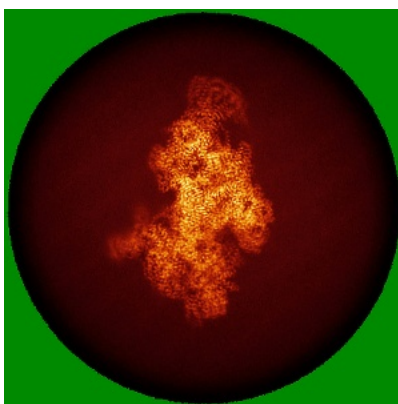
The images above show the largest variance slices of the map in three orthogonal directions.

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

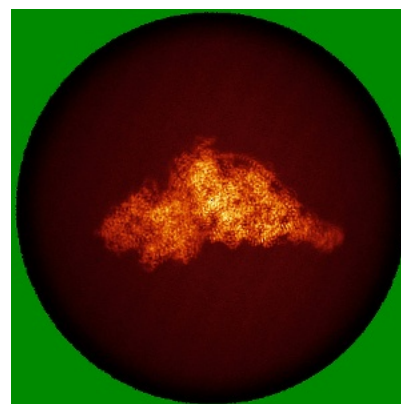
6.4.1 Primary map



X

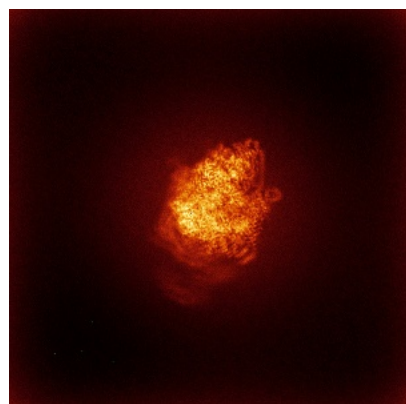


Y

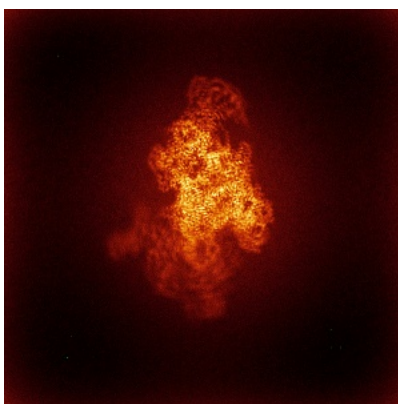


Z

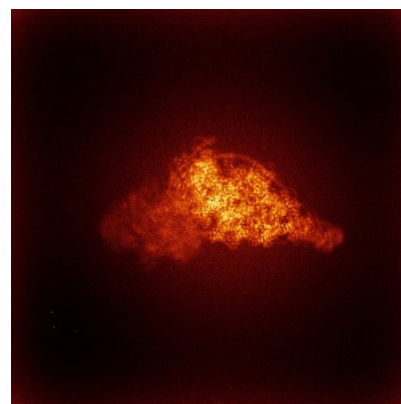
6.4.2 Raw map



X



Y

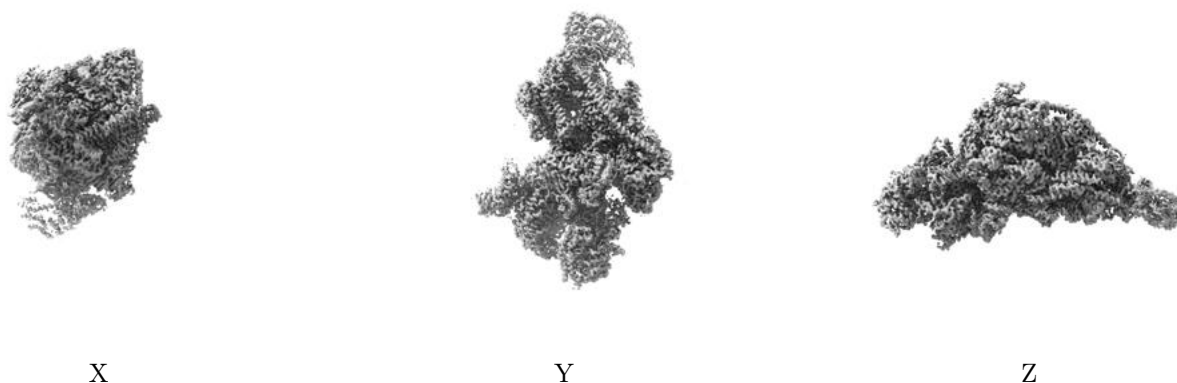


Z

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.

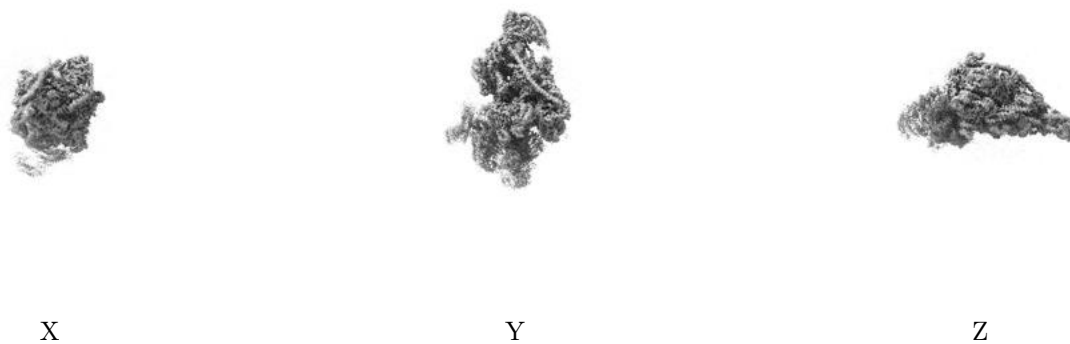
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.51. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

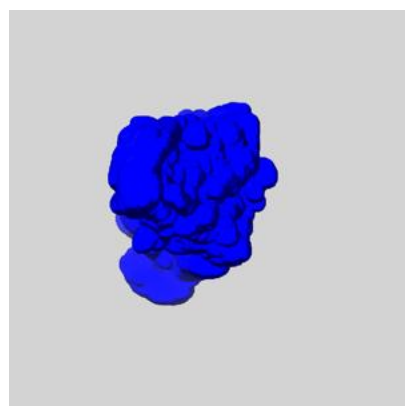
6.6 Mask visualisation [i](#)

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

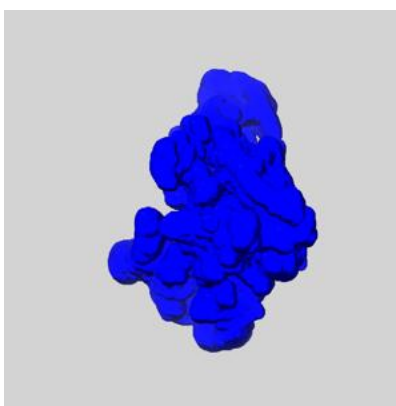
A mask typically either:

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

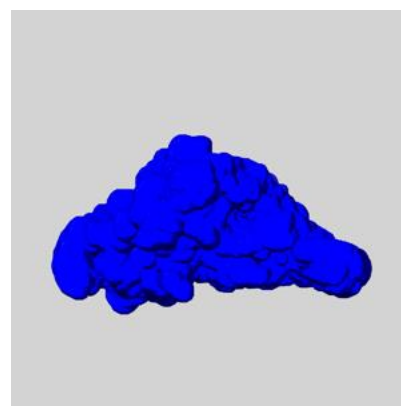
6.6.1 emd_52117_msk_1.map [i](#)



X



Y

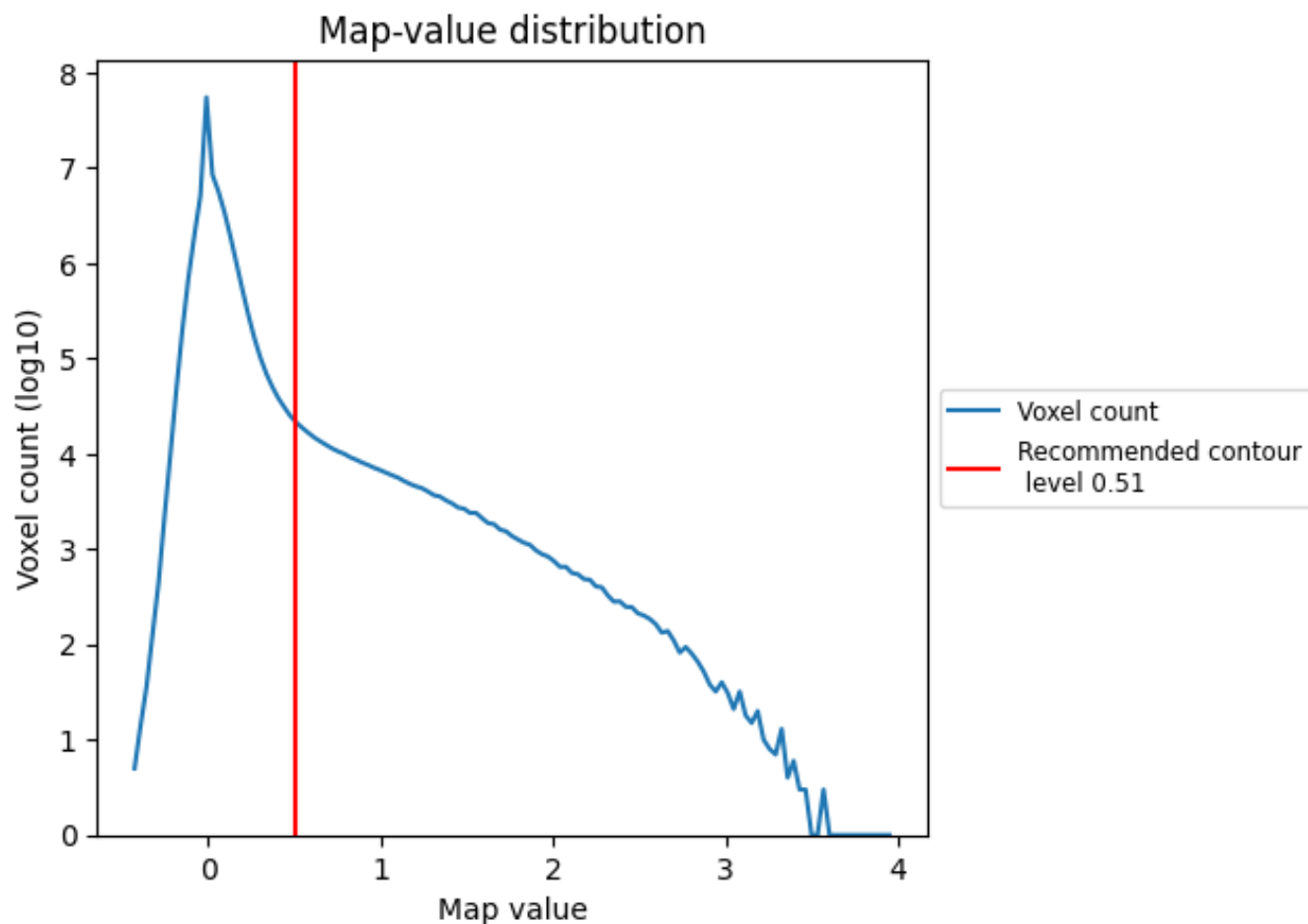


Z

7 Map analysis [i](#)

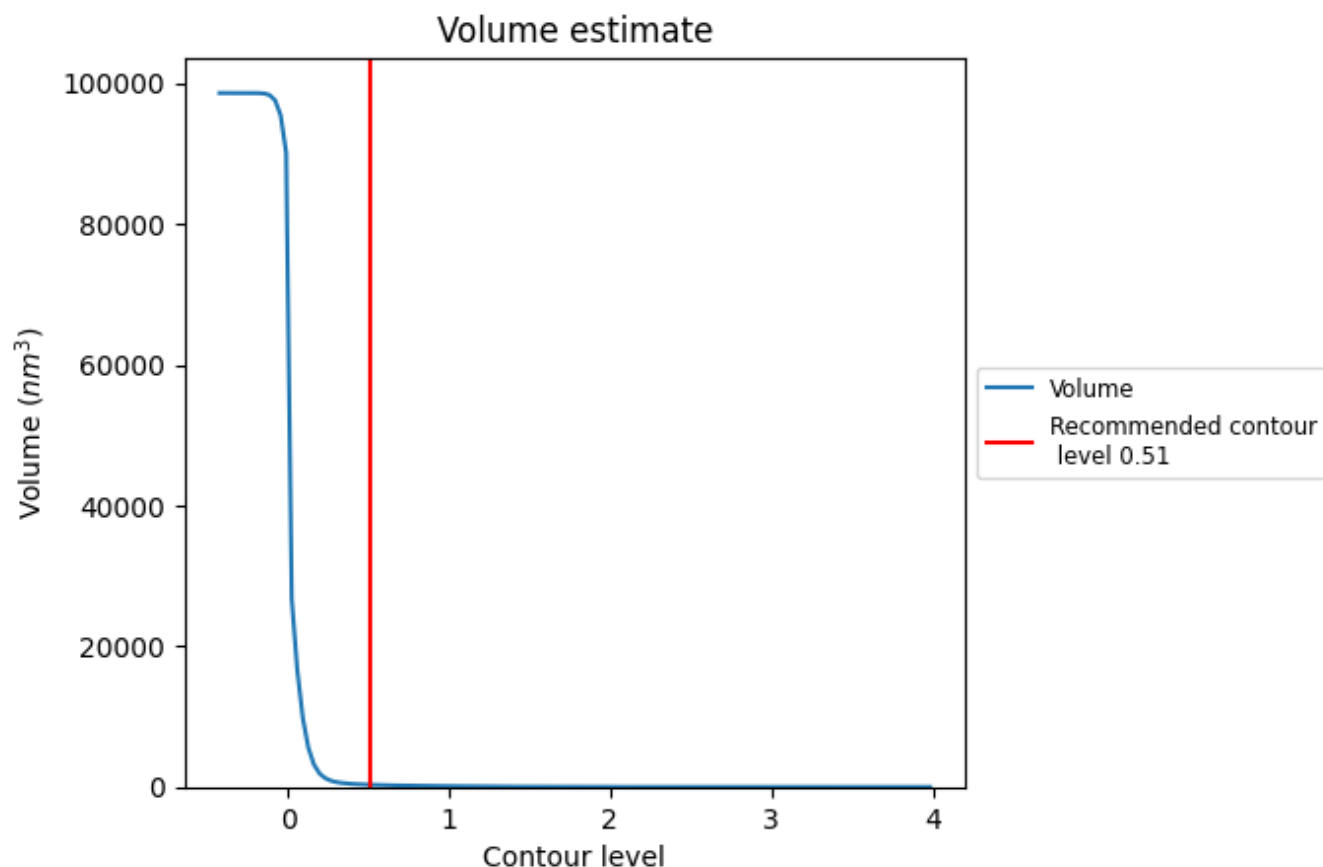
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

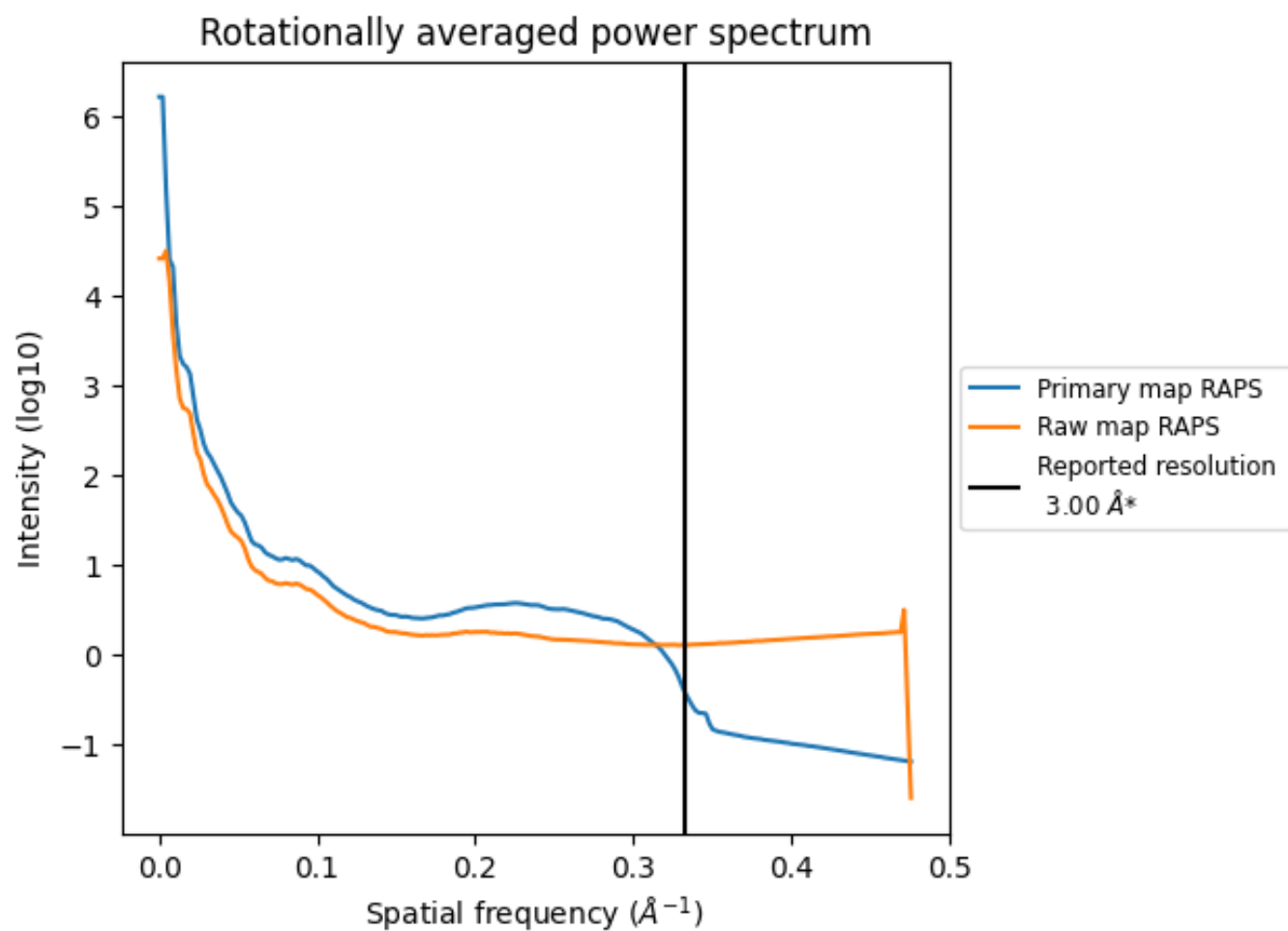
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 311 nm^3 ; this corresponds to an approximate mass of 281 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

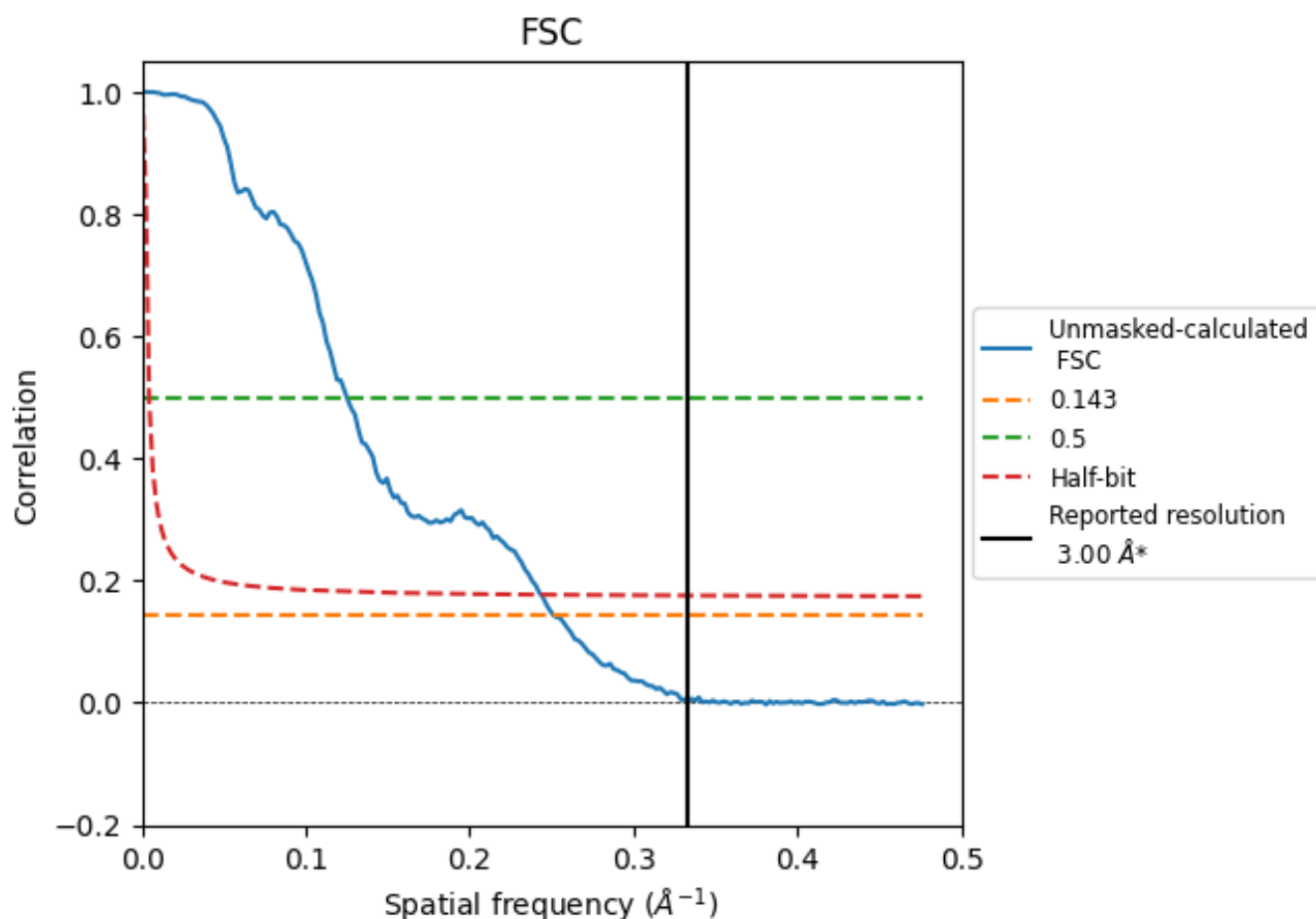


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

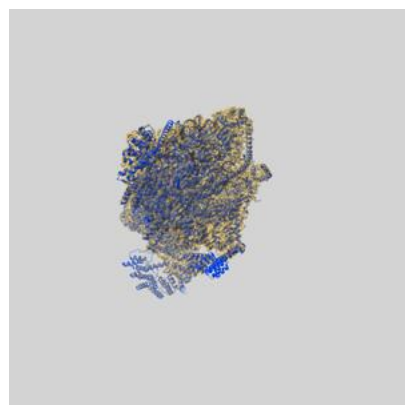
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	8.01	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.0 by more than 10 %

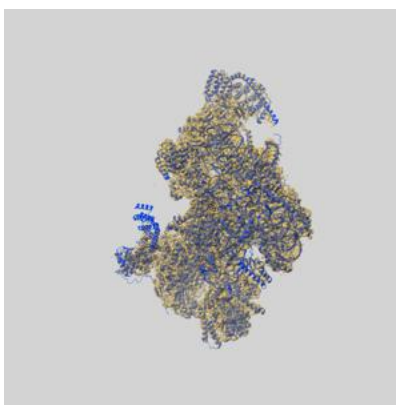
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52117 and PDB model 9HFM. Per-residue inclusion information can be found in section [3](#) on page [13](#).

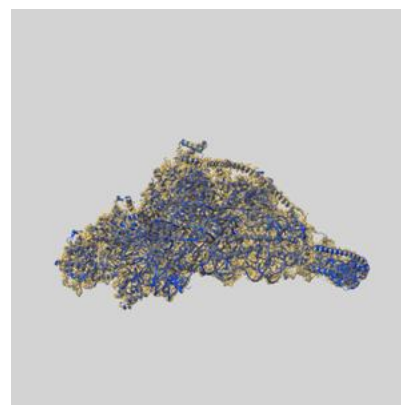
9.1 Map-model overlay [i](#)



X



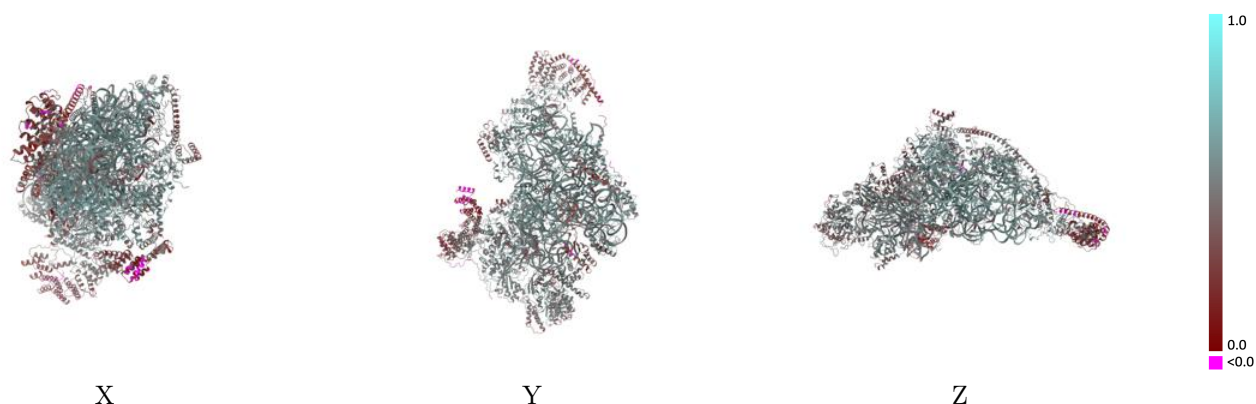
Y



Z

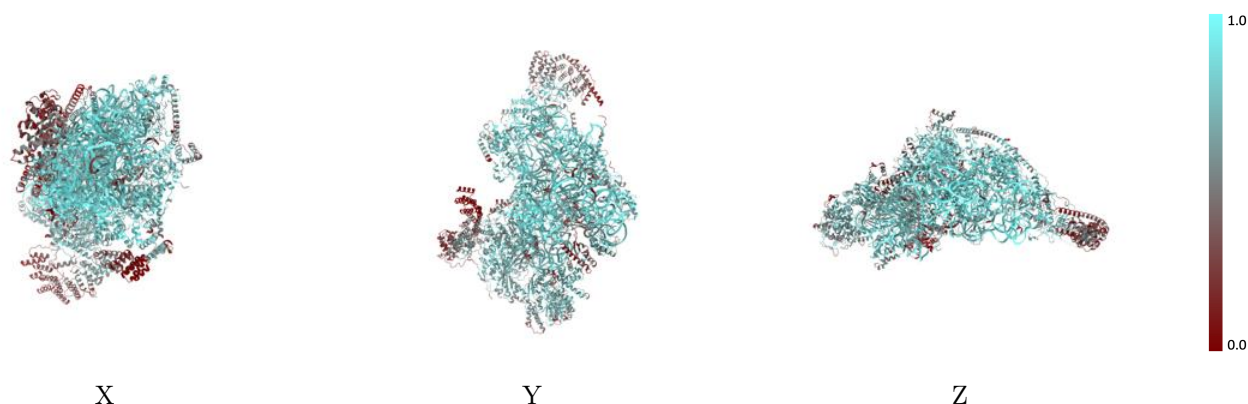
The images above show the 3D surface view of the map at the recommended contour level 0.51 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



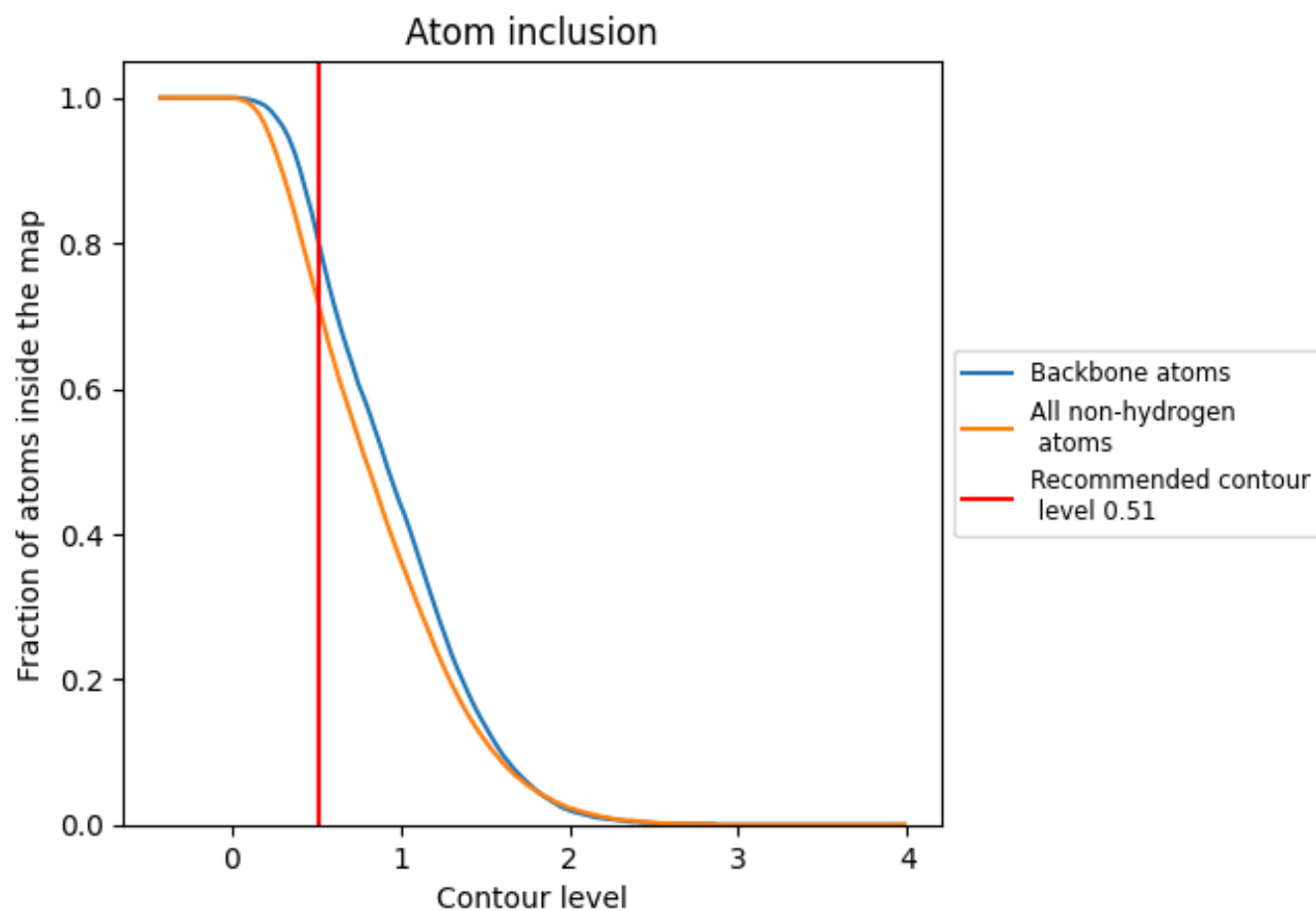
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.51).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.51) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.4930
0	 0.6820	 0.4940
1	 0.6570	 0.4740
2	 0.4170	 0.4230
3	 0.7170	 0.5240
4	 0.3310	 0.3030
8	 0.3040	 0.3070
A	 0.8860	 0.5520
B	 0.8680	 0.5580
C	 0.7620	 0.5500
D	 0.7080	 0.5190
E	 0.7040	 0.5150
F	 0.6110	 0.4600
G	 0.7040	 0.4880
H	 0.7120	 0.5150
I	 0.6840	 0.4870
J	 0.7600	 0.5410
K	 0.8090	 0.5430
L	 0.7340	 0.4960
M	 0.8650	 0.5770
N	 0.8460	 0.5670
O	 0.8370	 0.5600
P	 0.8050	 0.5410
Q	 0.7860	 0.5450
R	 0.7670	 0.5070
S	 0.6870	 0.4790
T	 0.8150	 0.5440
U	 0.7080	 0.4770
V	 0.3500	 0.3000
W	 0.7970	 0.5370
X	 0.6540	 0.4710
Y	 0.5390	 0.4070
Z	 0.6510	 0.4850

