



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 10:25 PM UTC

PDB ID : 9G5B / pdb_00009g5b
EMDB ID : EMD-51083
Title : Assembly intermediate of human mitochondrial ribosome small subunit (State A)
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 : 7PO1, 8CSR, 8CSP

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

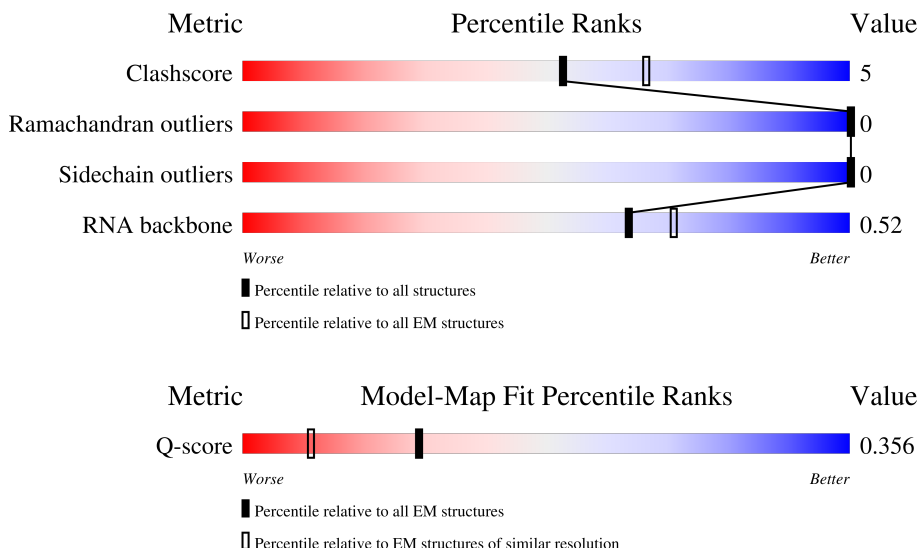
1 Overall quality at a glance i

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 $\leq 5\%$. 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	9% 87% 11%
2	1	323	9% 72% 13% 15%
3	4	689	29% 72% 13% 14%

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Mol	Chain	Length	Quality of chain
4	9	706	
5	A	955	
6	B	296	
7	C	167	
8	D	430	
9	E	125	
10	F	242	
11	G	396	
12	H	201	
13	I	194	
14	J	138	
15	K	128	
16	L	257	
17	M	137	
18	N	130	
19	O	258	
20	P	142	
21	Q	86	
22	R	360	
23	S	190	
24	T	173	
25	U	205	
26	V	414	
27	W	187	
28	X	398	

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Mol	Chain	Length	Quality of chain
29	Y	395	7%33%5%62%
30	Z	106	20%82%8%9%
31	a	343	6%30%68%
32	c	346	36%77%10%14%

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 68040 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 Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	592	Total	C	N	O	S	0	0
			4795	3070	812	885	28		

- Molecule 4 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	363	Total	C	N	O	S	0	0
			2885	1868	494	515	8		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	699	ASP	-	expression tag	UNP Q8NC60
9	700	TYR	-	expression tag	UNP Q8NC60
9	701	LYS	-	expression tag	UNP Q8NC60
9	702	ASP	-	expression tag	UNP Q8NC60
9	703	ASP	-	expression tag	UNP Q8NC60
9	704	ASP	-	expression tag	UNP Q8NC60
9	705	ASP	-	expression tag	UNP Q8NC60
9	706	LYS	-	expression tag	UNP Q8NC60

- Molecule 5 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	816	Total	C	N	O	P	0	0
			17344	7775	3133	5620	816		

- Molecule 6 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 7 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 8 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	331	Total	C	N	O	S	0	0
			2631	1651	496	471	13		

- Molecule 9 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 10 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	202	Total	C	N	O	S	0	0
			1666	1066	298	291	11		

- Molecule 11 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 12 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 13 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 14 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 15 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 16 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	156	Total	C	N	O	S	0	0
			1311	837	236	231	7		

- Molecule 17 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 18 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 19 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 20 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 21 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	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 22 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 23 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 24 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 25 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 26 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 27 is a protein called 28S ribosomal protein S28, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	349	Total	C	N	O	S	0	0
			2829	1810	496	512	11		

- Molecule 29 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 30 is a protein called 28S ribosomal protein S33, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	109	Total	C	N	O	S	0	0
			854	538	152	159	5		

- Molecule 32 is a protein called Dimethyladenosine transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	299	Total	C	N	O	S	0	0
			2417	1553	433	420	11		

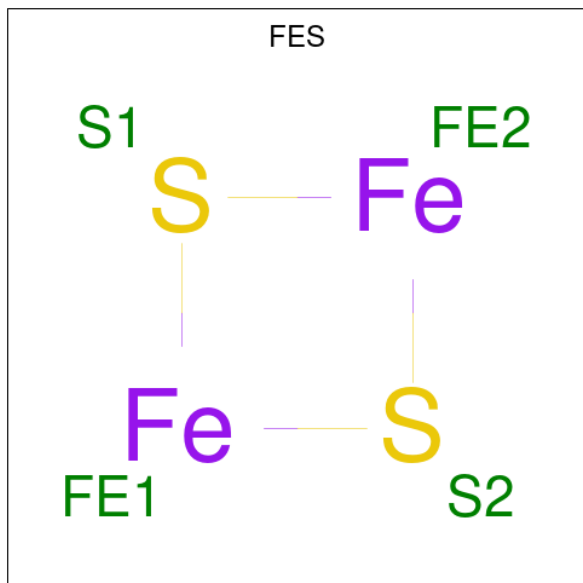
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	A	10	Total	Mg	0
			10	10	
33	B	1	Total	Mg	0
			1	1	
33	X	1	Total	Mg	0
			1	1	

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

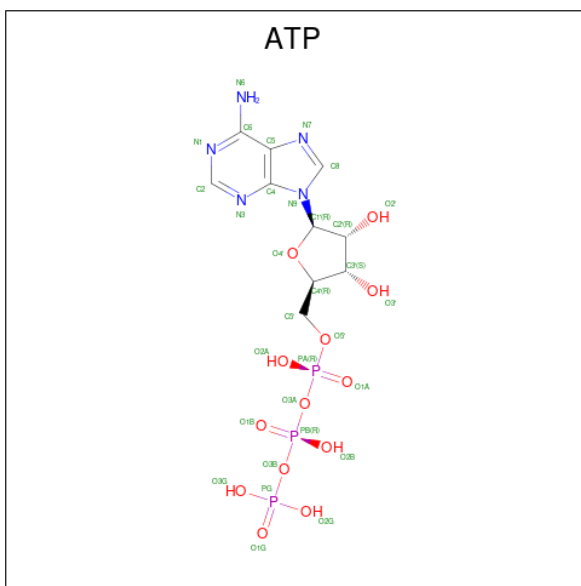
Mol	Chain	Residues	Atoms		AltConf
34	O	1	Total	Zn	0
			1	1	

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



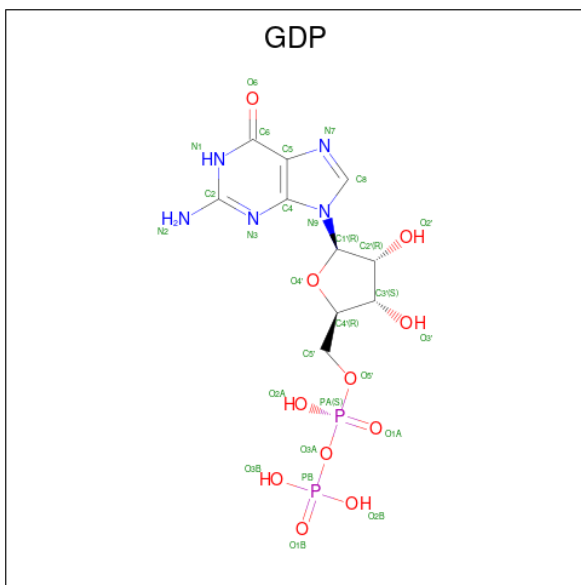
Mol	Chain	Residues	Atoms			AltConf
35	P	1	Total	Fe	S	0
			4	2	2	
35	T	1	Total	Fe	S	0
			4	2	2	

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



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

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

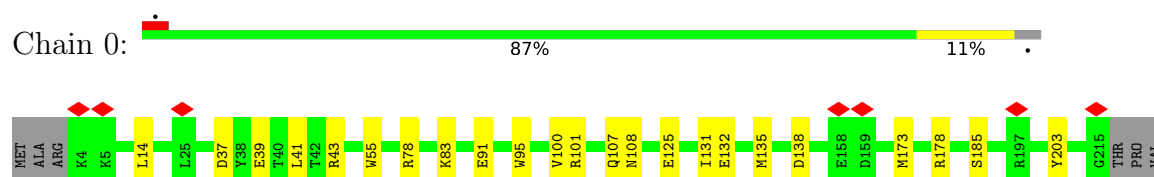


Mol	Chain	Residues	Atoms					AltConf
37	X	1	Total	C	N	O	P	0
			28	10	5	11	2	

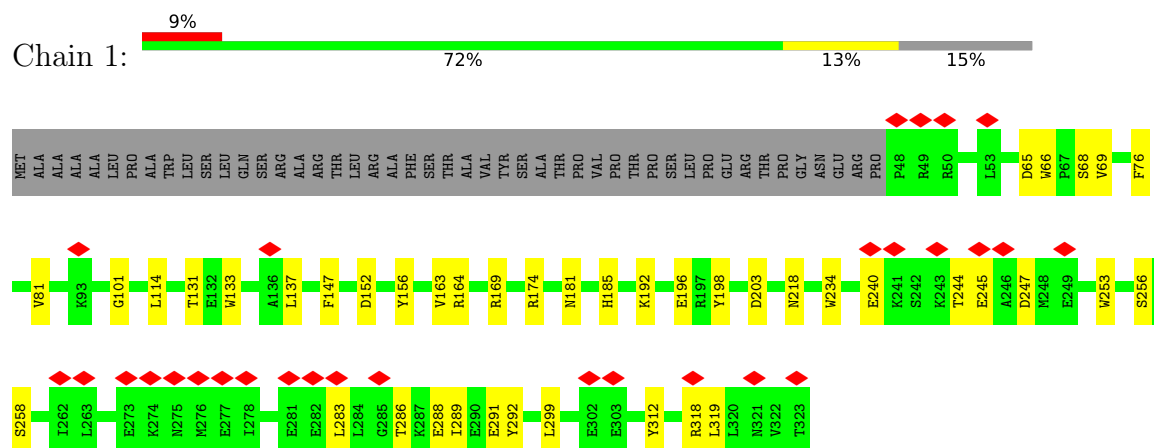
3 Residue-property plots

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.

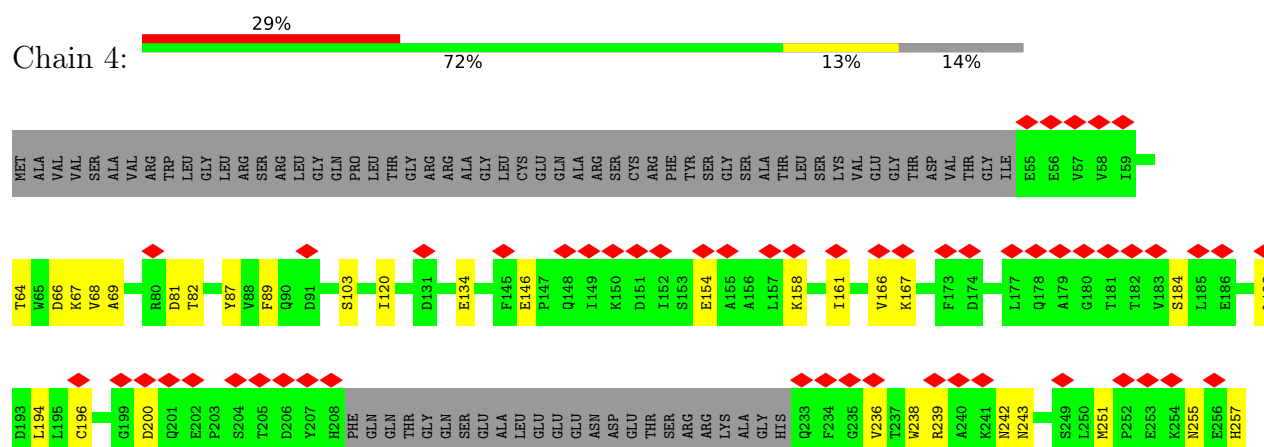
- Molecule 1: 28S ribosomal protein S34, mitochondrial

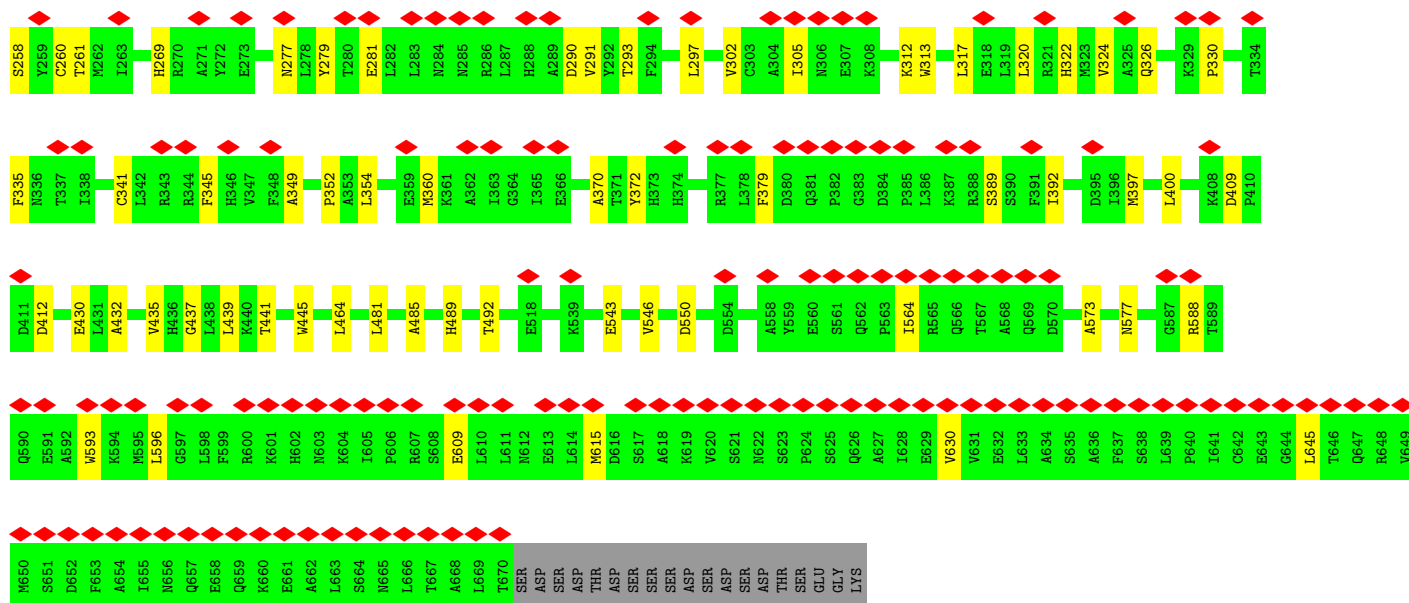


- Molecule 2: 28S ribosomal protein S35, mitochondrial

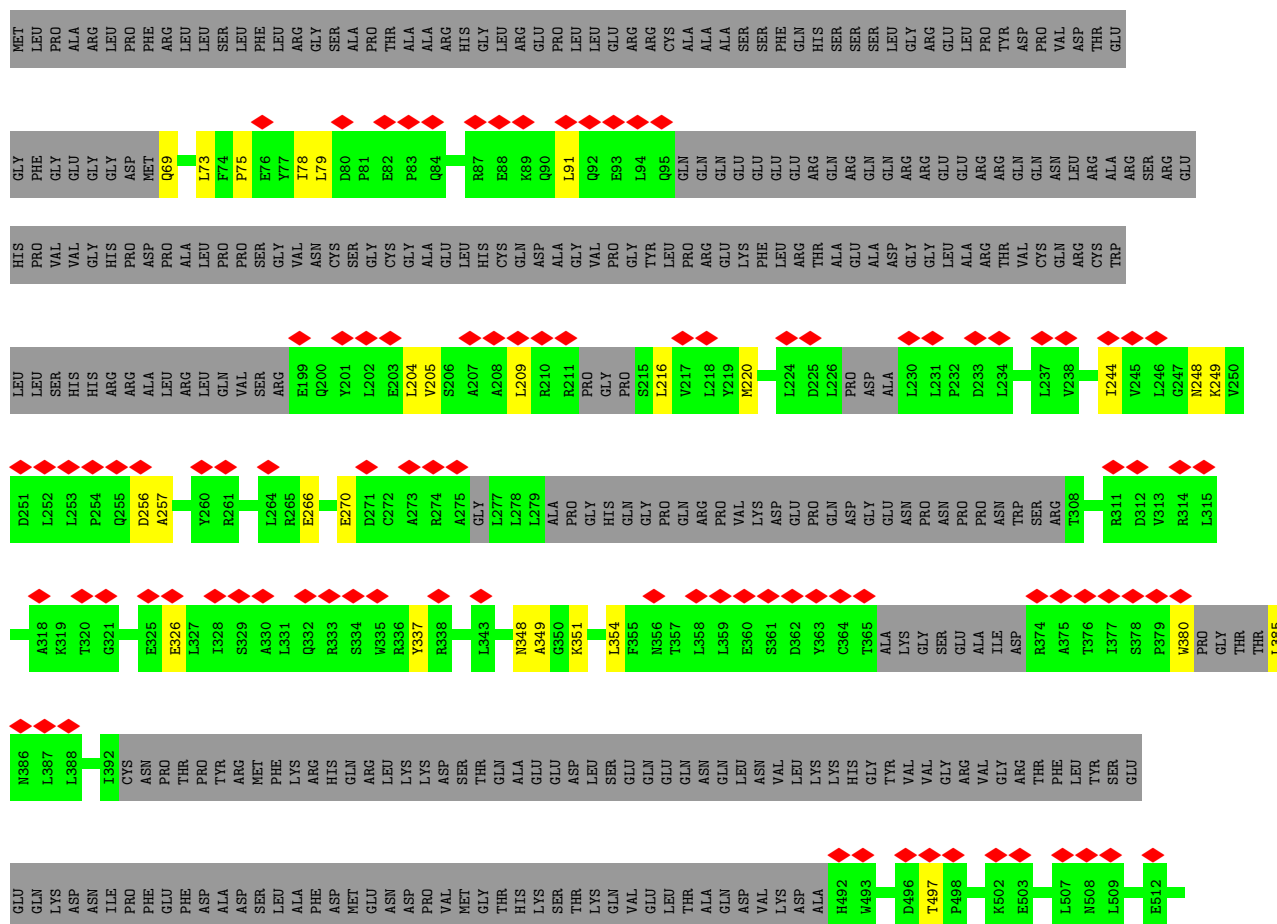
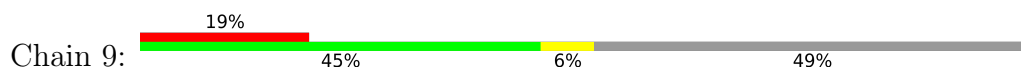


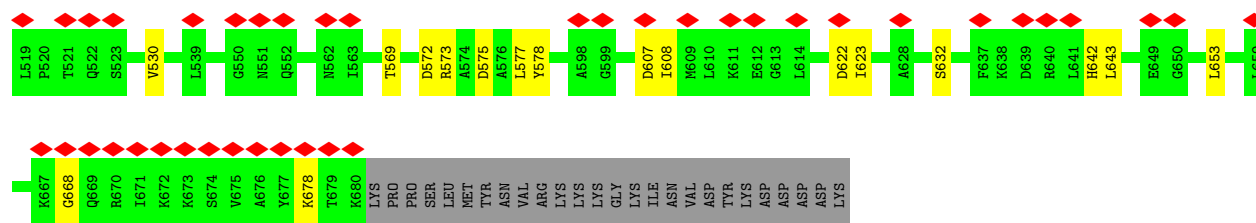
- Molecule 3: Pentatricopeptide repeat domain-containing protein 3, mitochondrial





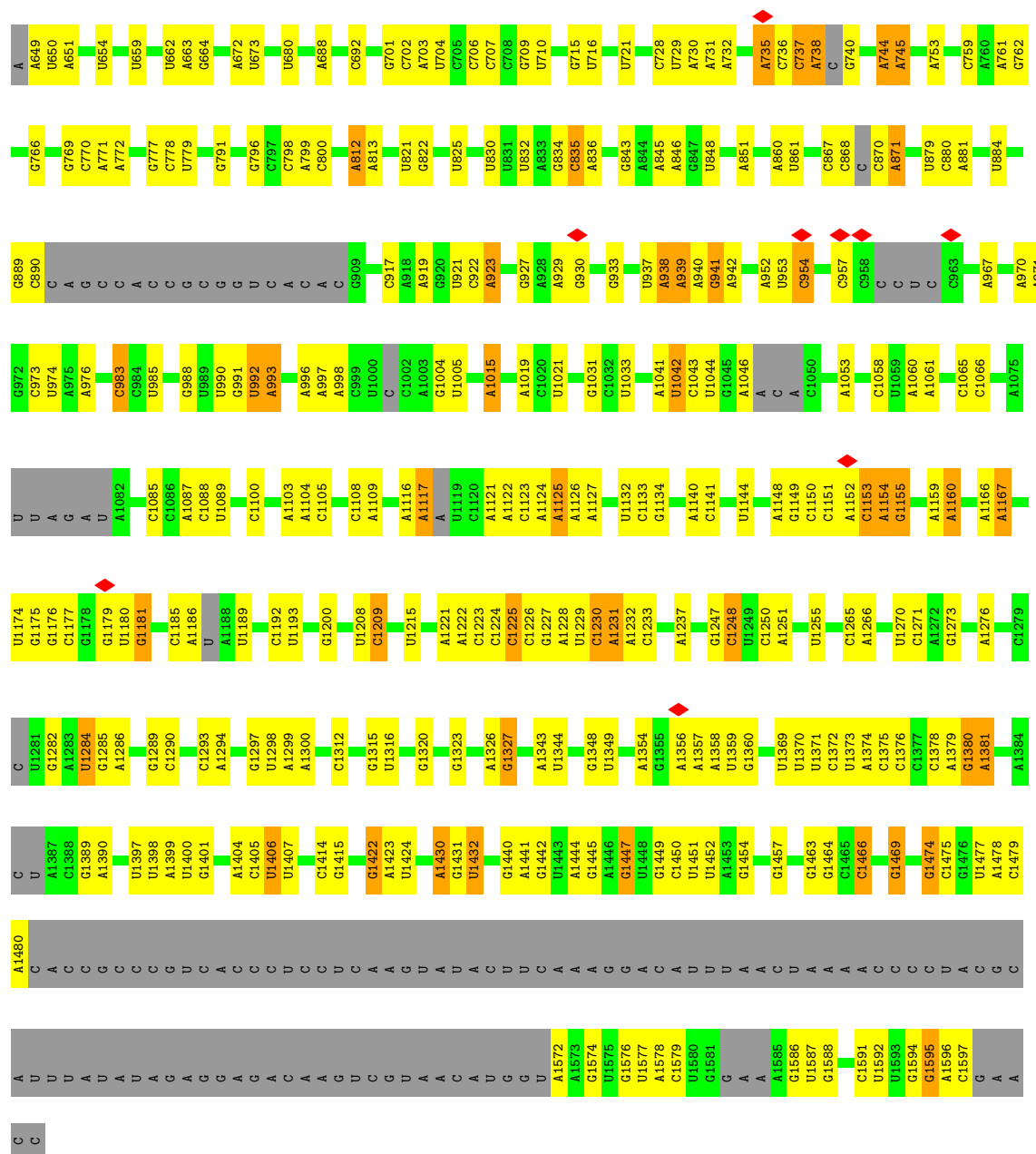
• Molecule 4: Nitric oxide-associated protein 1





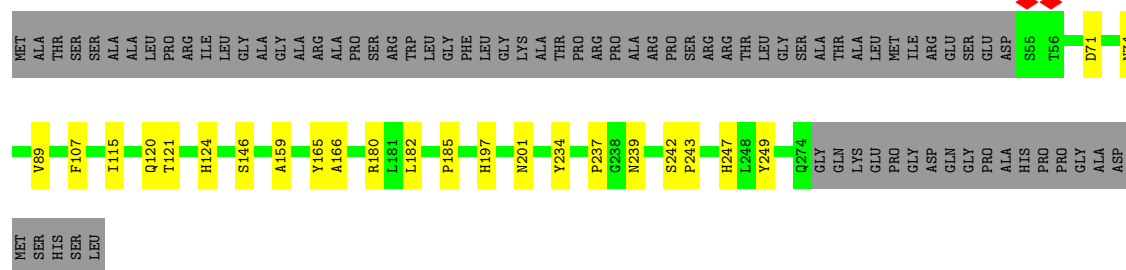
• Molecule 5: 12S mitochondrial rRNA

Chain A: 53% 28% 5% 15%



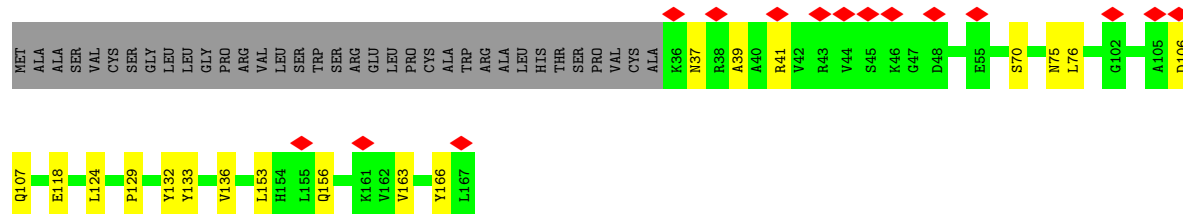
• Molecule 6: 28S ribosomal protein S2, mitochondrial

Chain B: 



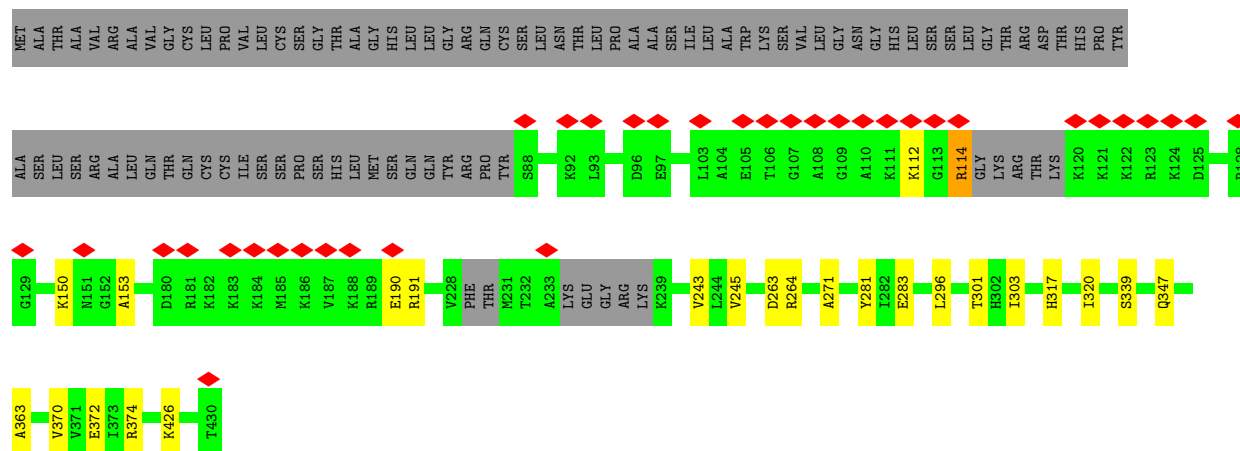
- Molecule 7: 28S ribosomal protein S24, mitochondrial

Chain C: 



- Molecule 8: 28S ribosomal protein S5, mitochondrial

Chain D: 

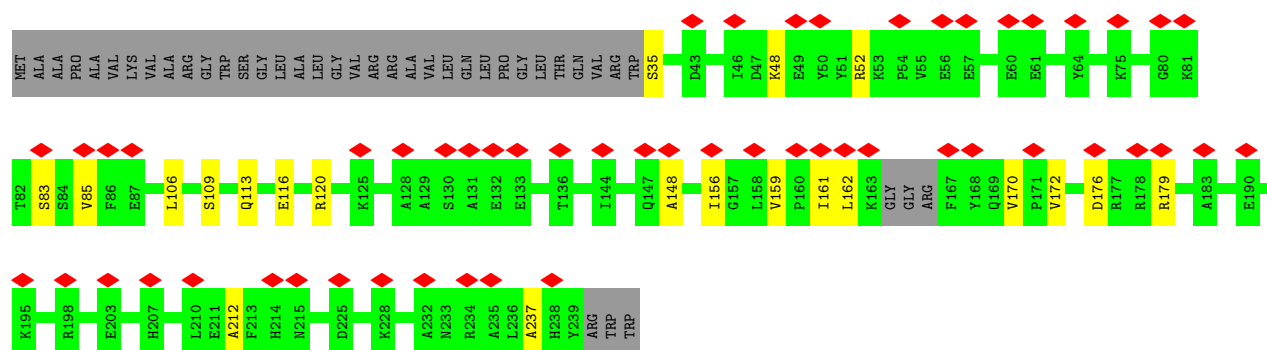
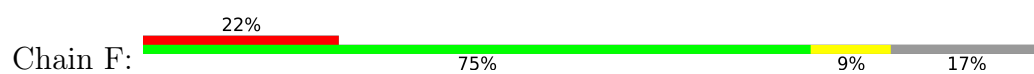


- Molecule 9: 28S ribosomal protein S6, mitochondrial

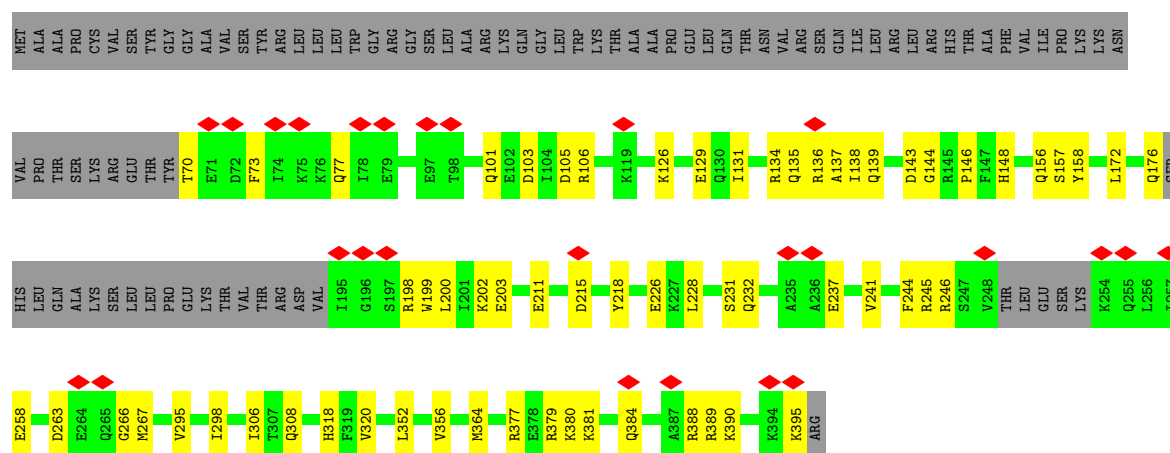
Chain E: 



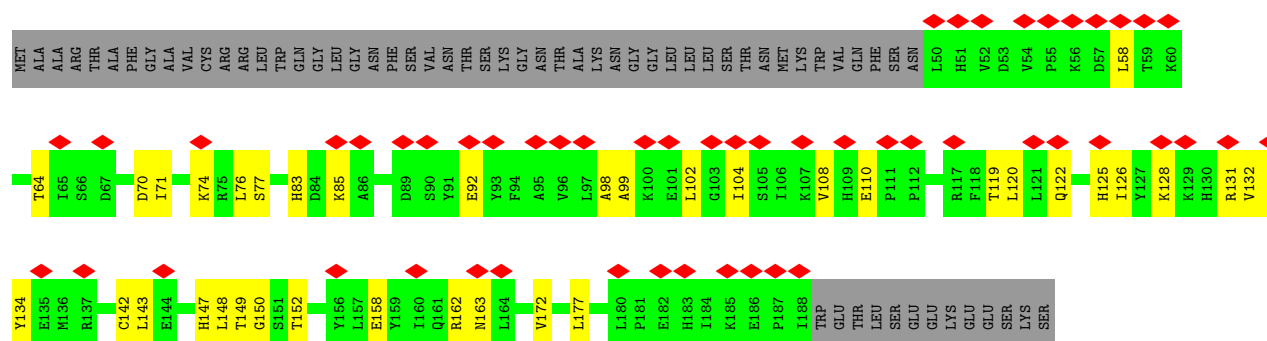
- Molecule 10: 28S ribosomal protein S7, mitochondrial



• Molecule 11: 28S ribosomal protein S9, mitochondrial



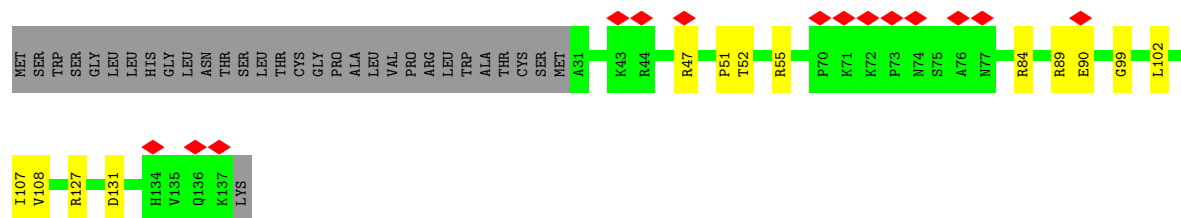
• Molecule 12: 28S ribosomal protein S10, mitochondrial



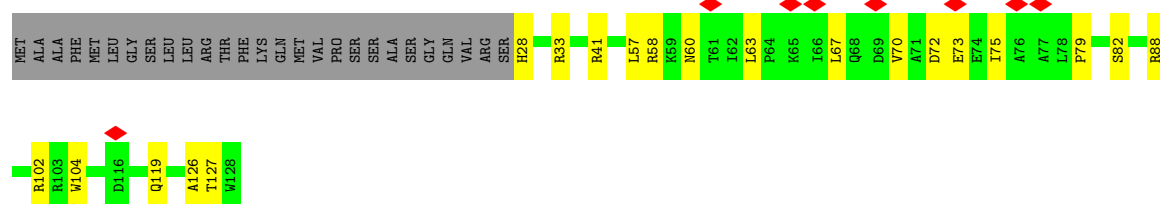
• Molecule 13: 28S ribosomal protein S11, mitochondrial



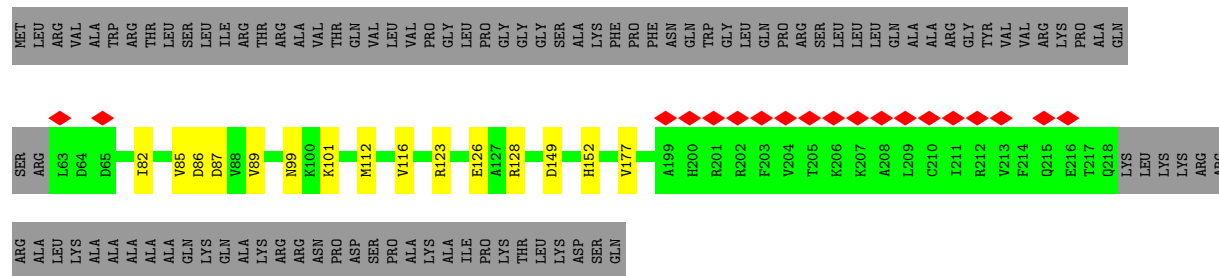
- Molecule 14: 28S ribosomal protein S12, mitochondrial



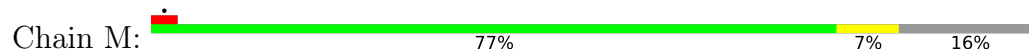
- Molecule 15: 28S ribosomal protein S14, mitochondrial



- Molecule 16: 28S ribosomal protein S15, mitochondrial



- Molecule 17: 28S ribosomal protein S16, mitochondrial



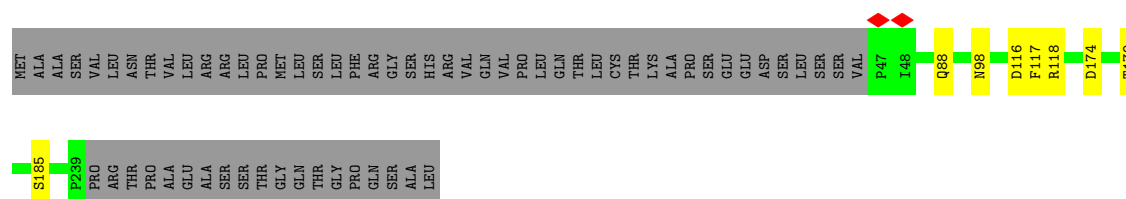
- Molecule 18: 28S ribosomal protein S17, mitochondrial

Chain N: 



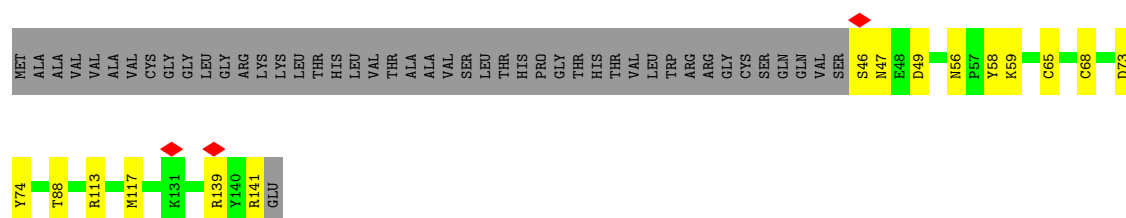
- Molecule 19: 28S ribosomal protein S18b, mitochondrial

Chain O: 

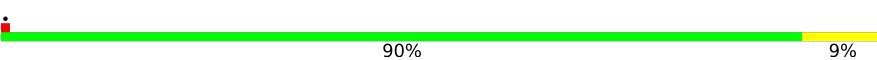


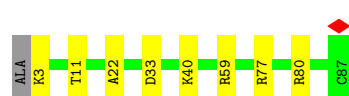
- Molecule 20: 28S ribosomal protein S18c, mitochondrial

Chain P: 



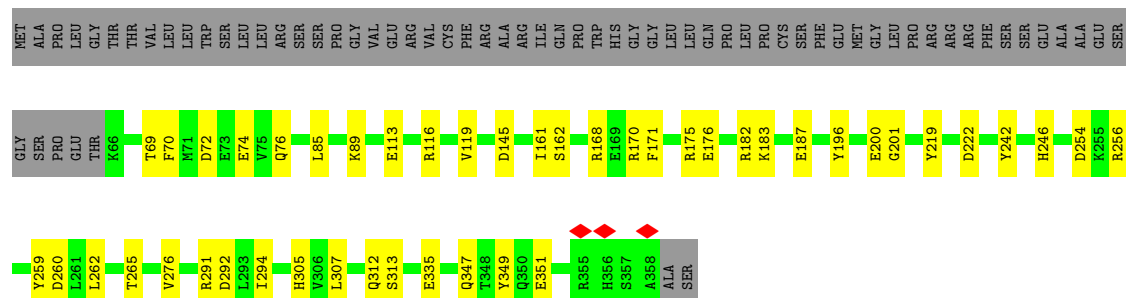
- Molecule 21: 28S ribosomal protein S21, mitochondrial

Chain Q: 

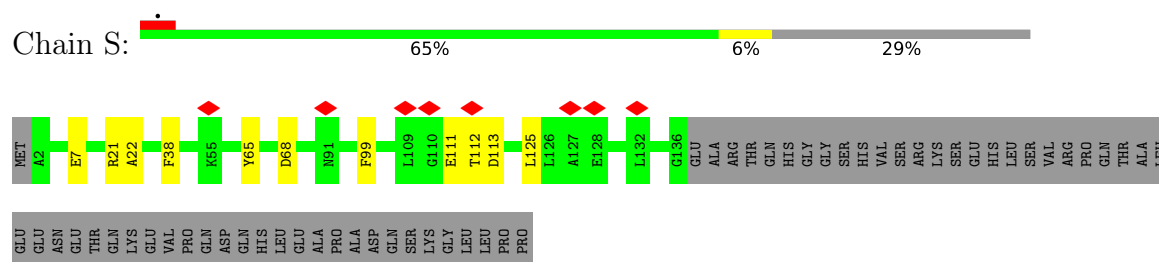


- Molecule 22: 28S ribosomal protein S22, mitochondrial

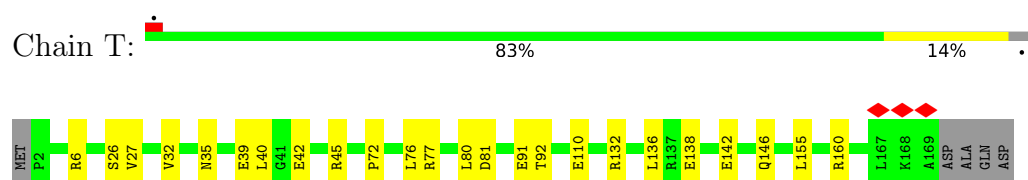
Chain R: 



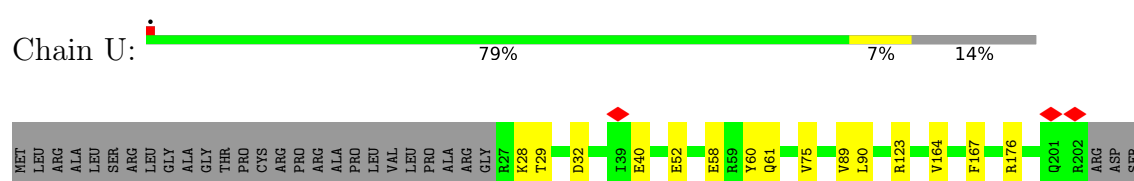
- Molecule 23: 28S ribosomal protein S23, mitochondrial



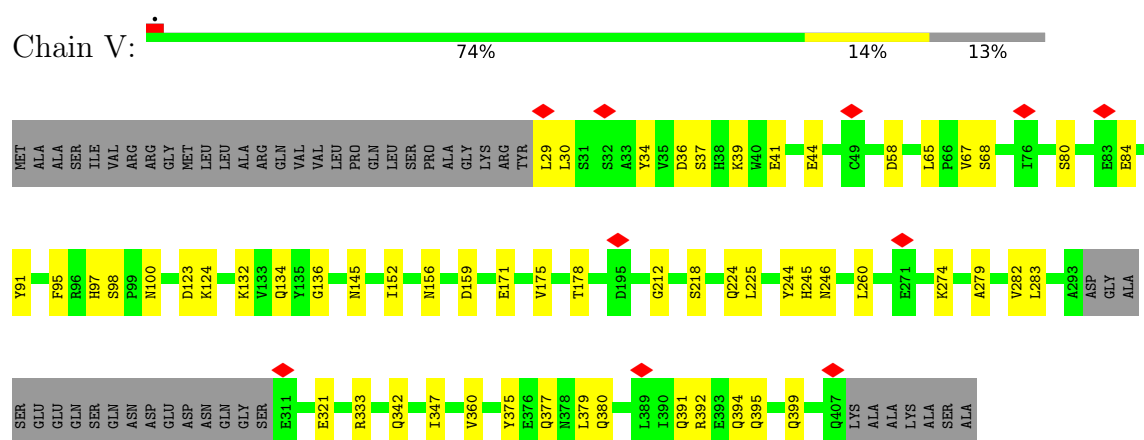
- Molecule 24: 28S ribosomal protein S25, mitochondrial



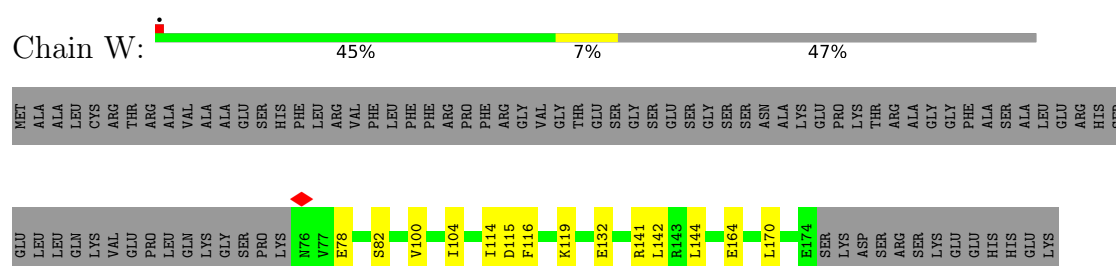
- Molecule 25: 28S ribosomal protein S26, mitochondrial



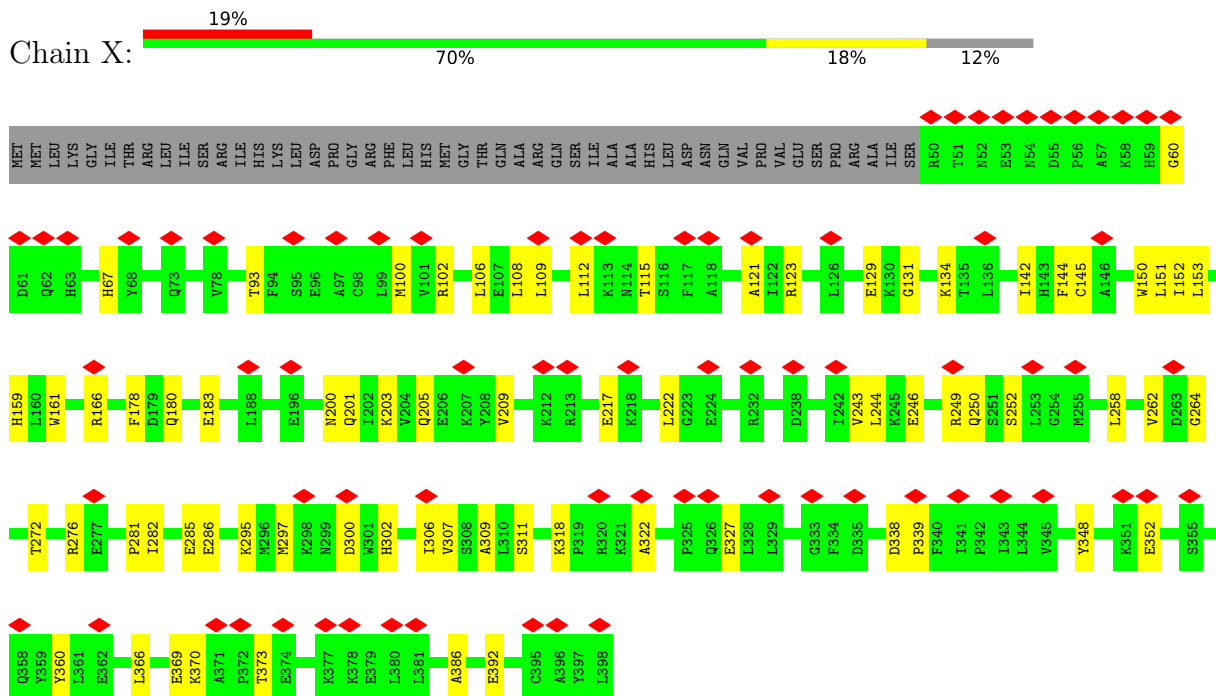
- Molecule 26: 28S ribosomal protein S27, mitochondrial



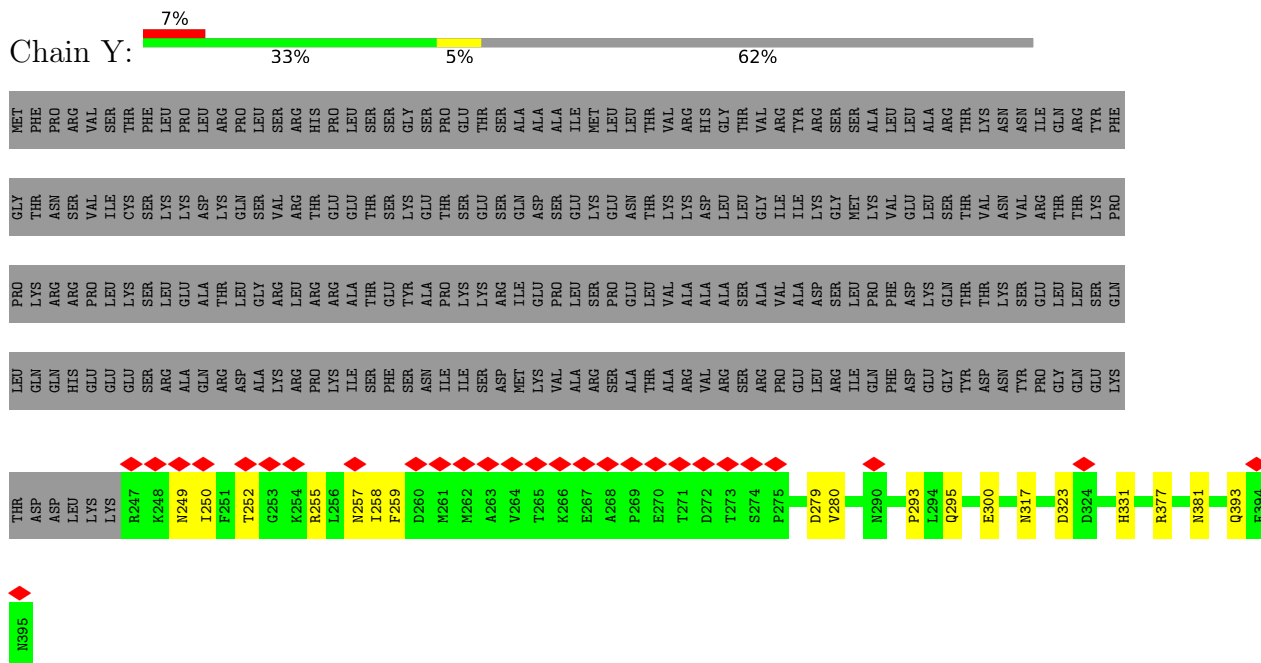
- Molecule 27: 28S ribosomal protein S28, mitochondrial



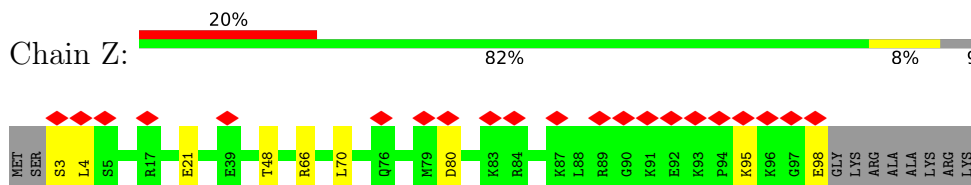
Chain X:

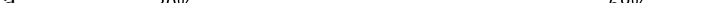


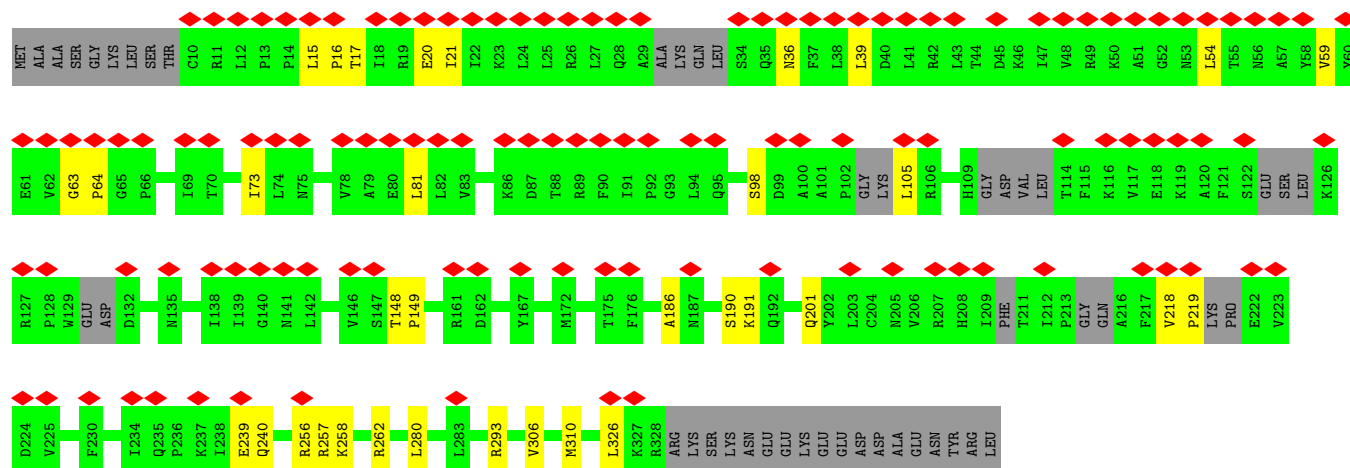
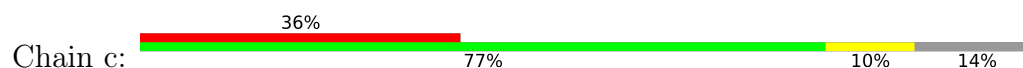
Chain Y:



Chain Z:



- Chain a: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36440	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	1.723	Depositor
Minimum map value	-0.318	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.296	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, ATP, MG, ZN, FES

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	0.18	0/1811	0.26	0/2452
2	1	0.14	0/2285	0.25	0/3090
3	4	0.14	0/4904	0.25	0/6636
4	9	0.14	0/2942	0.29	0/3990
5	A	0.21	0/19393	0.26	0/30167
6	B	0.21	0/1832	0.26	0/2480
7	C	0.18	0/1113	0.28	0/1505
8	D	0.20	0/2679	0.29	0/3585
9	E	0.17	0/989	0.28	0/1335
10	F	0.15	0/1703	0.27	0/2286
11	G	0.16	0/2544	0.27	0/3408
12	H	0.16	0/1162	0.34	0/1575
13	I	0.15	0/1039	0.26	0/1400
14	J	0.17	0/845	0.29	0/1137
15	K	0.16	0/880	0.26	0/1182
16	L	0.17	0/1335	0.24	0/1789
17	M	0.23	0/934	0.27	0/1255
18	N	0.19	0/877	0.25	0/1187
19	O	0.20	0/1648	0.25	0/2243
20	P	0.17	0/788	0.26	0/1058
21	Q	0.17	0/748	0.25	0/994
22	R	0.20	0/2440	0.26	0/3295
23	S	0.17	0/1138	0.24	0/1533
24	T	0.20	0/1402	0.26	0/1883
25	U	0.17	0/1510	0.24	0/2025
26	V	0.14	0/3030	0.25	0/4093
27	W	0.17	0/795	0.24	0/1071
28	X	0.15	0/2901	0.28	0/3928
29	Y	0.18	0/1280	0.30	0/1725
30	Z	0.15	0/828	0.23	0/1104
31	a	0.15	0/868	0.28	0/1179
32	c	0.15	0/2463	0.32	0/3324

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.18	0/71106	0.27	0/99914

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	114	ARG	Sidechain

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	17	0
2	1	2238	0	2269	30	0
3	4	4795	0	4796	59	0
4	9	2885	0	2976	29	0
5	A	17344	0	8813	180	0
6	B	1789	0	1781	15	0
7	C	1083	0	1088	13	0
8	D	2631	0	2688	17	0
9	E	972	0	1000	9	0
10	F	1666	0	1716	15	0
11	G	2491	0	2473	45	0
12	H	1138	0	1173	36	0
13	I	1019	0	1059	18	0
14	J	829	0	874	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	862	0	885	17	0
16	L	1311	0	1368	8	0
17	M	913	0	943	9	0
18	N	859	0	922	8	0
19	O	1592	0	1557	7	0
20	P	771	0	800	11	0
21	Q	736	0	749	10	0
22	R	2393	0	2415	28	0
23	S	1111	0	1115	8	0
24	T	1371	0	1393	18	0
25	U	1488	0	1499	11	0
26	V	2969	0	2961	37	0
27	W	783	0	797	10	0
28	X	2829	0	2821	47	0
29	Y	1246	0	1197	14	0
30	Z	810	0	824	6	0
31	a	854	0	866	8	0
32	c	2417	0	2495	29	0
33	A	10	0	0	0	0
33	B	1	0	0	0	0
33	X	1	0	0	0	0
34	O	1	0	0	0	0
35	P	4	0	0	0	0
35	T	4	0	0	0	0
36	X	31	0	12	2	0
37	X	28	0	12	1	0
All	All	68040	0	60110	674	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 5.

All (674) 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)
28:X:295:LYS:NZ	37:X:502:GDP:O1A	1.93	1.02
5:A:1454:G:OP2	11:G:377:ARG:NH1	2.06	0.89
3:4:260:CYS:SG	3:4:293:THR:OG1	2.33	0.87
5:A:1381:A:O3'	28:X:166:ARG:NH2	2.07	0.86
5:A:1154:A:OP2	32:c:293:ARG:NH2	2.10	0.85
5:A:1053:A:N1	5:A:1100:C:O2'	2.07	0.84
5:A:1415:G:OP2	5:A:1415:G:N2	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:272:THR:OG1	28:X:282:ILE:O	1.98	0.82
28:X:200:ASN:O	28:X:203:LYS:NZ	2.13	0.82
5:A:1294:A:OP1	6:B:201:ASN:ND2	2.12	0.82
24:T:155:LEU:O	24:T:160:ARG:NH1	2.14	0.81
32:c:17:THR:OG1	32:c:20:GLU:OE1	1.96	0.81
3:4:64:THR:OG1	12:H:64:THR:OG1	2.00	0.80
15:K:79:PRO:O	15:K:82:SER:OG	1.98	0.80
26:V:80:SER:N	26:V:84:GLU:OE1	2.15	0.79
5:A:1021:U:O4	21:Q:59:ARG:NH1	2.16	0.78
12:H:77:SER:OG	12:H:142:CYS:SG	2.42	0.78
28:X:276:ARG:NH1	28:X:281:PRO:O	2.16	0.77
32:c:191:LYS:O	32:c:256:ARG:NH2	2.18	0.77
12:H:92:GLU:CD	12:H:108:VAL:HG11	2.10	0.77
28:X:370:LYS:O	28:X:373:THR:OG1	2.03	0.77
5:A:927:G:OP1	14:J:47:ARG:NH1	2.17	0.76
22:R:254:ASP:OD1	22:R:259:TYR:OH	2.01	0.76
5:A:1224:C:N4	11:G:395:LYS:O	2.17	0.76
3:4:200:ASP:OD2	3:4:243:ASN:N	2.19	0.76
23:S:65:TYR:N	23:S:68:ASP:OD2	2.20	0.75
32:c:190:SER:O	32:c:293:ARG:NH1	2.20	0.75
2:1:286:THR:OG1	2:1:288:GLU:OE1	2.05	0.75
3:4:260:CYS:HG	3:4:293:THR:HG1	1.35	0.75
15:K:57:LEU:O	15:K:60:ASN:ND2	2.20	0.74
5:A:952:A:N3	5:A:954:C:N4	2.36	0.74
27:W:132:GLU:N	27:W:132:GLU:OE1	2.21	0.73
2:1:137:LEU:HD12	2:1:137:LEU:O	1.87	0.73
2:1:196:GLU:N	2:1:196:GLU:OE1	2.20	0.73
1:0:39:GLU:N	1:0:39:GLU:OE1	2.21	0.73
1:0:178:ARG:NH2	1:0:185:SER:O	2.21	0.73
28:X:205:GLN:N	28:X:246:GLU:OE2	2.22	0.72
5:A:1124:A:N6	5:A:1127:A:OP1	2.23	0.72
3:4:573:ALA:O	3:4:577:ASN:ND2	2.23	0.72
14:J:84:ARG:NH1	14:J:90:GLU:OE2	2.22	0.72
6:B:180:ARG:NH1	6:B:185:PRO:O	2.23	0.72
5:A:812:A:O2'	5:A:813:A:O4'	2.05	0.71
5:A:744:A:O2'	5:A:745:A:O5'	2.07	0.71
2:1:65:ASP:OD2	2:1:68:SER:OG	2.04	0.71
27:W:78:GLU:N	27:W:78:GLU:OE1	2.24	0.70
5:A:1033:U:O2'	9:E:93:ILE:O	2.08	0.70
4:9:205:VAL:HG12	4:9:209:LEU:HD13	1.72	0.70
26:V:218:SER:OG	26:V:274:LYS:O	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:58:ASP:OD1	26:V:91:TYR:OH	2.05	0.70
29:Y:323:ASP:OD2	29:Y:331:HIS:NE2	2.24	0.70
32:c:36:ASN:HD22	32:c:219:PRO:HB2	1.56	0.70
23:S:7:GLU:N	23:S:7:GLU:OE1	2.25	0.69
5:A:941:G:O2'	5:A:1109:A:OP2	2.09	0.69
5:A:1389:G:O6	5:A:1415:G:O2'	2.09	0.69
4:9:572:ASP:OD1	4:9:573:ARG:N	2.26	0.69
22:R:200:GLU:OE1	22:R:201:GLY:N	2.26	0.69
5:A:1422:G:O2'	5:A:1423:A:O4'	2.10	0.69
5:A:1237:A:O4'	15:K:33:ARG:NH2	2.25	0.69
13:I:71:SER:O	13:I:74:ARG:NH1	2.26	0.69
5:A:702:C:OP1	5:A:848:U:O2'	2.11	0.68
5:A:1289:G:O2'	5:A:1297:G:OP2	2.07	0.68
28:X:285:GLU:OE1	28:X:285:GLU:N	2.26	0.68
20:P:56:ASN:OD1	20:P:59:LYS:N	2.25	0.68
1:0:91:GLU:OE1	1:0:91:GLU:N	2.27	0.68
11:G:103:ASP:OD1	11:G:106:ARG:NH2	2.26	0.68
29:Y:255:ARG:O	29:Y:257:ASN:ND2	2.27	0.68
4:9:249:LYS:NZ	4:9:348:ASN:O	2.26	0.68
11:G:203:GLU:N	11:G:203:GLU:OE1	2.27	0.67
28:X:200:ASN:OD1	28:X:201:GLN:N	2.27	0.67
5:A:1176:G:H1	5:A:1477:U:H3	1.40	0.67
26:V:36:ASP:OD2	26:V:39:LYS:NZ	2.20	0.67
5:A:1225:C:HO2'	5:A:1449:G:HO2'	1.43	0.67
12:H:158:GLU:OE2	12:H:162:ARG:NH2	2.27	0.67
11:G:200:LEU:O	11:G:218:TYR:OH	2.11	0.67
3:4:320:LEU:O	3:4:324:VAL:HG23	1.95	0.67
27:W:141:ARG:NH2	27:W:170:LEU:O	2.27	0.66
15:K:58:ARG:NE	15:K:72:ASP:OD1	2.25	0.66
5:A:798:C:OP1	17:M:10:LYS:N	2.28	0.66
5:A:1221:A:OP2	5:A:1222:A:O2'	2.13	0.66
10:F:116:GLU:OE2	10:F:120:ARG:NH2	2.26	0.66
5:A:843:G:N2	5:A:846:A:OP2	2.29	0.66
12:H:108:VAL:HG13	12:H:143:LEU:HD23	1.77	0.65
15:K:41:ARG:NH1	30:Z:48:THR:O	2.28	0.65
7:C:124:LEU:O	7:C:132:TYR:OH	2.13	0.65
12:H:71:ILE:O	12:H:150:GLY:N	2.29	0.65
2:1:164:ARG:NH2	3:4:134:GLU:OE1	2.30	0.65
3:4:409:ASP:N	3:4:412:ASP:OD2	2.29	0.64
6:B:71:ASP:OD1	6:B:74:ASN:N	2.30	0.64
21:Q:77:ARG:NH1	27:W:164:GLU:OE2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:145:ASP:OD2	22:R:175:ARG:NH1	2.28	0.64
28:X:318:LYS:NZ	28:X:327:GLU:O	2.30	0.64
5:A:1116:A:H61	5:A:1127:A:H2	1.44	0.64
5:A:1285:G:O2'	5:A:1286:A:O4'	2.09	0.64
11:G:263:ASP:OD1	11:G:267:MET:N	2.30	0.64
1:O:135:MET:SD	1:O:135:MET:N	2.70	0.64
25:U:40:GLU:N	25:U:40:GLU:OE1	2.31	0.64
12:H:92:GLU:OE2	12:H:108:VAL:HG11	1.97	0.63
22:R:69:THR:N	22:R:72:ASP:OD2	2.31	0.63
5:A:1431:G:O2'	5:A:1457:G:O6	2.12	0.63
5:A:654:U:O2'	5:A:1167:A:OP2	2.14	0.63
16:L:149:ASP:OD2	16:L:152:HIS:ND1	2.32	0.62
3:4:161:ILE:HD12	3:4:194:LEU:HD22	1.80	0.62
5:A:1159:A:O2'	5:A:1160:A:O4'	2.16	0.62
11:G:258:GLU:OE1	11:G:258:GLU:N	2.30	0.62
14:J:51:PRO:O	14:J:89:ARG:NH2	2.32	0.62
4:9:622:ASP:OD1	4:9:632:SER:OG	2.09	0.62
3:4:322:HIS:ND1	3:4:326:GLN:OE1	2.32	0.62
22:R:74:GLU:OE1	22:R:74:GLU:N	2.30	0.62
22:R:305:HIS:NE2	22:R:313:SER:OG	2.28	0.62
2:1:253:TRP:O	2:1:256:SER:OG	2.12	0.62
1:O:125:GLU:OE2	1:O:203:TYR:OH	2.14	0.62
12:H:126:ILE:O	12:H:128:LYS:N	2.32	0.62
5:A:1293:C:N4	21:Q:80:ARG:O	2.33	0.61
4:9:256:ASP:OD1	4:9:257:ALA:N	2.34	0.61
7:C:106:ASP:OD1	7:C:107:GLN:N	2.33	0.61
14:J:107:ILE:N	14:J:131:ASP:OD2	2.32	0.61
20:P:73:ASP:OD1	20:P:74:TYR:N	2.34	0.61
9:E:100:GLN:N	9:E:100:GLN:OE1	2.32	0.61
5:A:1248:C:O2	15:K:28:HIS:N	2.34	0.61
5:A:769:G:OP2	18:N:73:ARG:NH2	2.33	0.61
32:c:280:LEU:HB2	32:c:310:MET:HE1	1.82	0.61
11:G:198:ARG:NH1	11:G:199:TRP:O	2.30	0.60
5:A:1104:A:OP1	5:A:1591:C:O2'	2.17	0.60
19:O:116:ASP:OD1	19:O:117:PHE:N	2.34	0.60
24:T:91:GLU:OE2	25:U:123:ARG:NH2	2.34	0.60
25:U:29:THR:N	25:U:32:ASP:OD2	2.34	0.60
32:c:36:ASN:ND2	32:c:219:PRO:HB2	2.16	0.60
5:A:825:U:O3'	14:J:55:ARG:NH2	2.35	0.60
6:B:239:ASN:ND2	6:B:242:SER:OG	2.35	0.60
5:A:1379:A:O2'	5:A:1380:G:O5'	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:44:GLU:OE1	26:V:44:GLU:N	2.34	0.59
13:I:177:ASP:OD1	13:I:178:ASN:N	2.36	0.59
28:X:123:ARG:NH1	28:X:297:MET:O	2.35	0.59
6:B:121:THR:OG1	6:B:237:PRO:O	2.21	0.59
22:R:294:ILE:HD11	22:R:349:TYR:CZ	2.36	0.59
28:X:369:GLU:OE1	28:X:369:GLU:N	2.31	0.59
10:F:109:SER:OG	10:F:113:GLN:OE1	2.19	0.59
26:V:225:LEU:HD11	26:V:283:LEU:HD22	1.84	0.59
32:c:36:ASN:HA	32:c:219:PRO:HG2	1.84	0.59
3:4:154:GLU:OE2	3:4:184:SER:N	2.30	0.59
4:9:266:GLU:O	4:9:270:GLU:OE1	2.21	0.59
22:R:187:GLU:N	22:R:187:GLU:OE1	2.31	0.59
29:Y:393:GLN:OE1	29:Y:393:GLN:N	2.34	0.59
19:O:185:SER:O	22:R:183:LYS:NZ	2.36	0.59
24:T:92:THR:O	24:T:92:THR:HG22	2.03	0.59
23:S:111:GLU:OE2	23:S:113:ASP:N	2.34	0.58
9:E:99:THR:OG1	9:E:100:GLN:OE1	2.18	0.58
16:L:86:ASP:OD1	16:L:87:ASP:N	2.36	0.58
5:A:1005:U:OP1	13:I:152:LYS:NZ	2.31	0.58
16:L:89:VAL:HG22	25:U:164:VAL:HG21	1.86	0.58
3:4:481:LEU:O	3:4:485:ALA:N	2.31	0.58
1:0:107:GLN:O	26:V:97:HIS:NE2	2.37	0.58
11:G:320:VAL:HG21	11:G:352:LEU:HD21	1.85	0.58
5:A:1430:A:OP2	10:F:35:SER:N	2.37	0.57
31:a:125:SER:N	31:a:139:TYR:O	2.37	0.57
3:4:550:ASP:OD1	3:4:588:ARG:NH2	2.36	0.57
28:X:217:GLU:N	28:X:217:GLU:OE1	2.37	0.57
5:A:953:U:OP1	24:T:6:ARG:NH2	2.38	0.57
7:C:70:SER:OG	15:K:119:GLN:O	2.15	0.57
23:S:111:GLU:OE2	23:S:112:THR:N	2.38	0.57
28:X:286:GLU:N	28:X:286:GLU:OE1	2.36	0.57
11:G:263:ASP:OD1	11:G:266:GLY:N	2.37	0.57
5:A:1108:C:H4'	5:A:1109:A:OP2	2.05	0.57
11:G:245:ARG:O	11:G:246:ARG:NH1	2.35	0.57
22:R:162:SER:O	22:R:170:ARG:NH1	2.36	0.57
2:1:152:ASP:OD2	2:1:174:ARG:NH2	2.38	0.56
4:9:204:LEU:HD23	4:9:385:LEU:HD11	1.87	0.56
5:A:1430:A:OP1	11:G:388:ARG:NH1	2.37	0.56
10:F:85:VAL:HG21	28:X:370:LYS:HG3	1.88	0.56
5:A:1231:A:OP1	15:K:88:ARG:NH2	2.35	0.56
17:M:67:ALA:HB2	22:R:196:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:146:GLU:N	3:4:146:GLU:OE1	2.38	0.56
26:V:95:PHE:O	26:V:98:SER:OG	2.18	0.56
28:X:142:ILE:HG23	28:X:152:ILE:HG21	1.87	0.56
8:D:245:VAL:HG22	8:D:271:ALA:HB1	1.88	0.56
24:T:138:GLU:N	24:T:142:GLU:OE2	2.39	0.56
26:V:67:VAL:O	26:V:100:ASN:ND2	2.39	0.56
28:X:112:LEU:O	28:X:115:THR:HG22	2.04	0.56
12:H:70:ASP:OD1	12:H:71:ILE:N	2.36	0.56
22:R:347:GLN:NE2	22:R:351:GLU:OE2	2.38	0.56
26:V:29:LEU:HD12	26:V:360:VAL:HG11	1.87	0.56
26:V:123:ASP:OD1	26:V:124:LYS:N	2.39	0.56
3:4:66:ASP:OD1	3:4:69:ALA:N	2.39	0.56
3:4:372:TYR:CE2	3:4:400:LEU:HD21	2.41	0.56
24:T:132:ARG:NH1	24:T:136:LEU:O	2.38	0.56
5:A:1227:G:OP2	5:A:1228:A:O2'	2.16	0.56
5:A:1578:A:H2'	5:A:1579:C:C6	2.41	0.55
30:Z:66:ARG:NH2	30:Z:80:ASP:OD2	2.36	0.55
5:A:771:A:O2'	5:A:772:A:O4'	2.24	0.55
28:X:108:LEU:HD21	28:X:307:VAL:HG11	1.88	0.55
30:Z:21:GLU:N	30:Z:21:GLU:OE1	2.38	0.55
3:4:302:VAL:HG11	3:4:341:CYS:HB3	1.89	0.55
7:C:118:GLU:N	7:C:118:GLU:OE1	2.40	0.55
5:A:1231:A:O2'	5:A:1233:C:OP2	2.25	0.54
6:B:239:ASN:OD1	27:W:119:LYS:NZ	2.40	0.54
24:T:32:VAL:HG13	24:T:76:LEU:HD23	1.89	0.54
2:1:192:LYS:NZ	2:1:247:ASP:O	2.36	0.54
22:R:176:GLU:OE2	22:R:182:ARG:NE	2.35	0.54
4:9:248:ASN:ND2	4:9:349:ALA:O	2.39	0.54
2:1:114:LEU:HD22	12:H:163:ASN:OD1	2.08	0.54
4:9:205:VAL:HG12	4:9:209:LEU:CD1	2.38	0.54
5:A:744:A:HO2'	5:A:745:A:P	2.31	0.54
5:A:769:G:N2	5:A:772:A:OP2	2.30	0.54
22:R:222:ASP:OD1	22:R:256:ARG:NH2	2.39	0.54
26:V:29:LEU:HD23	26:V:152:ILE:HG21	1.89	0.54
28:X:102:ARG:NE	28:X:352:GLU:OE1	2.40	0.54
14:J:52:THR:OG1	14:J:55:ARG:O	2.25	0.54
2:1:76:PHE:CE1	2:1:81:VAL:HG21	2.43	0.54
5:A:922:C:O2'	5:A:923:A:OP2	2.19	0.54
15:K:126:ALA:O	15:K:127:THR:HG23	2.07	0.54
3:4:335:PHE:CB	3:4:360:MET:HE2	2.38	0.53
8:D:372:GLU:OE2	8:D:374:ARG:NE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:76:LEU:HD22	12:H:148:LEU:HD11	1.89	0.53
3:4:277:ASN:O	3:4:281:GLU:OE1	2.27	0.53
22:R:219:TYR:O	22:R:256:ARG:NH1	2.38	0.53
29:Y:249:ASN:O	29:Y:252:THR:OG1	2.26	0.53
32:c:21:ILE:HD12	32:c:39:LEU:HD11	1.91	0.53
3:4:313:TRP:NE1	3:4:317:LEU:HD11	2.23	0.53
5:A:1089:U:H5'	32:c:326:LEU:HD13	1.89	0.53
13:I:83:ILE:O	13:I:148:ARG:NH2	2.39	0.53
25:U:167:PHE:O	25:U:176:ARG:NH1	2.41	0.53
4:9:642:HIS:C	4:9:643:LEU:HD12	2.33	0.53
5:A:1180:U:H2'	5:A:1181:G:C8	2.43	0.53
26:V:375:TYR:CE2	26:V:379:LEU:HD11	2.44	0.53
4:9:326:GLU:N	4:9:326:GLU:OE1	2.41	0.53
22:R:262:LEU:O	22:R:265:THR:OG1	2.21	0.53
3:4:609:GLU:N	3:4:609:GLU:OE1	2.38	0.53
3:4:279:TYR:HB2	3:4:297:LEU:HD21	1.91	0.53
5:A:1015:A:O5'	13:I:184:ASN:ND2	2.42	0.53
5:A:1232:A:OP1	5:A:1445:G:N1	2.33	0.53
26:V:175:VAL:HG13	26:V:178:THR:H	1.73	0.53
28:X:203:LYS:O	28:X:250:GLN:NE2	2.42	0.53
11:G:101:GLN:NE2	11:G:105:ASP:OD1	2.41	0.53
5:A:664:G:O2'	5:A:1166:A:N1	2.33	0.52
5:A:1004:G:OP1	13:I:89:LYS:NZ	2.42	0.52
3:4:196:CYS:O	3:4:269:HIS:NE2	2.40	0.52
4:9:244:ILE:HD11	4:9:337:TYR:CZ	2.44	0.52
5:A:1369:U:O4'	10:F:106:LEU:HD21	2.10	0.52
5:A:1414:C:O5'	5:A:1415:G:N2	2.43	0.52
12:H:76:LEU:HD11	12:H:172:VAL:CG2	2.39	0.52
26:V:212:GLY:O	26:V:224:GLN:NE2	2.42	0.52
3:4:615:MET:HE2	3:4:630:VAL:HB	1.91	0.52
10:F:170:VAL:HG13	10:F:237:ALA:HA	1.92	0.52
8:D:150:LYS:N	8:D:153:ALA:O	2.41	0.52
12:H:132:VAL:HG12	12:H:134:TYR:CE1	2.44	0.52
4:9:75:PRO:O	4:9:78:ILE:HD11	2.10	0.52
5:A:917:C:O2'	5:A:921:U:OP1	2.28	0.52
10:F:120:ARG:NH1	28:X:93:THR:OG1	2.42	0.52
15:K:72:ASP:O	15:K:75:ILE:HG22	2.10	0.52
28:X:264:GLY:N	28:X:309:ALA:O	2.42	0.52
12:H:125:HIS:CG	12:H:126:ILE:H	2.27	0.52
3:4:430:GLU:N	3:4:430:GLU:OE1	2.43	0.52
22:R:113:GLU:OE2	22:R:116:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:123:ARG:O	16:L:128:ARG:NH1	2.43	0.51
5:A:1230:C:N4	5:A:1447:G:OP2	2.43	0.51
11:G:126:LYS:O	11:G:131:ILE:HD11	2.09	0.51
8:D:112:LYS:HE3	8:D:114:ARG:NH2	2.25	0.51
25:U:58:GLU:OE1	25:U:61:GLN:NE2	2.44	0.51
28:X:151:LEU:HD22	28:X:258:LEU:CD1	2.41	0.51
5:A:1060:A:OP2	32:c:262:ARG:NH2	2.44	0.51
11:G:137:ALA:O	11:G:139:GLN:N	2.38	0.51
1:O:83:LYS:N	1:O:138:ASP:O	2.39	0.51
3:4:89:PHE:HZ	3:4:103:SER:HG	1.59	0.51
5:A:1132:U:H2'	5:A:1133:C:C6	2.46	0.51
8:D:283:GLU:OE2	23:S:21:ARG:NH2	2.44	0.51
2:1:169:ARG:O	2:1:218:ASN:ND2	2.42	0.51
5:A:1320:G:OP2	7:C:37:ASN:ND2	2.41	0.51
10:F:176:ASP:OD2	10:F:179:ARG:NH2	2.44	0.51
22:R:291:ARG:O	22:R:292:ASP:OD1	2.29	0.51
17:M:55:ASP:OD2	24:T:146:GLN:NE2	2.41	0.51
20:P:49:ASP:OD2	27:W:82:SER:OG	2.24	0.51
22:R:70:PHE:O	22:R:76:GLN:NE2	2.39	0.51
27:W:114:ILE:HG21	27:W:142:LEU:HD11	1.93	0.51
3:4:291:VAL:HG23	3:4:330:PRO:HA	1.92	0.50
5:A:939:A:O2'	5:A:940:A:O4'	2.23	0.50
32:c:239:GLU:O	32:c:240:GLN:NE2	2.44	0.50
2:1:291:GLU:OE1	2:1:318:ARG:NH1	2.44	0.50
25:U:89:VAL:HG23	25:U:90:LEU:HD12	1.94	0.50
8:D:263:ASP:OD1	8:D:264:ARG:N	2.43	0.50
11:G:380:LYS:NZ	11:G:384:GLN:O	2.39	0.50
28:X:205:GLN:OE1	28:X:249:ARG:NE	2.44	0.50
5:A:1400:U:O2'	5:A:1444:A:N3	2.44	0.50
5:A:1466:C:O4'	10:F:162:LEU:HD21	2.10	0.50
16:L:82:ILE:O	16:L:85:VAL:HG22	2.12	0.50
31:a:125:SER:OG	31:a:139:TYR:O	2.23	0.50
4:9:575:ASP:O	4:9:578:TYR:N	2.44	0.50
16:L:126:GLU:HG2	16:L:177:VAL:HG11	1.92	0.50
18:N:93:ASP:O	18:N:97:GLY:N	2.43	0.50
10:F:83:SER:OG	11:G:318:HIS:CE1	2.64	0.50
28:X:161:TRP:O	28:X:180:GLN:NE2	2.42	0.50
5:A:738:A:H2'	5:A:740:G:C4	2.45	0.50
5:A:1058:C:OP1	32:c:258:LYS:NZ	2.42	0.50
5:A:1089:U:C5'	32:c:326:LEU:HD13	2.41	0.50
6:B:243:PRO:O	6:B:247:HIS:ND1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:300:ASP:N	28:X:300:ASP:OD1	2.44	0.50
32:c:98:SER:HB2	32:c:105:LEU:HD23	1.93	0.50
23:S:99:PHE:HA	23:S:125:LEU:HD11	1.94	0.50
24:T:26:SER:O	24:T:81:ASP:N	2.39	0.50
3:4:615:MET:HE3	3:4:645:LEU:HD21	1.94	0.49
5:A:1192:C:N4	5:A:1463:G:O6	2.45	0.49
11:G:134:ARG:O	11:G:135:GLN:HG3	2.11	0.49
13:I:136:ALA:HB1	13:I:170:LEU:HD13	1.93	0.49
4:9:73:LEU:HD11	26:V:65:LEU:HD22	1.94	0.49
11:G:138:ILE:O	11:G:139:GLN:HB2	2.12	0.49
26:V:375:TYR:CZ	26:V:379:LEU:HD11	2.47	0.49
5:A:1282:G:N1	5:A:1286:A:OP2	2.39	0.49
1:0:78:ARG:NH1	26:V:171:GLU:OE1	2.45	0.49
2:1:131:THR:N	12:H:152:THR:OG1	2.37	0.49
2:1:163:VAL:HG22	2:1:163:VAL:O	2.13	0.49
9:E:44:GLU:OE2	9:E:60:ARG:NE	2.46	0.49
26:V:156:ASN:ND2	26:V:159:ASP:OD2	2.43	0.49
8:D:363:ALA:HB2	8:D:370:VAL:HG23	1.94	0.49
11:G:143:ASP:OD1	11:G:144:GLY:N	2.45	0.49
3:4:324:VAL:HG22	29:Y:259:PHE:CE1	2.47	0.49
16:L:112:MET:O	16:L:116:VAL:HG22	2.12	0.49
2:1:198:TYR:OH	2:1:203:ASP:OD1	2.27	0.49
5:A:1085:C:OP1	13:I:189:ARG:NH2	2.44	0.49
28:X:338:ASP:OD1	28:X:339:PRO:HA	2.13	0.49
3:4:335:PHE:HB2	3:4:360:MET:HE2	1.95	0.49
21:Q:40:LYS:CD	31:a:170:GLN:HG2	2.43	0.49
5:A:821:U:H2'	5:A:822:G:H8	1.78	0.48
5:A:1372:C:H2'	5:A:1373:U:C6	2.48	0.48
11:G:138:ILE:C	11:G:139:GLN:OE1	2.55	0.48
29:Y:279:ASP:OD1	29:Y:280:VAL:N	2.46	0.48
5:A:1406:U:H5'	5:A:1407:U:H5	1.78	0.48
32:c:306:VAL:HG12	32:c:310:MET:HE2	1.94	0.48
16:L:99:ASN:OD1	16:L:101:LYS:N	2.37	0.48
5:A:730:A:C4	5:A:731:A:C8	3.02	0.48
5:A:976:A:OP1	21:Q:3:LYS:N	2.46	0.48
11:G:306:ILE:HG22	11:G:308:GLN:H	1.78	0.48
5:A:845:A:H2'	5:A:846:A:C8	2.48	0.48
5:A:1200:G:H5'	5:A:1422:G:O6	2.14	0.48
2:1:181:ASN:O	2:1:234:TRP:NE1	2.43	0.48
3:4:437:GLY:O	3:4:441:THR:OG1	2.28	0.48
5:A:735:A:C6	5:A:736:C:C5	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:183:GLU:OE1	28:X:183:GLU:N	2.39	0.48
32:c:186:ALA:O	32:c:201:GLN:NE2	2.41	0.48
1:0:131:ILE:HG22	1:0:132:GLU:N	2.28	0.48
6:B:107:PHE:N	6:B:115:ILE:O	2.45	0.48
20:P:139:ARG:NE	20:P:141:ARG:O	2.44	0.48
1:0:100:VAL:HG12	1:0:101:ARG:N	2.29	0.48
4:9:607:ASP:OD1	4:9:608:ILE:N	2.46	0.48
11:G:202:LYS:NZ	11:G:215:ASP:OD1	2.43	0.48
2:1:244:THR:N	2:1:247:ASP:OD2	2.47	0.47
26:V:132:LYS:O	26:V:136:GLY:N	2.36	0.47
2:1:133:TRP:CE2	12:H:147:HIS:HA	2.48	0.47
4:9:623:ILE:CG2	4:9:653:LEU:HD11	2.44	0.47
5:A:1578:A:O3'	32:c:257:ARG:HD2	2.14	0.47
11:G:157:SER:N	11:G:211:GLU:OE2	2.42	0.47
13:I:101:SER:O	13:I:104:ASN:N	2.42	0.47
13:I:176:THR:HG23	21:Q:11:THR:OG1	2.13	0.47
4:9:569:THR:HG21	4:9:577:LEU:HD22	1.97	0.47
5:A:1226:C:O2'	12:H:126:ILE:HG22	2.14	0.47
7:C:39:ALA:O	7:C:41:ARG:NH1	2.48	0.47
24:T:110:GLU:OE1	24:T:110:GLU:N	2.43	0.47
3:4:87:TYR:OH	29:Y:300:GLU:OE1	2.23	0.47
5:A:1450:C:O3'	12:H:131:ARG:NH2	2.48	0.47
28:X:153:LEU:HD21	28:X:244:LEU:CD2	2.44	0.47
2:1:289:ILE:HD13	2:1:319:LEU:HD21	1.97	0.47
5:A:1266:A:N6	5:A:1327:G:C6	2.83	0.47
5:A:1379:A:H2'	5:A:1380:G:C8	2.49	0.47
13:I:153:GLY:O	13:I:158:ARG:NH1	2.48	0.47
13:I:183:HIS:O	13:I:184:ASN:ND2	2.47	0.47
19:O:98:ASN:OD1	19:O:98:ASN:C	2.58	0.47
20:P:56:ASN:OD1	20:P:58:TYR:N	2.47	0.47
26:V:395:GLN:O	26:V:399:GLN:NE2	2.48	0.47
32:c:54:LEU:HD12	32:c:59:VAL:HG22	1.95	0.47
1:0:43:ARG:NE	5:A:706:C:OP1	2.43	0.47
5:A:728:C:H2'	5:A:729:U:O4'	2.15	0.47
28:X:109:LEU:HD22	28:X:144:PHE:CG	2.50	0.47
4:9:351:LYS:NZ	4:9:497:THR:O	2.46	0.47
8:D:243:VAL:HG12	8:D:245:VAL:HG13	1.96	0.47
15:K:67:LEU:O	15:K:70:VAL:HG12	2.15	0.46
17:M:39:ASN:OD1	17:M:40:LYS:N	2.48	0.46
20:P:46:SER:OG	20:P:47:ASN:N	2.43	0.46
28:X:262:VAL:HG21	28:X:297:MET:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:66:TRP:CZ3	2:1:69:VAL:HG11	2.50	0.46
5:A:1379:A:C2'	5:A:1380:G:O5'	2.64	0.46
21:Q:40:LYS:HD3	31:a:170:GLN:HG2	1.96	0.46
32:c:73:ILE:HG22	32:c:81:LEU:HD12	1.96	0.46
10:F:159:VAL:HG12	10:F:172:VAL:HG11	1.96	0.46
11:G:200:LEU:HD22	11:G:244:PHE:HB3	1.98	0.46
5:A:672:A:H2'	5:A:673:U:C6	2.51	0.46
5:A:778:C:OP1	18:N:27:LYS:NZ	2.45	0.46
12:H:119:THR:OG1	12:H:133:GLN:OE1	2.21	0.46
17:M:109:ARG:NE	25:U:52:GLU:OE2	2.42	0.46
18:N:67:ARG:NH1	18:N:80:GLU:OE2	2.48	0.46
29:Y:249:ASN:OD1	29:Y:250:ILE:N	2.49	0.46
5:A:649:A:O3'	5:A:650:U:H3'	2.16	0.46
5:A:1450:C:O2'	12:H:131:ARG:NH2	2.47	0.46
8:D:112:LYS:CE	8:D:114:ARG:HH21	2.28	0.46
22:R:276:VAL:HG11	22:R:307:LEU:HD12	1.98	0.46
9:E:94:VAL:CG1	20:P:117:MET:HE1	2.45	0.46
27:W:115:ASP:OD1	27:W:116:PHE:N	2.49	0.46
26:V:29:LEU:CD2	26:V:152:ILE:HG21	2.45	0.46
26:V:67:VAL:HG12	26:V:68:SER:N	2.31	0.46
28:X:145:CYS:HB3	28:X:150:TRP:HB2	1.98	0.46
5:A:770:C:N4	5:A:771:A:N1	2.64	0.46
27:W:100:VAL:HG11	27:W:144:LEU:HD11	1.98	0.46
5:A:1186:A:C2	5:A:1469:G:C2	3.04	0.46
9:E:80:GLU:OE1	9:E:84:ARG:NE	2.49	0.46
11:G:136:ARG:NH2	11:G:156:GLN:HG2	2.31	0.46
4:9:244:ILE:HD11	4:9:337:TYR:CE1	2.50	0.45
5:A:1375:C:H2'	5:A:1376:C:O4'	2.16	0.45
11:G:134:ARG:HA	11:G:134:ARG:NE	2.30	0.45
11:G:295:VAL:N	11:G:298:ILE:O	2.39	0.45
32:c:148:THR:HB	32:c:149:PRO:HD3	1.98	0.45
3:4:335:PHE:HB3	3:4:360:MET:HE2	1.98	0.45
2:1:244:THR:HG22	2:1:245:GLU:N	2.32	0.45
3:4:120:ILE:HD11	30:Z:70:LEU:CD1	2.47	0.45
32:c:63:GLY:N	32:c:64:PRO:HD3	2.32	0.45
4:9:530:VAL:O	4:9:530:VAL:HG13	2.17	0.45
5:A:990:U:H2'	5:A:991:G:O4'	2.16	0.45
5:A:1087:A:H2'	5:A:1088:C:O4'	2.17	0.45
8:D:281:TYR:CE1	23:S:22:ALA:HB2	2.51	0.45
8:D:301:THR:OG1	8:D:339:SER:O	2.20	0.45
11:G:389:ARG:NH1	11:G:390:LYS:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:342:GLN:HB3	26:V:347:ILE:HD12	1.98	0.45
29:Y:258:ILE:O	29:Y:259:PHE:CD1	2.69	0.45
31:a:125:SER:HG	31:a:139:TYR:C	2.21	0.45
3:4:81:ASP:OD1	3:4:82:THR:N	2.49	0.45
3:4:397:MET:SD	3:4:435:VAL:HG22	2.57	0.45
24:T:32:VAL:HG22	24:T:76:LEU:HD22	1.99	0.45
3:4:67:LYS:HG3	3:4:68:VAL:HG13	1.97	0.45
4:9:91:LEU:C	4:9:91:LEU:HD23	2.41	0.45
5:A:1200:G:N3	5:A:1200:G:H2'	2.31	0.45
5:A:1400:U:H2'	5:A:1401:G:O4'	2.15	0.45
11:G:70:THR:HG23	11:G:73:PHE:H	1.80	0.45
21:Q:40:LYS:HE2	31:a:112:GLU:OE2	2.17	0.45
2:1:114:LEU:HD13	12:H:163:ASN:OD1	2.16	0.45
5:A:1041:A:H2'	5:A:1042:U:H4'	1.99	0.45
5:A:1229:U:O2'	5:A:1442:G:O4'	2.34	0.45
5:A:1232:A:C2	5:A:1404:A:C4	3.05	0.45
18:N:62:ASP:OD1	18:N:88:VAL:N	2.41	0.45
1:0:37:ASP:O	1:0:41:LEU:N	2.46	0.45
5:A:702:C:H2'	5:A:703:A:O4'	2.16	0.45
5:A:799:A:H2'	5:A:800:C:C6	2.52	0.45
5:A:834:G:H2'	5:A:835:C:O4'	2.17	0.45
5:A:867:C:O2'	5:A:870:C:N4	2.49	0.45
11:G:379:ARG:O	11:G:381:LYS:NZ	2.45	0.45
1:0:14:LEU:HB2	4:9:91:LEU:CD1	2.47	0.45
5:A:1108:C:H2'	5:A:1125:A:N6	2.32	0.45
5:A:1572:A:N1	5:A:1595:G:N7	2.65	0.45
10:F:161:ILE:HD12	10:F:170:VAL:HG11	1.97	0.45
26:V:279:ALA:O	26:V:282:VAL:HG12	2.17	0.45
3:4:192:LEU:HD11	3:4:251:MET:CE	2.47	0.44
6:B:159:ALA:CB	6:B:166:ALA:HB2	2.47	0.44
8:D:317:HIS:O	8:D:320:ILE:N	2.50	0.44
17:M:67:ALA:HB2	22:R:196:TYR:CE1	2.52	0.44
28:X:131:GLY:HA2	36:X:501:ATP:O1A	2.17	0.44
5:A:1225:C:O2'	5:A:1449:G:O2'	2.19	0.44
17:M:67:ALA:HB1	22:R:161:ILE:HG21	2.00	0.44
28:X:178:PHE:N	28:X:286:GLU:O	2.44	0.44
5:A:1108:C:H2'	5:A:1125:A:H61	1.82	0.44
5:A:1154:A:O2'	5:A:1155:G:O5'	2.20	0.44
5:A:1440:G:H2'	5:A:1441:A:C8	2.52	0.44
11:G:356:VAL:HG21	11:G:364:MET:HE2	1.98	0.44
26:V:30:LEU:HD13	26:V:34:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:252:SER:O	28:X:302:HIS:NE2	2.50	0.44
5:A:996:A:C4	5:A:997:A:C8	3.06	0.44
24:T:32:VAL:HG13	24:T:76:LEU:CD2	2.47	0.44
2:1:131:THR:OG1	12:H:149:THR:OG1	2.17	0.44
9:E:11:LYS:O	9:E:13:MET:HG2	2.17	0.44
9:E:96:HIS:O	9:E:99:THR:OG1	2.36	0.44
10:F:148:ALA:HB1	10:F:212:ALA:HB3	1.98	0.44
11:G:129:GLU:O	11:G:134:ARG:NH1	2.36	0.44
13:I:175:ILE:HD12	21:Q:22:ALA:HB3	2.00	0.44
3:4:305:ILE:O	3:4:312:LYS:NZ	2.48	0.44
3:4:324:VAL:HG22	29:Y:259:PHE:HE1	1.81	0.44
5:A:715:G:H2'	5:A:716:U:C6	2.53	0.44
8:D:426:LYS:N	19:O:88:GLN:OE1	2.50	0.44
10:F:48:LYS:O	10:F:52:ARG:HG2	2.18	0.44
24:T:35:ASN:ND2	24:T:72:PRO:O	2.50	0.44
13:I:104:ASN:C	13:I:104:ASN:OD1	2.61	0.44
2:1:101:GLY:N	7:C:156:GLN:OE1	2.51	0.44
2:1:156:TYR:O	29:Y:317:ASN:ND2	2.43	0.44
5:A:735:A:H2'	5:A:735:A:N3	2.32	0.44
8:D:296:LEU:HD11	8:D:303:ILE:HD12	1.99	0.44
22:R:85:LEU:HD21	22:R:119:VAL:HG13	1.98	0.44
28:X:360:TYR:HB2	28:X:366:LEU:HD11	1.99	0.44
3:4:389:SER:HA	3:4:392:ILE:HG22	2.00	0.44
5:A:736:C:C4	5:A:737:C:C4	3.05	0.44
26:V:391:GLN:O	26:V:394:GLN:HG2	2.18	0.44
5:A:983:C:H2'	5:A:983:C:O2	2.18	0.43
5:A:1208:U:H2'	5:A:1209:C:C6	2.53	0.43
3:4:489:HIS:O	3:4:492:THR:OG1	2.21	0.43
12:H:99:ALA:HB1	12:H:104:ILE:HB	1.98	0.43
26:V:245:HIS:O	26:V:246:ASN:HB2	2.18	0.43
28:X:67:HIS:HA	28:X:100:MET:HA	1.99	0.43
3:4:370:ALA:N	3:4:412:ASP:OD1	2.44	0.43
3:4:564:ILE:HG22	3:4:564:ILE:O	2.18	0.43
20:P:65:CYS:SG	20:P:68:CYS:HB2	2.58	0.43
32:c:36:ASN:ND2	32:c:219:PRO:O	2.51	0.43
5:A:1148:A:H2'	5:A:1149:G:H8	1.84	0.43
7:C:75:ASN:OD1	15:K:104:TRP:NE1	2.47	0.43
19:O:179:THR:HG22	19:O:179:THR:O	2.18	0.43
28:X:150:TRP:HB2	28:X:152:ILE:HD11	2.00	0.43
32:c:218:VAL:HB	32:c:219:PRO:HD3	2.01	0.43
3:4:345:PHE:HB2	3:4:349:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1122:A:H2'	5:A:1123:C:C6	2.54	0.43
5:A:1233:C:O2	5:A:1233:C:H2'	2.18	0.43
20:P:113:ARG:HG3	20:P:117:MET:HE3	1.99	0.43
5:A:662:U:OP2	8:D:339:SER:OG	2.37	0.43
5:A:1154:A:C4	5:A:1155:G:C8	3.07	0.43
11:G:156:GLN:HG3	11:G:157:SER:N	2.34	0.43
32:c:54:LEU:HD12	32:c:59:VAL:CG2	2.48	0.43
13:I:90:ALA:O	13:I:155:GLY:N	2.52	0.43
15:K:70:VAL:HA	15:K:73:GLU:HG2	2.00	0.43
26:V:34:TYR:OH	26:V:145:ASN:HB2	2.18	0.43
5:A:731:A:C4	5:A:732:A:C8	3.07	0.43
5:A:937:U:H5''	5:A:938:A:OP2	2.19	0.43
5:A:1315:G:H2'	5:A:1316:U:O4'	2.19	0.43
4:9:78:ILE:HG22	4:9:79:LEU:N	2.32	0.43
1:0:173:MET:HG2	22:R:171:PHE:CE2	2.54	0.42
5:A:1441:A:H2	5:A:1449:G:H1	1.59	0.42
3:4:239:ARG:O	3:4:242:ASN:ND2	2.42	0.42
5:A:1284:U:OP1	8:D:347:GLN:NE2	2.52	0.42
12:H:58:LEU:HD23	12:H:58:LEU:H	1.84	0.42
18:N:58:CYS:SG	18:N:81:LEU:HD22	2.59	0.42
2:1:258:SER:OG	2:1:292:TYR:OH	2.24	0.42
7:C:163:VAL:HG11	7:C:166:TYR:CZ	2.54	0.42
15:K:63:LEU:HD13	15:K:67:LEU:CD2	2.50	0.42
19:O:116:ASP:OD2	19:O:118:ARG:NH2	2.43	0.42
22:R:89:LYS:NZ	22:R:260:ASP:O	2.52	0.42
22:R:242:TYR:CZ	22:R:246:HIS:CE1	3.08	0.42
5:A:1298:U:H2'	5:A:1299:A:O4'	2.20	0.42
5:A:1576:G:H2'	5:A:1577:U:O4'	2.20	0.42
31:a:111:PRO:HA	31:a:118:TYR:HB2	2.02	0.42
3:4:290:ASP:OD1	3:4:293:THR:OG1	2.37	0.42
3:4:354:LEU:HD21	3:4:379:PHE:HE2	1.84	0.42
5:A:1088:C:O2'	5:A:1089:U:H5'	2.19	0.42
3:4:257:HIS:O	3:4:261:THR:HG23	2.19	0.42
5:A:762:G:N1	5:A:779:U:C4	2.87	0.42
5:A:1265:C:P	7:C:39:ALA:HB2	2.59	0.42
5:A:1348:G:H2'	5:A:1349:U:C6	2.55	0.42
5:A:1578:A:H2'	5:A:1579:C:H6	1.83	0.42
32:c:15:LEU:HD12	32:c:16:PRO:HD2	2.01	0.42
5:A:1116:A:H2'	5:A:1117:A:O4'	2.19	0.42
11:G:137:ALA:C	11:G:139:GLN:H	2.24	0.42
28:X:129:GLU:O	28:X:134:LYS:NZ	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:299:LEU:HD11	2:1:312:TYR:HB2	2.02	0.42
5:A:663:A:H2'	5:A:664:G:C8	2.55	0.42
5:A:710:U:O2'	25:U:28:LYS:O	2.37	0.42
5:A:992:U:O2'	5:A:993:A:O5'	2.18	0.42
5:A:1152:A:H4'	5:A:1153:C:O5'	2.20	0.42
5:A:1174:U:H2'	5:A:1175:G:H8	1.85	0.42
5:A:1180:U:O2	5:A:1474:G:N2	2.48	0.42
5:A:1327:G:P	5:A:1327:G:H3'	2.59	0.42
5:A:1451:U:H5'	12:H:131:ARG:CZ	2.49	0.42
10:F:156:ILE:CD1	31:a:193:LEU:HD13	2.50	0.42
11:G:148:HIS:ND1	11:G:156:GLN:HB2	2.35	0.42
11:G:158:TYR:N	11:G:211:GLU:OE1	2.48	0.42
14:J:99:GLY:O	14:J:127:ARG:NH2	2.50	0.42
26:V:244:TYR:CD1	26:V:244:TYR:C	2.98	0.42
5:A:1380:G:H2'	5:A:1381:A:C8	2.55	0.42
5:A:1452:U:OP1	12:H:133:GLN:NE2	2.52	0.42
5:A:1596:A:H2'	5:A:1597:C:C6	2.55	0.42
12:H:133:GLN:H	15:K:126:ALA:CB	2.32	0.42
28:X:159:HIS:NE2	28:X:311:SER:O	2.46	0.42
15:K:63:LEU:HD13	15:K:67:LEU:HD22	2.00	0.42
24:T:92:THR:O	24:T:92:THR:CG2	2.67	0.42
28:X:392:GLU:CD	36:X:501:ATP:H4'	2.44	0.42
5:A:1066:C:O2'	13:I:187:ARG:O	2.38	0.41
5:A:1359:U:H2'	5:A:1360:G:H8	1.85	0.41
6:B:120:GLN:O	6:B:124:HIS:ND1	2.39	0.41
6:B:165:TYR:OH	11:G:146:PRO:O	2.23	0.41
20:P:88:THR:OG1	21:Q:33:ASP:OD2	2.28	0.41
5:A:970:A:H2'	5:A:971:A:C8	2.55	0.41
5:A:973:C:O2'	5:A:974:U:H5'	2.19	0.41
11:G:199:TRP:NE1	11:G:226:GLU:OE2	2.48	0.41
17:M:78:GLY:O	25:U:75:VAL:HG22	2.19	0.41
17:M:100:HIS:H	17:M:103:MET:HE3	1.86	0.41
27:W:104:ILE:HG12	27:W:114:ILE:HG12	2.01	0.41
32:c:190:SER:C	32:c:293:ARG:HH12	2.28	0.41
5:A:997:A:C4	5:A:998:A:C8	3.08	0.41
5:A:1192:C:H2'	5:A:1193:U:O4'	2.20	0.41
12:H:98:ALA:O	12:H:102:LEU:HG	2.20	0.41
26:V:260:LEU:HD12	26:V:333:ARG:CZ	2.51	0.41
29:Y:293:PRO:O	29:Y:295:GLN:NE2	2.48	0.41
1:0:95:TRP:CD2	1:0:131:ILE:CD1	3.04	0.41
3:4:432:ALA:HB2	3:4:464:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:69:GLN:OE1	26:V:392:ARG:NH1	2.52	0.41
5:A:659:U:O2'	5:A:1285:G:H1'	2.20	0.41
12:H:119:THR:HG22	12:H:120:LEU:N	2.35	0.41
13:I:147:ILE:HG21	13:I:170:LEU:HD23	2.03	0.41
2:1:185:HIS:NE2	2:1:240:GLU:OE1	2.54	0.41
3:4:236:VAL:HG12	3:4:238:TRP:H	1.86	0.41
5:A:879:U:OP2	5:A:880:C:O2'	2.36	0.41
5:A:1060:A:O2'	5:A:1061:A:H5'	2.21	0.41
5:A:701:G:C6	5:A:709:G:N1	2.88	0.41
5:A:870:C:O2'	5:A:871:A:OP2	2.25	0.41
5:A:1150:C:C4	5:A:1151:C:C2	3.08	0.41
5:A:1357:A:H2'	5:A:1358:A:C8	2.55	0.41
6:B:234:TYR:OH	23:S:38:PHE:O	2.32	0.41
28:X:222:LEU:HD11	28:X:243:VAL:HG22	2.02	0.41
3:4:166:VAL:HG23	3:4:167:LYS:N	2.36	0.41
3:4:439:LEU:O	3:4:445:TRP:N	2.54	0.41
26:V:321:GLU:OE1	26:V:321:GLU:N	2.42	0.41
32:c:21:ILE:CD1	32:c:39:LEU:HD11	2.51	0.41
1:0:108:ASN:OD1	26:V:134:GLN:NE2	2.53	0.41
4:9:380:TRP:N	4:9:385:LEU:O	2.48	0.41
5:A:1444:A:OP2	15:K:102:ARG:NH1	2.48	0.41
5:A:1574:G:N1	5:A:1592:U:C4	2.89	0.41
5:A:1578:A:N6	5:A:1588:G:O6	2.54	0.41
6:B:146:SER:HG	6:B:197:HIS:CG	2.30	0.41
12:H:85:LYS:NZ	12:H:110:GLU:OE2	2.46	0.41
28:X:60:GLY:HA2	28:X:106:LEU:HD22	2.03	0.41
32:c:293:ARG:NH1	32:c:293:ARG:HB3	2.36	0.41
4:9:216:LEU:HD21	4:9:244:ILE:HD12	2.03	0.41
5:A:737:C:H2'	5:A:738:A:O4'	2.21	0.41
5:A:1298:U:O2'	6:B:182:LEU:HD23	2.21	0.41
6:B:89:VAL:HG13	6:B:249:TYR:OH	2.21	0.41
7:C:76:LEU:HD21	12:H:83:HIS:NE2	2.36	0.41
11:G:237:GLU:O	11:G:241:VAL:HG23	2.21	0.41
19:O:174:ASP:OD2	22:R:168:ARG:NE	2.47	0.41
22:R:312:GLN:N	22:R:335:GLU:OE2	2.54	0.41
26:V:37:SER:OG	26:V:41:GLU:OE1	2.34	0.41
26:V:377:GLN:O	26:V:380:GLN:HG3	2.21	0.41
28:X:322:ALA:HB1	28:X:327:GLU:HG3	2.03	0.41
28:X:348:TYR:O	28:X:386:ALA:HB1	2.21	0.41
29:Y:258:ILE:O	29:Y:259:PHE:HD1	2.03	0.41
30:Z:95:LYS:N	30:Z:98:GLU:OE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:158:LYS:O	3:4:161:ILE:HG22	2.20	0.41
3:4:291:VAL:CG2	3:4:330:PRO:HA	2.50	0.41
5:A:941:G:C6	5:A:1134:G:N1	2.89	0.41
5:A:1140:A:H2'	5:A:1141:C:O4'	2.21	0.41
5:A:1374:A:H2'	5:A:1375:C:O4'	2.21	0.41
5:A:1401:G:N1	5:A:1404:A:OP2	2.54	0.41
7:C:129:PRO:O	7:C:133:TYR:CD2	2.74	0.41
7:C:136:VAL:HG22	7:C:153:LEU:HD23	2.03	0.41
9:E:94:VAL:HG11	20:P:117:MET:HE1	2.02	0.41
12:H:172:VAL:O	12:H:172:VAL:HG13	2.21	0.41
13:I:169:GLY:C	13:I:170:LEU:HD12	2.46	0.41
18:N:51:ALA:CB	18:N:66:LEU:HD22	2.51	0.41
1:0:41:LEU:HD13	1:0:55:TRP:CG	2.56	0.40
5:A:701:G:C6	5:A:709:G:C2	3.09	0.40
5:A:1177:C:O2	5:A:1477:U:O2	2.38	0.40
11:G:139:GLN:O	11:G:146:PRO:HA	2.22	0.40
11:G:231:SER:O	11:G:232:GLN:C	2.64	0.40
24:T:27:VAL:HG22	24:T:80:LEU:CD2	2.51	0.40
29:Y:377:ARG:O	29:Y:381:ASN:ND2	2.55	0.40
3:4:349:ALA:HA	3:4:352:PRO:HG2	2.03	0.40
8:D:190:GLU:O	8:D:191:ARG:C	2.63	0.40
12:H:74:LYS:HB2	12:H:177:LEU:HD21	2.03	0.40
2:1:147:PHE:CD2	12:H:177:LEU:HD13	2.56	0.40
3:4:255:ASN:OD1	3:4:258:SER:N	2.45	0.40
4:9:220:MET:HE2	4:9:354:LEU:HD22	2.02	0.40
5:A:1358:A:H2'	5:A:1359:U:O4'	2.22	0.40
5:A:1370:U:C2	5:A:1371:U:C5	3.08	0.40
5:A:1397:U:H2'	5:A:1398:U:H6	1.86	0.40
5:A:1430:A:O4'	5:A:1432:U:C6	2.74	0.40
11:G:73:PHE:O	11:G:77:GLN:HG2	2.22	0.40
11:G:172:LEU:HD12	11:G:228:LEU:HD12	2.04	0.40
11:G:176:GLN:NE2	11:G:232:GLN:OE1	2.55	0.40
26:V:80:SER:HG	26:V:84:GLU:CD	2.29	0.40
30:Z:3:SER:OG	30:Z:4:LEU:N	2.54	0.40
2:1:283:LEU:O	2:1:286:THR:HG22	2.21	0.40
3:4:543:GLU:O	3:4:546:VAL:HG12	2.22	0.40
3:4:593:TRP:CE3	3:4:596:LEU:HD12	2.57	0.40
4:9:668:GLY:N	4:9:678:LYS:O	2.55	0.40
5:A:1398:U:H2'	5:A:1399:A:H8	1.86	0.40
12:H:122:GLN:HA	12:H:132:VAL:HG23	2.04	0.40
12:H:125:HIS:CE1	12:H:126:ILE:HG23	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:102:LEU:HD22	14:J:108:VAL:CG1	2.51	0.40
24:T:42:GLU:OE1	24:T:45:ARG:NH2	2.48	0.40
5:A:662:U:H2'	5:A:663:A:O4'	2.22	0.40
5:A:812:A:HO2'	5:A:813:A:C4'	2.30	0.40
5:A:845:A:H4'	25:U:60:TYR:CE2	2.57	0.40
5:A:1180:U:H5''	5:A:1181:G:OP1	2.22	0.40
5:A:1586:G:H2'	5:A:1587:U:O4'	2.22	0.40
18:N:85:VAL:HG13	24:T:77:ARG:NH2	2.37	0.40
24:T:39:GLU:HG2	24:T:40:LEU:N	2.36	0.40
28:X:121:ALA:HB1	28:X:306:ILE:HD12	2.03	0.40
28:X:209:VAL:O	28:X:209:VAL:HG23	2.21	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%)	201 (96%)	9 (4%)	0	100	100
2	1	274/323 (85%)	268 (98%)	6 (2%)	0	100	100
3	4	588/689 (85%)	570 (97%)	18 (3%)	0	100	100
4	9	345/706 (49%)	332 (96%)	13 (4%)	0	100	100
6	B	218/296 (74%)	211 (97%)	7 (3%)	0	100	100
7	C	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
8	D	323/430 (75%)	311 (96%)	12 (4%)	0	100	100
9	E	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
10	F	198/242 (82%)	191 (96%)	7 (4%)	0	100	100
11	G	297/396 (75%)	283 (95%)	14 (5%)	0	100	100
12	H	137/201 (68%)	132 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	135/194 (70%)	126 (93%)	9 (7%)	0	100	100
14	J	105/138 (76%)	97 (92%)	8 (8%)	0	100	100
15	K	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
16	L	154/257 (60%)	149 (97%)	5 (3%)	0	100	100
17	M	113/137 (82%)	111 (98%)	2 (2%)	0	100	100
18	N	107/130 (82%)	100 (94%)	7 (6%)	0	100	100
19	O	191/258 (74%)	186 (97%)	5 (3%)	0	100	100
20	P	94/142 (66%)	93 (99%)	1 (1%)	0	100	100
21	Q	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
22	R	291/360 (81%)	278 (96%)	13 (4%)	0	100	100
23	S	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
24	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
25	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
26	V	358/414 (86%)	348 (97%)	10 (3%)	0	100	100
27	W	97/187 (52%)	92 (95%)	5 (5%)	0	100	100
28	X	347/398 (87%)	340 (98%)	7 (2%)	0	100	100
29	Y	147/395 (37%)	142 (97%)	5 (3%)	0	100	100
30	Z	94/106 (89%)	92 (98%)	2 (2%)	0	100	100
31	a	107/343 (31%)	104 (97%)	3 (3%)	0	100	100
32	c	281/346 (81%)	278 (99%)	3 (1%)	0	100	100
All	All	6116/8380 (73%)	5926 (97%)	190 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	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	4	529/609 (87%)	529 (100%)	0	100	100
4	9	316/608 (52%)	316 (100%)	0	100	100
6	B	194/249 (78%)	194 (100%)	0	100	100
7	C	115/143 (80%)	115 (100%)	0	100	100
8	D	276/357 (77%)	276 (100%)	0	100	100
9	E	104/107 (97%)	104 (100%)	0	100	100
10	F	181/209 (87%)	181 (100%)	0	100	100
11	G	262/342 (77%)	262 (100%)	0	100	100
12	H	129/180 (72%)	129 (100%)	0	100	100
13	I	105/147 (71%)	105 (100%)	0	100	100
14	J	92/118 (78%)	92 (100%)	0	100	100
15	K	91/113 (80%)	91 (100%)	0	100	100
16	L	146/226 (65%)	146 (100%)	0	100	100
17	M	94/113 (83%)	94 (100%)	0	100	100
18	N	95/115 (83%)	95 (100%)	0	100	100
19	O	174/230 (76%)	174 (100%)	0	100	100
20	P	87/123 (71%)	87 (100%)	0	100	100
21	Q	78/78 (100%)	78 (100%)	0	100	100
22	R	262/318 (82%)	262 (100%)	0	100	100
23	S	116/164 (71%)	116 (100%)	0	100	100
24	T	153/157 (98%)	153 (100%)	0	100	100
25	U	152/174 (87%)	152 (100%)	0	100	100
26	V	325/364 (89%)	325 (100%)	0	100	100
27	W	86/158 (54%)	86 (100%)	0	100	100
28	X	309/351 (88%)	309 (100%)	0	100	100
29	Y	137/357 (38%)	137 (100%)	0	100	100
30	Z	88/95 (93%)	88 (100%)	0	100	100
31	a	93/288 (32%)	93 (100%)	0	100	100
32	c	270/309 (87%)	270 (100%)	0	100	100
All	All	5498/7283 (76%)	5498 (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 (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	137	HIS
3	4	545	GLN
3	4	612	ASN
4	9	386	ASN
4	9	504	ASN
4	9	551	ASN
4	9	669	GLN
6	B	69	HIS
6	B	148	ASN
6	B	265	GLN
8	D	151	ASN
10	F	169	GLN
10	F	215	ASN
11	G	176	GLN
11	G	318	HIS
13	I	184	ASN
15	K	68	GLN
15	K	117	HIS
16	L	146	HIS
19	O	80	ASN
19	O	166	HIS
20	P	78	GLN
22	R	350	GLN
24	T	54	GLN
24	T	56	GLN
25	U	61	GLN
26	V	237	GLN
26	V	245	HIS
26	V	246	ASN
26	V	324	GLN
27	W	110	ASN
28	X	52	ASN
28	X	73	GLN
28	X	110	HIS
28	X	257	HIS
29	Y	381	ASN
31	a	151	HIS
31	a	157	GLN
31	a	175	ASN

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Mol	Chain	Res	Type
32	c	36	ASN
32	c	53	ASN
32	c	137	HIS
32	c	171	GLN
32	c	208	HIS
32	c	254	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	802/955 (83%)	119 (14%)	3 (0%)

All (119) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	651	A
5	A	680	U
5	A	688	A
5	A	692	C
5	A	704	U
5	A	707	C
5	A	721	U
5	A	735	A
5	A	737	C
5	A	738	A
5	A	745	A
5	A	753	A
5	A	759	C
5	A	761	A
5	A	766	G
5	A	777	G
5	A	791	G
5	A	796	G
5	A	812	A
5	A	830	U
5	A	832	U
5	A	835	C
5	A	836	A
5	A	851	A
5	A	860	A
5	A	861	U

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Mol	Chain	Res	Type
5	A	868	C
5	A	871	A
5	A	881	A
5	A	884	U
5	A	889	G
5	A	890	C
5	A	919	A
5	A	923	A
5	A	929	A
5	A	930	G
5	A	933	G
5	A	938	A
5	A	939	A
5	A	941	G
5	A	942	A
5	A	954	C
5	A	957	C
5	A	967	A
5	A	983	C
5	A	985	U
5	A	988	G
5	A	993	A
5	A	1015	A
5	A	1019	A
5	A	1031	G
5	A	1042	U
5	A	1043	C
5	A	1044	U
5	A	1046	A
5	A	1065	C
5	A	1103	A
5	A	1105	C
5	A	1117	A
5	A	1121	A
5	A	1125	A
5	A	1126	A
5	A	1144	U
5	A	1153	C
5	A	1154	A
5	A	1155	G
5	A	1160	A
5	A	1167	A

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Mol	Chain	Res	Type
5	A	1179	G
5	A	1181	G
5	A	1185	C
5	A	1189	U
5	A	1209	C
5	A	1215	U
5	A	1223	C
5	A	1225	C
5	A	1230	C
5	A	1231	A
5	A	1247	G
5	A	1248	C
5	A	1250	C
5	A	1251	A
5	A	1255	U
5	A	1270	U
5	A	1271	C
5	A	1273	G
5	A	1276	A
5	A	1284	U
5	A	1290	C
5	A	1300	A
5	A	1312	C
5	A	1323	G
5	A	1326	A
5	A	1327	G
5	A	1343	A
5	A	1344	U
5	A	1354	A
5	A	1356	A
5	A	1378	C
5	A	1380	G
5	A	1381	A
5	A	1390	A
5	A	1405	C
5	A	1406	U
5	A	1422	G
5	A	1424	U
5	A	1430	A
5	A	1432	U
5	A	1447	G
5	A	1464	G

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Mol	Chain	Res	Type
5	A	1466	C
5	A	1469	G
5	A	1474	G
5	A	1475	C
5	A	1478	A
5	A	1479	C
5	A	1480	A
5	A	1594	G
5	A	1595	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	744	A
5	A	992	U
5	A	1154	A

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 17 ligands modelled in this entry, 13 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	ATP	X	501	33	32,33,33	0.36	0	48,52,52	0.72	1 (2%)
37	GDP	X	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	FES	T	201	24,17	0,4,4	-	-	-		
35	FES	P	201	9,20	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	GDP	X	502	-	-	3/16/32/32	0/3/3/3
35	FES	P	201	9,20	-	-	0/1/1/1
35	FES	T	201	24,17	-	-	0/1/1/1
36	ATP	X	501	33	-	7/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	502	GDP	C5-C4	2.97	1.46	1.38
37	X	502	GDP	C6-N1	-2.46	1.34	1.38
37	X	502	GDP	C5-N7	-2.14	1.34	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	X	502	GDP	C5-C4-N3	-5.96	118.91	128.39
37	X	502	GDP	C2-N3-C4	4.87	120.69	112.30
37	X	502	GDP	N9-C4-N3	4.30	134.55	125.95
37	X	502	GDP	C6-C5-N7	3.23	136.18	130.29
37	X	502	GDP	C4-C5-N7	-2.59	106.56	110.67
37	X	502	GDP	C3'-C2'-C1'	2.43	106.05	101.46
36	X	501	ATP	O3'-C3'-C2'	-2.03	105.30	111.82
37	X	502	GDP	O6-C6-C5	-2.02	121.20	126.53

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	X	501	ATP	PB-O3B-PG-O2G
36	X	501	ATP	C5'-O5'-PA-O2A
36	X	501	ATP	C5'-O5'-PA-O3A
37	X	502	GDP	C5'-O5'-PA-O3A

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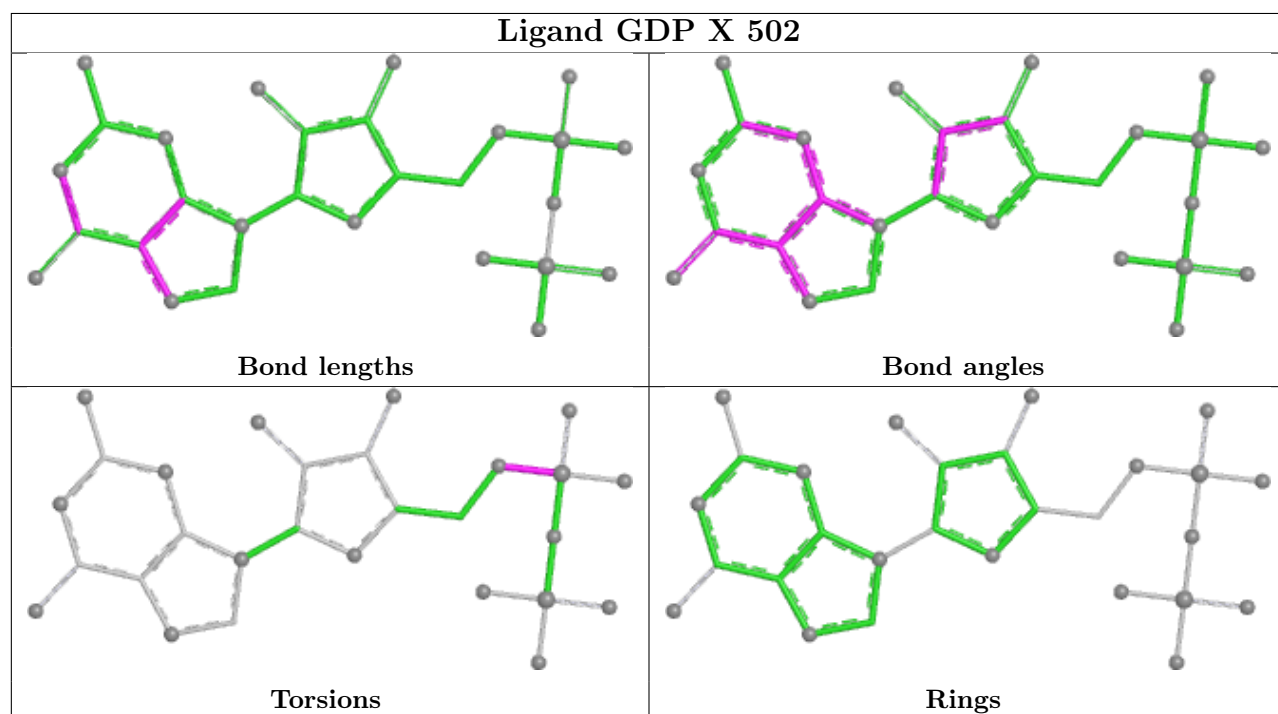
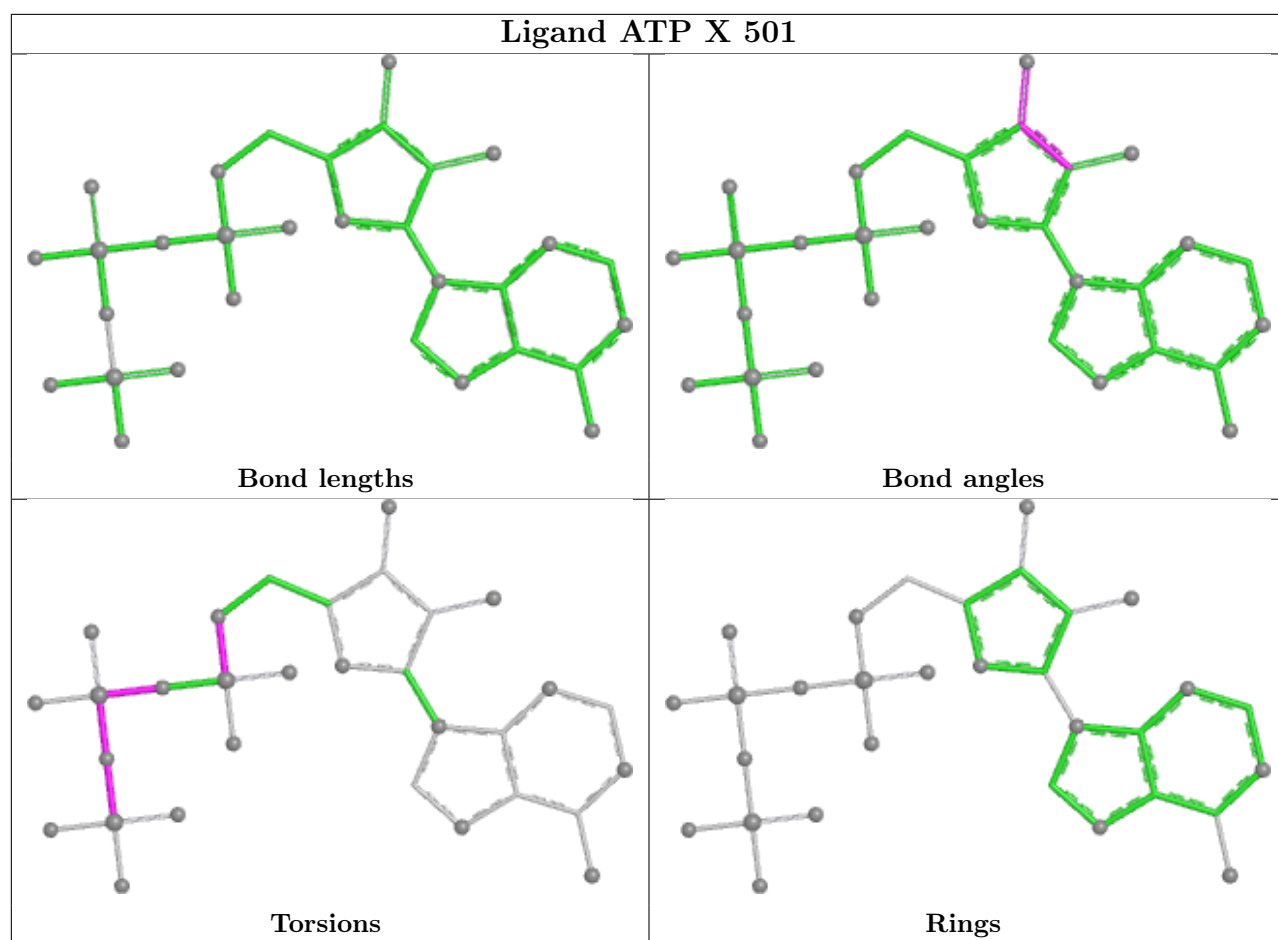
Mol	Chain	Res	Type	Atoms
37	X	502	GDP	C5'-O5'-PA-O1A
37	X	502	GDP	C5'-O5'-PA-O2A
36	X	501	ATP	PB-O3B-PG-O3G
36	X	501	ATP	PB-O3B-PG-O1G
36	X	501	ATP	PG-O3B-PB-O2B
36	X	501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	X	501	ATP	2	0
37	X	502	GDP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

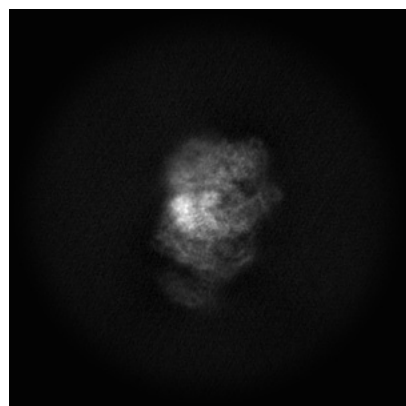
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51083. These allow visual inspection of the internal detail of the map and identification of artifacts.

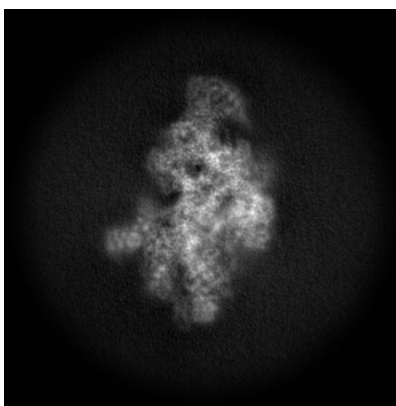
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

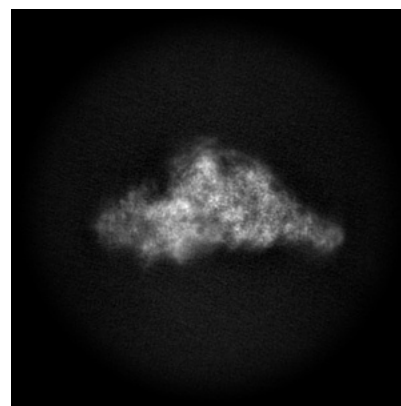
6.1.1 Primary map



X

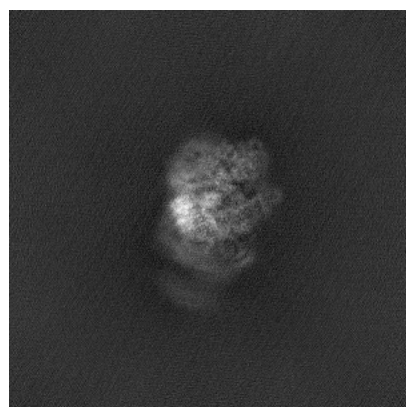


Y

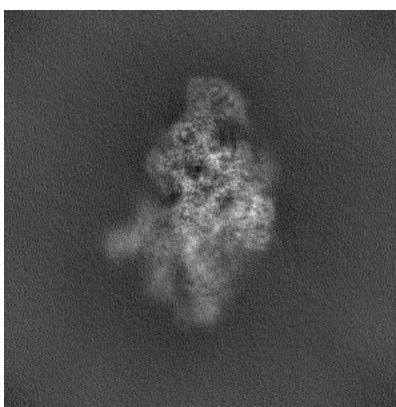


Z

6.1.2 Raw map



X



Y

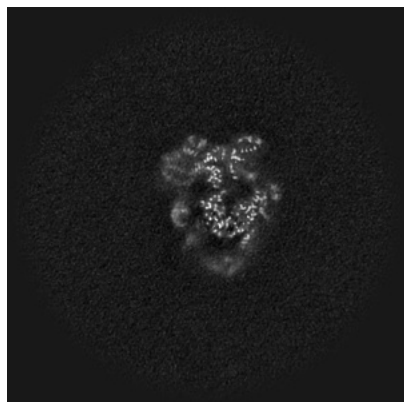


Z

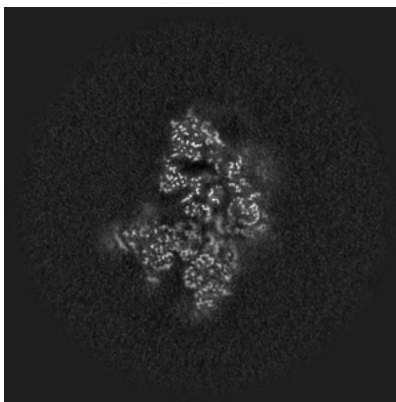
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

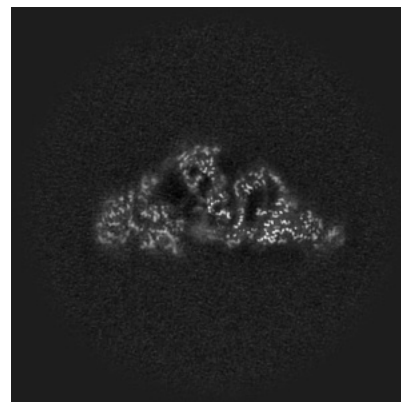
6.2.1 Primary map



X Index: 220

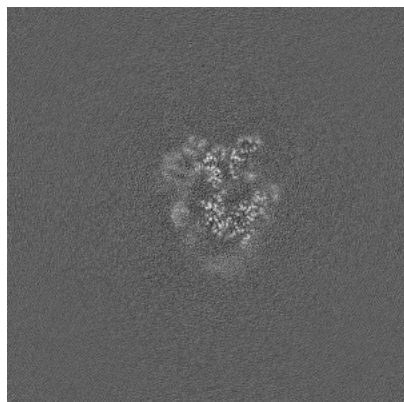


Y Index: 220

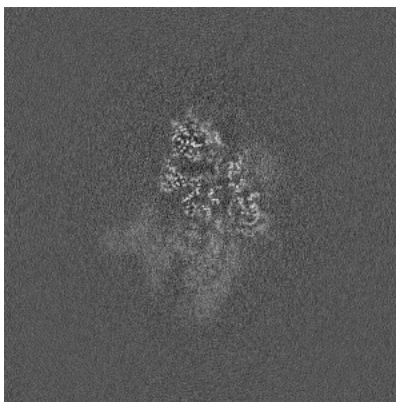


Z Index: 220

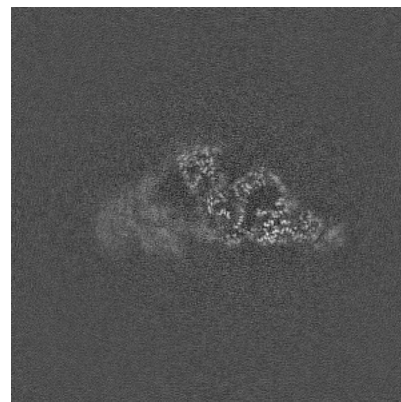
6.2.2 Raw map



X Index: 220



Y Index: 220

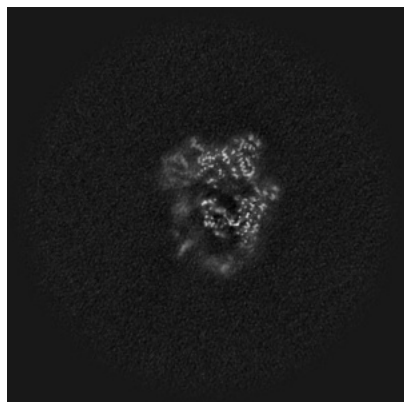


Z Index: 220

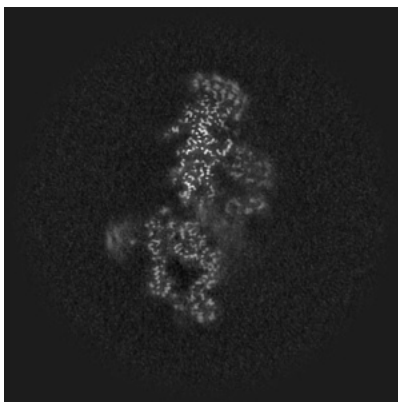
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

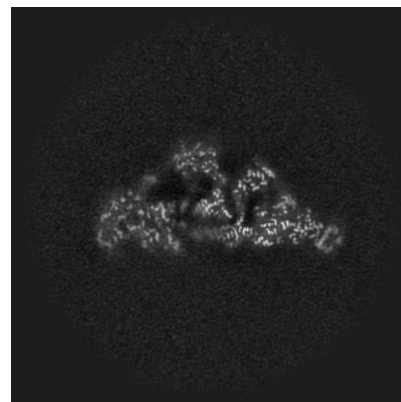
6.3.1 Primary map



X Index: 215



Y Index: 195

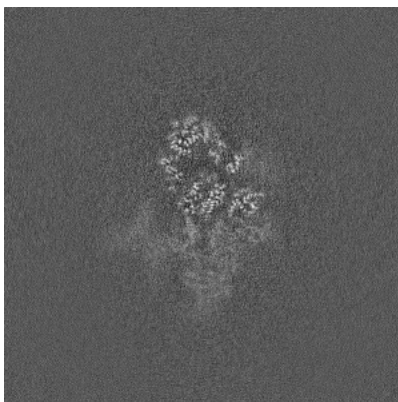


Z Index: 224

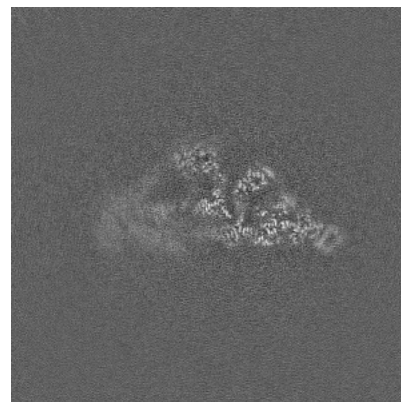
6.3.2 Raw map



X Index: 215



Y Index: 224

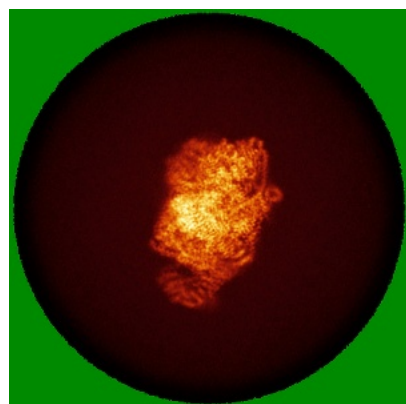


Z Index: 224

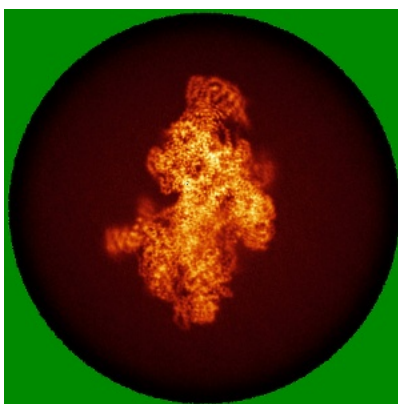
The images above show the largest variance slices of the map in three orthogonal directions.

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

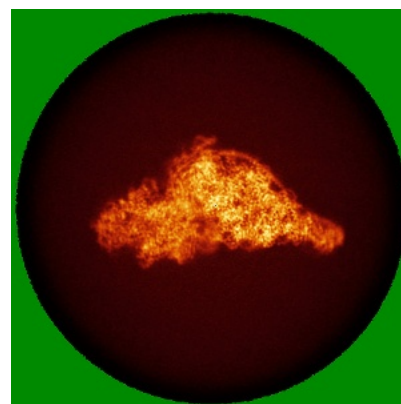
6.4.1 Primary map



X

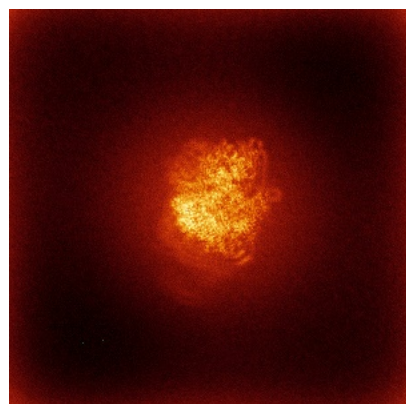


Y

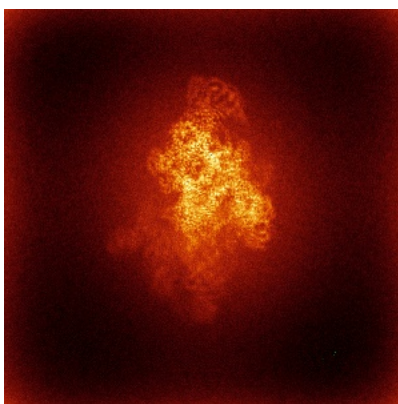


Z

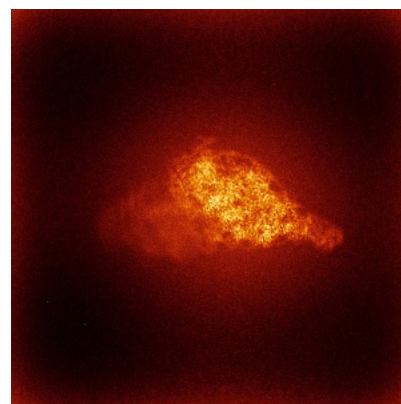
6.4.2 Raw map



X



Y

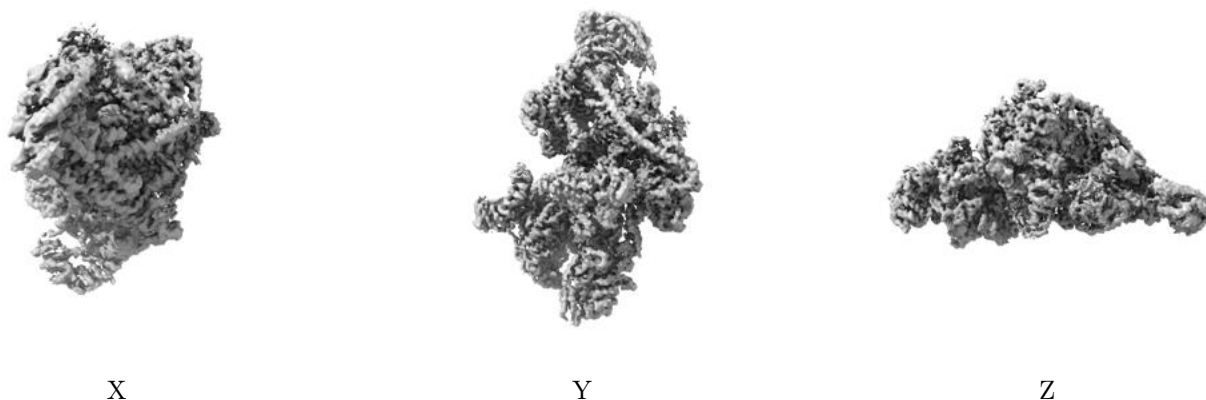


Z

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.

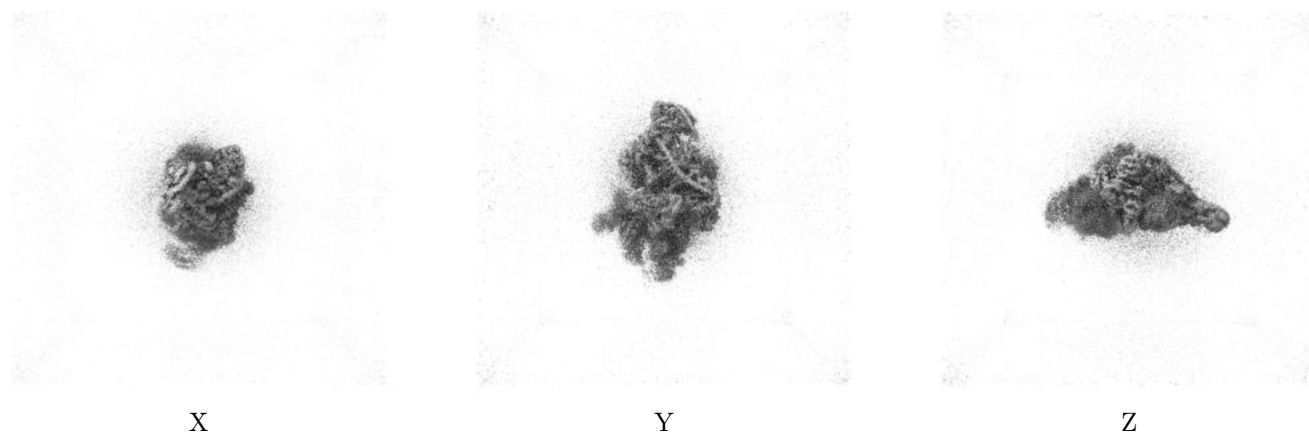
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.296. 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.

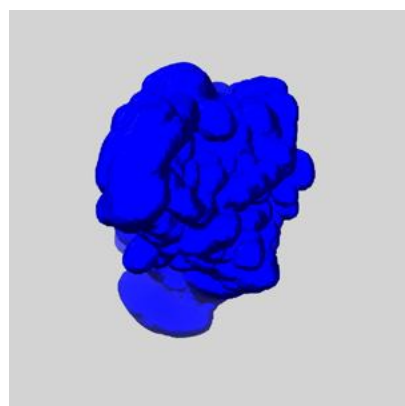
6.6 Mask visualisation [i](#)

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

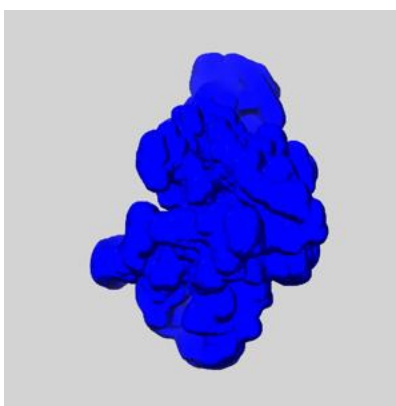
A mask typically either:

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

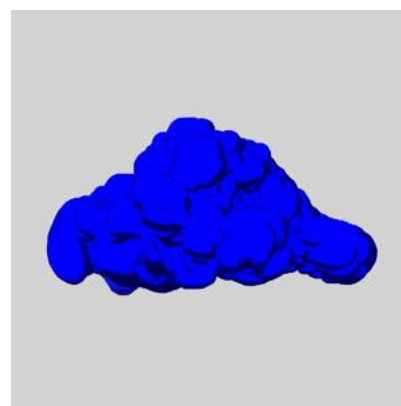
6.6.1 emd_51083_msk_1.map [i](#)



X



Y

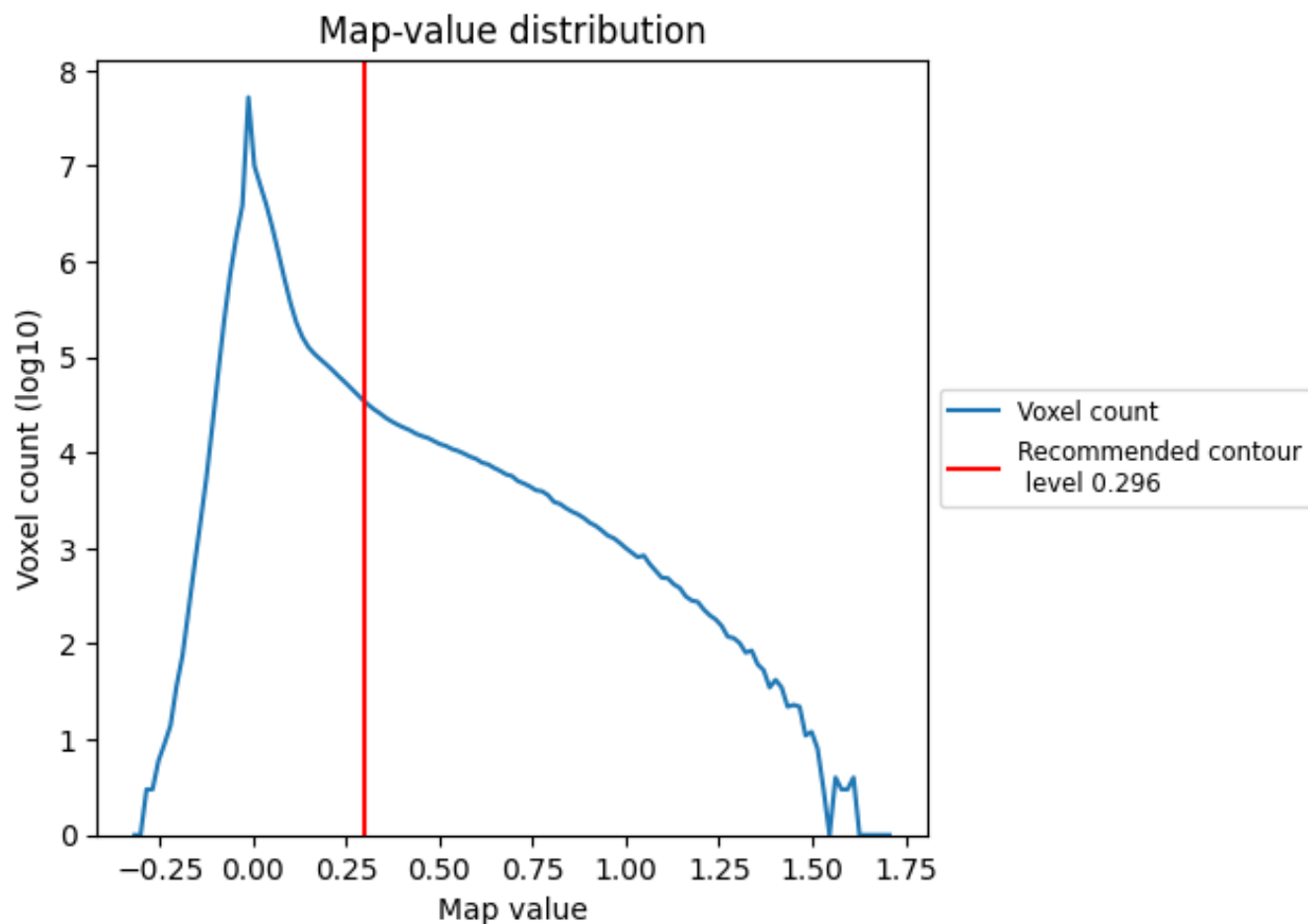


Z

7 Map analysis [i](#)

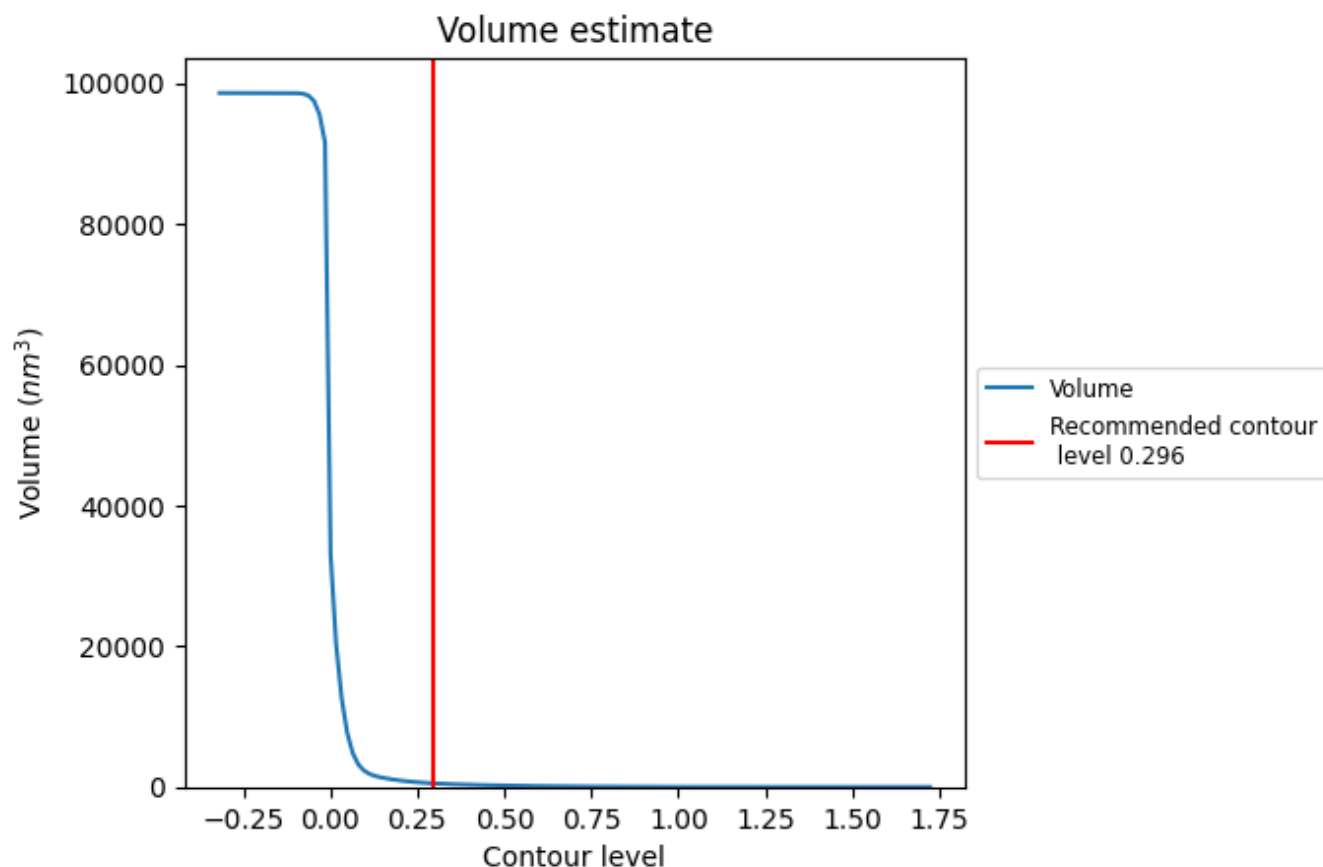
This section contains the results of statistical analysis of the map.

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.

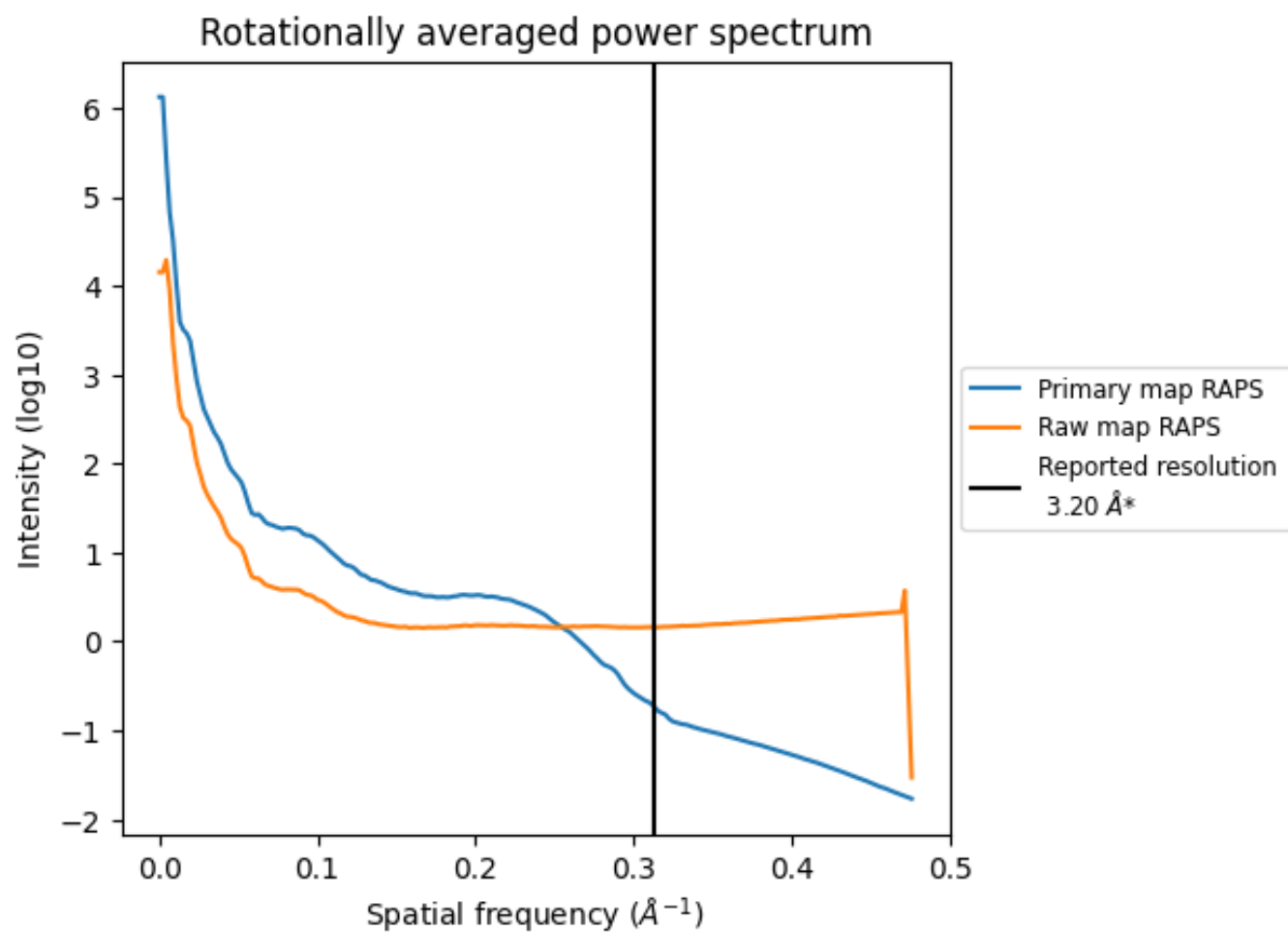
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 515 nm^3 ; this corresponds to an approximate mass of 465 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 ⓘ

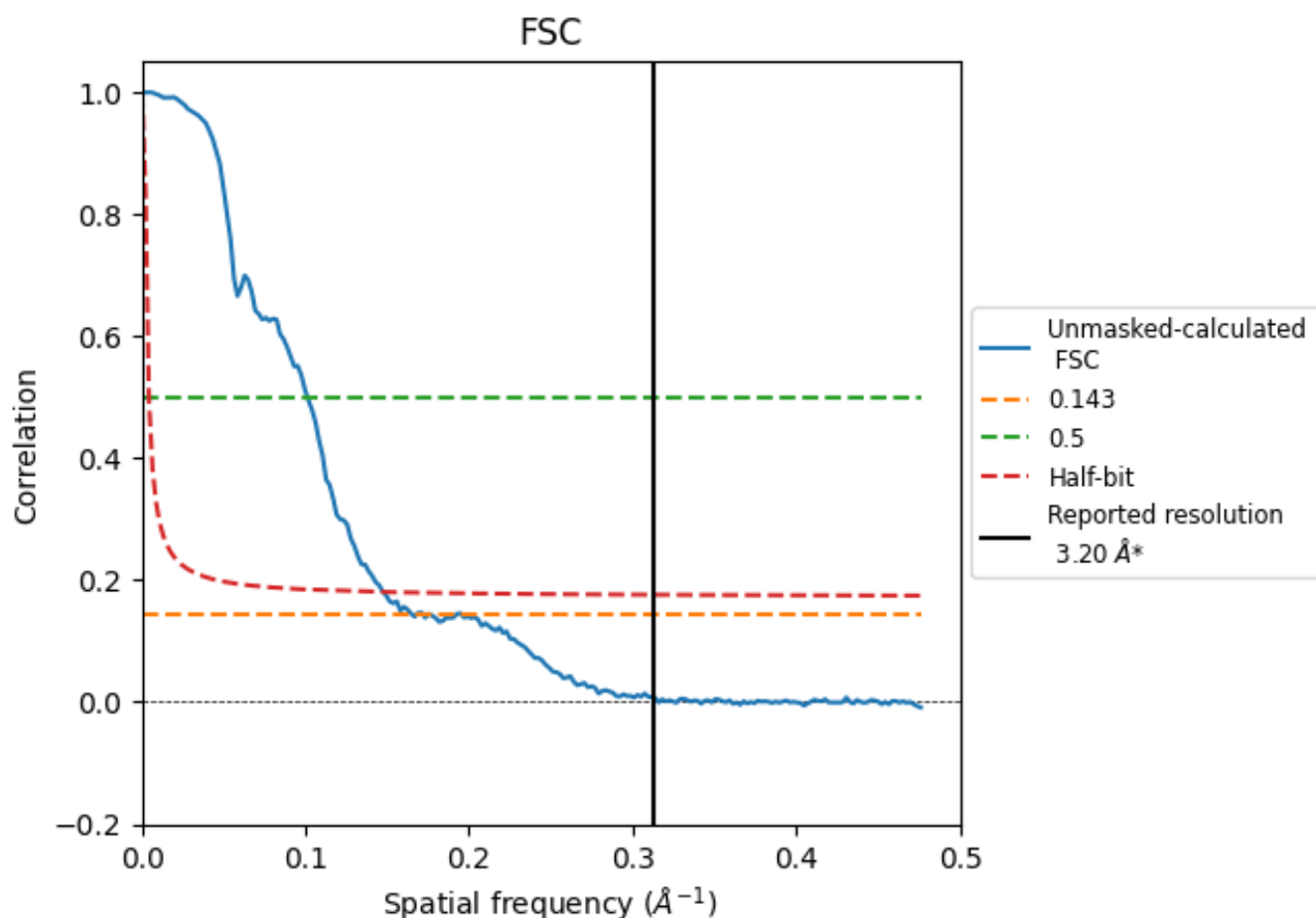


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

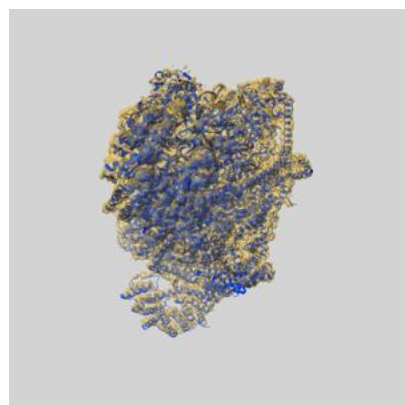
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.05	9.89	6.78

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

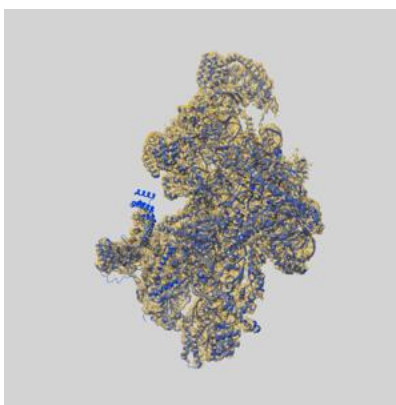
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51083 and PDB model 9G5B. Per-residue inclusion information can be found in section [3](#) on page [12](#).

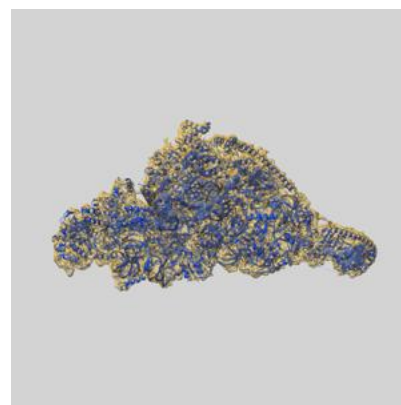
9.1 Map-model overlay [i](#)



X



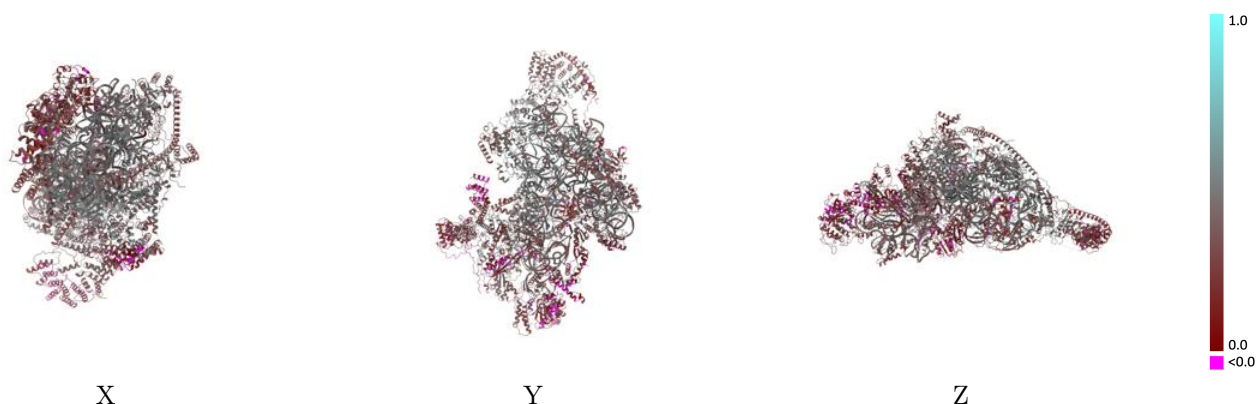
Y



Z

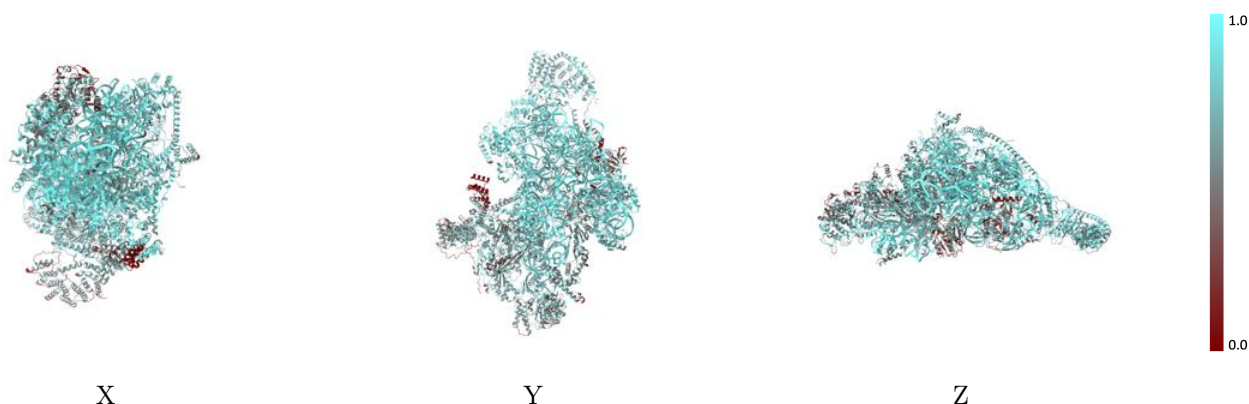
The images above show the 3D surface view of the map at the recommended contour level 0.296 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



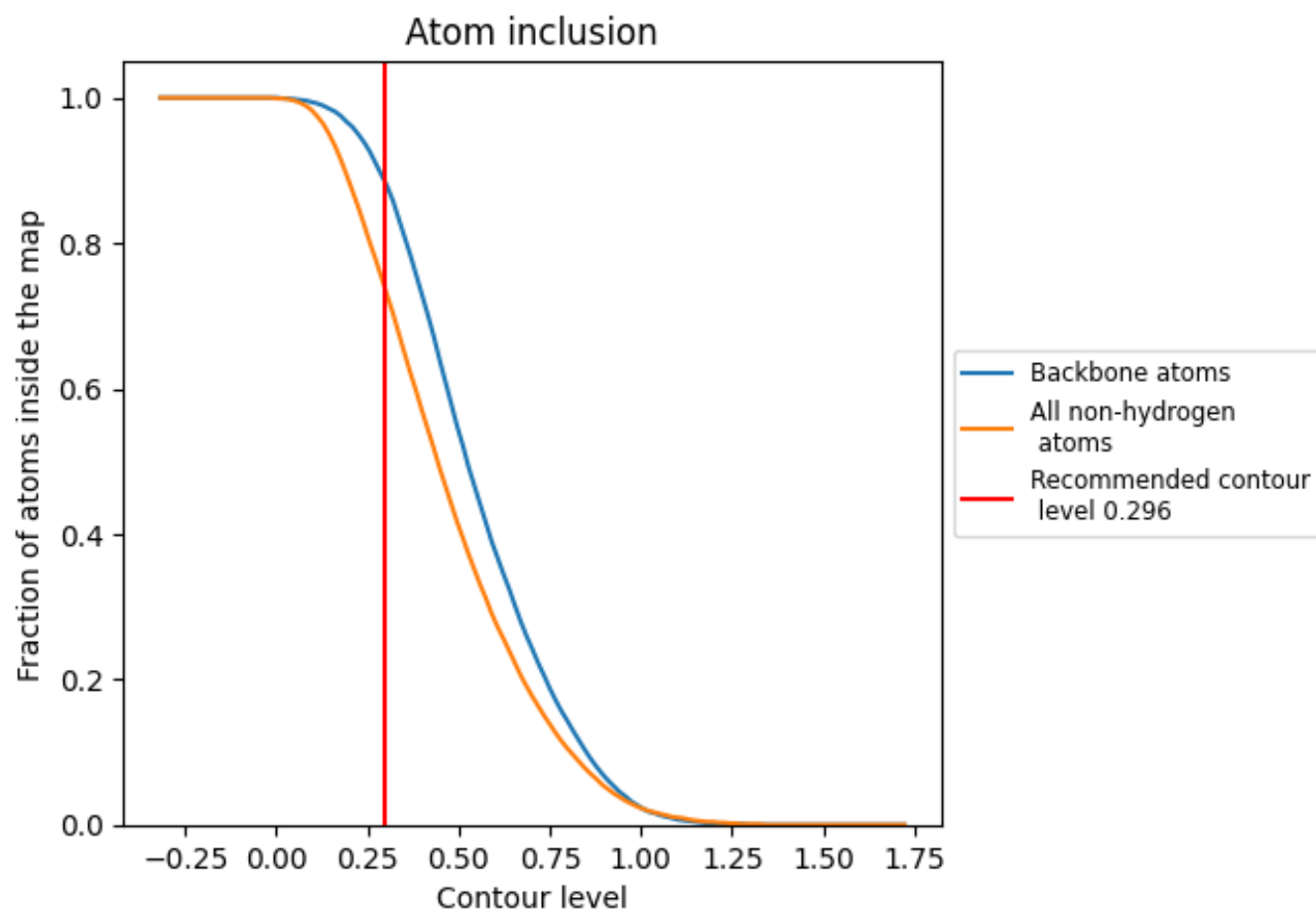
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.296).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 74% 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 (0.296) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7400	 0.3560
0	 0.7990	 0.4300
1	 0.6730	 0.3460
4	 0.4900	 0.2070
9	 0.4710	 0.2880
A	 0.9280	 0.4330
B	 0.8610	 0.4450
C	 0.6610	 0.3590
D	 0.7260	 0.4240
E	 0.6970	 0.3550
F	 0.5610	 0.1650
G	 0.6940	 0.3090
H	 0.4570	 0.1250
I	 0.7200	 0.3150
J	 0.6910	 0.3550
K	 0.7490	 0.3680
L	 0.7160	 0.3790
M	 0.8680	 0.4760
N	 0.8630	 0.4720
O	 0.8720	 0.4720
P	 0.8030	 0.4210
Q	 0.7540	 0.3990
R	 0.8400	 0.4340
S	 0.7640	 0.3670
T	 0.8300	 0.4620
U	 0.7740	 0.3800
V	 0.7130	 0.2920
W	 0.8000	 0.4200
X	 0.6110	 0.2000
Y	 0.6090	 0.3290
Z	 0.6170	 0.3000
a	 0.5930	 0.3090
c	 0.4650	 0.2190

