



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:59 PM UTC

PDB ID : 8OIS / pdb_00008ois
EMDB ID : EMD-16898
Title : 28S human mitochondrial small ribosomal subunit with mtRF1 and P-site tRNA
Authors : Saurer, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Ban, N.
Deposited on : 2023-03-23
Resolution : 3.00 Å (reported)
Based on initial models : 7QI4, .

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 EMD 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

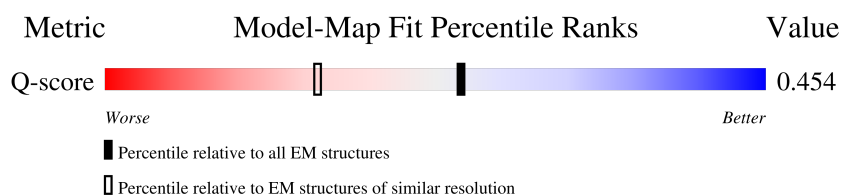
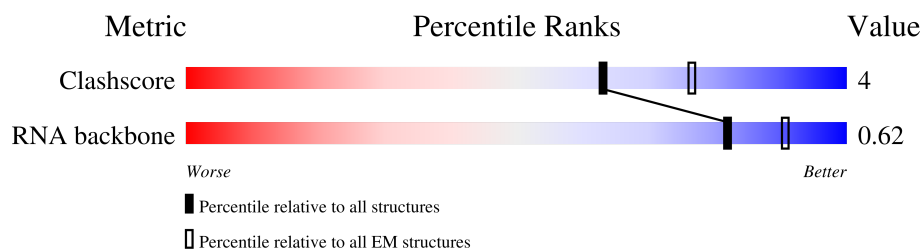
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

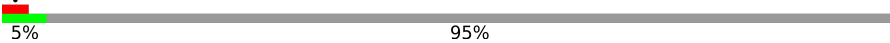
The reported resolution of this entry is 3.00 Å.

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	-
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	BX	292	
2	Bd	128	
3	AA	955	
4	AB	323	
5	AC	167	

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Mol	Chain	Length	Quality of chain
6	AD	199	
7	AE	125	
8	AF	242	
9	AG	71	
10	AH	201	
11	AI	33	
12	AJ	138	
13	AK	128	
14	AL	257	
15	AM	137	
16	AN	130	
17	AO	258	
18	AP	142	
19	AQ	87	
20	AR	360	
21	AS	190	
22	AT	173	
23	AU	205	
24	AV	414	
25	AW	187	
26	AX	398	
27	AY	395	
28	AZ	106	
29	Aa	484	
30	Ab	296	

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Mol	Chain	Length	Quality of chain
31	Ac	118	
32	Ad	430	
33	Ae	689	
34	Ag	396	
35	Ai	194	
36	Aj	218	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 72671 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 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	BX	14	Total	C	N	O	0	0
			113	74	22	17		

- Molecule 2 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Bd	26	Total	C	N	O	0	0
			241	150	45	46		

- Molecule 3 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AA	955	Total	C	N	O	P	0	0
			20283	9098	3652	6578	955		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	62	G	A	variant	GB OM714795.1

- Molecule 4 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AB	279	Total	C	N	O	S	0	0
			2265	1435	387	432	11		

- Molecule 5 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 6 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AD	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 7 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 8 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AF	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 9 is a RNA chain called P-site Met-tRNA(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AG	71	Total	C	N	O	P	0	0
			1504	674	264	495	71		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	69	C	-	insertion	GB NC_012920.1
AG	70	C	-	insertion	GB NC_012920.1

- Molecule 10 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AH	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 11 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AI	33	Total	C	N	O	P	0	0
			463	198	29	203	33		

- Molecule 12 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 13 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 14 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AL	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 15 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 16 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AN	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 17 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 18 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AP	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 19 is a protein called 28S ribosomal protein S21, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 20 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AR	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 21 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 22 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 23 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 24 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 25 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AW	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 26 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 27 is a protein called 28S ribosomal protein S31, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AZ	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 29 is a protein called Peptide chain release factor 1, mitochondrial,mtRF1(AAQ).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aa	381	Total	C	N	O	S	0	0
			3114	1940	569	592	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	311	ALA	GLY	engineered mutation	UNP O75570
Aa	312	ALA	GLY	engineered mutation	UNP O75570

- Molecule 30 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ab	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 31 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ac	117	Total	C	N	O	S	0	0
			935	579	182	166	8		

- Molecule 32 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ad	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 33 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ae	588	Total	C	N	O	S	0	0
			4768	3053	808	879	28		

- Molecule 34 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ag	327	Total	C	N	O	S	0	0
			2688	1710	477	487	14		

- Molecule 35 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ai	137	Total	C	N	O	S	0	0
			1020	642	192	182	4		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 36 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Aj	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

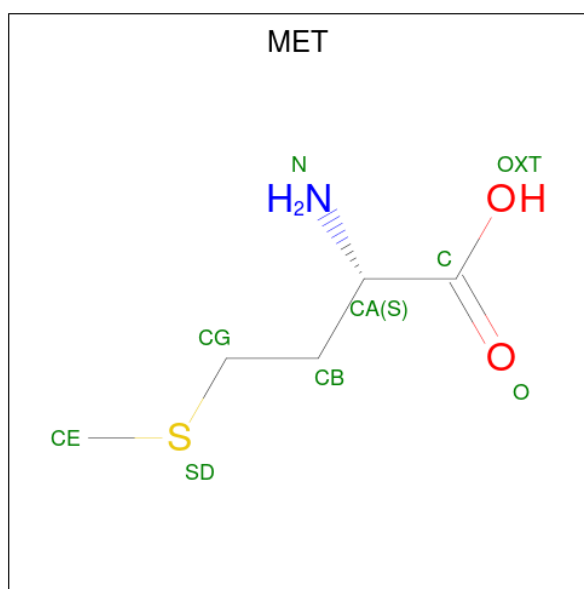
- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
37	AA	16	Total	K	0
			16	16	
37	Ae	1	Total	K	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
38	AA	120	Total	Mg	0
			120	120	
38	AD	1	Total	Mg	0
			1	1	
38	AG	1	Total	Mg	0
			1	1	
38	AU	1	Total	Mg	0
			1	1	
38	AX	1	Total	Mg	0
			1	1	
38	Ab	1	Total	Mg	0
			1	1	
38	Ad	1	Total	Mg	0
			1	1	

- Molecule 39 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).

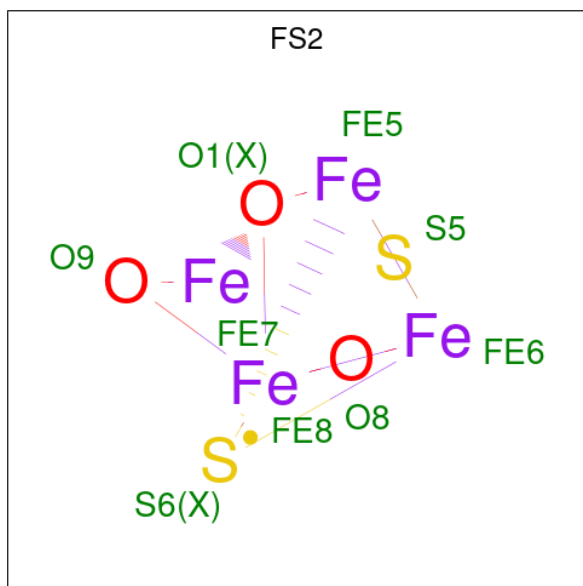


Mol	Chain	Residues	Atoms					AltConf
39	AG	1	Total	C	N	O	S	0
			8	5	1	1	1	

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

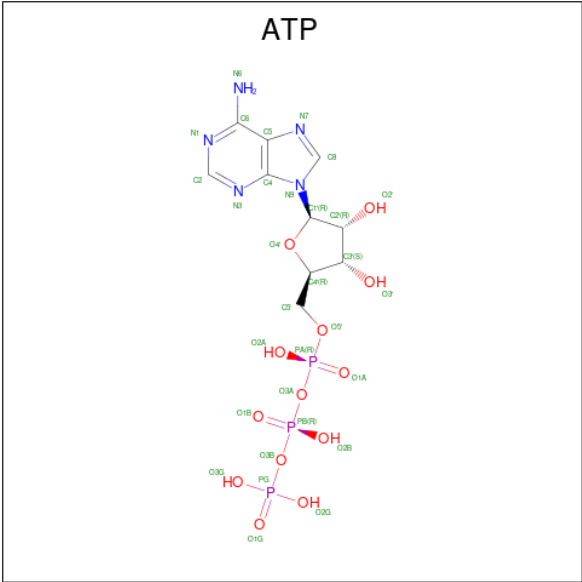
Mol	Chain	Residues	Atoms		AltConf
40	AO	1	Total	Zn	0
			1	1	

- Molecule 41 is FE-S-O HYBRID CLUSTER (CCD ID: FS2) (formula: Fe₄O₃S₂).



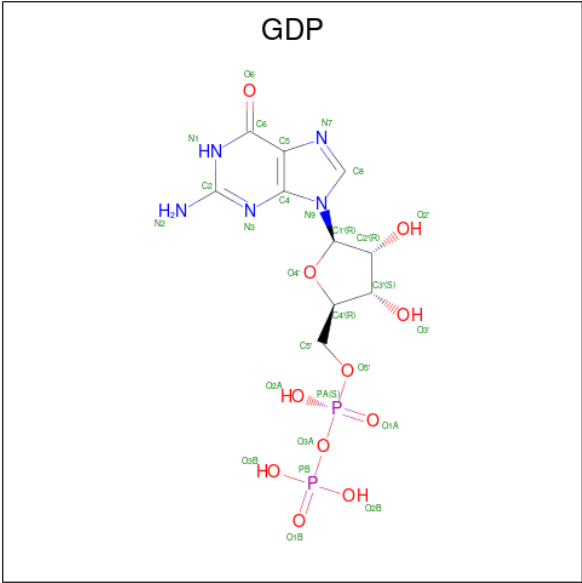
Mol	Chain	Residues	Atoms			AltConf
41	AP	1	Total	Fe	S	0
			4	2	2	
41	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 42 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

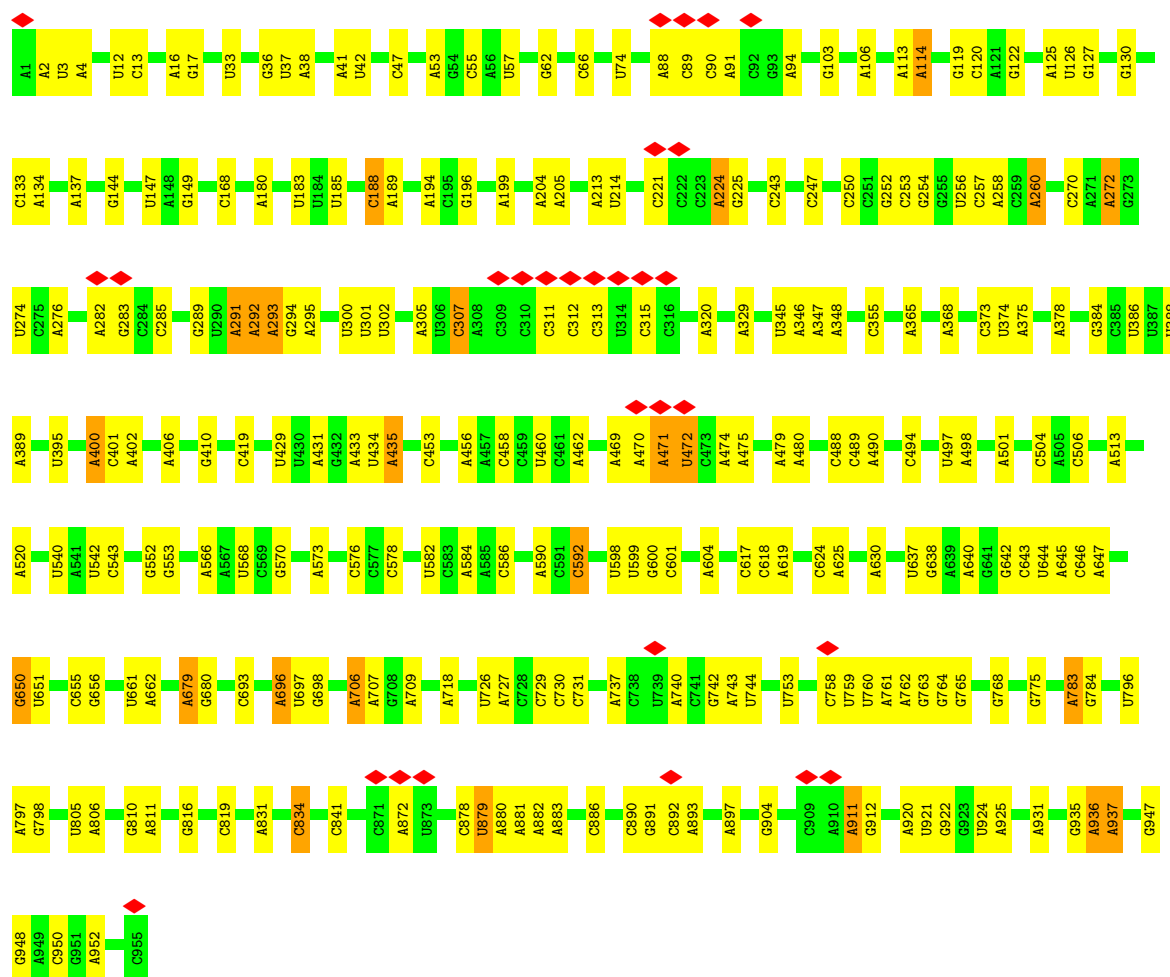
- Molecule 43 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



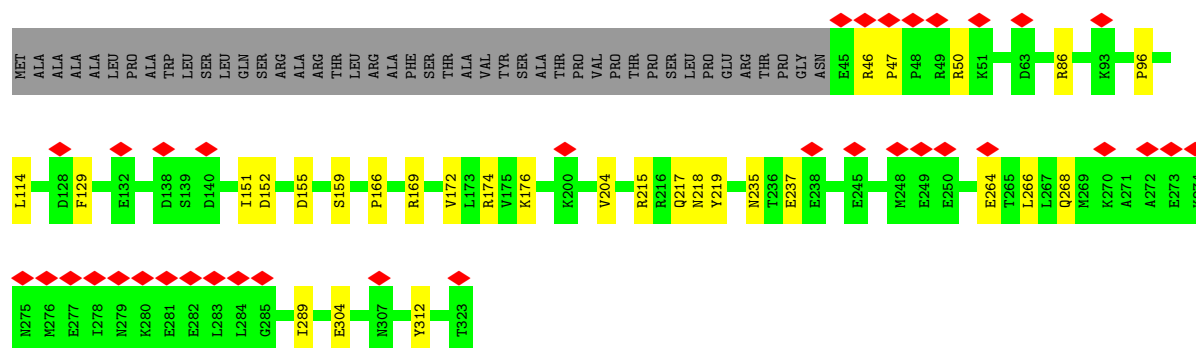
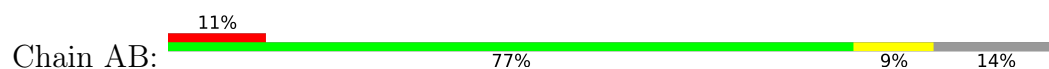
Mol	Chain	Residues	Atoms					AltConf
43	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 44 is water.

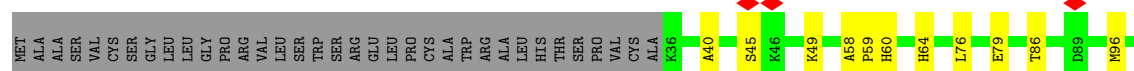
Mol	Chain	Residues	Atoms		AltConf
44	AX	3	Total 3	O 3	0



• Molecule 4: 28S ribosomal protein S35, mitochondrial

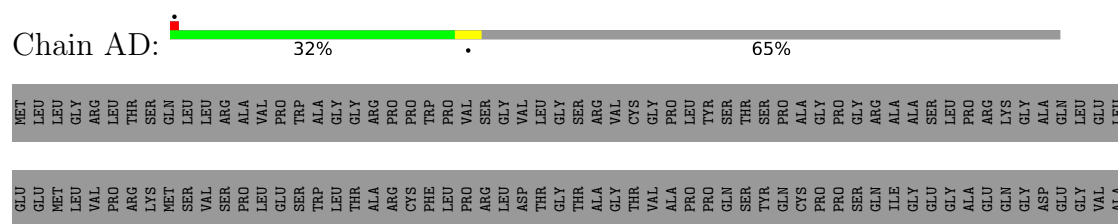


• Molecule 5: 28S ribosomal protein S24, mitochondrial

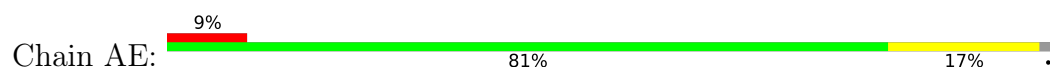




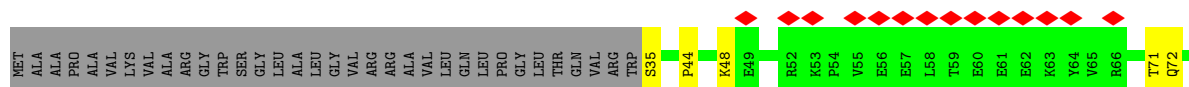
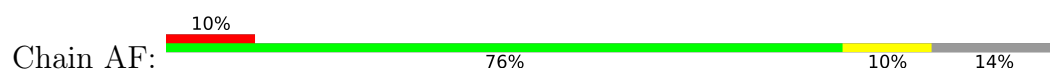
- Molecule 6: Aurora kinase A-interacting protein



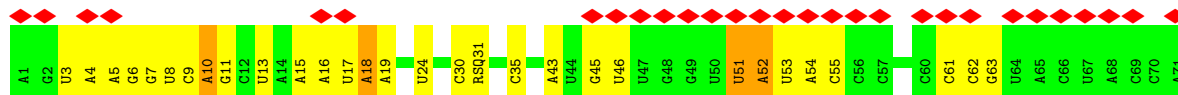
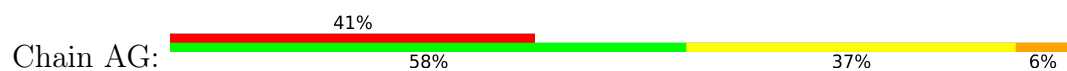
- Molecule 7: 28S ribosomal protein S6, mitochondrial



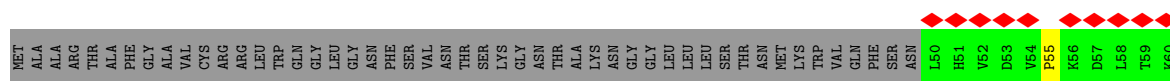
- Molecule 8: 28S ribosomal protein S7, mitochondrial

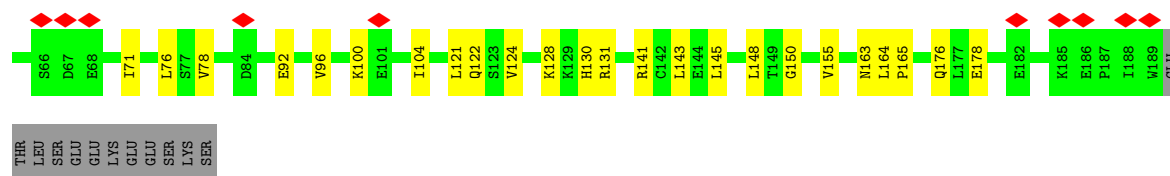


- Molecule 9: P-site Met-tRNA(Met)

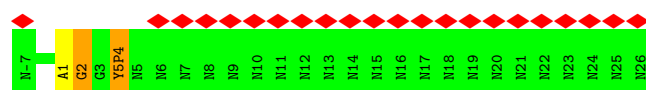
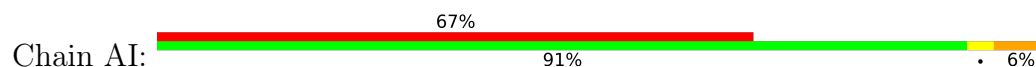


- Molecule 10: 28S ribosomal protein S10, mitochondrial

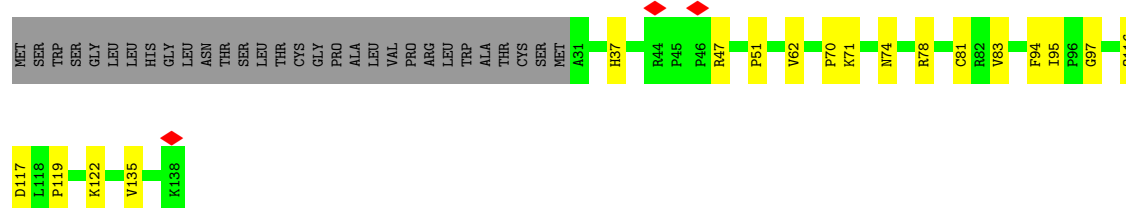




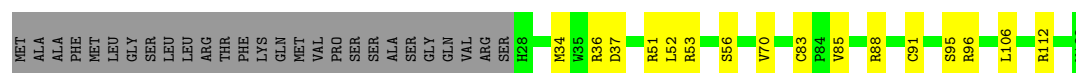
- Molecule 11: mRNA



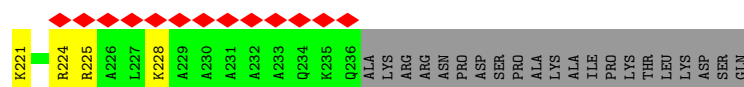
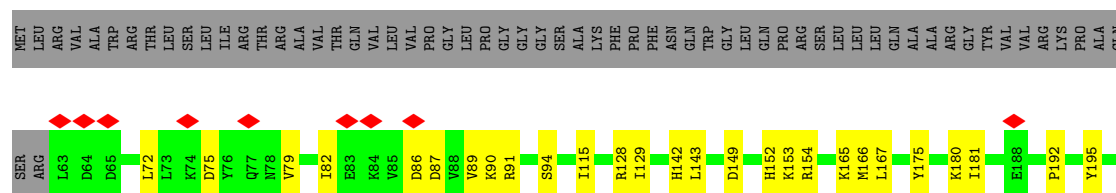
- Molecule 12: 28S ribosomal protein S12, mitochondrial



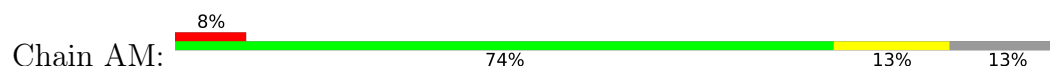
- Molecule 13: 28S ribosomal protein S14, mitochondrial



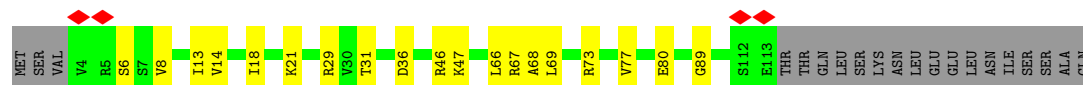
- Molecule 14: 28S ribosomal protein S15, mitochondrial



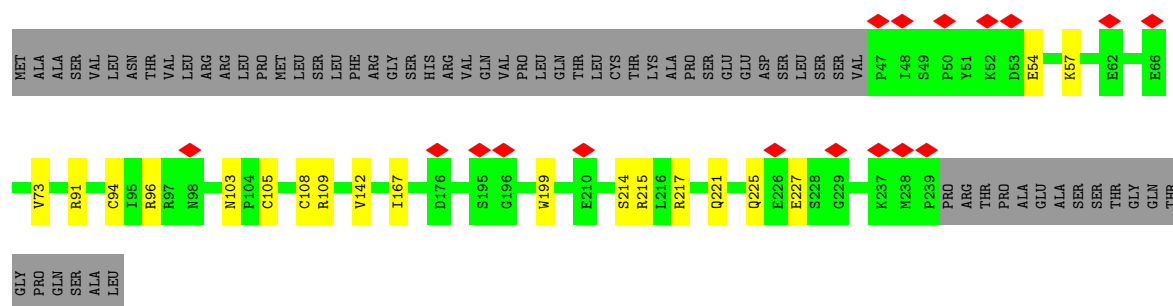
- Molecule 15: 28S ribosomal protein S16, mitochondrial



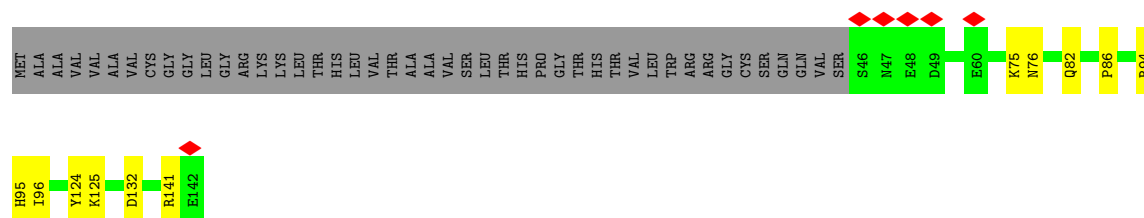
- Molecule 16: 28S ribosomal protein S17, mitochondrial



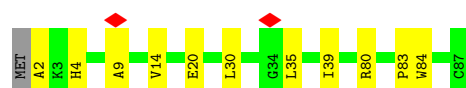
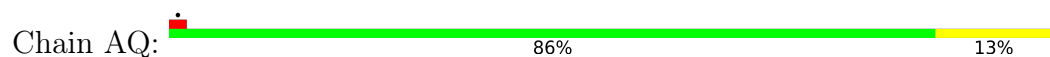
- Molecule 17: 28S ribosomal protein S18b, mitochondrial



- Molecule 18: 28S ribosomal protein S18c, mitochondrial

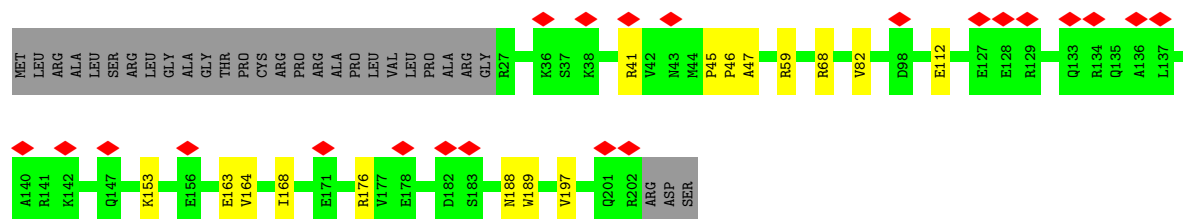
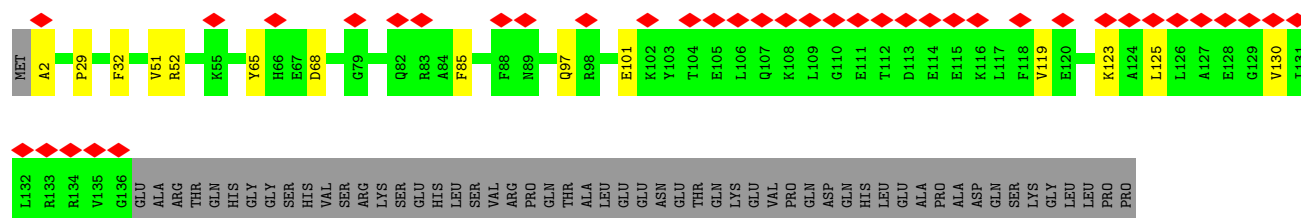
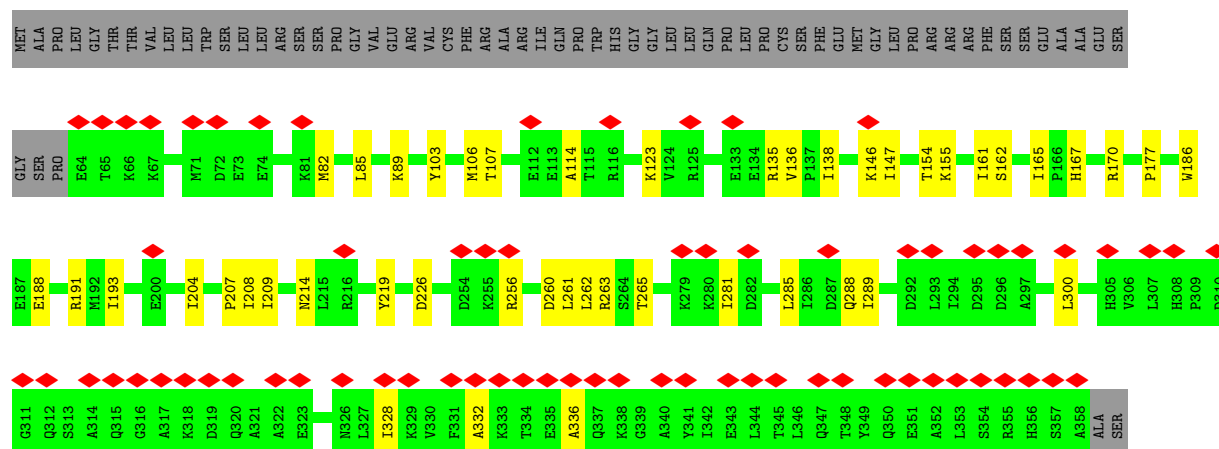


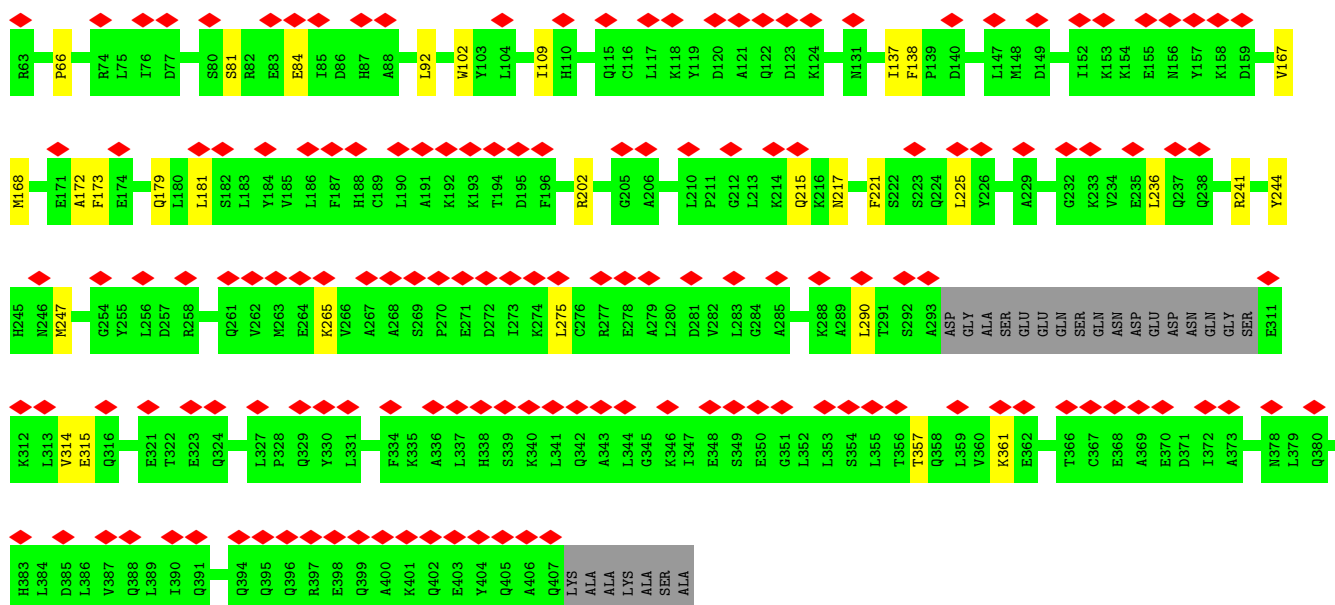
- Molecule 19: 28S ribosomal protein S21, mitochondrial



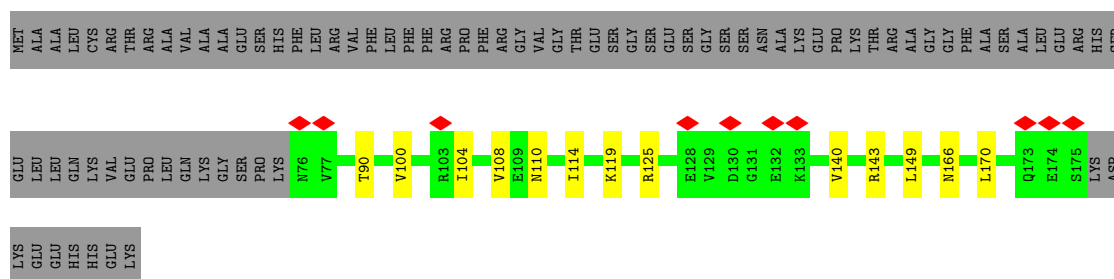
- Molecule 20: 28S ribosomal protein S22, mitochondrial



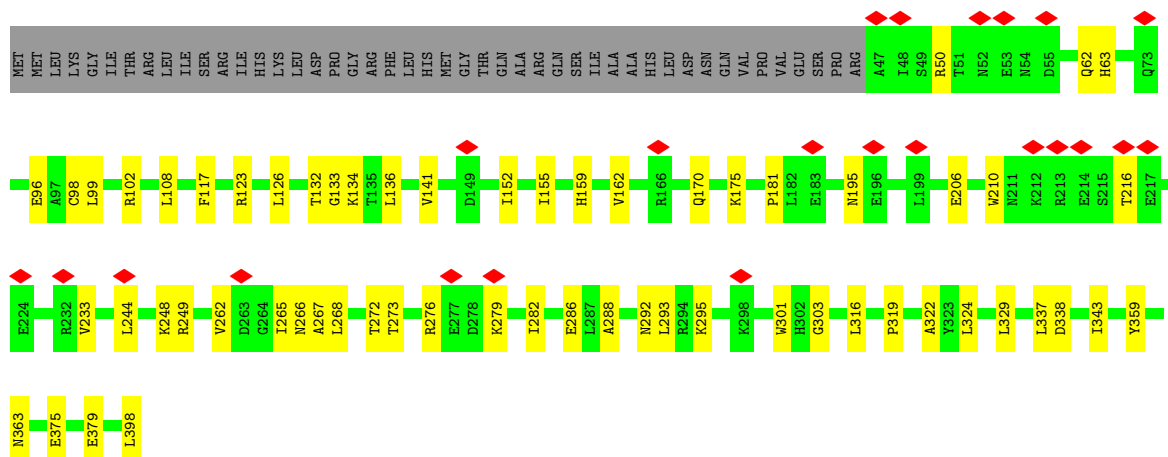
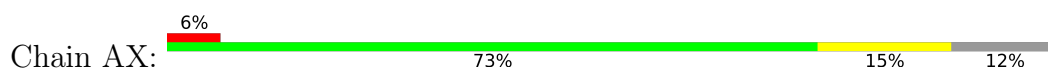




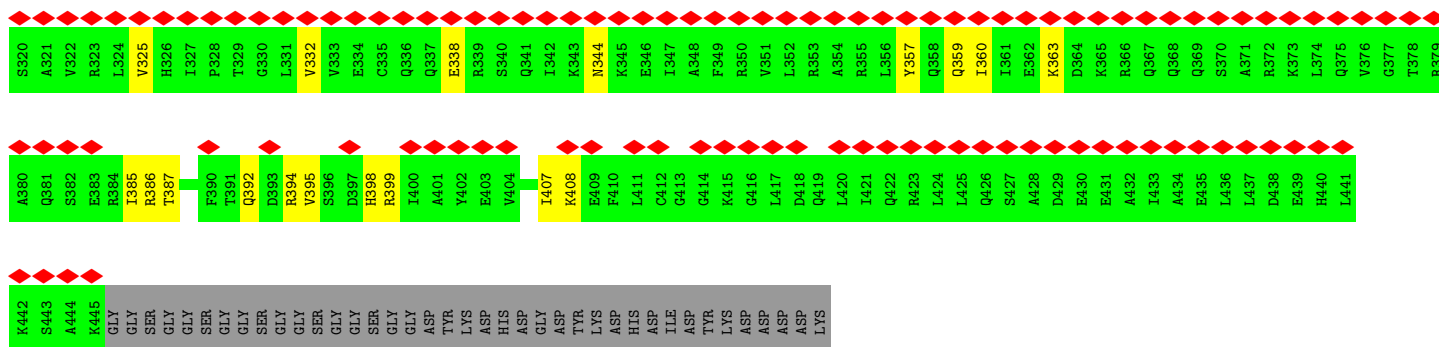
- Molecule 25: 28S ribosomal protein S28, mitochondrial



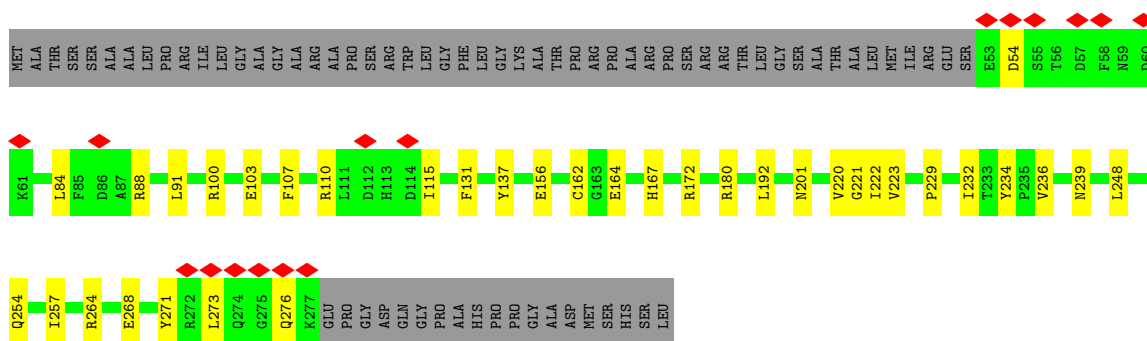
- Molecule 26: 28S ribosomal protein S29, mitochondrial



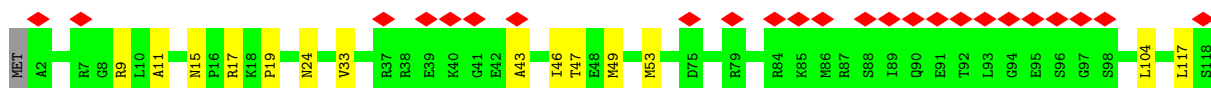
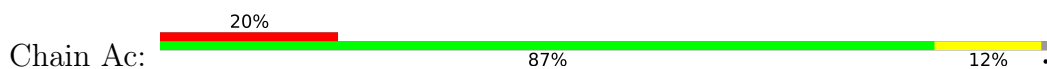
- Molecule 27: 28S ribosomal protein S31, mitochondrial



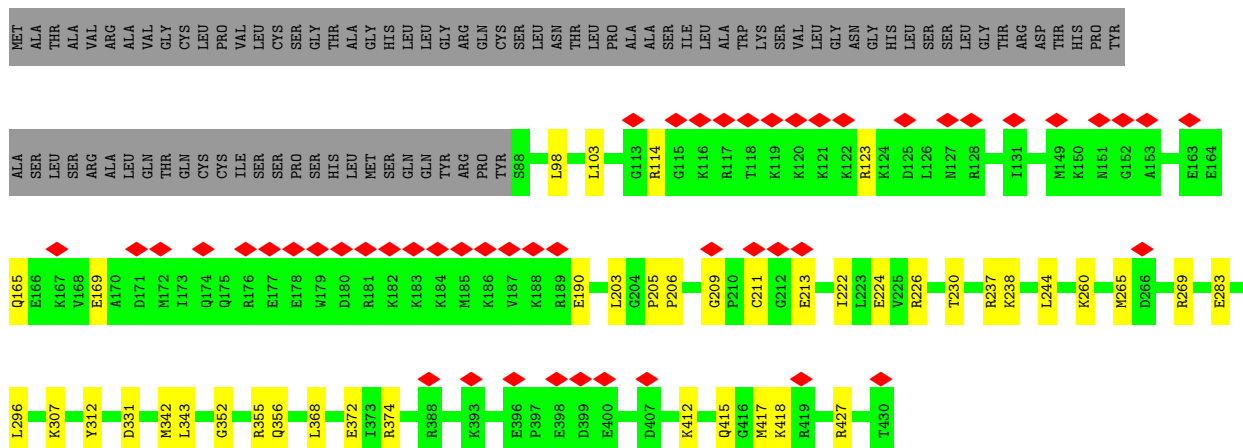
- Molecule 30: 28S ribosomal protein S2, mitochondrial



- Molecule 31: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

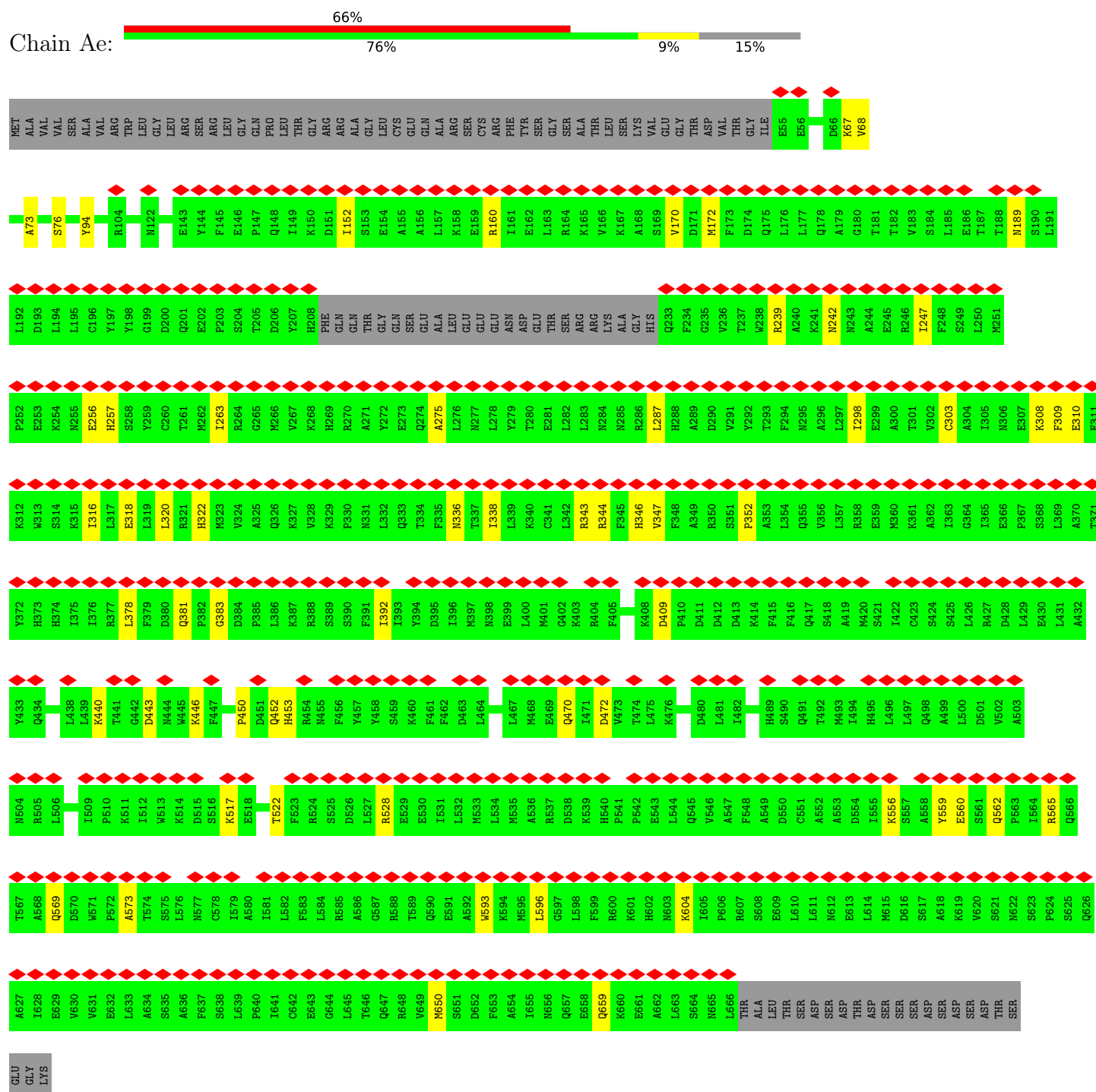


- Molecule 32: 28S ribosomal protein S5, mitochondrial



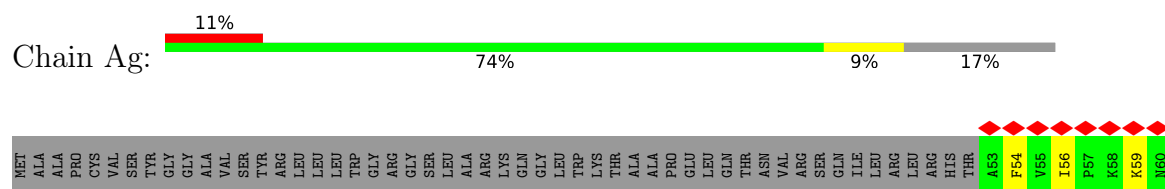
• Molecule 33: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

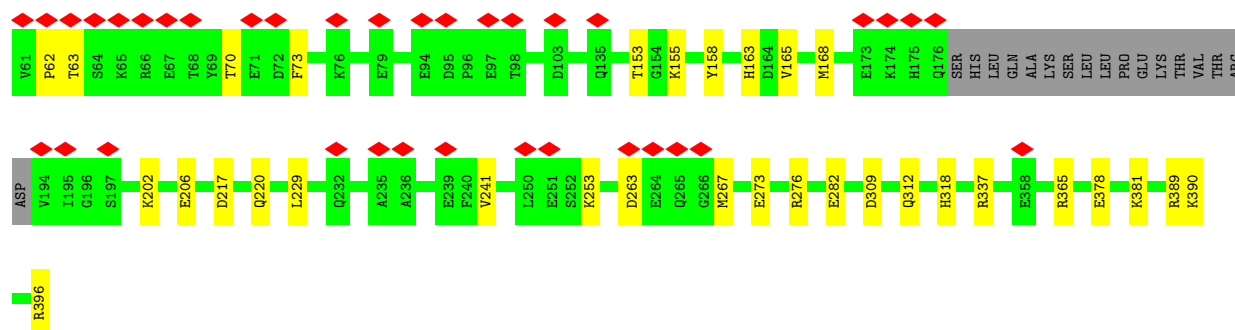
Chain Ae:



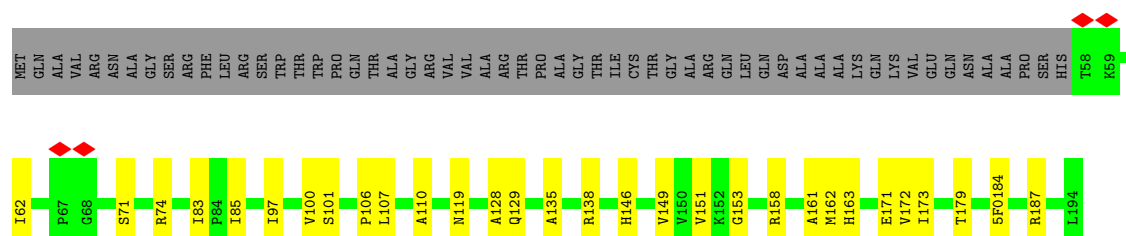
• Molecule 34: 28S ribosomal protein S9, mitochondrial

Chain Ag:

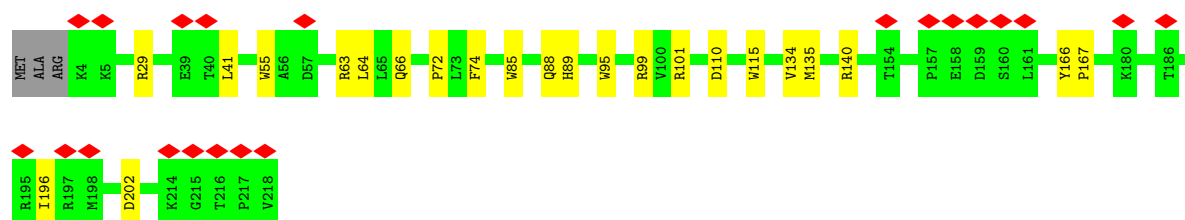
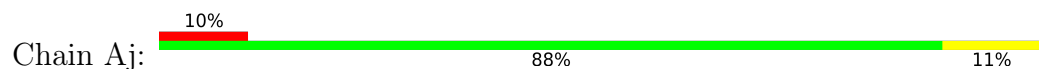




- Molecule 35: 28S ribosomal protein S11, mitochondrial



- Molecule 36: 28S ribosomal protein S34, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.409	Depositor
Minimum map value	-1.537	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.115	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, Y5P, 5MU, 5MC, RSQ, MG, K, GDP, PSU, FS2, 5F0, AYA, MA6, B8T, ATP

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	BX	0.06	0/118	0.19	0/162
2	Bd	0.06	0/246	0.20	0/329
3	AA	0.09	0/22563	0.13	0/35124
4	AB	0.08	0/2313	0.18	0/3129
5	AC	0.09	0/1113	0.20	0/1505
6	AD	0.08	0/636	0.18	0/839
7	AE	0.08	0/989	0.19	0/1335
8	AF	0.07	0/1767	0.17	0/2373
9	AG	0.06	0/1588	0.13	0/2466
10	AH	0.09	0/1178	0.22	0/1598
11	AI	0.07	0/149	0.13	0/231
12	AJ	0.09	0/855	0.20	0/1148
13	AK	0.09	0/880	0.18	0/1182
14	AL	0.07	0/1477	0.16	0/1974
15	AM	0.09	0/963	0.19	0/1295
16	AN	0.09	0/886	0.21	0/1199
17	AO	0.08	0/1648	0.20	0/2243
18	AP	0.08	0/798	0.20	0/1070
19	AQ	0.08	0/748	0.18	0/994
20	AR	0.07	0/2456	0.17	0/3317
21	AS	0.07	0/1138	0.15	0/1533
22	AT	0.09	0/1402	0.19	0/1883
23	AU	0.06	0/1510	0.15	0/2025
24	AV	0.06	0/3030	0.16	0/4093
25	AW	0.08	0/801	0.18	0/1079
26	AX	0.08	0/2921	0.19	0/3954
27	AY	0.06	0/1280	0.16	0/1725
28	AZ	0.08	0/857	0.17	0/1141
29	Aa	0.07	0/3162	0.17	0/4253
30	Ab	0.09	0/1871	0.20	0/2531
31	Ac	0.07	0/941	0.18	0/1257
32	Ad	0.09	0/2783	0.19	0/3724

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ae	0.06	0/4877	0.18	0/6598
34	Ag	0.08	0/2746	0.17	0/3681
35	Ai	0.08	0/1030	0.19	0/1386
36	Aj	0.08	0/1834	0.20	0/2484
All	All	0.08	0/75554	0.17	0/106860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BX	113	0	121	0	0
2	Bd	241	0	223	2	0
3	AA	20283	0	10300	128	0
4	AB	2265	0	2294	19	0
5	AC	1083	0	1088	13	0
6	AD	625	0	699	6	0
7	AE	972	0	1000	15	0
8	AF	1725	0	1769	18	0
9	AG	1504	0	764	18	0
10	AH	1152	0	1183	17	0
11	AI	463	0	286	1	0
12	AJ	839	0	887	13	0
13	AK	862	0	885	14	0
14	AL	1453	0	1540	25	0
15	AM	942	0	965	15	0
16	AN	868	0	928	15	0
17	AO	1592	0	1557	14	0
18	AP	781	0	806	11	0
19	AQ	744	0	758	10	0
20	AR	2409	0	2428	31	0
21	AS	1111	0	1115	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AT	1371	0	1393	10	0
23	AU	1488	0	1499	13	0
24	AV	2969	0	2961	22	0
25	AW	789	0	802	9	0
26	AX	2849	0	2843	42	0
27	AY	1246	0	1197	7	0
28	AZ	839	0	858	8	0
29	Aa	3114	0	3115	30	0
30	Ab	1828	0	1815	23	0
31	Ac	935	0	971	11	0
32	Ad	2731	0	2804	31	0
33	Ae	4768	0	4764	35	0
34	Ag	2688	0	2687	24	0
35	Ai	1020	0	1053	20	0
36	Aj	1787	0	1796	19	0
37	AA	16	0	0	0	0
37	Ae	1	0	0	0	0
38	AA	120	0	0	0	0
38	AD	1	0	0	0	0
38	AG	1	0	0	0	0
38	AU	1	0	0	0	0
38	AX	1	0	0	0	0
38	Ab	1	0	0	0	0
38	Ad	1	0	0	0	0
39	AG	8	0	8	0	0
40	AO	1	0	0	0	0
41	AP	4	0	0	0	0
41	AT	4	0	0	0	0
42	AX	31	0	12	1	0
43	AX	28	0	12	2	0
44	AX	3	0	0	0	0
All	All	72671	0	62186	549	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 (549) 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)
3:AA:389:A:HO2'	14:AL:142:HIS:HD1	1.32	0.77
3:AA:640:A:OP2	32:Ad:260:LYS:NZ	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AR:85:LEU:HD21	20:AR:123:LYS:HG3	1.71	0.71
35:AI:97:ILE:HD11	35:AI:161:ALA:HB1	1.72	0.71
32:AD:244:LEU:HD22	32:AD:343:LEU:HD23	1.71	0.71
4:AB:152:ASP:OD2	4:AB:174:ARG:NH1	2.23	0.70
20:AR:207:PRO:HB2	20:AR:209:ILE:HG22	1.74	0.69
32:AD:103:LEU:HD11	32:AD:123:ARG:HB2	1.74	0.69
18:AP:82:GLN:HE21	18:AP:132:ASP:HB3	1.57	0.69
29:AA:293:VAL:HG22	29:AA:360:ILE:HD12	1.76	0.68
32:AD:283:GLU:O	32:AD:356:GLN:NE2	2.27	0.68
33:AE:239:ARG:O	33:AE:242:ASN:ND2	2.25	0.67
3:AA:122:G:OP2	16:AN:73:ARG:NH2	2.28	0.67
29:AA:70:TRP:HA	29:AA:75:LEU:HD23	1.76	0.66
22:AT:21:VAL:HG22	22:AT:103:ARG:HB2	1.76	0.66
3:AA:647:A:OP1	30:AB:201:ASN:ND2	2.28	0.66
8:AF:119:LYS:NZ	26:AX:398:LEU:O	2.29	0.65
3:AA:783:A:OP2	8:AF:35:SER:N	2.30	0.65
7:AE:35:ILE:HD11	14:AL:91:ARG:HD3	1.76	0.65
7:AE:49:TYR:OH	7:AE:90:ARG:NH1	2.29	0.65
33:AE:443:ASP:HB3	33:AE:446:LYS:HE2	1.79	0.65
31:AC:11:ALA:HB2	31:AC:19:PRO:HB3	1.78	0.65
33:AE:189:ASN:HB3	33:AE:257:HIS:HD2	1.62	0.65
21:AS:51:VAL:HG13	31:AC:117:LEU:HD11	1.78	0.65
12:AJ:74:ASN:ND2	12:AJ:117:ASP:OD1	2.30	0.64
8:AF:79:ALA:O	34:AG:312:GLN:NE2	2.31	0.64
32:AD:296:LEU:HD11	32:AD:352:GLY:HA3	1.78	0.64
26:AX:155:ILE:HB	26:AX:262:VAL:HA	1.79	0.64
3:AA:625:A:N1	3:AA:656:G:O2'	2.30	0.64
26:AX:288:ALA:O	26:AX:292:ASN:ND2	2.30	0.64
3:AA:598:U:O2'	28:AZ:96:LYS:NZ	2.30	0.64
26:AX:50:ARG:NH2	26:AX:96:GLU:OE2	2.31	0.63
3:AA:881:A:OP1	36:AJ:101:ARG:NH2	2.31	0.63
26:AX:295:LYS:NZ	43:AX:503:GDP:O1A	2.31	0.63
33:AE:160:ARG:NH1	33:AE:172:MET:SD	2.72	0.63
24:AV:36:ASP:OD1	24:AV:38:HIS:ND1	2.32	0.63
3:AA:882:A:HI'	24:AV:66:PRO:HD3	1.80	0.62
32:AD:412:LYS:HG2	32:AD:418:LYS:HB2	1.81	0.62
3:AA:345:U:O2'	3:AA:347:A:OP2	2.17	0.62
7:AE:26:ILE:HG23	7:AE:36:VAL:HG21	1.81	0.62
3:AA:247:C:N4	12:AJ:117:ASP:OD2	2.32	0.62
8:AF:48:LYS:NZ	26:AX:375:GLU:OE2	2.31	0.62
10:AH:121:LEU:HD21	10:AH:128:LYS:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ad:165:GLN:NE2	32:Ad:169:GLU:OE2	2.33	0.62
3:AA:374:U:OP2	31:Ac:9:ARG:NH2	2.32	0.61
12:Aj:37:HIS:ND1	16:AN:36:ASP:OD2	2.33	0.61
5:AC:100:PHE:HB3	5:AC:103:CYS:HB2	1.83	0.61
26:AX:276:ARG:NH2	26:AX:286:GLU:OE1	2.34	0.61
3:AA:122:G:N2	3:AA:125:A:OP2	2.33	0.61
3:AA:552:G:N1	3:AA:775:G:OP2	2.33	0.61
25:AW:119:LYS:NZ	30:Ab:239:ASN:OD1	2.33	0.61
14:AL:128:ARG:HH21	14:AL:166:MET:HE2	1.64	0.60
20:AR:155:LYS:HB3	20:AR:177:PRO:HD3	1.83	0.60
34:Ag:273:GLU:HG2	34:Ag:282:GLU:HG2	1.81	0.60
8:AF:72:GLN:O	34:Ag:365:ARG:NH2	2.34	0.60
21:AS:97:GLN:NE2	21:AS:101:GLU:OE2	2.33	0.60
15:AM:104:ILE:HG23	20:AR:147:ILE:HG12	1.83	0.60
23:AU:68:ARG:HD2	36:Aj:196:ILE:HG23	1.83	0.60
4:AB:86:ARG:HB3	4:AB:96:PRO:HB2	1.82	0.60
10:AH:71:ILE:O	10:AH:150:GLY:N	2.35	0.59
15:AM:108:GLU:OE2	23:AU:59:ARG:NH2	2.30	0.59
17:AO:199:TRP:NE1	36:Aj:166:TYR:O	2.34	0.59
24:AV:167:VAL:HG13	24:AV:172:ALA:HB3	1.84	0.59
17:AO:215:ARG:NH1	36:Aj:88:GLN:O	2.35	0.59
21:AS:85:PHE:HB2	25:AW:100:VAL:HG12	1.84	0.59
9:AG:18:A:H61	9:AG:43:A:H2'	1.68	0.59
15:AM:19:ILE:HB	15:AM:83:LEU:HD23	1.84	0.59
3:AA:472:U:HO2'	3:AA:480:A:HO2'	1.48	0.58
34:Ag:59:LYS:HE2	34:Ag:62:PRO:HA	1.85	0.58
26:AX:268:LEU:HD21	26:AX:293:LEU:HD23	1.83	0.58
33:Ae:470:GLN:NE2	33:Ae:472:ASP:OD2	2.36	0.58
34:Ag:378:GLU:OE2	34:Ag:381:LYS:NZ	2.36	0.58
34:Ag:229:LEU:HD21	34:Ag:241:VAL:HG11	1.85	0.58
8:AF:176:ASP:OD2	8:AF:180:ARG:NH1	2.36	0.58
29:Aa:205:ARG:HA	29:Aa:235:LEU:HD12	1.84	0.58
36:Aj:63:ARG:NH2	36:Aj:110:ASP:OD2	2.36	0.58
3:AA:194:A:OP1	15:AM:39:ASN:ND2	2.37	0.58
34:Ag:155:LYS:NZ	34:Ag:217:ASP:OD2	2.37	0.58
3:AA:655:C:OP1	5:AC:165:LYS:NZ	2.31	0.58
33:Ae:565:ARG:NH1	33:Ae:569:GLN:OE1	2.37	0.58
3:AA:283:G:O6	12:Aj:47:ARG:NH2	2.38	0.57
3:AA:291:A:OP1	6:AD:128:LYS:NZ	2.37	0.57
3:AA:329:A:H5''	19:AQ:2:AYA:HM3	1.86	0.57
13:AK:34:MET:HE3	13:AK:95:SER:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AO:105:CYS:HB2	17:AO:142:VAL:HA	1.87	0.57
3:AA:292:A:OP1	6:AD:132:LYS:NZ	2.34	0.57
10:AH:76:LEU:HB2	10:AH:145:LEU:HB2	1.87	0.57
3:AA:590:A:OP1	13:AK:36:ARG:NH2	2.34	0.57
3:AA:706:A:H5'	3:AA:707:A:H5'	1.85	0.57
27:AY:255:ARG:NH1	27:AY:256:LEU:O	2.38	0.57
10:AH:104:ILE:HG23	10:AH:148:LEU:HD21	1.86	0.57
16:AN:31:THR:HG22	16:AN:46:ARG:HG2	1.85	0.57
9:AG:9:C:O2'	9:AG:10:A:N7	2.32	0.57
24:AV:102:TRP:HD1	36:Aj:74:PHE:HD2	1.52	0.57
9:AG:51:PSU:H3'	9:AG:52:A:H8	1.69	0.57
33:Ae:256:GLU:HG2	33:Ae:287:LEU:HB3	1.86	0.57
7:AE:5:GLU:OE2	18:AP:75:LYS:NZ	2.30	0.56
12:AJ:70:PRO:HB3	12:AJ:117:ASP:HB3	1.87	0.56
19:AQ:14:VAL:HG21	35:Ai:172:VAL:HG12	1.86	0.56
22:AT:139:CYS:HB3	22:AT:141:CYS:SG	2.44	0.56
35:Ai:149:VAL:HG11	35:Ai:162:MET:HE2	1.87	0.56
3:AA:768:G:OP2	3:AA:768:G:N2	2.29	0.56
33:Ae:318:GLU:OE2	33:Ae:322:HIS:NE2	2.37	0.56
16:AN:67:ARG:NH1	16:AN:80:GLU:OE2	2.39	0.56
5:AC:115:ASN:ND2	27:AY:309:LYS:O	2.39	0.56
20:AR:167:HIS:HB3	20:AR:193:ILE:HD13	1.86	0.56
30:Ab:220:VAL:HG22	30:Ab:234:TYR:HB2	1.87	0.56
34:Ag:389:ARG:NH1	34:Ag:390:LYS:O	2.39	0.56
20:AR:162:SER:O	20:AR:170:ARG:NH1	2.37	0.56
25:AW:104:ILE:HG12	25:AW:114:ILE:HG12	1.86	0.56
36:Aj:110:ASP:OD1	36:Aj:110:ASP:N	2.36	0.55
3:AA:729:C:H4'	3:AA:730:C:H5'	1.87	0.55
13:AK:51:ARG:NH2	13:AK:83:CYS:SG	2.79	0.55
21:AS:29:PRO:HG2	21:AS:32:PHE:HB2	1.86	0.55
30:Ab:162:CYS:HB3	30:Ab:254:GLN:HG3	1.86	0.55
4:AB:114:LEU:HD11	10:AH:163:ASN:HB3	1.89	0.55
15:AM:29:ARG:HD2	15:AM:57:LEU:HD12	1.88	0.55
17:AO:221:GLN:NE2	24:AV:314:VAL:O	2.33	0.55
20:AR:188:GLU:HG2	20:AR:191:ARG:HH22	1.72	0.55
36:Aj:135:MET:SD	36:Aj:135:MET:N	2.79	0.55
21:AS:119:VAL:HG12	21:AS:123:LYS:HE3	1.88	0.55
33:Ae:170:VAL:HG23	33:Ae:247:ILE:HD11	1.88	0.55
3:AA:378:A:OP1	14:AL:154:ARG:NH2	2.38	0.55
8:AF:44:PRO:HD3	8:AF:75:LYS:HB2	1.89	0.55
19:AQ:20:GLU:OE2	35:Ai:163:HIS:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AS:2:ALA:N	32:Ad:213:GLU:OE2	2.39	0.55
27:AY:383:LYS:HD2	27:AY:386:ILE:HD12	1.88	0.55
20:AR:219:TYR:O	20:AR:256:ARG:NH2	2.38	0.54
24:AV:236:LEU:HD12	24:AV:290:LEU:HD13	1.87	0.54
24:AV:244:TYR:OH	24:AV:315:GLU:OE2	2.26	0.54
3:AA:494:C:OP1	6:AD:139:ASN:ND2	2.41	0.54
29:Aa:325:VAL:HG22	29:Aa:332:VAL:HG22	1.90	0.54
18:AP:124:TYR:HB3	19:AQ:9:ALA:HB2	1.89	0.54
29:Aa:387:THR:OG1	29:Aa:398:HIS:NE2	2.38	0.54
29:Aa:395:VAL:HG23	29:Aa:407:ILE:HG12	1.89	0.54
3:AA:642:G:O2'	3:AA:650:G:OP2	2.19	0.54
9:AG:6:G:H1	9:AG:62:C:H42	1.55	0.54
29:Aa:189:VAL:HG12	29:Aa:282:VAL:HG22	1.89	0.54
6:AD:173:LEU:HD22	14:AL:209:LEU:HD22	1.89	0.54
3:AA:796:U:O2'	3:AA:798:G:N7	2.28	0.54
4:AB:129:PHE:HB3	10:AH:155:VAL:HG21	1.90	0.54
9:AG:16:A:O2'	9:AG:54:A:O2'	2.25	0.54
14:AL:149:ASP:OD2	14:AL:152:HIS:ND1	2.40	0.54
32:Ad:415:GLN:NE2	32:Ad:417:MET:SD	2.81	0.54
4:AB:176:LYS:HG2	4:AB:204:VAL:HG22	1.90	0.53
20:AR:103:TYR:OH	32:Ad:307:LYS:NZ	2.41	0.53
4:AB:235:ASN:ND2	4:AB:237:GLU:OE2	2.38	0.53
24:AV:357:THR:HG22	24:AV:361:LYS:HE3	1.89	0.53
3:AA:302:U:O2'	16:AN:46:ARG:NH1	2.42	0.53
5:AC:86:THR:HG21	13:AK:106:LEU:HD11	1.89	0.53
26:AX:206:GLU:HG3	26:AX:249:ARG:HH12	1.74	0.53
9:AG:15:A:H2	9:AG:18:A:H1'	1.74	0.53
3:AA:196:G:N2	3:AA:199:A:OP2	2.40	0.53
14:AL:75:ASP:HB3	23:AU:153:LYS:HE3	1.89	0.53
16:AN:29:ARG:HD3	16:AN:46:ARG:HD2	1.90	0.53
29:Aa:241:ARG:NE	29:Aa:287:GLN:OE1	2.39	0.53
32:Ad:209:GLY:N	32:Ad:213:GLU:O	2.41	0.53
15:AM:21:LEU:HB3	15:AM:32:TYR:HB3	1.90	0.53
29:Aa:301:ARG:HH21	29:Aa:325:VAL:HG21	1.73	0.53
33:Ae:308:LYS:HE3	33:Ae:310:GLU:HB3	1.89	0.53
33:Ae:556:LYS:NZ	33:Ae:560:GLU:OE2	2.41	0.53
33:Ae:452:GLN:HG2	33:Ae:453:HIS:HD2	1.74	0.53
3:AA:252:G:O2'	3:AA:260:A:N1	2.40	0.53
3:AA:289:G:O6	3:AA:475:A:N6	2.42	0.53
4:AB:169:ARG:O	4:AB:218:ASN:ND2	2.38	0.53
10:AH:92:GLU:OE1	10:AH:141:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AX:108:LEU:HD23	26:AX:141:VAL:HG21	1.91	0.53
26:AX:319:PRO:HG2	26:AX:322:ALA:HB2	1.91	0.53
3:AA:66:C:H5'	15:AM:42:PRO:HG3	1.92	0.52
15:AM:63:GLU:HG2	20:AR:155:LYS:HE2	1.91	0.52
3:AA:646:C:N4	19:AQ:80:ARG:O	2.42	0.52
4:AB:155:ASP:OD1	4:AB:215:ARG:NH1	2.35	0.52
10:AH:176:GLN:NE2	10:AH:178:GLU:OE2	2.43	0.52
3:AA:113:A:N1	3:AA:133:C:O2'	2.35	0.52
35:AI:83:ILE:HG21	35:AI:173:ILE:HD11	1.90	0.52
3:AA:293:A:O2'	3:AA:488:C:O2'	2.22	0.52
4:AB:166:PRO:O	4:AB:169:ARG:NH1	2.43	0.52
14:AL:175:TYR:HB2	16:AN:89:GLY:HA3	1.92	0.52
17:AO:214:SER:OG	17:AO:217:ARG:NH2	2.42	0.52
3:AA:250:C:OP2	12:AJ:116:GLN:NE2	2.43	0.52
34:AG:155:LYS:HB3	34:AG:158:TYR:HB3	1.91	0.52
35:AI:153:GLY:O	35:AI:158:ARG:NH1	2.41	0.52
5:AC:45:SER:HB2	5:AC:49:LYS:HE3	1.92	0.51
30:AB:180:ARG:NH2	32:AD:211:CYS:SG	2.83	0.51
4:AB:264:GLU:HG2	4:AB:268:GLN:HE21	1.76	0.51
17:AO:225:GLN:NE2	23:AU:47:ALA:O	2.43	0.51
3:AA:114:A:O2'	3:AA:137:A:N1	2.42	0.51
24:AV:92:LEU:HD21	24:AV:137:ILE:HD11	1.92	0.51
3:AA:470:A:H2'	3:AA:471:A:H8	1.75	0.51
24:AV:315:GLU:OE2	36:AJ:140:ARG:NH2	2.40	0.51
14:AL:72:LEU:HD13	14:AL:82:ILE:HD13	1.93	0.51
26:AX:152:ILE:O	26:AX:195:ASN:ND2	2.42	0.51
29:AA:392:GLN:OE1	29:AA:394:ARG:NH2	2.43	0.51
36:AJ:63:ARG:HB2	36:AJ:66:GLN:HG3	1.92	0.51
24:AV:109:ILE:HD13	24:AV:138:PHE:H	1.76	0.51
26:AX:273:THR:HG23	26:AX:316:LEU:HD13	1.93	0.51
29:AA:254:GLU:OE1	29:AA:386:ARG:NH2	2.44	0.51
3:AA:311:C:H4'	3:AA:312:C:H5'	1.92	0.51
7:AE:96:HIS:HB3	7:AE:99:THR:HG23	1.93	0.51
10:AH:164:LEU:HD12	10:AH:165:PRO:HD2	1.93	0.51
3:AA:811:A:OP1	8:AF:104:LYS:NZ	2.38	0.51
4:AB:151:ILE:HG13	4:AB:219:TYR:HE1	1.76	0.51
20:AR:106:MET:HE1	20:AR:114:ALA:HB2	1.92	0.51
32:AD:203:LEU:HD22	34:AG:56:ILE:HD11	1.93	0.51
4:AB:266:LEU:HD11	4:AB:289:ILE:HD11	1.93	0.50
13:AK:37:ASP:OD2	28:AZ:52:TYR:OH	2.26	0.50
20:AR:82:MET:HE3	20:AR:288:GLN:HE22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AT:132:ARG:NH1	22:AT:136:LEU:O	2.43	0.50
30:Ab:273:LEU:HA	30:Ab:276:GLN:HE21	1.76	0.50
32:Ad:203:LEU:HD21	32:Ad:222:ILE:HD11	1.94	0.50
35:Ai:128:ALA:HB1	35:Ai:161:ALA:HB2	1.93	0.50
3:AA:388:U:OP1	7:AE:95:LYS:NZ	2.35	0.50
15:AM:64:LYS:HE3	20:AR:154:THR:HB	1.92	0.50
3:AA:693:C:O3'	28:AZ:101:ARG:NH2	2.45	0.50
3:AA:256:U:H2'	29:Aa:392:GLN:HE22	1.76	0.50
3:AA:784:G:O6	34:Ag:276:ARG:NH2	2.44	0.50
16:AN:13:ILE:HG13	16:AN:66:LEU:HB2	1.93	0.50
22:AT:78:PHE:HB2	22:AT:86:VAL:HB	1.93	0.50
31:Ac:33:VAL:HG21	31:Ac:104:LEU:HD23	1.93	0.50
32:Ad:190:GLU:CD	32:Ad:190:GLU:H	2.20	0.50
3:AA:718:A:H4'	3:AA:742:G:H4'	1.94	0.50
33:Ae:309:PHE:HZ	33:Ae:352:PRO:HG2	1.76	0.50
36:Aj:41:LEU:HD13	36:Aj:55:TRP:CG	2.47	0.50
8:AF:147:GLN:NE2	8:AF:151:ASN:OD1	2.45	0.50
26:AX:272:THR:OG1	26:AX:282:ILE:O	2.29	0.50
33:Ae:336:ASN:ND2	33:Ae:409:ASP:OD2	2.44	0.50
24:AV:202:ARG:HD2	24:AV:247:MET:HG3	1.94	0.49
3:AA:305:A:N3	3:AA:307:C:N4	2.60	0.49
9:AG:30:C:OP2	34:Ag:396:ARG:NH1	2.43	0.49
34:Ag:165:VAL:HA	34:Ag:168:MET:HE2	1.94	0.49
3:AA:618:C:OP1	13:AK:112:ARG:NH2	2.35	0.49
11:AI:1:A:N3	11:AI:2:G:N1	2.55	0.49
7:AE:6:LEU:HB3	7:AE:66:VAL:HB	1.94	0.49
3:AA:431:A:OP1	9:AG:35:C:O2'	2.20	0.49
9:AG:13:U:H3	9:AG:19:A:H61	1.59	0.49
12:AJ:78:ARG:HB3	12:AJ:94:PHE:HE1	1.77	0.49
14:AL:115:ILE:HG23	14:AL:180:LYS:HG2	1.93	0.49
3:AA:617:C:H1'	10:AH:124:VAL:HG13	1.95	0.49
17:AO:91:ARG:NH1	17:AO:103:ASN:O	2.45	0.49
3:AA:42:U:OP1	3:AA:180:A:O2'	2.30	0.49
22:AT:101:HIS:HE1	23:AU:112:GLU:HG2	1.76	0.49
3:AA:586:C:OP1	3:AA:706:A:N6	2.45	0.49
7:AE:40:GLU:HB2	7:AE:65:LEU:HB2	1.95	0.49
21:AS:65:TYR:N	21:AS:68:ASP:OD2	2.40	0.49
33:Ae:343:ARG:HA	33:Ae:378:LEU:HD13	1.95	0.49
5:AC:96:MET:HB2	5:AC:108:LEU:HD11	1.94	0.48
15:AM:95:GLY:O	36:Aj:167:PRO:HB2	2.13	0.48
30:Ab:131:PHE:HE2	30:Ab:192:LEU:HD13	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AG:3:U:H2'	9:AG:4:A:C8	2.48	0.48
12:AJ:71:LYS:HD3	12:AJ:119:PRO:HG3	1.95	0.48
34:Ag:59:LYS:HE2	34:Ag:63:THR:H	1.78	0.48
34:Ag:70:THR:HG23	34:Ag:73:PHE:H	1.77	0.48
33:Ae:528:ARG:HH12	33:Ae:562:GLN:HE21	1.60	0.48
3:AA:419:C:O2'	35:Ai:187:ARG:O	2.31	0.48
5:AC:76:LEU:HB2	5:AC:79:GLU:HG3	1.94	0.48
9:AG:3:U:H2'	9:AG:4:A:H8	1.79	0.48
26:AX:123:ARG:NH2	26:AX:337:LEU:O	2.47	0.48
29:Aa:89:LEU:HD22	29:Aa:106:LEU:HD22	1.95	0.48
8:AF:161:ILE:HD12	8:AF:170:VAL:HG21	1.96	0.48
35:Ai:151:VAL:HG21	35:Ai:158:ARG:HG3	1.95	0.48
17:AO:94:CYS:HB2	17:AO:108:CYS:SG	2.53	0.48
22:AT:26:SER:O	22:AT:81:ASP:N	2.46	0.48
3:AA:497:U:H2'	3:AA:498:A:H8	1.78	0.48
3:AA:53:A:N1	3:AA:62:G:O2'	2.43	0.47
3:AA:292:A:N3	3:AA:489:C:O2'	2.43	0.47
3:AA:406:A:N1	3:AA:453:C:O2'	2.40	0.47
14:AL:72:LEU:HA	14:AL:94:SER:HA	1.96	0.47
16:AN:18:ILE:HD13	16:AN:29:ARG:HB2	1.96	0.47
17:AO:217:ARG:NH1	17:AO:227:GLU:OE2	2.45	0.47
24:AV:81:SER:HB3	24:AV:84:GLU:HG3	1.96	0.47
29:Aa:227:TYR:CZ	29:Aa:235:LEU:HD21	2.48	0.47
3:AA:12:U:OP1	32:Ad:226:ARG:HD3	2.14	0.47
3:AA:696:A:O2'	3:AA:698:G:N7	2.36	0.47
14:AL:89:VAL:HG22	23:AU:164:VAL:HG21	1.95	0.47
25:AW:114:ILE:HD13	25:AW:140:VAL:HG21	1.95	0.47
26:AX:102:ARG:HH22	26:AX:133:GLY:HA3	1.79	0.47
33:Ae:450:PRO:HD2	33:Ae:453:HIS:CG	2.49	0.47
7:AE:29:LEU:HB3	7:AE:34:ALA:HB3	1.96	0.47
20:AR:191:ARG:HG3	20:AR:204:ILE:HG23	1.97	0.47
26:AX:50:ARG:NH1	26:AX:98:CYS:SG	2.87	0.47
29:Aa:359:GLN:O	29:Aa:363:LYS:N	2.42	0.47
30:Ab:264:ARG:NE	30:Ab:268:GLU:OE2	2.47	0.47
33:Ae:593:TRP:HA	33:Ae:596:LEU:HD23	1.95	0.47
3:AA:586:C:H42	13:AK:85:VAL:HG12	1.80	0.47
3:AA:834:C:OP1	32:Ad:237:ARG:NH2	2.37	0.47
33:Ae:152:ILE:HA	33:Ae:172:MET:HE3	1.96	0.47
33:Ae:559:TYR:HA	33:Ae:562:GLN:HG3	1.97	0.47
14:AL:87:ASP:HA	14:AL:90:LYS:HE3	1.96	0.47
26:AX:162:VAL:HB	26:AX:272:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bd:109:GLU:O	28:AZ:13:ARG:NH1	2.48	0.47
8:AF:172:VAL:HG12	8:AF:240:ARG:HD2	1.97	0.47
24:AV:30:LEU:HD21	24:AV:181:LEU:HD11	1.97	0.47
29:Aa:338:GLU:O	29:Aa:344:ASN:ND2	2.43	0.47
30:Ab:223:VAL:HG11	30:Ab:229:PRO:HB3	1.96	0.47
35:Ai:146:HIS:NE2	35:Ai:171:GLU:OE1	2.48	0.47
8:AF:84:SER:OG	26:AX:379:GLU:OE1	2.33	0.47
26:AX:265:ILE:HD13	26:AX:337:LEU:HD11	1.97	0.47
4:AB:50:ARG:NH1	33:Ae:94:TYR:O	2.47	0.47
8:AF:71:THR:O	34:Ag:253:LYS:NZ	2.48	0.47
19:AQ:83:PRO:HA	25:AW:108:VAL:HG21	1.97	0.47
4:AB:159:SER:HB2	5:AC:112:ARG:HB3	1.97	0.46
10:AH:78:VAL:HB	10:AH:143:LEU:HB2	1.96	0.46
19:AQ:39:ILE:HD13	35:Ai:179:THR:HG21	1.97	0.46
3:AA:566:A:N3	3:AA:592:C:O2'	2.46	0.46
13:AK:52:LEU:HD11	28:AZ:36:LEU:HB3	1.96	0.46
33:Ae:73:ALA:O	33:Ae:76:SER:OG	2.29	0.46
3:AA:13:C:OP2	32:Ad:226:ARG:NH1	2.49	0.46
3:AA:651:U:H4'	30:Ab:172:ARG:HH21	1.81	0.46
7:AE:37:ARG:NH2	23:AU:163:GLU:OE1	2.49	0.46
3:AA:47:C:H2'	3:AA:168:C:H41	1.80	0.46
30:Ab:221:GLY:HA3	30:Ab:232:ILE:HD13	1.96	0.46
3:AA:293:A:HO2'	3:AA:488:C:HO2'	1.60	0.46
25:AW:110:ASN:HB2	25:AW:125:ARG:HH21	1.80	0.46
26:AX:266:ASN:HA	26:AX:329:LEU:HD23	1.98	0.46
27:AY:250:ILE:HG21	33:Ae:392:ILE:HD13	1.98	0.46
32:Ad:312:TYR:N	32:Ad:331:ASP:OD2	2.48	0.46
10:AH:55:PRO:HA	33:Ae:440:LYS:HB3	1.98	0.46
13:AK:52:LEU:HD22	28:AZ:41:PRO:HG3	1.97	0.46
15:AM:54:TYR:HD1	15:AM:66:VAL:HG22	1.80	0.46
35:Ai:71:SER:O	35:Ai:74:ARG:NH1	2.36	0.46
3:AA:879:U:H2'	36:Aj:99:ARG:HD3	1.97	0.46
9:AG:18:A:H2'	9:AG:43:A:N6	2.31	0.46
9:AG:51:PSU:H3'	9:AG:52:A:C8	2.51	0.46
10:AH:128:LYS:HE2	10:AH:131:ARG:NH2	2.30	0.46
17:AO:167:ILE:HD12	20:AR:226:ASP:HB3	1.98	0.46
35:Ai:85:ILE:N	35:Ai:100:VAL:O	2.45	0.46
3:AA:126:U:OP2	14:AL:225:ARG:NH2	2.47	0.46
20:AR:332:ALA:HA	20:AR:336:ALA:HB3	1.98	0.46
22:AT:34:TYR:CZ	22:AT:68:LYS:HG2	2.50	0.46
20:AR:208:ILE:O	20:AR:214:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AG:61:C:H2'	9:AG:62:C:C6	2.51	0.45
29:Aa:394:ARG:H	29:Aa:407:ILE:HD11	1.81	0.45
3:AA:950:C:OP2	31:Ac:24:ASN:ND2	2.49	0.45
27:AY:323:ASP:OD1	27:AY:323:ASP:N	2.49	0.45
33:Ae:298:ILE:HG21	33:Ae:338:ILE:HG12	1.99	0.45
35:Ai:110:ALA:HB2	35:Ai:138:ARG:HH21	1.81	0.45
3:AA:472:U:O2'	3:AA:480:A:O2'	2.23	0.45
3:AA:737:A:OP2	8:AF:198:ARG:NH1	2.50	0.45
26:AX:117:PHE:HB3	26:AX:303:GLY:HA2	1.99	0.45
3:AA:130:G:H5''	16:AN:21:LYS:HB3	1.99	0.45
3:AA:347:A:O2'	8:AF:166:ARG:NH1	2.50	0.45
24:AV:215:GLN:HB3	24:AV:217:ASN:HD21	1.82	0.45
26:AX:210:TRP:HE1	26:AX:216:THR:HG1	1.58	0.45
36:Aj:85:TRP:HH2	36:Aj:95:TRP:HE1	1.64	0.45
18:AP:141:ARG:HD2	35:Ai:62:ILE:HD13	1.98	0.45
24:AV:138:PHE:HB3	36:Aj:72:PRO:HG3	1.99	0.45
29:Aa:67:LYS:HG2	29:Aa:71:LYS:HE3	1.98	0.45
29:Aa:241:ARG:HE	29:Aa:287:GLN:CD	2.24	0.45
3:AA:134:A:OP2	14:AL:195:TYR:OH	2.16	0.45
3:AA:258:A:O2'	3:AA:260:A:OP1	2.34	0.45
3:AA:410:G:H4'	3:AA:931:A:H4'	1.99	0.45
3:AA:646:C:OP2	34:Ag:220:GLN:NE2	2.44	0.45
3:AA:661:U:O2'	5:AC:64:HIS:ND1	2.48	0.45
9:AG:31:RSQ:OP1	9:AG:31:RSQ:H10	2.17	0.45
3:AA:570:G:OP1	29:Aa:408:LYS:NZ	2.50	0.45
4:AB:312:TYR:OH	26:AX:338:ASP:OD1	2.23	0.45
8:AF:110:LEU:HD22	8:AF:202:PRO:HD3	1.98	0.45
26:AX:159:HIS:CD2	26:AX:267:ALA:HB2	2.52	0.45
3:AA:584:A:OP1	13:AK:88:ARG:NH2	2.50	0.44
3:AA:765:G:OP1	26:AX:279:LYS:NZ	2.31	0.44
12:Aj:62:VAL:HA	12:Aj:83:VAL:HG12	1.98	0.44
14:AL:143:LEU:HD11	14:AL:153:LYS:HA	1.99	0.44
14:AL:86:ASP:OD1	14:AL:87:ASP:N	2.50	0.44
3:AA:348:A:H5'	35:Ai:119:ASN:HD22	1.82	0.44
3:AA:433:A:O2'	3:AA:435:A:N7	2.42	0.44
31:Ac:47:THR:HG23	35:Ai:129:GLN:HE22	1.82	0.44
2:Bd:104:LYS:HB2	2:Bd:107:GLU:HG3	1.98	0.44
3:AA:375:A:OP2	31:Ac:17:ARG:NE	2.50	0.44
15:AM:30:PRO:HD2	15:AM:57:LEU:HD11	1.98	0.44
20:AR:136:VAL:O	20:AR:186:TRP:NE1	2.40	0.44
30:Ab:88:ARG:HB3	30:Ab:91:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:94:A:H4'	23:AU:82:VAL:HG21	2.00	0.44
26:AX:248:LYS:HE3	26:AX:301:TRP:CD1	2.53	0.44
33:Ae:517:LYS:HG2	33:Ae:522:THR:HG23	2.00	0.44
35:Ai:101:SER:HB3	35:Ai:107:LEU:HD11	1.98	0.44
31:Ac:43:ALA:HB1	31:Ac:46:ILE:HD11	2.00	0.44
34:Ag:309:ASP:OD1	34:Ag:337:ARG:NH1	2.50	0.44
36:Aj:64:LEU:HB3	36:Aj:134:VAL:HG13	1.99	0.44
4:AB:152:ASP:HB2	4:AB:172:VAL:HB	2.00	0.44
31:Ac:15:ASN:OD1	31:Ac:17:ARG:HG2	2.18	0.44
35:Ai:100:VAL:HG12	35:Ai:106:PRO:HA	1.99	0.44
7:AE:11:LYS:HD3	7:AE:58:HIS:HE1	1.82	0.44
16:AN:8:VAL:HB	16:AN:68:ALA:HB1	1.99	0.44
29:Aa:220:TRP:CH2	29:Aa:247:VAL:HA	2.53	0.44
16:AN:6:SER:OG	16:AN:69:LEU:O	2.34	0.44
18:AP:95:HIS:CD2	18:AP:96:ILE:HG13	2.53	0.44
29:Aa:253:TYR:O	29:Aa:399:ARG:NH1	2.32	0.44
35:Ai:110:ALA:HB3	35:Ai:135:ALA:HB2	1.99	0.44
20:AR:89:LYS:NZ	20:AR:261:LEU:O	2.47	0.43
26:AX:206:GLU:OE2	26:AX:249:ARG:NH2	2.50	0.43
3:AA:66:C:O2'	3:AA:205:A:O2'	2.32	0.43
3:AA:805:U:H2'	3:AA:806:A:C8	2.52	0.43
7:AE:90:ARG:HG2	7:AE:92:ASN:HD21	1.83	0.43
26:AX:62:GLN:HG2	26:AX:63:HIS:CD2	2.53	0.43
34:Ag:263:ASP:OD1	34:Ag:267:MET:N	2.51	0.43
3:AA:188:C:N4	3:AA:204:A:OP2	2.39	0.43
3:AA:753:U:O2'	3:AA:797:A:N3	2.48	0.43
12:AJ:97:GLY:HA3	12:AJ:135:VAL:HG11	2.00	0.43
13:AK:91:CYS:HB3	13:AK:96:ARG:H	1.81	0.43
33:Ae:650:MET:HE3	33:Ae:659:GLN:HB3	1.99	0.43
10:AH:122:GLN:O	13:AK:112:ARG:NH1	2.51	0.43
20:AR:260:ASP:HA	20:AR:263:ARG:HG3	1.98	0.43
26:AX:170:GLN:NE2	26:AX:175:LYS:O	2.52	0.43
3:AA:936:MA6:O5'	3:AA:936:MA6:H8	2.18	0.43
17:AO:54:GLU:OE1	17:AO:57:LYS:NZ	2.38	0.43
30:Ab:84:LEU:HD23	30:Ab:248:LEU:HD21	2.01	0.43
30:Ab:137:TYR:O	30:Ab:264:ARG:NH1	2.45	0.43
9:AG:5:A:H2'	9:AG:6:G:C8	2.52	0.43
14:AL:224:ARG:O	14:AL:228:LYS:HG2	2.19	0.43
17:AO:73:VAL:O	17:AO:109:ARG:NH2	2.52	0.43
26:AX:126:LEU:HD23	26:AX:343:ILE:HB	1.99	0.43
3:AA:469:A:P	30:Ab:100:ARG:HH22	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AC:104:LEU:HD23	5:AC:123:VAL:HG12	2.00	0.43
15:AM:111:ARG:NH2	20:AR:146:LYS:O	2.51	0.43
18:AP:124:TYR:HE2	19:AQ:4:HIS:HB3	1.84	0.43
24:AV:241:ARG:HA	24:AV:244:TYR:CE1	2.54	0.43
26:AX:181:PRO:HB2	26:AX:233:VAL:HG12	2.00	0.43
28:AZ:58:TYR:O	28:AZ:62:MET:HG2	2.19	0.43
3:AA:400:A:OP2	3:AA:402:A:N6	2.42	0.43
3:AA:270:C:O2'	3:AA:274:U:OP1	2.35	0.43
3:AA:373:C:H4'	18:AP:94:ARG:NH1	2.34	0.43
26:AX:244:LEU:HD12	26:AX:292:ASN:HB3	2.01	0.43
9:AG:62:C:H2'	9:AG:63:G:C8	2.54	0.43
20:AR:135:ARG:CZ	20:AR:186:TRP:HB3	2.48	0.43
30:Ab:156:GLU:OE1	34:Ag:163:HIS:ND1	2.52	0.43
3:AA:55:C:OP1	23:AU:41:ARG:NH2	2.39	0.42
5:AC:40:ALA:HB3	5:AC:59:PRO:HG3	2.01	0.42
10:AH:96:VAL:O	10:AH:100:LYS:HG2	2.19	0.42
15:AM:29:ARG:HH22	22:AT:140:ILE:HG23	1.83	0.42
29:Aa:385:ILE:HG22	29:Aa:399:ARG:HD3	2.00	0.42
34:Ag:202:LYS:NZ	34:Ag:206:GLU:OE2	2.43	0.42
3:AA:88:A:H2'	3:AA:89:C:O4'	2.20	0.42
18:AP:86:PRO:HA	18:AP:125:LYS:HB3	2.01	0.42
24:AV:225:LEU:HD22	24:AV:275:LEU:HD13	2.01	0.42
20:AR:107:THR:HG22	32:Ad:368:LEU:HD22	2.01	0.42
20:AR:289:ILE:HD11	20:AR:328:ILE:HD13	2.02	0.42
23:AU:168:ILE:HG12	23:AU:176:ARG:HG2	2.01	0.42
26:AX:379:GLU:OE2	34:Ag:318:HIS:NE2	2.52	0.42
31:Ac:49:MET:HG2	31:Ac:53:MET:HE2	2.01	0.42
3:AA:253:C:H4'	3:AA:260:A:C6	2.55	0.42
3:AA:272:A:OP2	17:AO:96:ARG:NH2	2.43	0.42
3:AA:386:U:H4'	7:AE:94:VAL:HG12	2.01	0.42
3:AA:471:A:H4'	32:Ad:355:ARG:NH1	2.35	0.42
29:Aa:280:MET:HE2	29:Aa:280:MET:HB2	1.96	0.42
30:Ab:54:ASP:OD1	30:Ab:271:TYR:OH	2.36	0.42
3:AA:16:A:H2'	3:AA:17:G:C8	2.55	0.42
3:AA:301:U:H4'	14:AL:192:PRO:HG3	2.02	0.42
3:AA:883:A:OP1	36:Aj:29:ARG:NH2	2.50	0.42
13:AK:53:ARG:O	13:AK:56:SER:OG	2.36	0.42
20:AR:262:LEU:O	20:AR:265:THR:OG1	2.29	0.42
29:Aa:206:GLU:CD	29:Aa:262:ARG:HH12	2.27	0.42
3:AA:3:U:C4	32:Ad:427:ARG:HD3	2.55	0.42
12:AJ:51:PRO:HG3	12:AJ:122:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AL:129:ILE:HD13	14:AL:167:LEU:HD23	2.02	0.42
14:AL:221:LYS:O	14:AL:225:ARG:HG2	2.20	0.42
20:AR:281:ILE:HB	20:AR:300:LEU:HD21	2.02	0.42
30:Ab:107:PHE:N	30:Ab:115:ILE:O	2.52	0.42
3:AA:619:A:H5''	10:AH:130:HIS:CE1	2.55	0.42
3:AA:805:U:H2'	3:AA:806:A:H8	1.85	0.42
6:AD:196:LEU:HD23	6:AD:196:LEU:HA	1.88	0.42
32:Ad:230:THR:HG23	32:Ad:238:LYS:HB3	2.01	0.42
33:Ae:346:HIS:CD2	33:Ae:347:VAL:HG23	2.55	0.42
3:AA:761:A:H2'	3:AA:762:A:C8	2.55	0.42
13:AK:70:VAL:HG21	27:AY:386:ILE:HD13	2.02	0.42
23:AU:45:PRO:HA	23:AU:46:PRO:HD3	1.94	0.42
25:AW:90:THR:O	30:Ab:110:ARG:NH2	2.47	0.42
26:AX:102:ARG:NH1	26:AX:132:THR:O	2.51	0.42
32:Ad:224:GLU:HB2	32:Ad:342:MET:HG2	2.02	0.42
32:Ad:265:MET:HE1	34:Ag:54:PHE:HZ	1.85	0.42
33:Ae:573:ALA:HB2	33:Ae:604:LYS:HD2	2.00	0.42
25:AW:143:ARG:HH12	25:AW:170:LEU:HD21	1.84	0.41
30:Ab:164:GLU:HG3	30:Ab:257:ILE:HD13	2.02	0.41
16:AN:14:VAL:O	22:AT:63:GLN:NE2	2.48	0.41
20:AR:285:LEU:HD21	20:AR:328:ILE:HG23	2.01	0.41
29:Aa:141:ASN:O	29:Aa:145:GLU:HG3	2.20	0.41
3:AA:224:A:H4'	3:AA:225:G:H5'	2.03	0.41
3:AA:726:U:H2'	3:AA:727:A:C8	2.55	0.41
15:AM:67:ALA:HB1	20:AR:161:ILE:HD13	2.01	0.41
26:AX:359:TYR:O	26:AX:363:ASN:ND2	2.47	0.41
28:AZ:75:HIS:ND1	32:Ad:98:LEU:HD11	2.35	0.41
3:AA:103:G:H5''	16:AN:47:LYS:NZ	2.35	0.41
3:AA:126:U:H2'	3:AA:127:G:C8	2.55	0.41
5:AC:58:ALA:HB3	5:AC:60:HIS:CE1	2.55	0.41
14:AL:115:ILE:HG21	14:AL:181:ILE:HD13	2.01	0.41
20:AR:138:ILE:HG13	20:AR:186:TRP:NE1	2.36	0.41
23:AU:189:TRP:CE3	23:AU:197:VAL:HG13	2.55	0.41
29:Aa:360:ILE:HA	29:Aa:363:LYS:HB3	2.02	0.41
32:Ad:205:PRO:HA	32:Ad:206:PRO:HD3	1.97	0.41
3:AA:300:U:OP1	14:AL:165:LYS:NZ	2.43	0.41
3:AA:784:G:O2'	3:AA:810:G:O6	2.32	0.41
29:Aa:293:VAL:HG21	29:Aa:357:TYR:HA	2.01	0.41
9:AG:5:A:H2	9:AG:63:G:H1	1.64	0.41
20:AR:281:ILE:HD12	20:AR:300:LEU:HG	2.02	0.41
3:AA:679:A:O4'	32:Ad:114:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AC:109:VAL:HB	5:AC:120:CYS:HB2	2.03	0.41
36:Aj:99:ARG:HB3	36:Aj:115:TRP:HB2	2.03	0.41
3:AA:726:U:H2'	3:AA:727:A:H8	1.85	0.41
14:AL:220:LEU:O	14:AL:224:ARG:HG2	2.21	0.41
20:AR:162:SER:HB2	20:AR:165:ILE:HD12	2.03	0.41
3:AA:36:G:OP1	22:AT:160:ARG:NH2	2.50	0.41
4:AB:46:ARG:HB2	4:AB:47:PRO:HD3	2.03	0.41
7:AE:17:GLU:OE1	7:AE:17:GLU:N	2.54	0.41
17:AO:91:ARG:HD2	17:AO:94:CYS:SG	2.61	0.41
18:AP:76:ASN:OD1	23:AU:188:ASN:HA	2.20	0.41
21:AS:125:LEU:HB3	21:AS:130:VAL:HB	2.01	0.41
26:AX:136:LEU:HD23	26:AX:136:LEU:HA	1.95	0.41
26:AX:248:LYS:HE3	26:AX:301:TRP:HD1	1.86	0.41
29:Aa:194:THR:OG1	29:Aa:279:THR:OG1	2.22	0.41
30:Ab:167:HIS:CD2	34:Ag:153:THR:HA	2.56	0.41
32:Ad:372:GLU:CD	32:Ad:374:ARG:HE	2.29	0.41
33:Ae:303:CYS:SG	33:Ae:344:ARG:NH2	2.94	0.41
3:AA:37:U:H2'	3:AA:38:A:H8	1.86	0.41
33:Ae:263:ILE:HG23	33:Ae:275:ALA:HB1	2.01	0.41
33:Ae:381:GLN:O	33:Ae:383:GLY:N	2.54	0.41
3:AA:501:A:P	6:AD:165:LYS:HE3	2.61	0.40
4:AB:217:GLN:NE2	27:AY:326:SER:O	2.54	0.40
8:AF:193:ASP:OD1	8:AF:194:LYS:N	2.54	0.40
21:AS:52:ARG:NH2	30:Ab:103:GLU:OE1	2.55	0.40
33:Ae:309:PHE:CZ	33:Ae:352:PRO:HG2	2.56	0.40
3:AA:630:A:OP1	32:Ad:269:ARG:NH2	2.55	0.40
3:AA:763:G:H2'	3:AA:764:G:H8	1.86	0.40
3:AA:783:A:N1	3:AA:811:A:H5''	2.36	0.40
24:AV:30:LEU:HD13	24:AV:34:TYR:CD1	2.56	0.40
26:AX:99:LEU:HD11	26:AX:136:LEU:HB3	2.01	0.40
26:AX:134:LYS:NZ	42:AX:501:ATP:O2B	2.45	0.40
33:Ae:67:LYS:HG3	33:Ae:68:VAL:HG13	2.02	0.40
36:Aj:89:HIS:NE2	36:Aj:202:ASP:OD2	2.46	0.40
3:AA:120:C:H5''	16:AN:77:VAL:HG23	2.04	0.40
3:AA:922:G:P	3:AA:925:A:H4'	2.61	0.40
7:AE:65:LEU:HD11	18:AP:75:LYS:HD2	2.04	0.40
12:AJ:81:CYS:HB3	12:AJ:95:ILE:HD11	2.03	0.40
30:Ab:222:ILE:HD13	30:Ab:236:VAL:HB	2.02	0.40
33:Ae:316:ILE:O	33:Ae:320:LEU:HG	2.22	0.40
3:AA:250:C:P	12:AJ:116:GLN:HE21	2.43	0.40
3:AA:618:C:H4'	10:AH:122:GLN:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:661:U:H2'	3:AA:662:A:H8	1.85	0.40
19:AQ:83:PRO:HG2	19:AQ:84:TRP:CD1	2.57	0.40
24:AV:168:MET:HA	24:AV:173:PHE:HE2	1.86	0.40
24:AV:173:PHE:O	24:AV:179:GLN:NE2	2.48	0.40
24:AV:221:PHE:HE2	24:AV:265:LYS:HD3	1.85	0.40
25:AW:149:LEU:HD11	25:AW:166:ASN:HB2	2.03	0.40
32:Ad:244:LEU:HD23	32:Ad:342:MET:HG3	2.02	0.40
3:AA:911:A:C6	29:Aa:195:THR:HA	2.56	0.40
4:AB:304:GLU:HG2	26:AX:324:LEU:HD13	2.04	0.40
8:AF:234:ARG:HB2	31:Ac:53:MET:HE1	2.02	0.40
14:AL:79:VAL:HG23	14:AL:82:ILE:HB	2.03	0.40
18:AP:75:LYS:HE3	18:AP:75:LYS:HB2	1.83	0.40
19:AQ:30:LEU:HD22	19:AQ:35:LEU:HD22	2.04	0.40
26:AX:295:LYS:NZ	43:AX:503:GDP:O1B	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AI	6/33 (18%)	2 (33%)	0
3	AA	954/955 (99%)	121 (12%)	1 (0%)
9	AG	70/71 (98%)	10 (14%)	0
All	All	1030/1059 (97%)	133 (12%)	1 (0%)

All (133) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	AA	2	A

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Mol	Chain	Res	Type
3	AA	4	A
3	AA	33	U
3	AA	41	A
3	AA	57	U
3	AA	74	U
3	AA	90	C
3	AA	91	A
3	AA	106	A
3	AA	114	A
3	AA	119	G
3	AA	144	G
3	AA	147	U
3	AA	149	G
3	AA	183	U
3	AA	185	U
3	AA	188	C
3	AA	189	A
3	AA	213	A
3	AA	214	U
3	AA	221	C
3	AA	224	A
3	AA	243	C
3	AA	254	G
3	AA	257	C
3	AA	260	A
3	AA	272	A
3	AA	276	A
3	AA	282	A
3	AA	285	C
3	AA	291	A
3	AA	292	A
3	AA	293	A
3	AA	294	G
3	AA	295	A
3	AA	307	C
3	AA	313	C
3	AA	315	C
3	AA	320	A
3	AA	346	A
3	AA	355	C
3	AA	365	A
3	AA	368	A

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Mol	Chain	Res	Type
3	AA	384	G
3	AA	395	U
3	AA	400	A
3	AA	401	C
3	AA	434	U
3	AA	435	A
3	AA	456	A
3	AA	458	C
3	AA	460	U
3	AA	462	A
3	AA	471	A
3	AA	472	U
3	AA	474	A
3	AA	479	A
3	AA	490	A
3	AA	504	C
3	AA	506	C
3	AA	513	A
3	AA	520	A
3	AA	540	U
3	AA	542	U
3	AA	543	C
3	AA	553	G
3	AA	568	U
3	AA	573	A
3	AA	576	C
3	AA	578	C
3	AA	582	U
3	AA	599	U
3	AA	600	G
3	AA	601	C
3	AA	604	A
3	AA	624	C
3	AA	637	U
3	AA	638	G
3	AA	643	C
3	AA	644	U
3	AA	645	A
3	AA	650	G
3	AA	679	A
3	AA	680	G
3	AA	696	A

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Mol	Chain	Res	Type
3	AA	697	U
3	AA	706	A
3	AA	709	A
3	AA	731	C
3	AA	740	A
3	AA	743	A
3	AA	744	U
3	AA	758	C
3	AA	759	U
3	AA	760	U
3	AA	783	A
3	AA	816	G
3	AA	819	C
3	AA	831	A
3	AA	834	C
3	AA	872	A
3	AA	878	C
3	AA	879	U
3	AA	880	A
3	AA	886	C
3	AA	890	C
3	AA	891	G
3	AA	892	C
3	AA	893	A
3	AA	897	A
3	AA	904	G
3	AA	911	A
3	AA	912	G
3	AA	920	A
3	AA	921	U
3	AA	924	U
3	AA	935	G
3	AA	937	MA6
3	AA	947	G
3	AA	948	G
3	AA	952	A
9	AG	7	G
9	AG	8	U
9	AG	10	A
9	AG	11	G
9	AG	17	U
9	AG	18	A

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Mol	Chain	Res	Type
9	AG	45	G
9	AG	52	A
9	AG	53	U
9	AG	55	C
11	AI	2	G
11	AI	4	Y5P

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	AA	592	C

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

13 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PSU	AG	51	9	18,21,22	1.37	2 (11%)	21,30,33	1.94	3 (14%)
3	MA6	AA	936	3	23,26,27	2.36	5 (21%)	33,38,41	3.78	12 (36%)
9	PSU	AG	46	9	18,21,22	1.35	2 (11%)	21,30,33	2.01	4 (19%)
3	MA6	AA	937	3	23,26,27	2.37	5 (21%)	33,38,41	3.78	12 (36%)
31	AYA	Ac	2	31	6,7,8	0.79	0	6,8,10	0.64	0
3	5MU	AA	429	3	19,22,23	1.39	6 (31%)	27,32,35	2.08	6 (22%)
35	5F0	Ai	184	35	8,8,9	1.45	2 (25%)	8,9,11	1.57	1 (12%)
3	B8T	AA	839	37,3	19,22,23	0.39	0	25,31,34	0.35	0
9	PSU	AG	24	9	18,21,22	1.35	2 (11%)	21,30,33	2.00	4 (19%)
9	RSQ	AG	31	9,11	19,23,24	0.35	0	25,33,36	0.54	0
19	AYA	AQ	2	19	6,7,8	0.76	0	6,8,10	0.61	0
3	5MC	AA	841	3	19,22,23	1.54	3 (15%)	26,32,35	1.08	2 (7%)
11	Y5P	AI	4	11	14,19,20	1.92	1 (7%)	18,26,29	0.53	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
9	PSU	AG	51	9	-	2/7/25/26	0/2/2/2
3	MA6	AA	936	3	-	0/11/29/30	0/3/3/3
9	PSU	AG	46	9	-	0/7/25/26	0/2/2/2
3	MA6	AA	937	3	-	2/11/29/30	0/3/3/3
31	AYA	Ac	2	31	-	2/5/6/8	-
3	5MU	AA	429	3	-	0/7/25/26	0/2/2/2
35	5F0	Ai	184	35	-	4/9/9/10	-
3	B8T	AA	839	37,3	-	0/7/27/28	0/2/2/2
9	PSU	AG	24	9	-	0/7/25/26	0/2/2/2
9	RSQ	AG	31	9,11	-	1/9/27/28	0/2/2/2
19	AYA	AQ	2	19	-	0/5/6/8	-
3	5MC	AA	841	3	-	0/7/25/26	0/2/2/2
11	Y5P	AI	4	11	-	5/7/33/34	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AI	4	Y5P	C2-N3	7.06	1.32	1.27
3	AA	937	MA6	C5-N7	7.00	1.51	1.39
3	AA	936	MA6	C5-N7	6.97	1.51	1.39
3	AA	937	MA6	C8-N9	-5.77	1.27	1.37
3	AA	936	MA6	C8-N9	-5.73	1.27	1.37
3	AA	841	5MC	C5-C4	5.50	1.48	1.44
3	AA	937	MA6	C4-N9	-4.03	1.29	1.37
3	AA	936	MA6	C4-N9	-3.93	1.29	1.37
9	AG	51	PSU	C6-C5	3.43	1.39	1.35
9	AG	46	PSU	C6-C5	3.41	1.39	1.35
3	AA	936	MA6	C5-C4	3.40	1.45	1.39
3	AA	937	MA6	C5-C4	3.38	1.45	1.39
9	AG	24	PSU	C6-C5	3.32	1.39	1.35
3	AA	936	MA6	C6-N6	3.26	1.45	1.36
3	AA	937	MA6	C6-N6	3.25	1.45	1.36
35	Ai	184	5F0	OD1-C1	2.83	1.40	1.33
3	AA	429	5MU	C6-C5	2.64	1.38	1.34
3	AA	429	5MU	C4-N3	-2.64	1.33	1.38
9	AG	24	PSU	C4-N3	-2.62	1.33	1.38
3	AA	841	5MC	C6-C5	2.62	1.38	1.34
9	AG	46	PSU	C4-N3	-2.55	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AG	51	PSU	C4-N3	-2.53	1.34	1.38
3	AA	429	5MU	C6-N1	-2.31	1.34	1.38
3	AA	841	5MC	C6-N1	-2.25	1.34	1.38
3	AA	429	5MU	C4-C5	2.24	1.48	1.44
35	Ai	184	5F0	OD1-CXT	-2.22	1.40	1.45
3	AA	429	5MU	C2-N3	-2.11	1.34	1.38
3	AA	429	5MU	C2-N1	2.10	1.41	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AA	937	MA6	C4-N9-C8	15.14	121.64	105.74
3	AA	936	MA6	C4-N9-C8	15.02	121.51	105.74
3	AA	936	MA6	N3-C4-N9	6.50	138.22	127.17
3	AA	937	MA6	N3-C4-N9	6.37	138.00	127.17
9	AG	46	PSU	N1-C2-N3	6.27	121.79	115.17
9	AG	24	PSU	N1-C2-N3	6.27	121.78	115.17
3	AA	937	MA6	C4-C5-N7	-6.27	103.42	110.58
3	AA	936	MA6	C4-C5-N7	-6.20	103.49	110.58
9	AG	51	PSU	N1-C2-N3	6.08	121.58	115.17
3	AA	937	MA6	N9-C8-N7	-5.70	105.84	113.94
3	AA	936	MA6	N9-C8-N7	-5.65	105.92	113.94
3	AA	936	MA6	C5-C4-N3	-5.42	119.25	126.72
3	AA	937	MA6	C5-C4-N3	-5.27	119.47	126.72
3	AA	429	5MU	C4-N3-C2	-5.08	120.68	127.34
3	AA	429	5MU	N3-C2-N1	4.93	121.31	114.89
3	AA	429	5MU	C5-C4-N3	4.41	119.15	115.32
3	AA	936	MA6	N1-C2-N3	-4.35	121.99	128.58
3	AA	937	MA6	N1-C2-N3	-4.23	122.18	128.58
3	AA	429	5MU	O4-C4-C5	-4.12	120.20	124.92
9	AG	24	PSU	C4-N3-C2	-4.06	120.78	126.37
9	AG	46	PSU	C4-N3-C2	-4.06	120.78	126.37
3	AA	936	MA6	C2-N1-C6	3.99	121.58	111.83
3	AA	937	MA6	C2-N1-C6	3.99	121.57	111.83
9	AG	51	PSU	C4-N3-C2	-3.76	121.19	126.37
3	AA	937	MA6	C6-C5-N7	3.58	139.14	133.43
9	AG	51	PSU	O2-C2-N1	-3.52	119.16	122.79
3	AA	936	MA6	C6-C5-N7	3.51	139.04	133.43
9	AG	46	PSU	O2-C2-N1	-3.51	119.17	122.79
9	AG	24	PSU	O2-C2-N1	-3.49	119.19	122.79
3	AA	429	5MU	C5-C6-N1	-3.45	119.56	123.31
3	AA	937	MA6	C1'-N9-C8	-3.45	119.44	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AA	936	MA6	C1'-N9-C8	-3.42	119.50	127.09
3	AA	936	MA6	C2-N3-C4	3.31	119.92	111.83
35	Ai	184	5F0	OD1-C1-CA	3.31	119.91	111.50
3	AA	937	MA6	C4-N9-C1'	-3.30	118.92	126.63
3	AA	936	MA6	C4-N9-C1'	-3.27	118.98	126.63
3	AA	937	MA6	C2-N3-C4	3.20	119.64	111.83
3	AA	841	5MC	C5-C6-N1	-3.19	119.84	123.31
3	AA	936	MA6	C5-C4-N9	-3.01	102.53	105.81
3	AA	937	MA6	C5-C4-N9	-3.01	102.53	105.81
3	AA	841	5MC	C5-C4-N3	-2.66	119.03	121.75
3	AA	429	5MU	O2-C2-N1	-2.51	119.53	122.80
9	AG	46	PSU	C5-C6-N1	-2.07	119.27	122.14
9	AG	24	PSU	C5-C6-N1	-2.04	119.31	122.14

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	AG	51	PSU	O4'-C1'-C5-C4
9	AG	51	PSU	O4'-C1'-C5-C6
35	Ai	184	5F0	OD1-C1-CA-CB
35	Ai	184	5F0	CA-C1-OD1-CXT
35	Ai	184	5F0	O1-C1-OD1-CXT
35	Ai	184	5F0	O1-C1-CA-CB
11	AI	4	Y5P	C2'-C1'-N1-C2
11	AI	4	Y5P	C2'-C1'-N1-C6
31	Ac	2	AYA	CM-CT-N-CA
11	AI	4	Y5P	O4'-C1'-N1-C2
3	AA	937	MA6	C3'-C4'-C5'-O5'
11	AI	4	Y5P	O4'-C4'-C5'-O5'
11	AI	4	Y5P	O4'-C1'-N1-C6
3	AA	937	MA6	C4'-C5'-O5'-P
31	Ac	2	AYA	OT-CT-N-CA
9	AG	31	RSQ	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AG	51	PSU	2	0
3	AA	936	MA6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AG	31	RSQ	1	0
19	AQ	2	AYA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 149 ligands modelled in this entry, 144 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
43	GDP	AX	503	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
39	MET	AG	101	9	6,7,8	0.49	0	2,7,9	0.13	0
42	ATP	AX	501	38	32,33,33	0.35	0	48,52,52	0.26	0
41	FS2	AT	201	15,22	0,5,14	-	-	-	-	-
41	FS2	AP	201	7,18	0,5,14	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	GDP	AX	503	-	-	4/16/32/32	0/3/3/3
39	MET	AG	101	9	-	0/5/6/8	-
42	ATP	AX	501	38	-	1/22/38/38	0/3/3/3
41	FS2	AT	201	15,22	-	-	0/2/2/6
41	FS2	AP	201	7,18	-	-	0/2/2/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	AX	503	GDP	C5-C4	3.14	1.47	1.38
43	AX	503	GDP	C6-N1	-2.42	1.34	1.38
43	AX	503	GDP	C5-N7	-2.10	1.34	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	AX	503	GDP	C5-C4-N3	-6.20	118.52	128.39
43	AX	503	GDP	C2-N3-C4	5.04	120.99	112.30
43	AX	503	GDP	N9-C4-N3	4.57	135.10	125.95
43	AX	503	GDP	C6-C5-N7	3.15	136.02	130.29
43	AX	503	GDP	C4-C5-N7	-2.57	106.59	110.67
43	AX	503	GDP	C3'-C2'-C1'	2.22	105.65	101.46
43	AX	503	GDP	O6-C6-C5	-2.07	121.06	126.53

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	AX	503	GDP	C5'-O5'-PA-O3A
43	AX	503	GDP	C5'-O5'-PA-O2A
43	AX	503	GDP	C3'-C4'-C5'-O5'
43	AX	503	GDP	O4'-C4'-C5'-O5'
42	AX	501	ATP	PA-O3A-PB-O2B

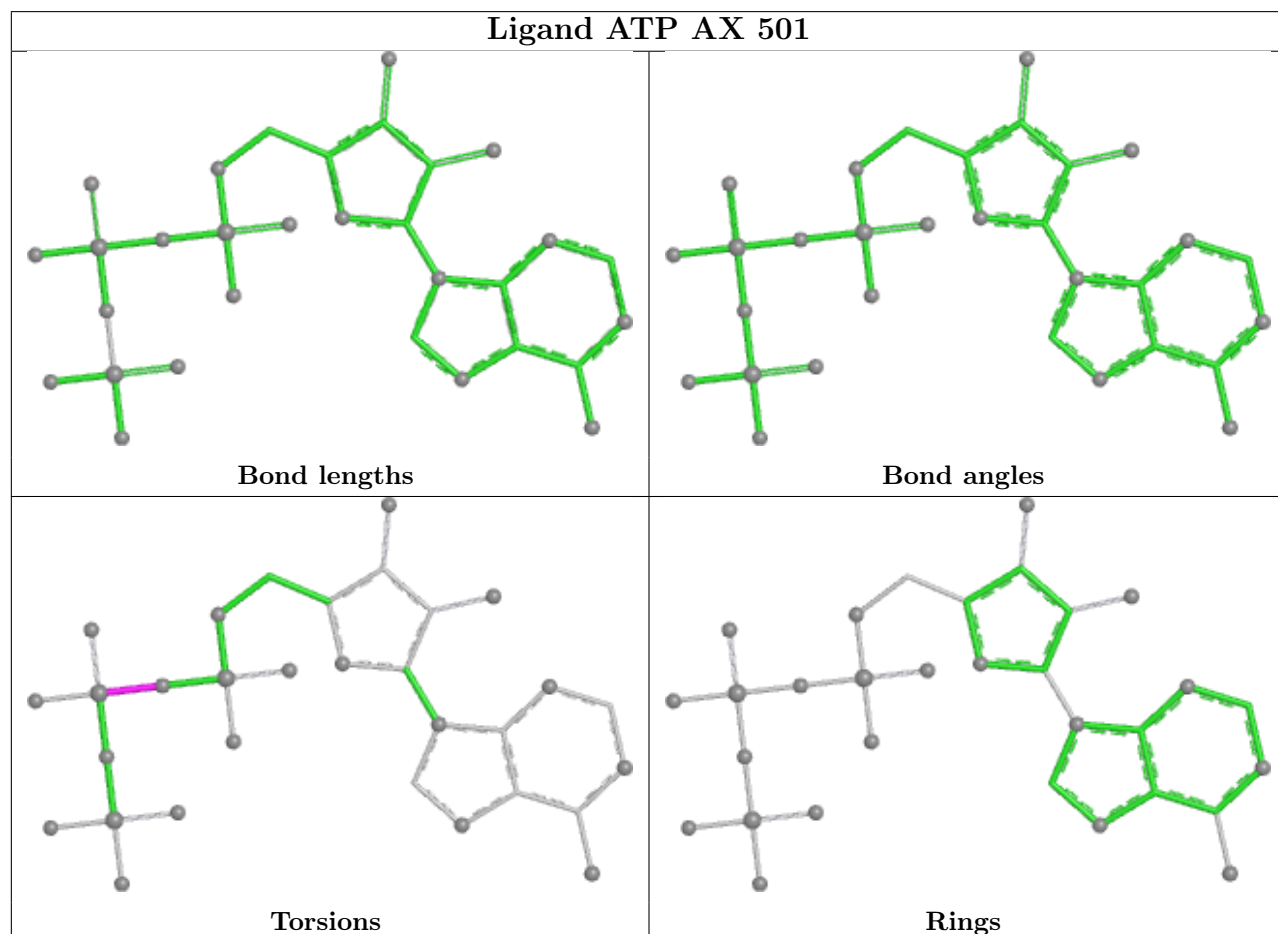
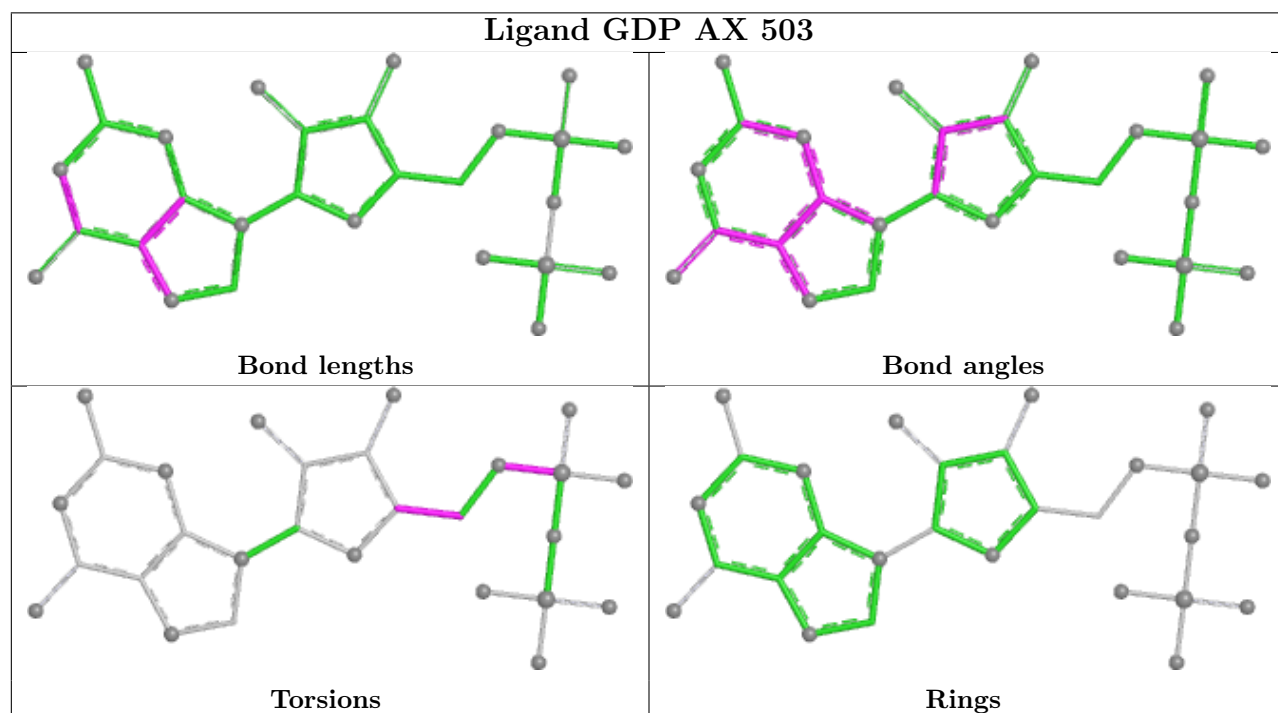
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	AX	503	GDP	2	0
42	AX	501	ATP	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

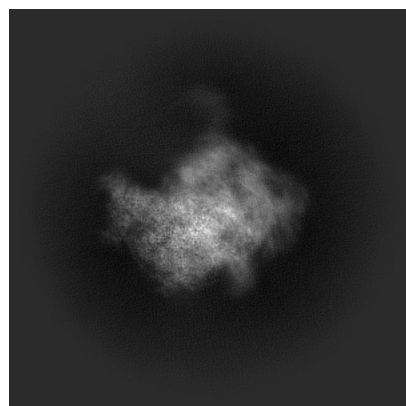
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16898. These allow visual inspection of the internal detail of the map and identification of artifacts.

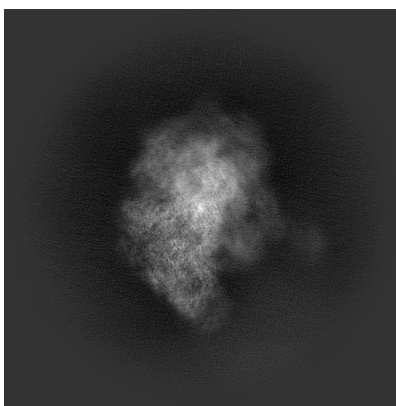
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

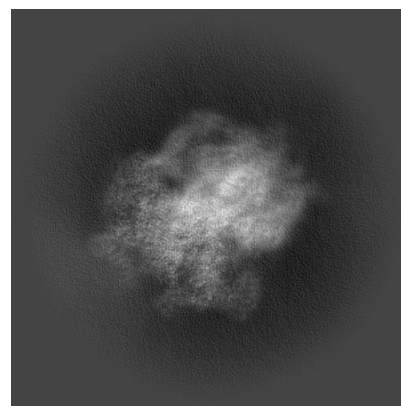
6.1.1 Primary map



X

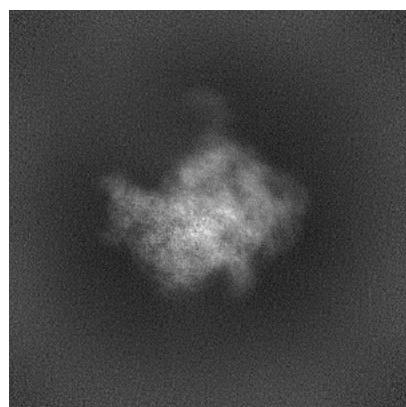


Y

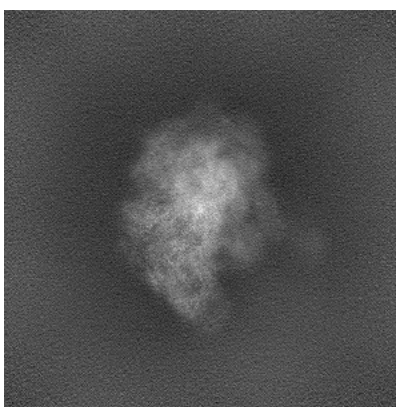


Z

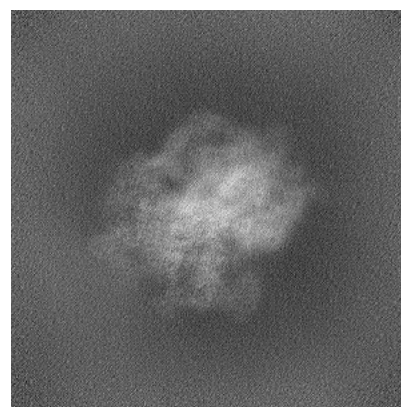
6.1.2 Raw map



X



Y

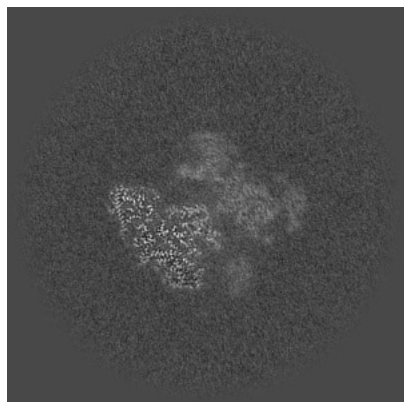


Z

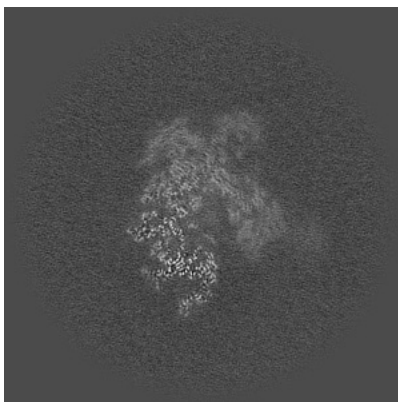
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

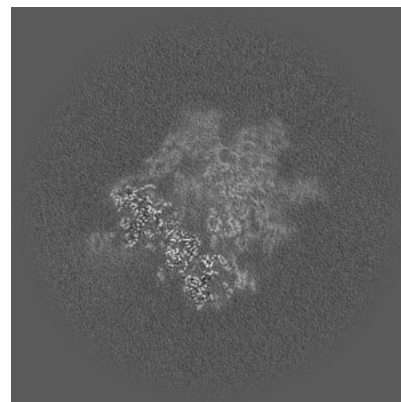
6.2.1 Primary map



X Index: 256

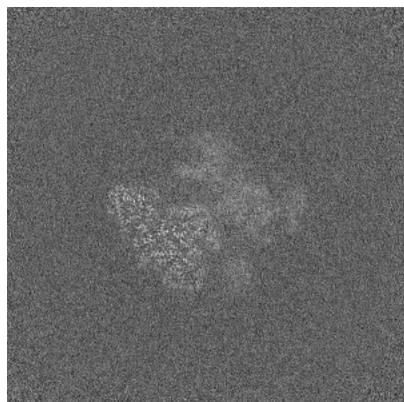


Y Index: 256

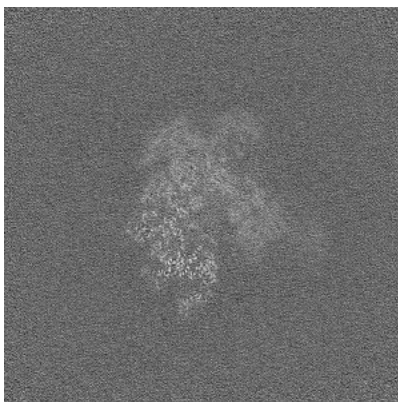


Z Index: 256

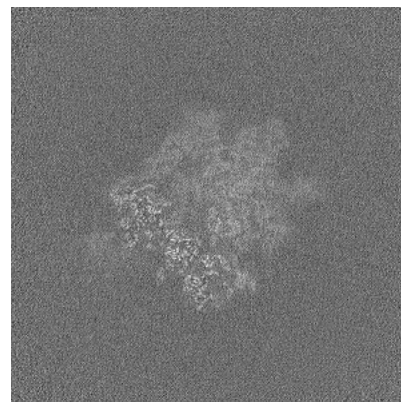
6.2.2 Raw map



X Index: 256



Y Index: 256

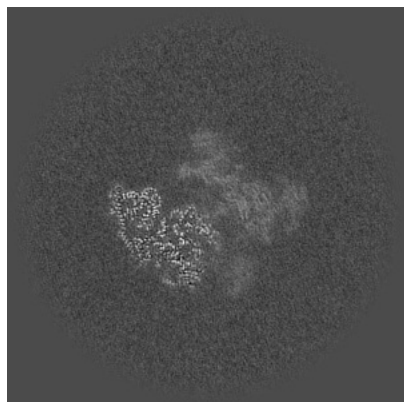


Z Index: 256

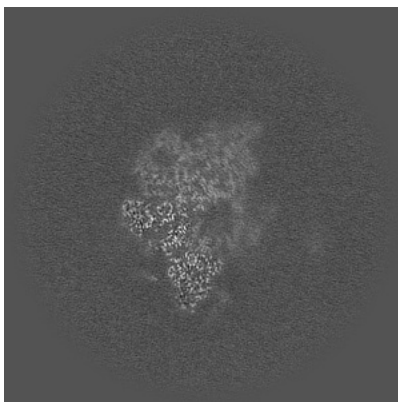
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

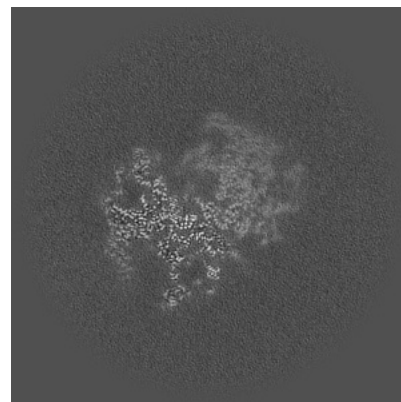
6.3.1 Primary map



X Index: 252

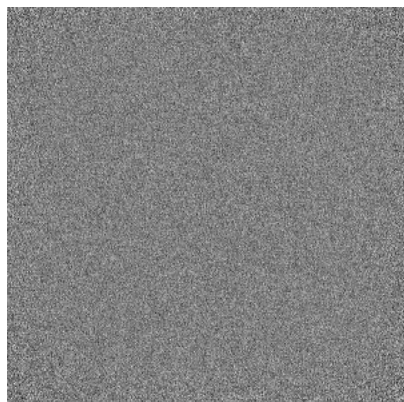


Y Index: 235

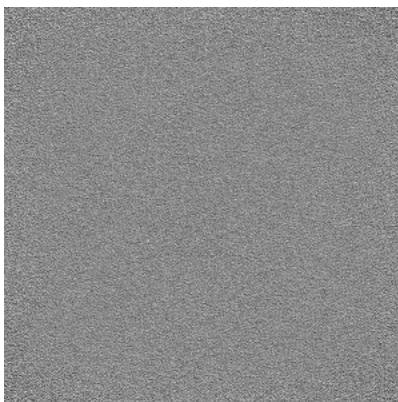


Z Index: 230

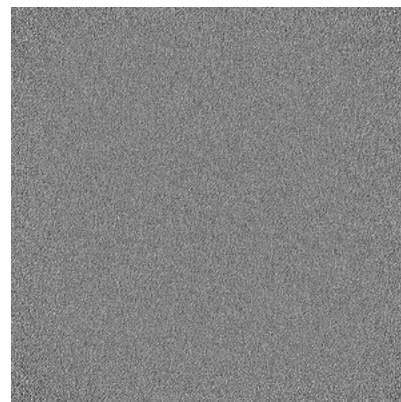
6.3.2 Raw map



X Index: 0



Y Index: 0

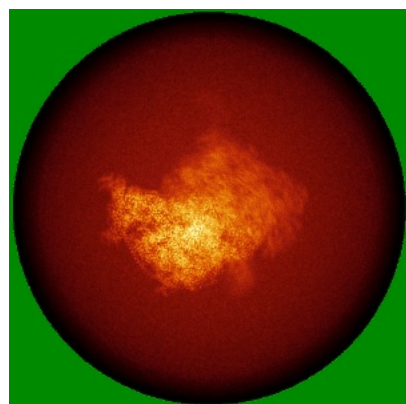


Z Index: 0

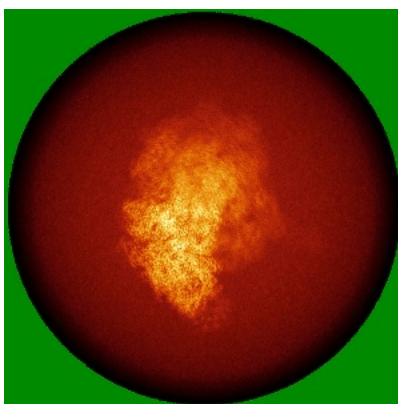
The images above show the largest variance slices of the map in three orthogonal directions.

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

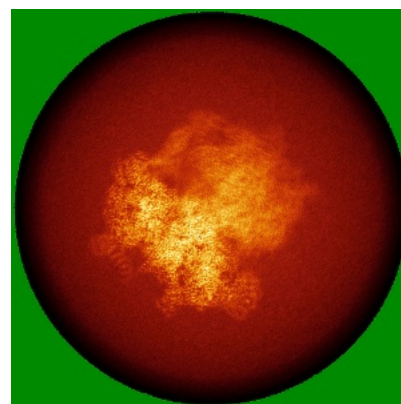
6.4.1 Primary map



X

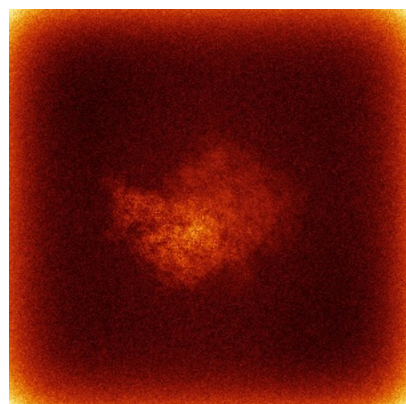


Y

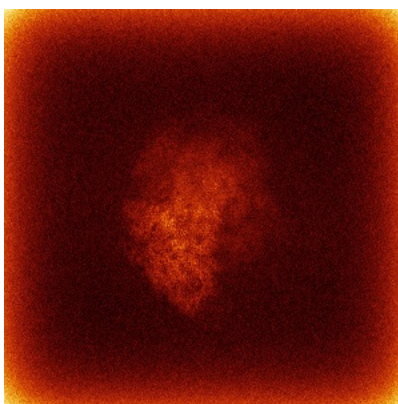


Z

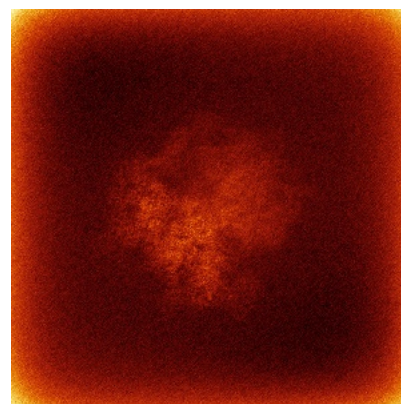
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



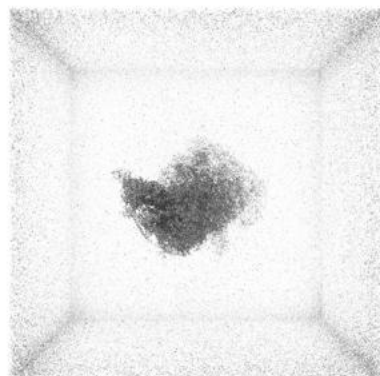
Y



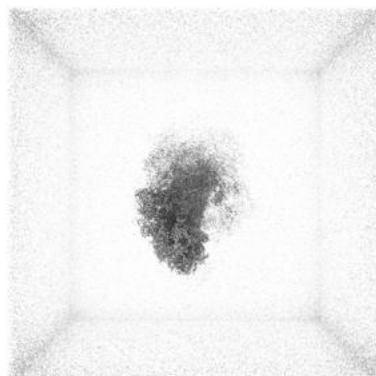
Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

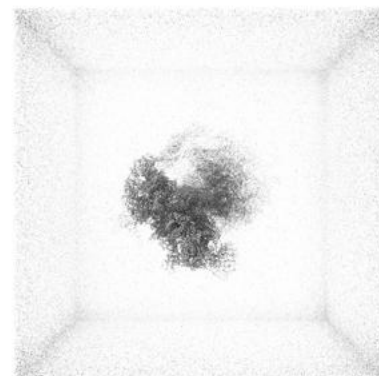
6.5.2 Raw map



X



Y



Z

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

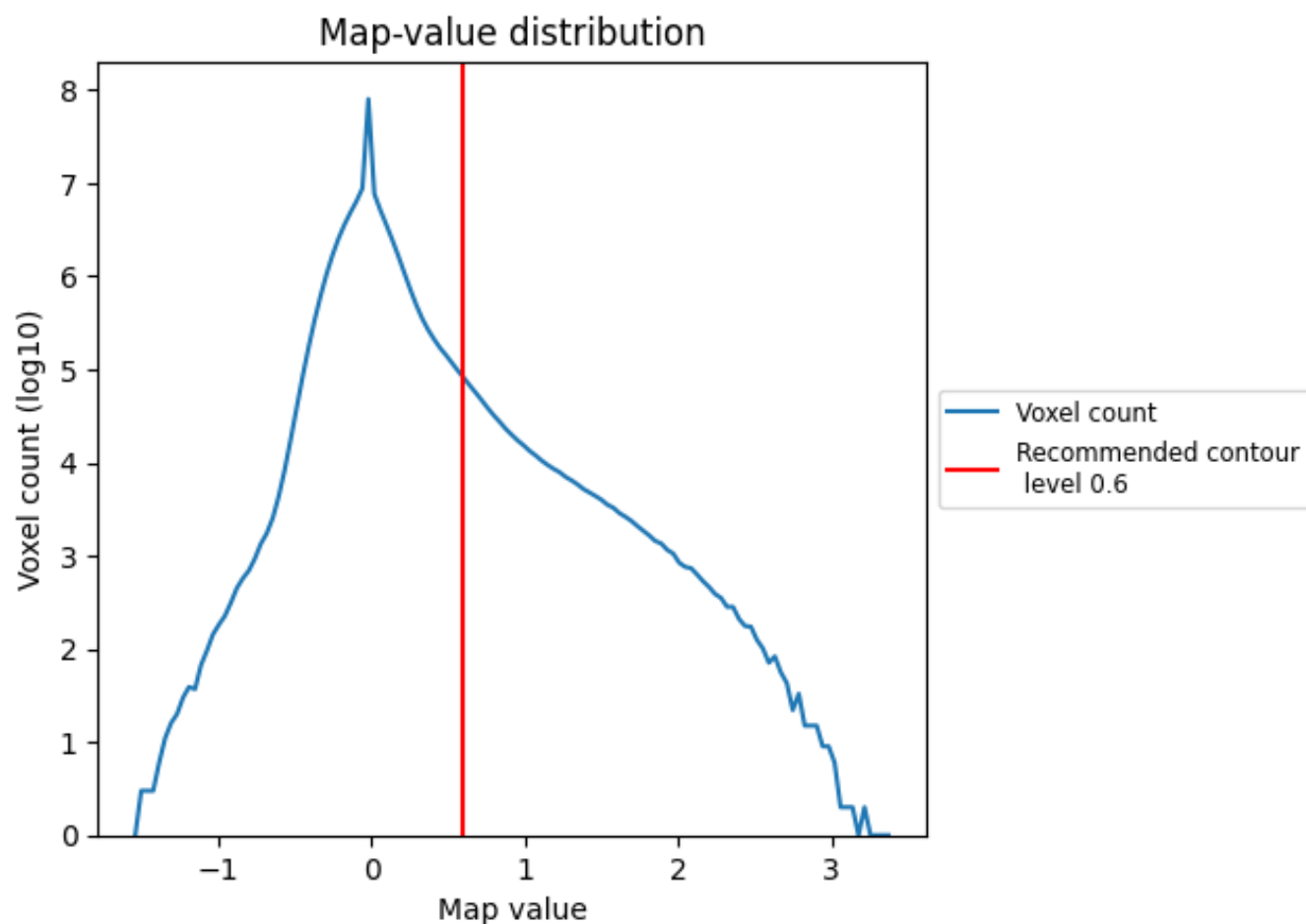
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

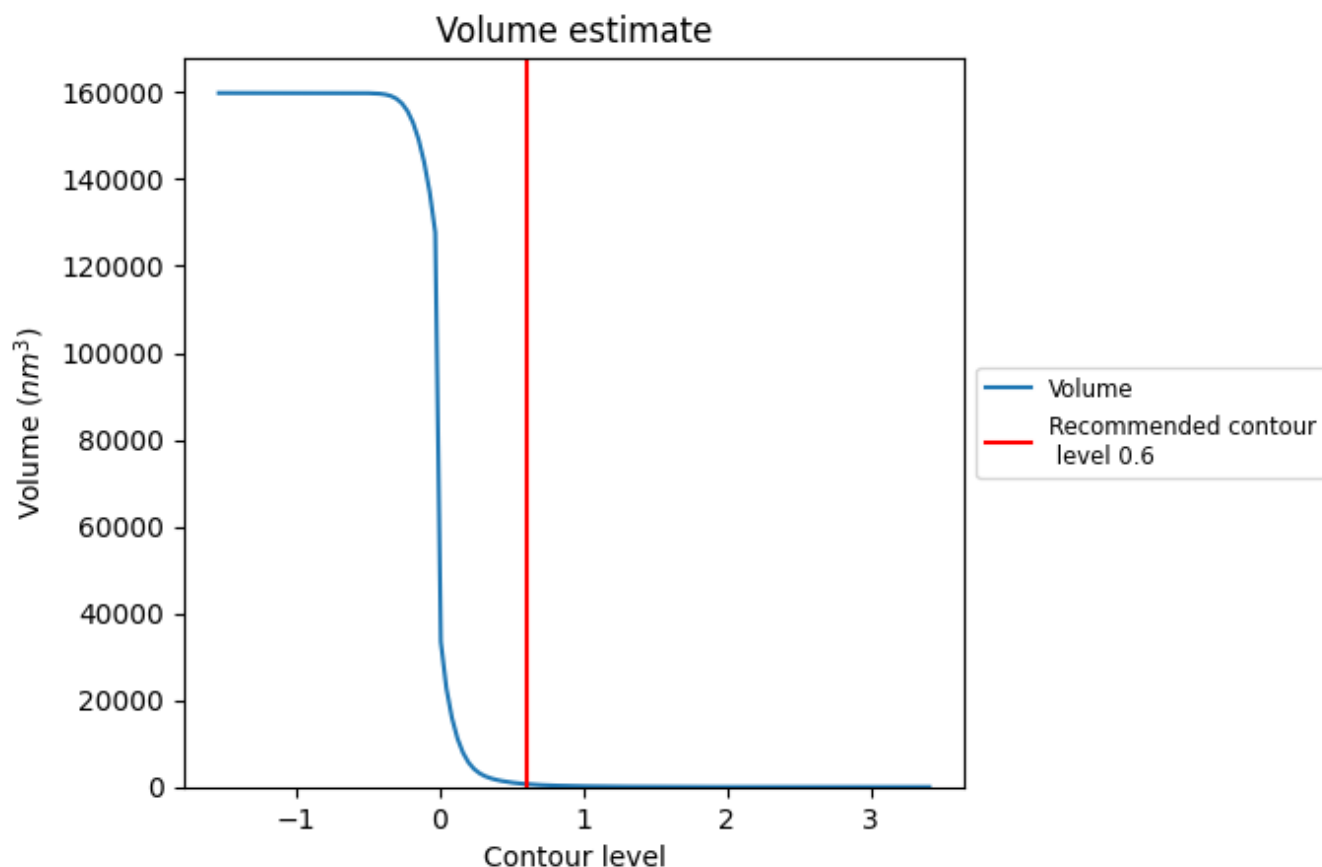
This section contains the results of statistical analysis of the map.

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.

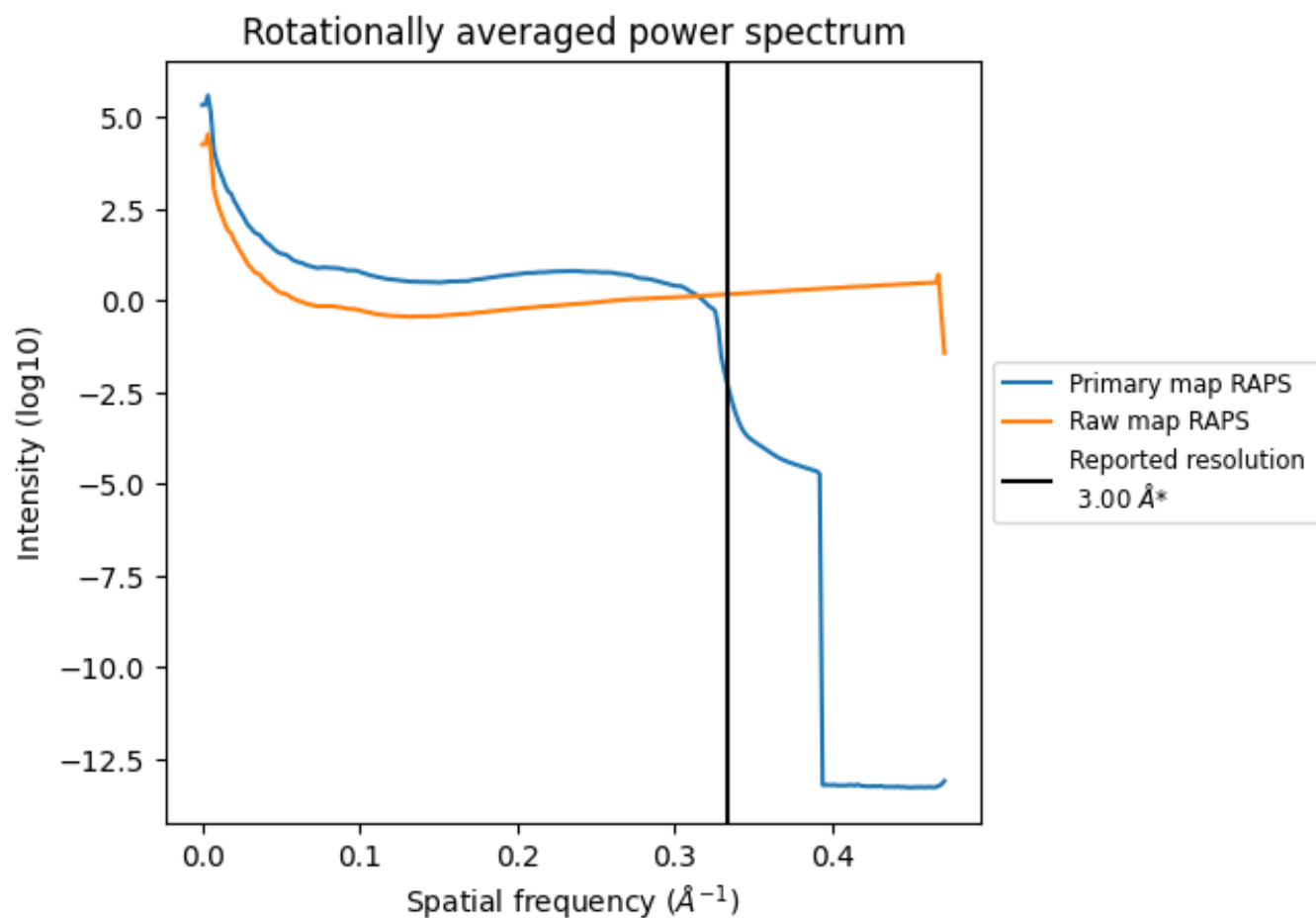
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 673 nm³; this corresponds to an approximate mass of 608 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 ⓘ

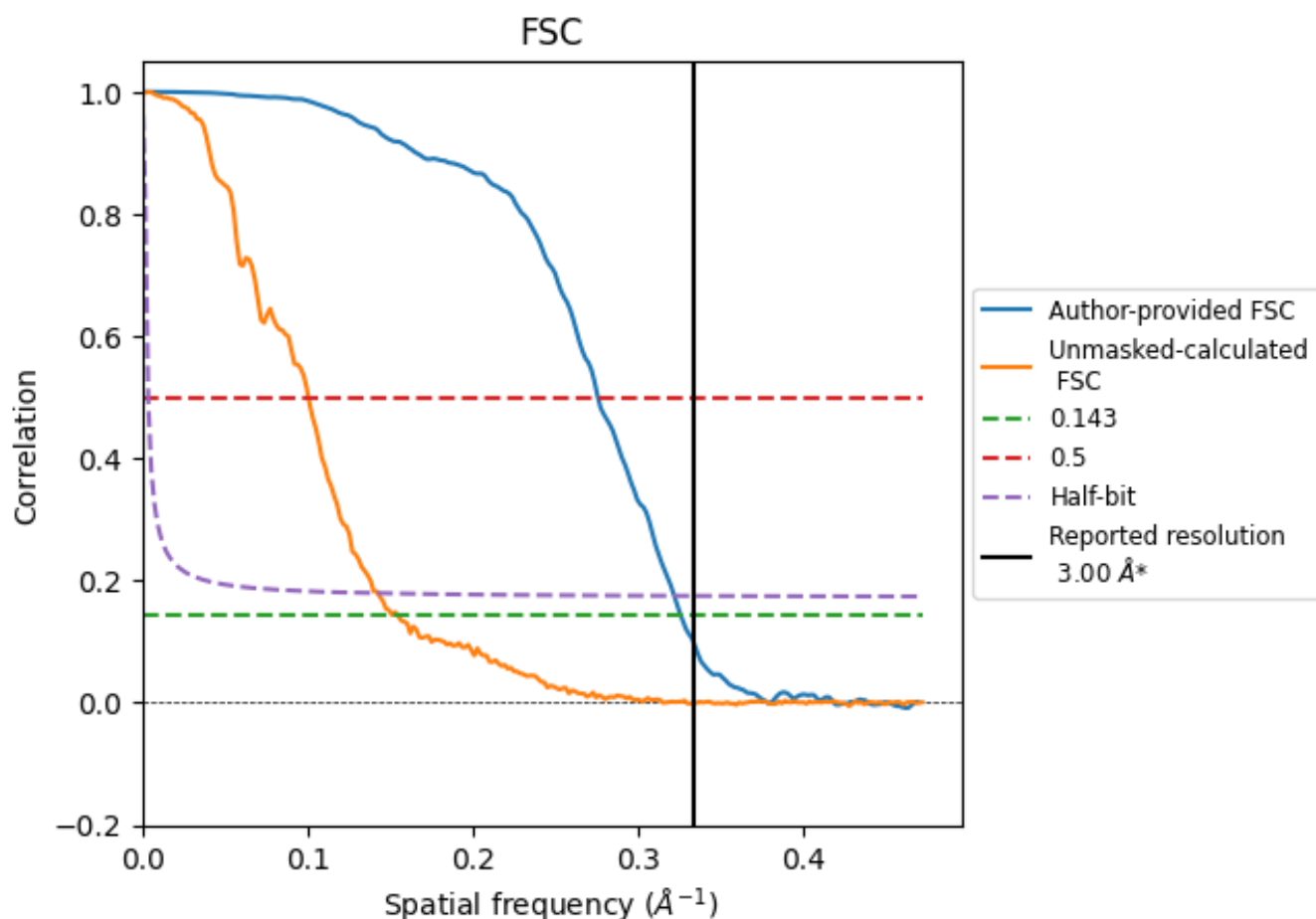


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 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	3.07	3.63	3.11
Unmasked-calculated*	6.47	9.95	7.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.47 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-16898 and PDB model 8OIS. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)

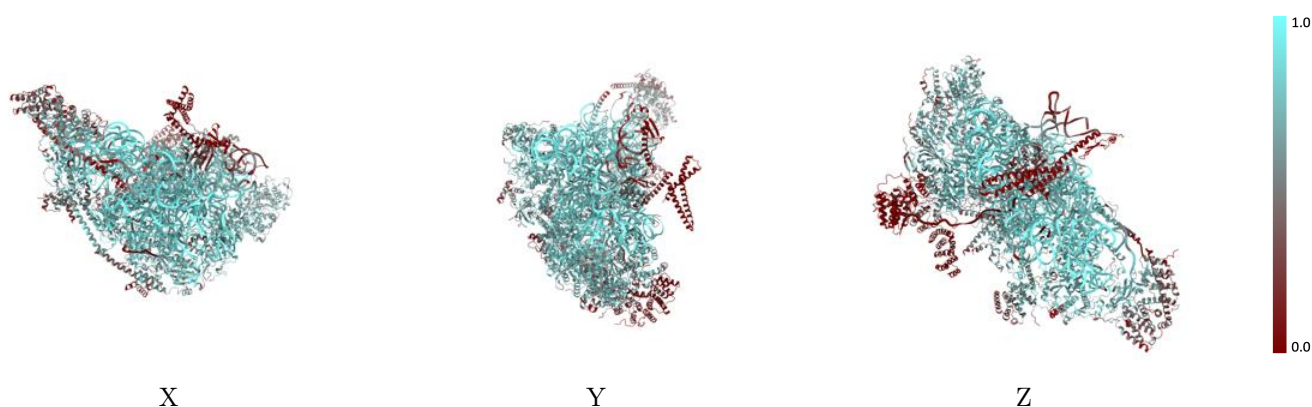
This section was not generated.

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



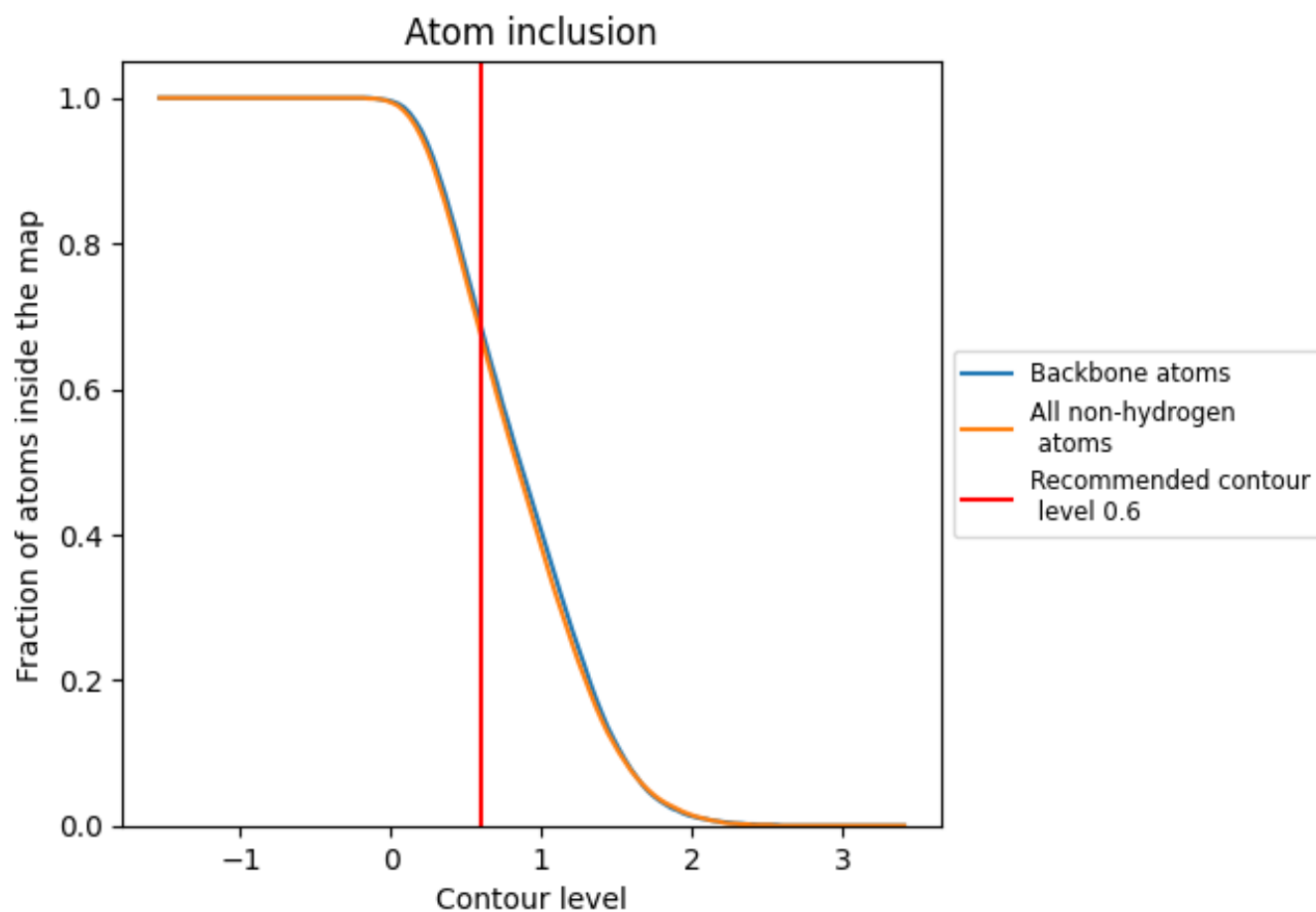
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 67% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6700	 0.4540
AA	 0.8940	 0.5270
AB	 0.6340	 0.4580
AC	 0.7940	 0.5400
AD	 0.7940	 0.5100
AE	 0.6910	 0.4520
AF	 0.6960	 0.4890
AG	 0.4860	 0.3040
AH	 0.6900	 0.5010
AI	 0.3560	 0.2740
AJ	 0.7590	 0.5270
AK	 0.8180	 0.5450
AL	 0.6770	 0.4580
AM	 0.7650	 0.5090
AN	 0.8090	 0.5350
AO	 0.7270	 0.4880
AP	 0.7470	 0.4760
AQ	 0.7890	 0.5170
AR	 0.5890	 0.4280
AS	 0.5920	 0.4360
AT	 0.7500	 0.5150
AU	 0.6330	 0.4560
AV	 0.4200	 0.3250
AW	 0.6780	 0.4740
AX	 0.6920	 0.4760
AY	 0.4890	 0.3660
AZ	 0.6900	 0.4880
Aa	 0.1550	 0.2160
Ab	 0.7450	 0.4960
Ac	 0.6420	 0.4490
Ad	 0.7010	 0.5070
Ae	 0.2010	 0.2500
Ag	 0.6640	 0.4760
Ai	 0.7550	 0.4840
Aj	 0.6870	 0.4720



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Chain	Atom inclusion	Q-score
BX	0.2070	0.1600
Bd	0.2260	0.2230