Full wwPDB EM Validation Report

Aug 27, 2026 – 12:28 am BST

PDB ID	:	9G5D / pdb_00009g5d
EMDB ID	:	EMD-51085
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit (State C)
Authors	:	Finke, A.F.; Heinrichs, M.; Aibara, S.; Richter-Dennerlein, R.; Hillen, H.S.
Deposited on	:	2024-07-16
Resolution	:	3.00 Å(reported)
Based on initial model	:	7PNX

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

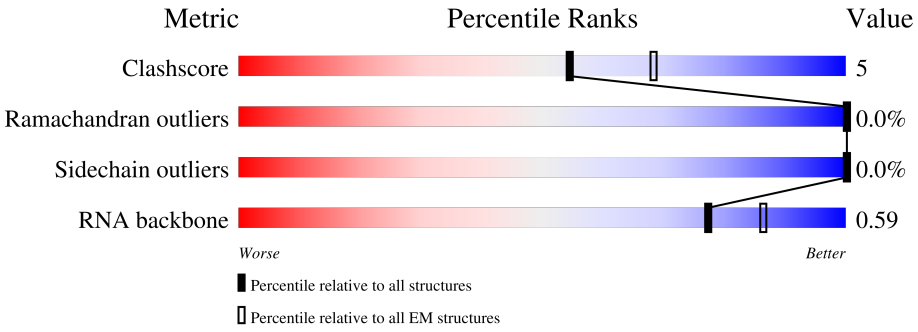
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

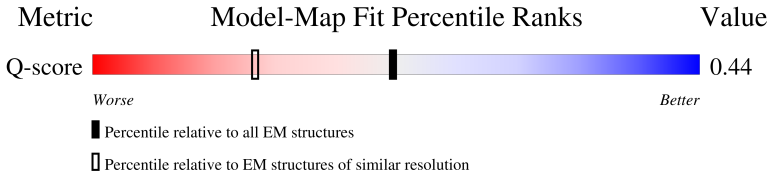
1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

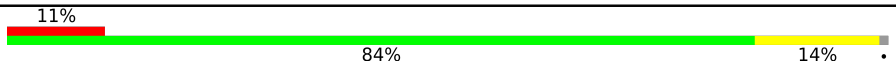
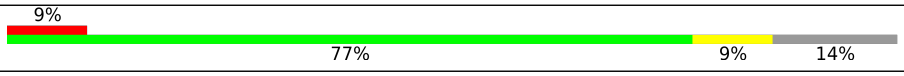
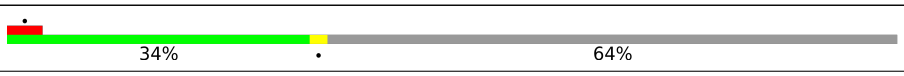
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	218	
2	1	323	
3	3	199	

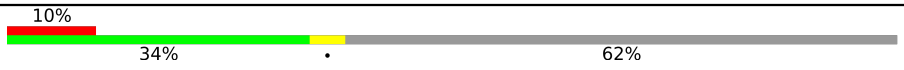
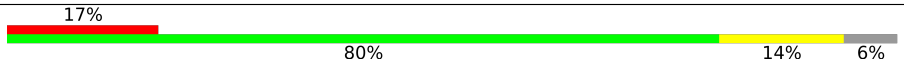
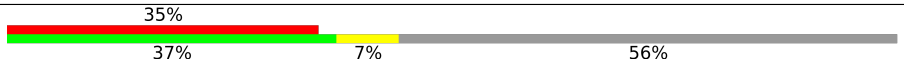
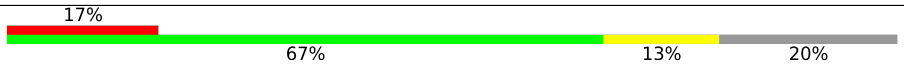
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Mol	Chain	Length	Quality of chain
4	4	689	39% 71% 15% 14%
5	A	955	66% 27%
6	B	296	65% 11% 24%
7	C	167	5% 59% 20% 21%
8	D	430	13% 69% 10% 20%
9	E	125	14% 85% 10% 6%
10	F	242	8% 74% 6% 19%
11	G	396	9% 66% 11% 23%
12	H	201	6% 58% 11% 30%
13	I	194	63% 8% 29%
14	J	138	7% 70% 9% 22%
15	K	128	66% 12% 21%
16	L	257	8% 61% 7% 32%
17	M	137	6% 75% 12% 13%
18	N	130	74% 11% 15%
19	O	258	67% 8% 25%
20	P	142	5% 61% 8% 32%
21	Q	87	6% 86% 11%
22	R	360	68% 14% 18%
23	S	190	12% 64% 7% 29%
24	T	173	6% 88% 9%
25	U	205	79% 7% 14%
26	V	414	34% 74% 14% 13%
27	W	187	42% 11% 47%
28	X	398	6% 71% 17% 12%

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Mol	Chain	Length	Quality of chain
29	Y	395	
30	Z	106	
31	a	343	
32	b	407	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 68801 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	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	278	Total	C	N	O	S	0	0
			2256	1430	386	429	11		

- Molecule 3 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 4 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	590	Total	C	N	O	S	0	0
			4775	3056	809	882	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	917	Total	C	N	O	P	0	0
			19474	8730	3508	6319	917		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	225	Total	C	N	O	S	0	0
			1828	1164	331	323	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	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	118	Total	C	N	O	S	0	0
			936	592	168	172	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	195	Total	C	N	O	S	0	0
			1604	1020	290	283	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	304	Total	C	N	O	S	0	0
			2500	1587	444	455	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	140	Total	C	N	O	S	0	0
			1152	745	194	210	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	108	Total	C	N	O	S	0	0
			839	521	169	143	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	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	110	Total	C	N	O	S	0	0
			868	562	156	147	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	97	Total	C	N	O	S	0	0
			781	501	134	138	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	295	Total	C	N	O	S	0	0
			2409	1533	413	455	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	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	352	Total	C	N	O	S	0	0
			2849	1822	499	517	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	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	150	Total	C	N	O	S	0	0
			1188	743	221	217	7		

- Molecule 32 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	326	Total	C	N	O	S	0	0
			2546	1610	456	466	14		

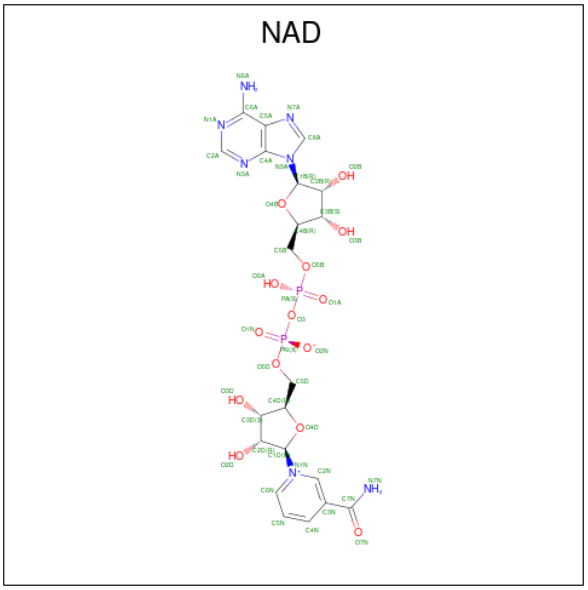
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	3	1	Total	Mg	0
			1	1	
33	A	8	Total	Mg	0
			8	8	
33	B	1	Total	Mg	0
			1	1	

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

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

- Molecule 35 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

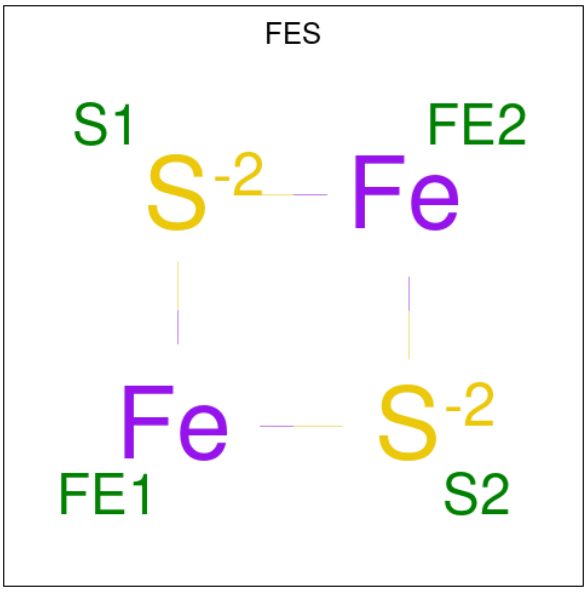


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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

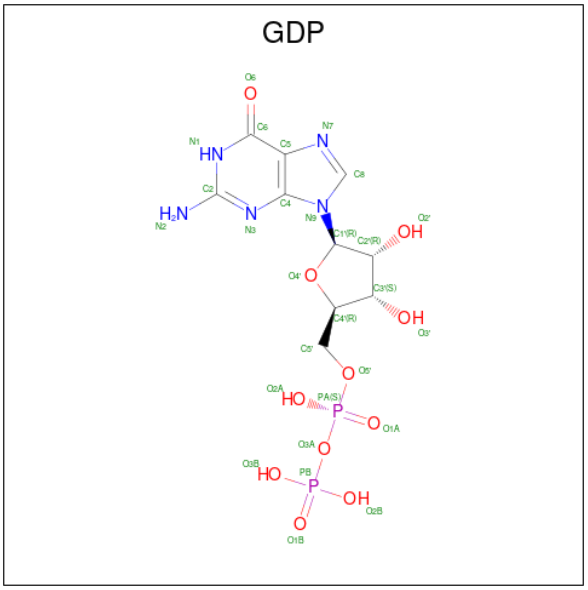
Mol	Chain	Residues	Atoms		AltConf
36	O	1	Total	Zn	0
			1	1	

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



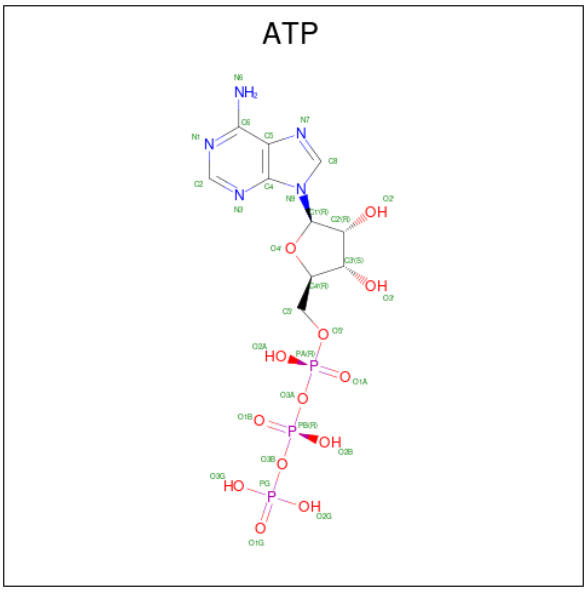
Mol	Chain	Residues	Atoms			AltConf
37	P	1	Total	Fe	S	0
			4	2	2	
37	T	1	Total	Fe	S	0
			4	2	2	

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



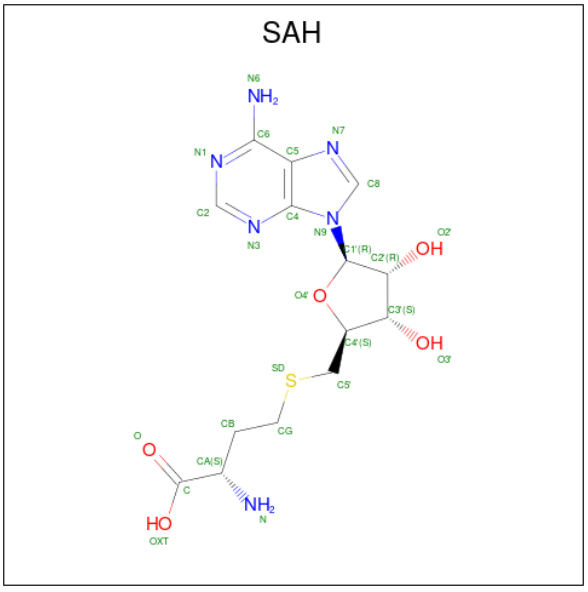
Mol	Chain	Residues	Atoms					AltConf
38	X	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 39 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 40 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



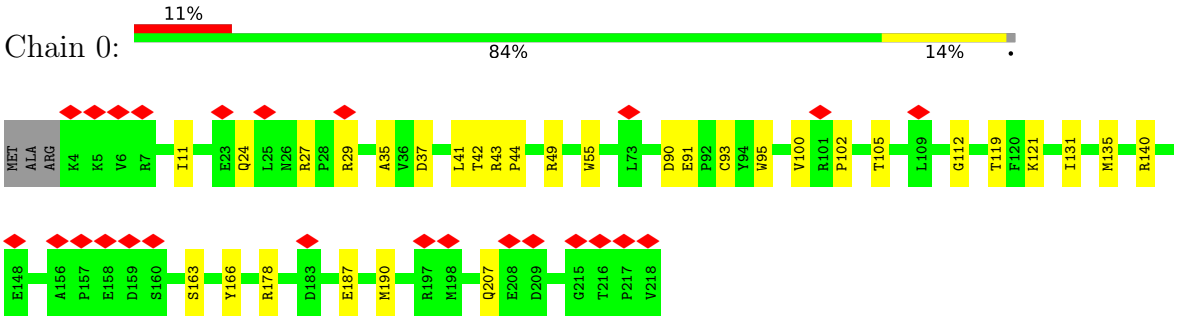
Mol	Chain	Residues	Atoms					AltConf
40	b	1	Total	C	N	O	S	0
			26	14	6	5	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

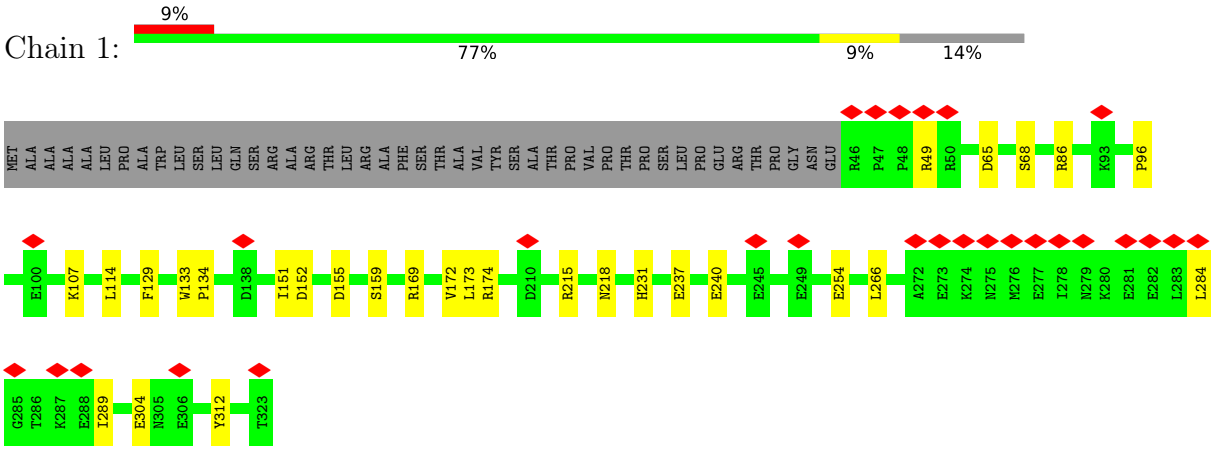
• Molecule 1: 28S ribosomal protein S34, mitochondrial

Chain 0:



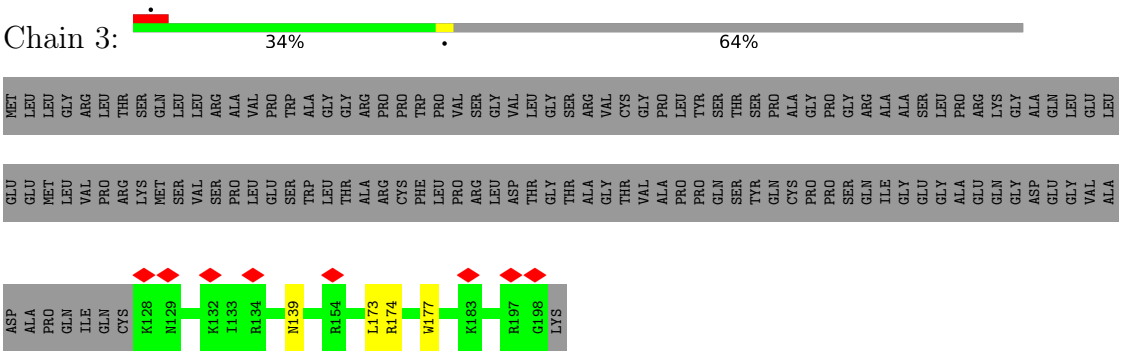
• Molecule 2: 28S ribosomal protein S35, mitochondrial

Chain 1:



• Molecule 3: Aurora kinase A-interacting protein

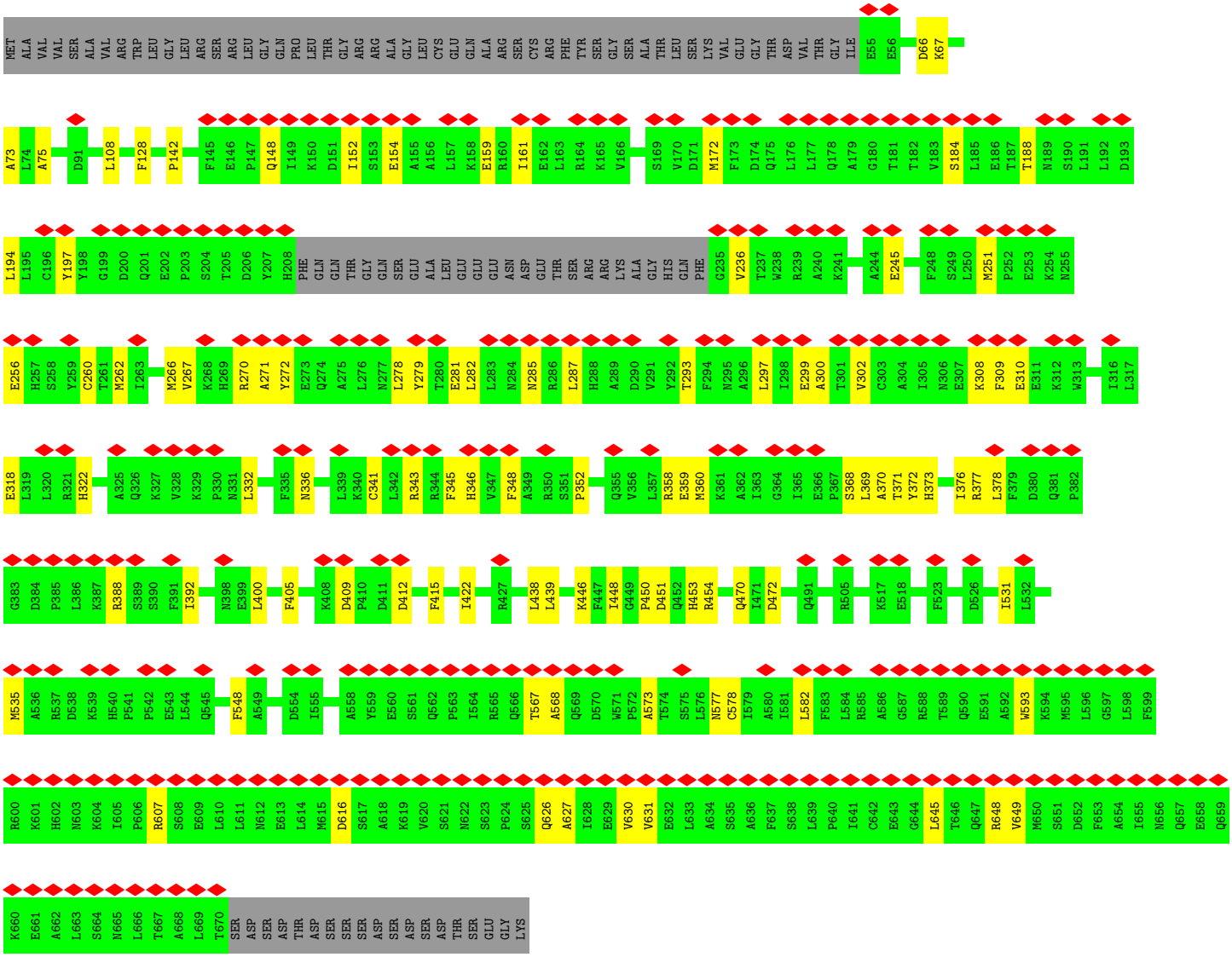
Chain 3:



• Molecule 4: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain 4:

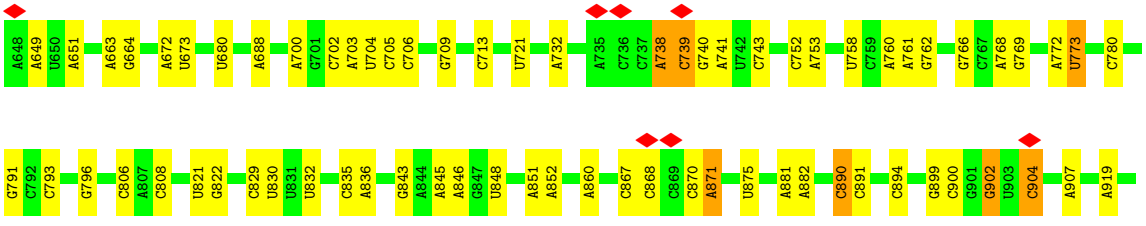


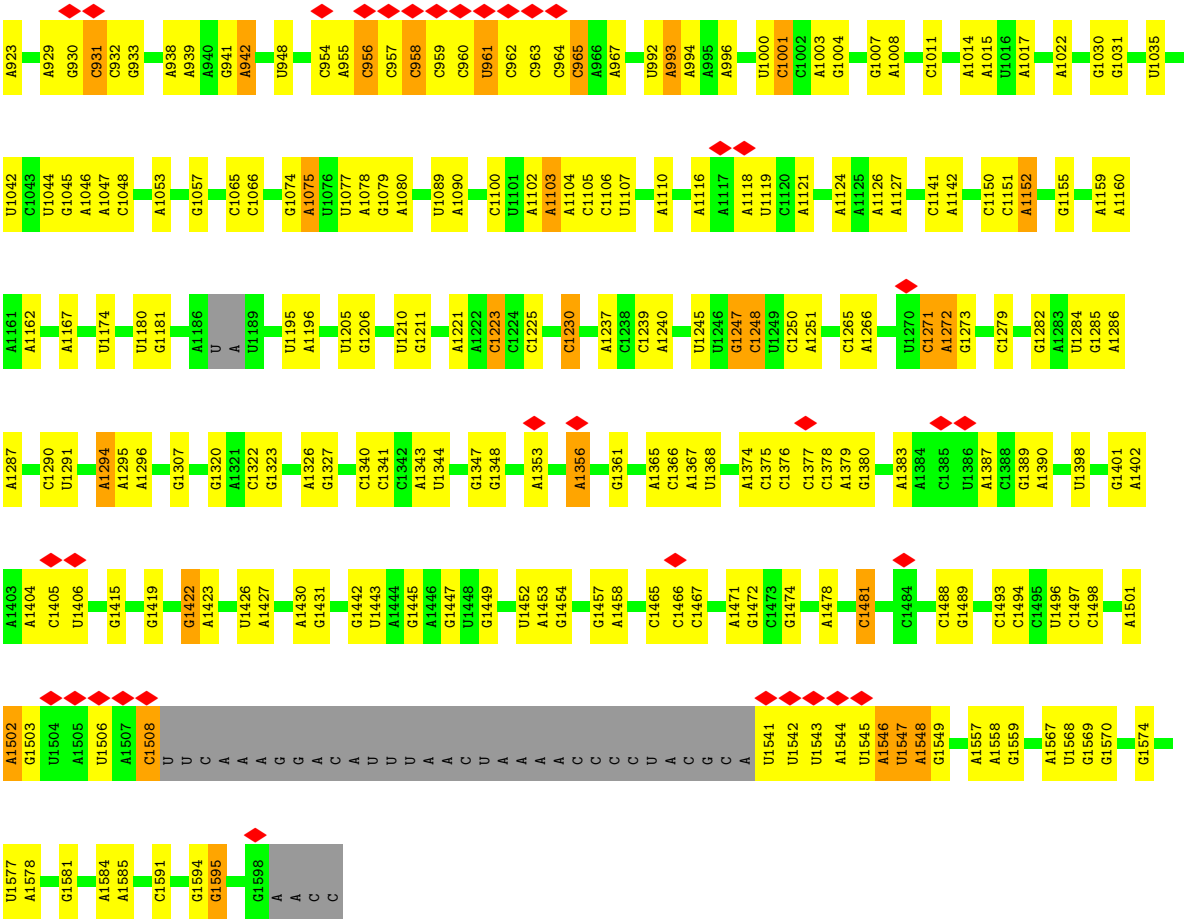


• Molecule 5: 12S mitochondrial rRNA

Chain A:



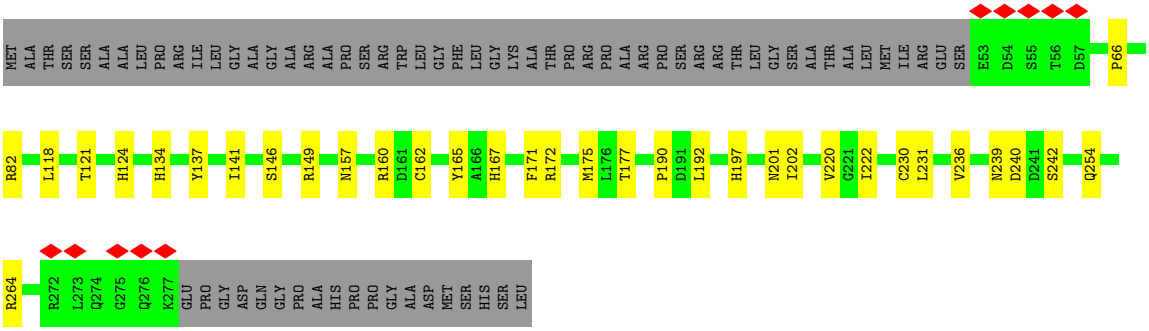




• Molecule 6: 28S ribosomal protein S2, mitochondrial

Chain B:

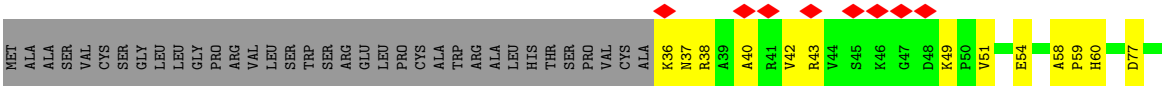


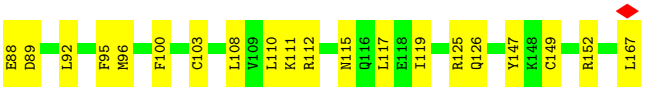


• Molecule 7: 28S ribosomal protein S24, mitochondrial

Chain C:

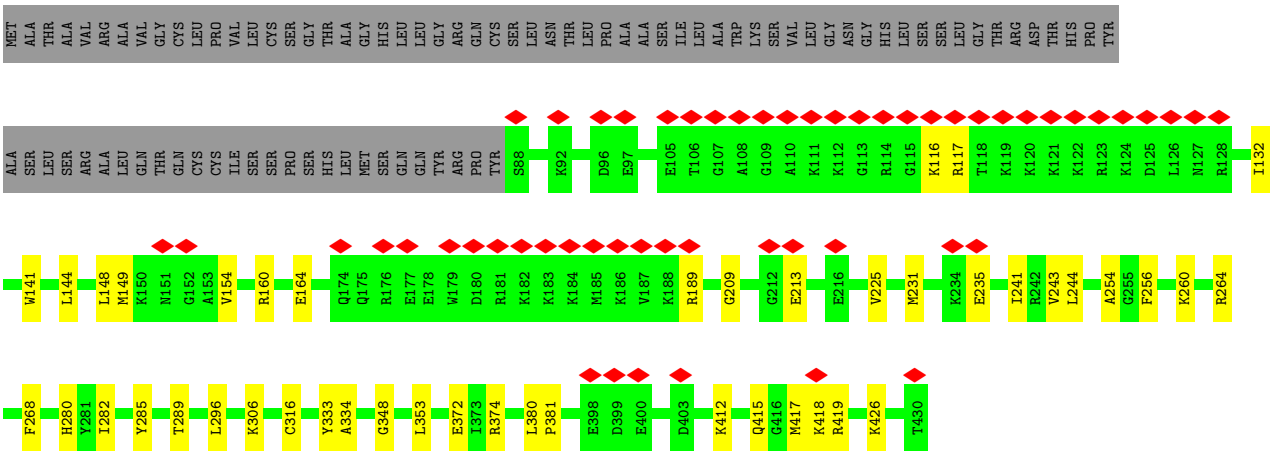




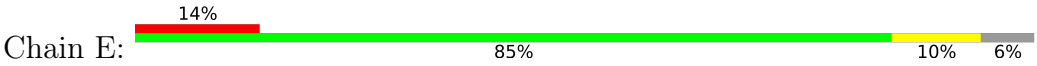


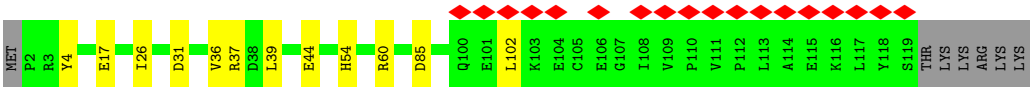
• Molecule 8: 28S ribosomal protein S5, mitochondrial



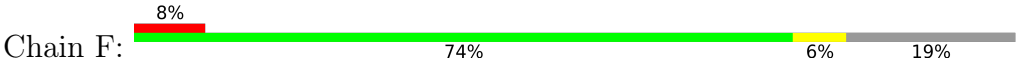


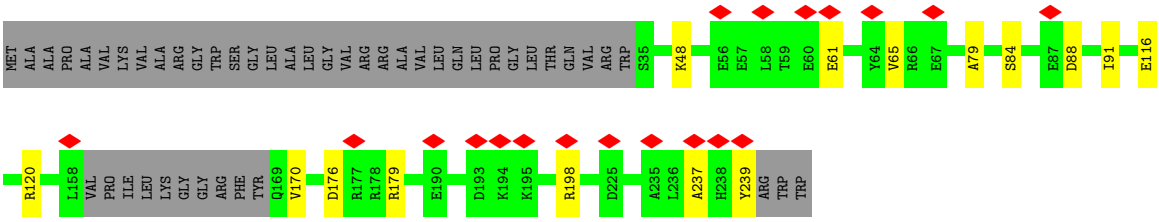
• Molecule 9: 28S ribosomal protein S6, mitochondrial





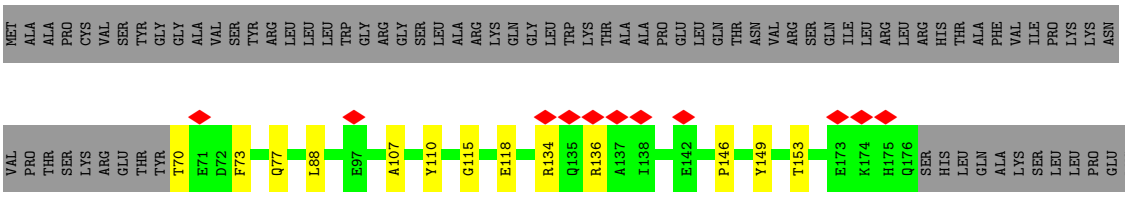
• Molecule 10: 28S ribosomal protein S7, mitochondrial

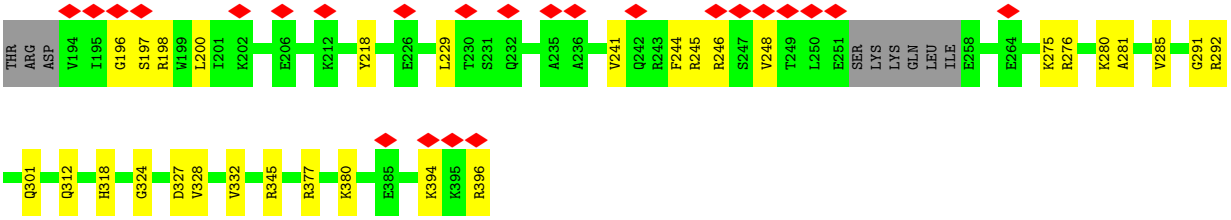




• Molecule 11: 28S ribosomal protein S9, mitochondrial



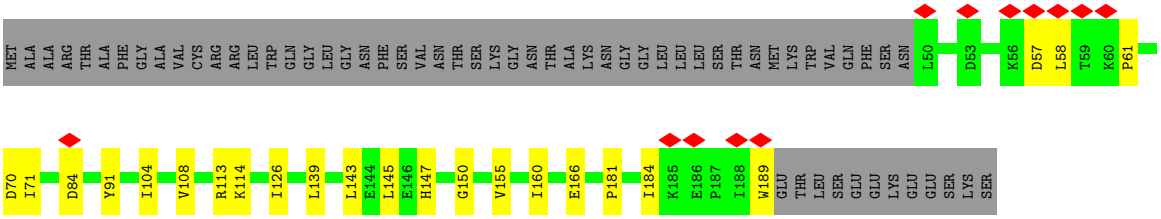




• Molecule 12: 28S ribosomal protein S10, mitochondrial

Chain H:

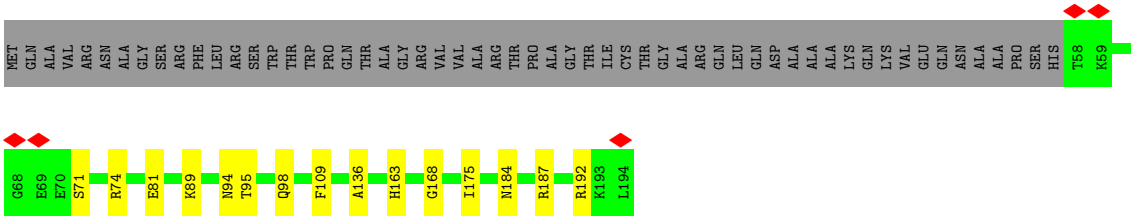




• Molecule 13: 28S ribosomal protein S11, mitochondrial

Chain I:

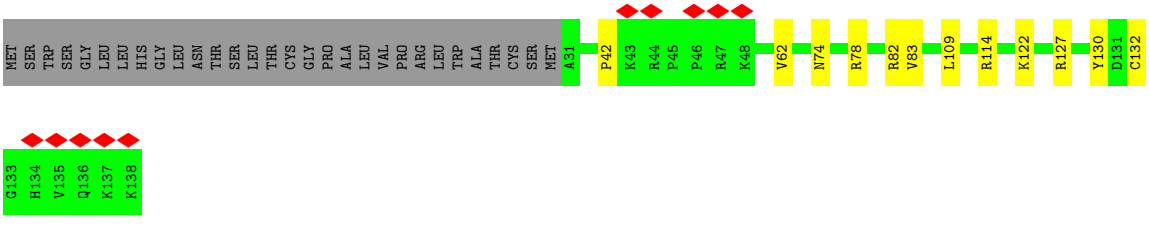




• Molecule 14: 28S ribosomal protein S12, mitochondrial

Chain J:

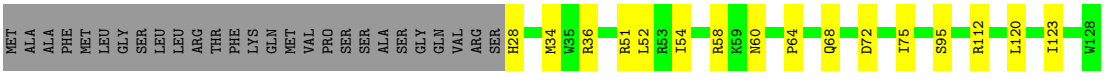




• Molecule 15: 28S ribosomal protein S14, mitochondrial

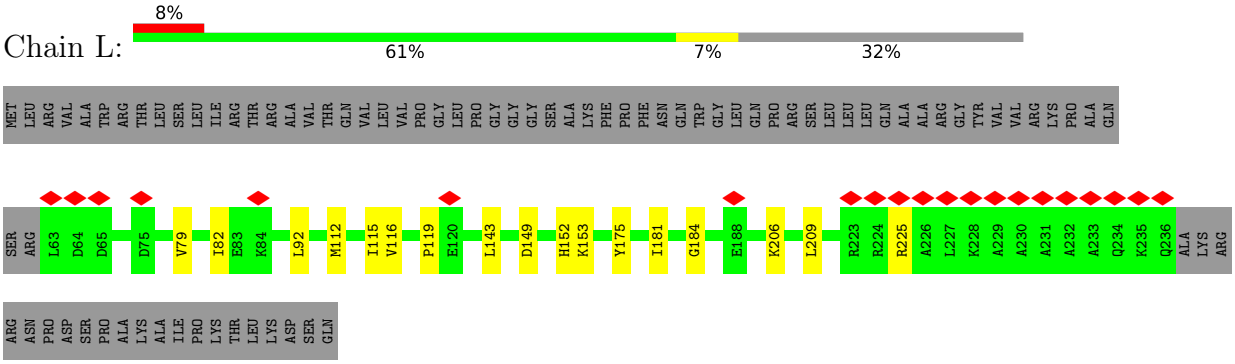
Chain K:





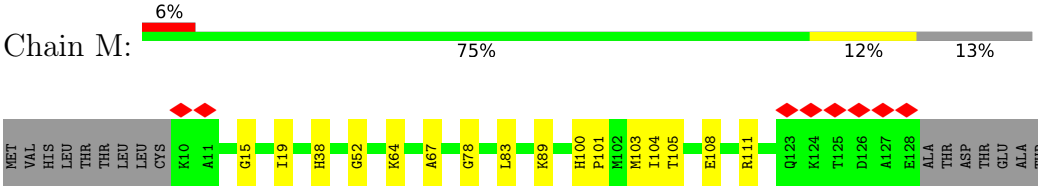
• Molecule 16: 28S ribosomal protein S15, mitochondrial

Chain L:



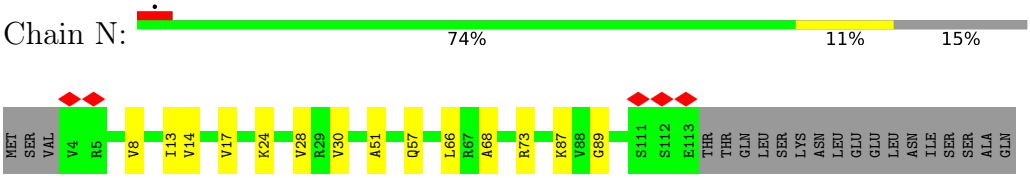
• Molecule 17: 28S ribosomal protein S16, mitochondrial

Chain M:



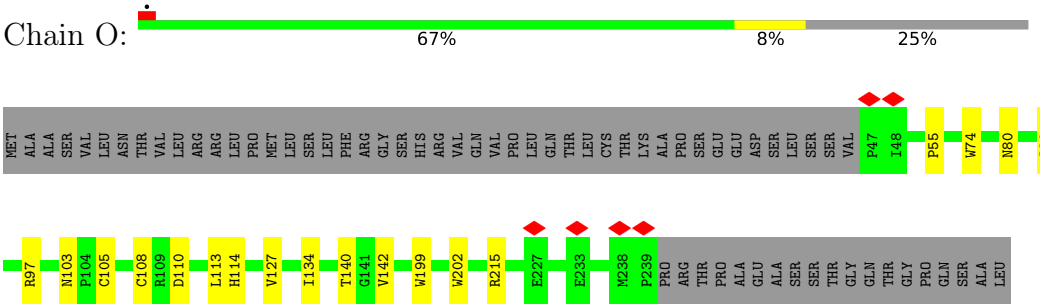
• Molecule 18: 28S ribosomal protein S17, mitochondrial

Chain N:



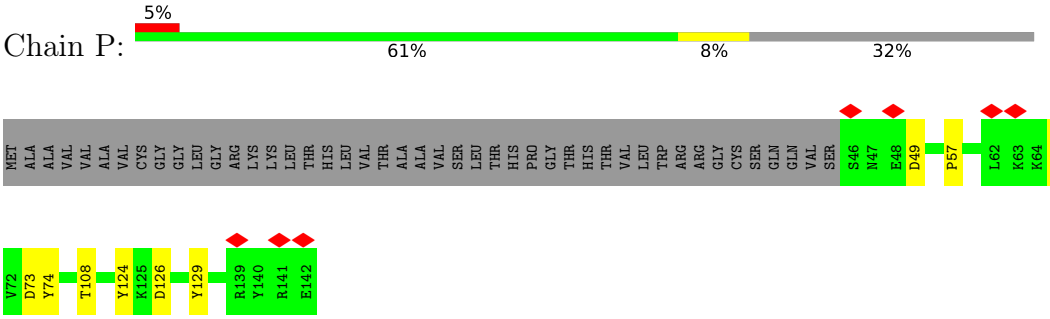
• Molecule 19: 28S ribosomal protein S18b, mitochondrial

Chain O:



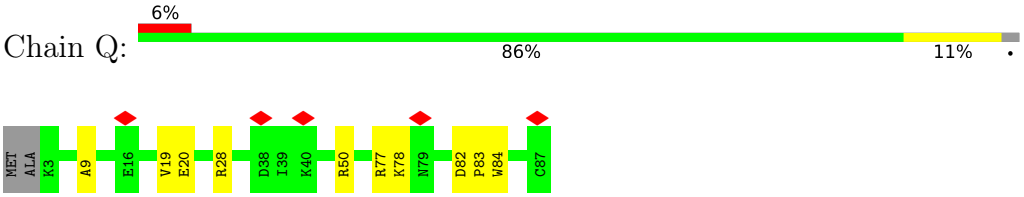
• Molecule 20: 28S ribosomal protein S18c, mitochondrial

Chain P:



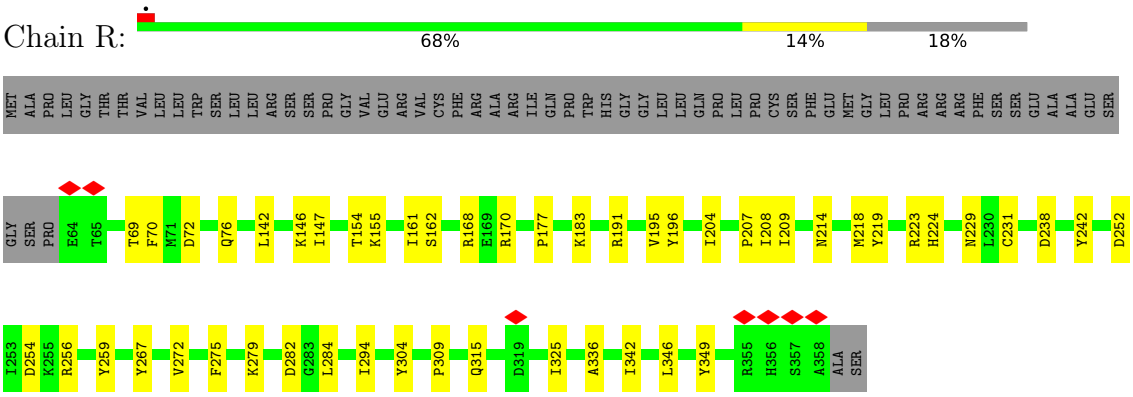
• Molecule 21: 28S ribosomal protein S21, mitochondrial

Chain Q:



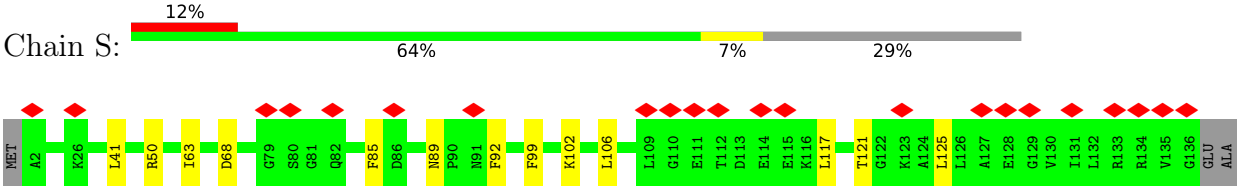
• Molecule 22: 28S ribosomal protein S22, mitochondrial

Chain R:



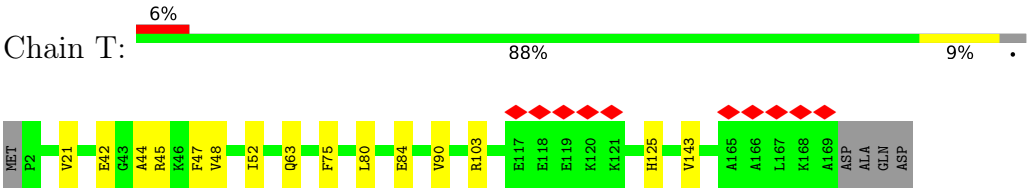
• Molecule 23: 28S ribosomal protein S23, mitochondrial

Chain S:



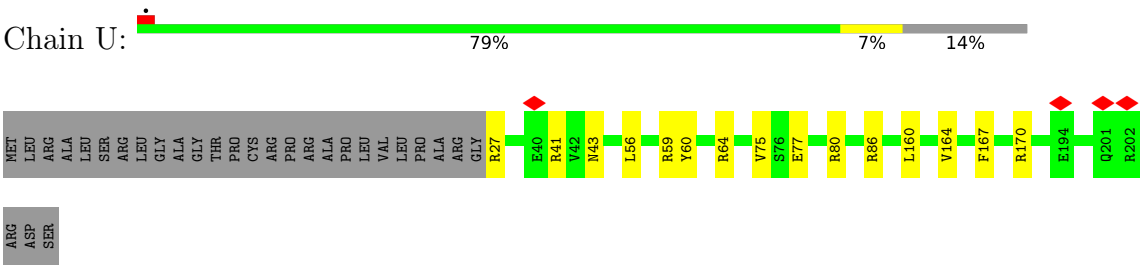
• Molecule 24: 28S ribosomal protein S25, mitochondrial

Chain T:



• Molecule 25: 28S ribosomal protein S26, mitochondrial

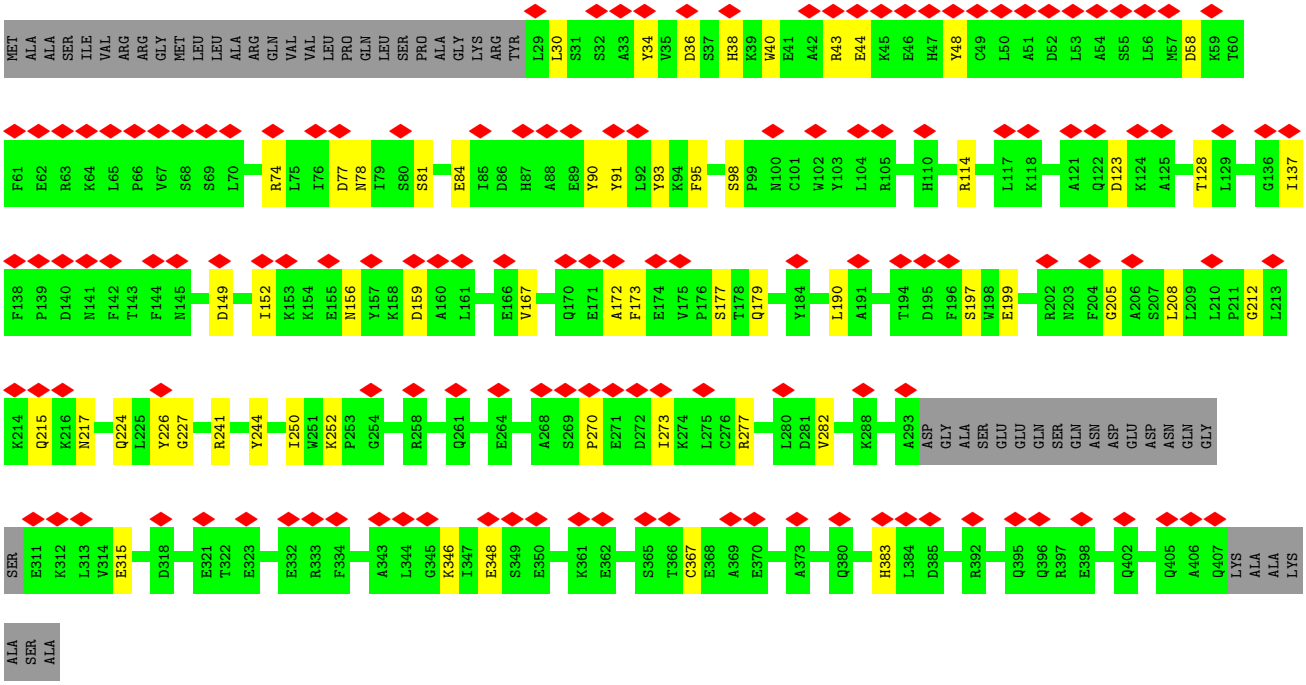
Chain U:



• Molecule 26: 28S ribosomal protein S27, mitochondrial

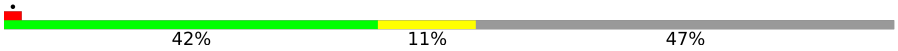
Chain V:

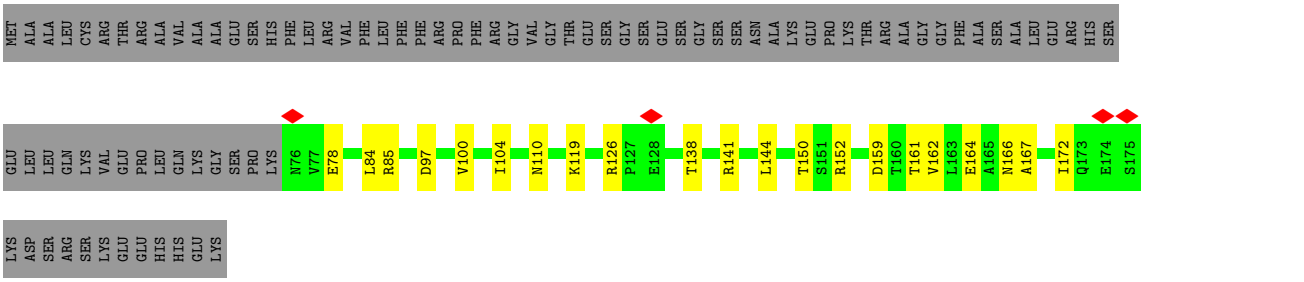




• Molecule 27: 28S ribosomal protein S28, mitochondrial

Chain W:

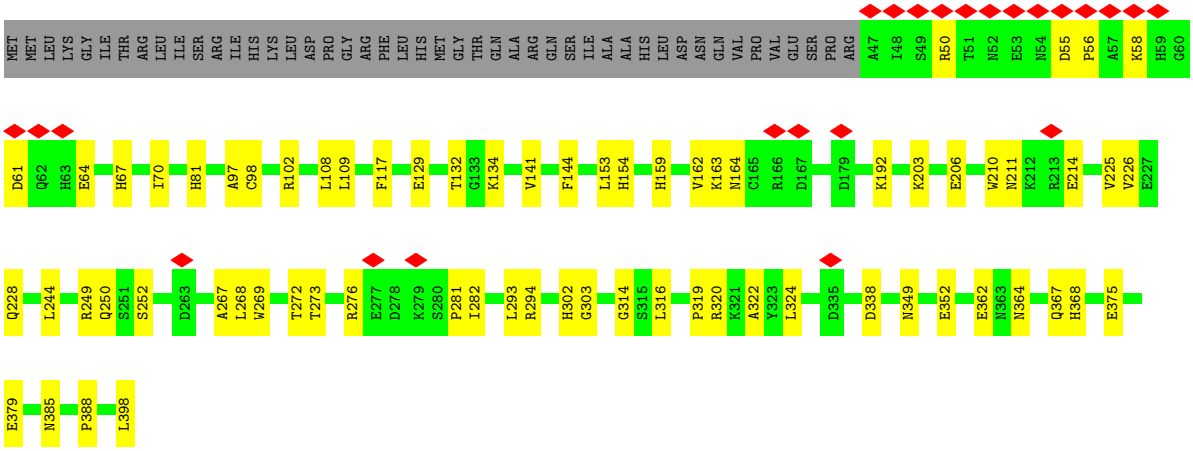




• Molecule 28: 28S ribosomal protein S29, mitochondrial

Chain X:

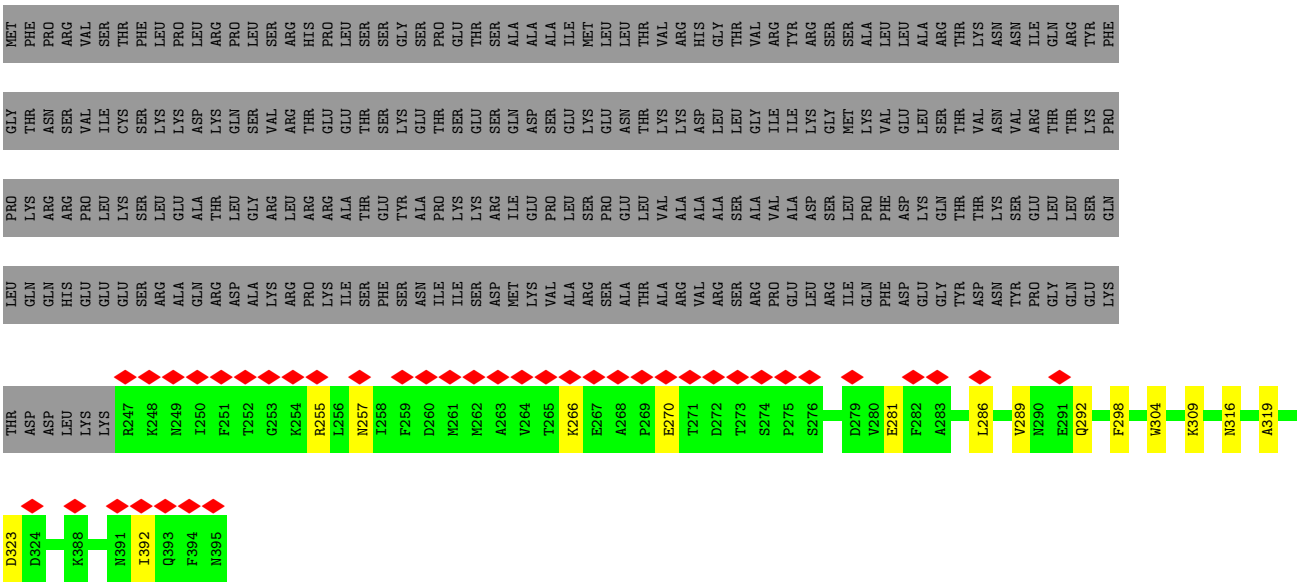




• Molecule 29: 28S ribosomal protein S31, mitochondrial

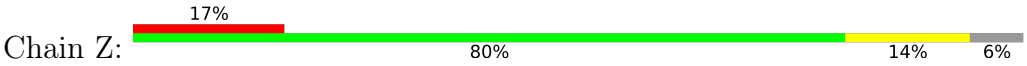
Chain Y:

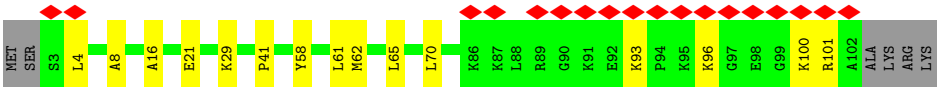




• Molecule 30: 28S ribosomal protein S33, mitochondrial

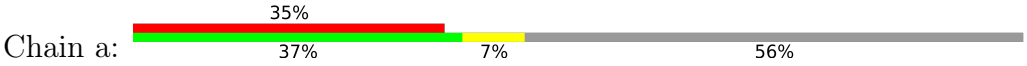
Chain Z:

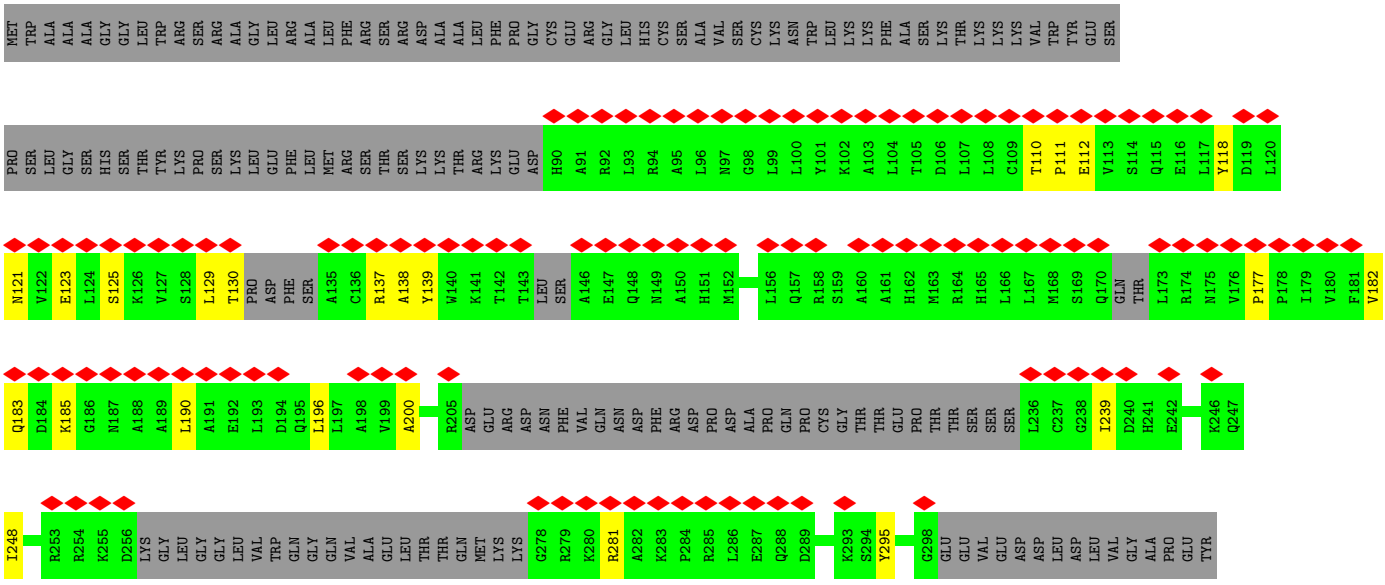




• Molecule 31: Putative ribosome-binding factor A, mitochondrial

Chain a:



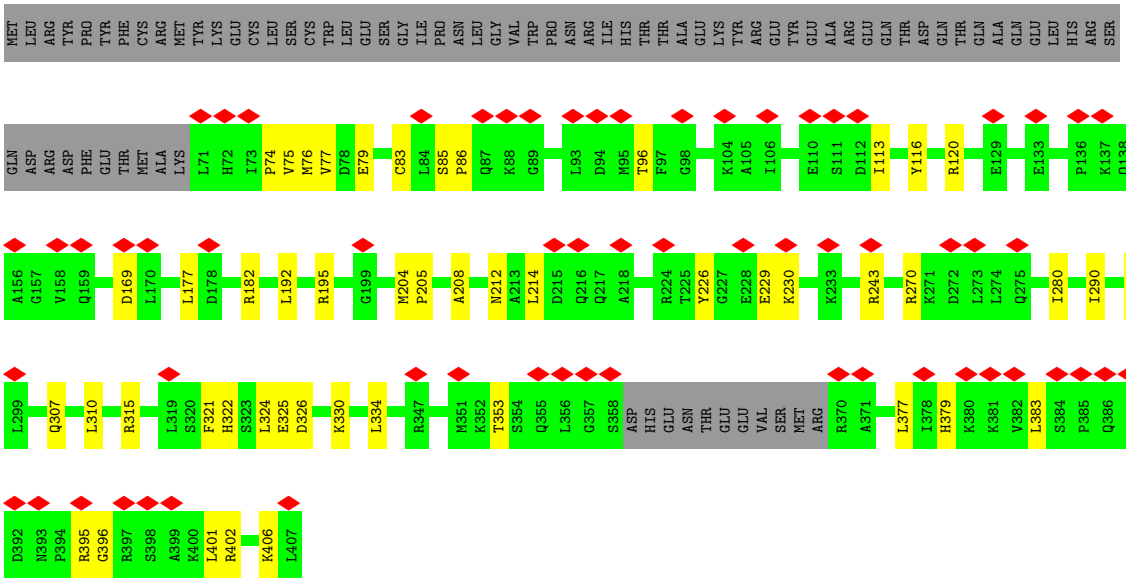




• Molecule 32: 12S rRNA N4-methylcytidine (m4C) methyltransferase

Chain b:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79037	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.113	Depositor
Minimum map value	-0.196	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.39	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.13	0/1834	0.27	0/2484
2	1	0.14	0/2304	0.24	0/3117
3	3	0.13	0/640	0.25	0/844
4	4	0.11	0/4883	0.26	0/6608
5	A	0.17	0/21782	0.18	0/33911
6	B	0.18	0/1871	0.31	0/2531
7	C	0.18	0/1113	0.27	0/1505
8	D	0.17	0/2783	0.28	0/3724
9	E	0.17	0/953	0.30	0/1289
10	F	0.12	0/1638	0.24	0/2197
11	G	0.14	0/2553	0.25	0/3420
12	H	0.17	0/1178	0.28	0/1598
13	I	0.14	0/1039	0.28	0/1400
14	J	0.16	0/855	0.26	0/1148
15	K	0.16	0/880	0.26	0/1182
16	L	0.16	0/1477	0.22	0/1974
17	M	0.20	0/963	0.27	0/1295
18	N	0.18	0/886	0.31	0/1199
19	O	0.17	0/1648	0.23	0/2243
20	P	0.15	0/798	0.26	0/1070
21	Q	0.13	0/748	0.21	0/994
22	R	0.15	0/2456	0.23	0/3317
23	S	0.13	0/1138	0.20	0/1533
24	T	0.17	0/1402	0.30	0/1883
25	U	0.15	0/1510	0.24	0/2025
26	V	0.10	0/3030	0.26	0/4093
27	W	0.14	0/801	0.23	0/1079
28	X	0.12	0/2921	0.28	0/3954
29	Y	0.13	0/1280	0.23	0/1725
30	Z	0.14	0/857	0.24	0/1141
31	a	0.08	0/1201	0.22	0/1610
32	b	0.11	0/2590	0.25	0/3492

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.15	0/72012	0.23	0/101585

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1787	0	1796	23	0
2	1	2256	0	2288	23	0
3	3	629	0	702	3	0
4	4	4775	0	4779	65	0
5	A	19474	0	9893	169	0
6	B	1828	0	1815	28	0
7	C	1083	0	1088	24	0
8	D	2731	0	2804	30	0
9	E	936	0	954	9	0
10	F	1604	0	1647	10	0
11	G	2500	0	2476	31	0
12	H	1152	0	1183	15	0
13	I	1019	0	1059	11	0
14	J	839	0	887	9	0
15	K	862	0	885	11	0
16	L	1453	0	1540	12	0
17	M	942	0	965	15	0
18	N	868	0	928	9	0
19	O	1592	0	1557	14	0
20	P	781	0	806	8	0
21	Q	736	0	749	11	0
22	R	2409	0	2428	30	0
23	S	1111	0	1115	10	0
24	T	1371	0	1393	10	0
25	U	1488	0	1499	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	V	2969	0	2961	32	0
27	W	789	0	802	16	0
28	X	2849	0	2844	42	0
29	Y	1246	0	1197	13	0
30	Z	839	0	858	14	0
31	a	1188	0	1212	16	0
32	b	2546	0	2615	34	0
33	3	1	0	0	0	0
33	A	8	0	0	0	0
33	B	1	0	0	0	0
34	A	1	0	0	0	0
35	A	44	0	26	1	0
36	O	1	0	0	0	0
37	P	4	0	0	0	0
37	T	4	0	0	0	0
38	X	28	0	12	0	0
39	X	31	0	12	0	0
40	b	26	0	19	1	0
All	All	68801	0	59794	619	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 (619) 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)
4:4:343:ARG:HA	4:4:378:LEU:HD13	1.66	0.75
5:A:1247:G:N7	30:Z:96:LYS:NZ	2.35	0.73
31:a:248:ILE:HG21	32:b:205:PRO:HB3	1.70	0.73
5:A:1294:A:OP1	6:B:201:ASN:ND2	2.22	0.72
5:A:1248:C:O2	15:K:28:HIS:N	2.24	0.71
32:b:195:ARG:NH1	32:b:204:MET:O	2.24	0.70
11:G:394:LYS:O	11:G:396:ARG:NH1	2.25	0.70
5:A:1508:C:O2	5:A:1542:U:N3	2.24	0.69
5:A:1287:A:OP2	8:D:260:LYS:NZ	2.26	0.68
5:A:996:A:N3	5:A:1074:G:O2'	2.27	0.67
4:4:616:ASP:OD1	4:4:648:ARG:NH2	2.24	0.67
7:C:100:PHE:HB3	7:C:103:CYS:HB2	1.76	0.67
22:R:208:ILE:O	22:R:214:ASN:ND2	2.26	0.67
1:0:93:CYS:HA	1:0:119:THR:O	1.95	0.67
5:A:1380:G:N3	28:X:164:ASN:ND2	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1508:C:N3	5:A:1542:U:O4	2.28	0.67
32:b:182:ARG:NH2	32:b:195:ARG:O	2.28	0.66
5:A:1501:A:H3'	5:A:1502:A:H5"	1.78	0.65
2:1:49:ARG:NH2	7:C:125:ARG:O	2.30	0.64
15:K:58:ARG:NE	15:K:72:ASP:OD1	2.30	0.64
5:A:1078:A:O2'	32:b:326:ASP:OD2	2.16	0.64
6:B:82:ARG:NH2	27:W:78:GLU:OE1	2.31	0.64
5:A:843:G:N2	5:A:846:A:OP2	2.30	0.64
1:0:140:ARG:NH2	26:V:244:TYR:OH	2.31	0.64
10:F:176:ASP:OD1	10:F:179:ARG:NH2	2.31	0.64
5:A:1230:C:OP2	5:A:1442:G:O2'	2.15	0.64
5:A:930:G:OP1	8:D:419:ARG:NH1	2.30	0.63
11:G:301:GLN:OE1	28:X:385:ASN:ND2	2.27	0.63
5:A:894:C:H41	14:J:78:ARG:HH21	1.46	0.63
8:D:415:GLN:NE2	8:D:417:MET:SD	2.71	0.63
13:I:71:SER:O	13:I:74:ARG:NH1	2.28	0.63
32:b:310:LEU:HD23	32:b:406:LYS:HB2	1.79	0.63
5:A:1581:G:N2	5:A:1584:A:OP2	2.31	0.63
5:A:1078:A:OP2	32:b:330:LYS:NZ	2.32	0.63
17:M:104:ILE:HG23	22:R:147:ILE:HG12	1.80	0.63
26:V:215:GLN:OE1	26:V:217:ASN:ND2	2.32	0.63
5:A:1465:C:O2	5:A:1467:C:N4	2.31	0.62
22:R:309:PRO:O	22:R:315:GLN:NE2	2.33	0.62
5:A:773:U:OP2	16:L:225:ARG:NH1	2.33	0.62
5:A:703:A:OP2	25:U:43:ASN:ND2	2.33	0.62
18:N:57:GLN:O	18:N:87:LYS:NZ	2.32	0.62
5:A:1431:G:O6	11:G:276:ARG:NH2	2.33	0.62
1:0:140:ARG:NH2	26:V:315:GLU:OE2	2.24	0.62
5:A:961:U:O2'	5:A:963:C:N4	2.29	0.62
26:V:48:TYR:N	26:V:78:ASN:OD1	2.29	0.61
5:A:1320:G:OP2	7:C:37:ASN:ND2	2.33	0.61
21:Q:78:LYS:HD3	27:W:162:VAL:HB	1.83	0.61
32:b:116:TYR:OH	32:b:140:ARG:NH1	2.33	0.61
5:A:867:C:O2	5:A:870:C:N4	2.34	0.61
16:L:149:ASP:OD2	16:L:152:HIS:ND1	2.34	0.61
18:N:13:ILE:HD12	18:N:30:VAL:HG21	1.83	0.61
5:A:1496:U:OP1	14:J:82:ARG:NH2	2.34	0.61
8:D:189:ARG:NH1	31:a:295:TYR:O	2.32	0.61
5:A:1341:C:O2	30:Z:93:LYS:NZ	2.33	0.61
6:B:239:ASN:ND2	6:B:242:SER:OG	2.34	0.60
5:A:1077:U:N3	5:A:1080:A:OP2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:290:ILE:HG23	32:b:295:GLU:HB2	1.82	0.60
22:R:325:ILE:HG23	22:R:346:LEU:HD21	1.83	0.60
28:X:108:LEU:HD23	28:X:141:VAL:HG21	1.82	0.60
5:A:1079:G:H2'	5:A:1080:A:H8	1.65	0.60
22:R:69:THR:N	22:R:72:ASP:OD2	2.34	0.60
26:V:74:ARG:O	26:V:78:ASN:ND2	2.35	0.60
1:0:166:TYR:O	19:O:199:TRP:NE1	2.30	0.60
4:4:578:CYS:SG	4:4:607:ARG:NH2	2.70	0.60
32:b:120:ARG:NH2	32:b:298:GLU:OE1	2.35	0.59
5:A:1543:U:H2'	5:A:1544:A:C8	2.37	0.59
5:A:1102:A:OP2	5:A:1104:A:N6	2.30	0.59
10:F:48:LYS:NZ	28:X:375:GLU:OE2	2.31	0.59
15:K:60:ASN:O	15:K:68:GLN:NE2	2.35	0.59
5:A:1245:U:H1'	30:Z:96:LYS:HE3	1.85	0.59
17:M:19:ILE:HB	17:M:83:LEU:HD23	1.84	0.59
26:V:167:VAL:HG13	26:V:172:ALA:HB3	1.85	0.59
9:E:26:ILE:HG23	9:E:36:VAL:HG21	1.85	0.59
16:L:115:ILE:HG21	16:L:181:ILE:HD13	1.84	0.58
11:G:134:ARG:O	11:G:136:ARG:NH1	2.37	0.58
11:G:200:LEU:O	11:G:218:TYR:OH	2.19	0.58
6:B:137:TYR:O	6:B:264:ARG:NH1	2.36	0.58
19:O:94:CYS:HB2	19:O:108:CYS:SG	2.43	0.58
28:X:102:ARG:NH1	28:X:132:THR:O	2.37	0.58
32:b:192:LEU:HB3	32:b:208:ALA:HB2	1.86	0.58
5:A:942:A:N6	5:A:1047:A:OP2	2.25	0.58
26:V:277:ARG:N	26:V:348:GLU:O	2.34	0.58
1:0:24:GLN:O	1:0:27:ARG:NH1	2.36	0.58
5:A:1180:U:OP1	5:A:1570:G:N2	2.24	0.58
5:A:904:C:N4	8:D:116:LYS:O	2.37	0.58
22:R:219:TYR:O	22:R:256:ARG:NH2	2.36	0.58
24:T:21:VAL:HG22	24:T:103:ARG:HB2	1.85	0.58
13:I:163:HIS:NE2	21:Q:20:GLU:OE2	2.37	0.57
4:4:627:ALA:HB1	4:4:649:VAL:HG22	1.85	0.57
5:A:1174:U:O2'	8:D:231:MET:O	2.22	0.57
5:A:1454:G:OP2	11:G:377:ARG:NH1	2.37	0.57
4:4:302:VAL:HG11	4:4:341:CYS:HB3	1.86	0.57
26:V:190:LEU:HD11	26:V:208:LEU:HD11	1.86	0.57
2:1:169:ARG:O	2:1:218:ASN:ND2	2.37	0.57
26:V:36:ASP:OD1	26:V:38:HIS:ND1	2.37	0.57
28:X:319:PRO:HG2	28:X:322:ALA:HB2	1.85	0.57
32:b:208:ALA:O	32:b:212:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1383:A:H2'	10:F:198:ARG:HD2	1.87	0.56
1:0:135:MET:SD	1:0:135:MET:N	2.76	0.56
4:4:343:ARG:HD3	4:4:377:ARG:HB3	1.87	0.56
26:V:90:TYR:O	26:V:93:TYR:HB3	2.05	0.56
22:R:229:ASN:OD1	22:R:267:TYR:OH	2.19	0.56
26:V:173:PHE:O	26:V:179:GLN:NE2	2.37	0.56
10:F:79:ALA:O	11:G:312:GLN:NE2	2.38	0.56
5:A:1340:C:O2'	30:Z:101:ARG:NH2	2.38	0.56
1:0:42:THR:HG22	1:0:49:ARG:HG2	1.87	0.56
8:D:225:VAL:HG22	8:D:243:VAL:HG22	1.86	0.56
15:K:52:LEU:HD22	30:Z:41:PRO:HG3	1.87	0.56
5:A:1044:U:OP1	5:A:1110:A:O2'	2.24	0.56
5:A:1211:G:N2	5:A:1353:A:OP1	2.39	0.56
7:C:111:LYS:NZ	12:H:166:GLU:OE2	2.31	0.56
21:Q:28:ARG:NH1	31:a:123:GLU:OE2	2.39	0.56
1:0:93:CYS:SG	1:0:121:LYS:N	2.73	0.56
5:A:1079:G:H2'	5:A:1080:A:C8	2.40	0.56
22:R:207:PRO:HB2	22:R:209:ILE:HG22	1.87	0.56
5:A:1543:U:H2'	5:A:1544:A:H8	1.70	0.55
14:J:62:VAL:HA	14:J:83:VAL:HG12	1.86	0.55
22:R:70:PHE:O	22:R:76:GLN:NE2	2.36	0.55
11:G:312:GLN:OE1	11:G:345:ARG:NH1	2.39	0.55
2:1:107:LYS:NZ	7:C:54:GLU:OE1	2.40	0.55
31:a:129:LEU:HD11	31:a:177:PRO:HG2	1.89	0.55
4:4:370:ALA:N	4:4:412:ASP:OD1	2.32	0.55
19:O:105:CYS:HB2	19:O:142:VAL:HA	1.89	0.55
7:C:49:LYS:N	7:C:167:LEU:OXT	2.40	0.54
5:A:1503:G:O6	5:A:1547:U:C2	2.60	0.54
26:V:270:PRO:O	26:V:346:LYS:NZ	2.40	0.54
26:V:81:SER:N	26:V:84:GLU:OE1	2.39	0.54
29:Y:266:LYS:NZ	29:Y:270:GLU:OE2	2.33	0.54
30:Z:16:ALA:HB1	30:Z:21:GLU:HB2	1.88	0.54
5:A:1271:C:O2'	5:A:1272:A:OP1	2.22	0.54
28:X:272:THR:OG1	28:X:282:ILE:O	2.23	0.54
28:X:364:ASN:O	28:X:367:GLN:NE2	2.34	0.54
4:4:439:LEU:HD21	4:4:448:ILE:HD12	1.90	0.54
5:A:1017:A:O2'	20:P:108:THR:OG1	2.21	0.54
5:A:899:G:O2'	5:A:907:A:N1	2.40	0.54
5:A:1481:C:O4'	31:a:281:ARG:NH1	2.40	0.54
5:A:1595:G:O6	21:Q:50:ARG:NH1	2.34	0.54
24:T:42:GLU:OE1	24:T:45:ARG:NH2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:83:CYS:HG	32:b:379:HIS:HE2	1.52	0.54
1:0:207:GLN:O	1:0:207:GLN:NE2	2.41	0.53
4:4:282:LEU:HG	4:4:287:LEU:HB2	1.91	0.53
5:A:700:A:N1	5:A:709:G:O2'	2.39	0.53
5:A:1279:C:O2'	5:A:1296:A:N1	2.41	0.53
5:A:760:A:N1	5:A:780:C:O2'	2.40	0.53
6:B:162:CYS:HB3	6:B:254:GLN:HG3	1.91	0.53
27:W:141:ARG:NH1	27:W:172:ILE:O	2.41	0.53
8:D:372:GLU:OE2	8:D:374:ARG:NE	2.40	0.53
5:A:1004:G:OP1	13:I:89:LYS:NZ	2.37	0.53
1:0:102:PRO:HA	1:0:112:GLY:HA3	1.90	0.53
18:N:14:VAL:O	24:T:63:GLN:NE2	2.38	0.53
5:A:713:C:N3	25:U:27:ARG:N	2.57	0.53
15:K:54:ILE:HG21	15:K:75:ILE:HB	1.91	0.53
4:4:400:LEU:HD22	4:4:405:PHE:HE1	1.74	0.52
4:4:631:VAL:HG22	4:4:645:LEU:HB3	1.90	0.52
8:D:426:LYS:N	19:O:88:GLN:OE1	2.42	0.52
32:b:307:GLN:O	32:b:406:LYS:NZ	2.36	0.52
4:4:236:VAL:HA	4:4:270:ARG:HB2	1.90	0.52
5:A:769:G:N2	5:A:772:A:OP2	2.38	0.52
5:A:1162:A:N3	5:A:1497:C:O2'	2.41	0.52
22:R:254:ASP:OD1	22:R:259:TYR:OH	2.27	0.52
28:X:252:SER:O	28:X:302:HIS:NE2	2.42	0.52
31:a:196:LEU:O	31:a:200:ALA:N	2.42	0.52
5:A:762:G:OP1	16:L:206:LYS:NZ	2.38	0.52
11:G:292:ARG:NH2	11:G:327:ASP:OD2	2.43	0.52
26:V:40:TRP:CD2	26:V:114:ARG:HG2	2.45	0.52
9:E:54:HIS:NE2	9:E:85:ASP:O	2.43	0.52
4:4:451:ASP:OD1	4:4:454:ARG:NH2	2.36	0.52
5:A:1046:A:O2'	5:A:1048:C:OP2	2.19	0.52
28:X:210:TRP:HH2	28:X:225:VAL:HG13	1.74	0.52
2:1:152:ASP:OD2	2:1:174:ARG:NH1	2.33	0.52
11:G:70:THR:HG23	11:G:73:PHE:H	1.75	0.52
32:b:229:GLU:OE1	32:b:230:LYS:N	2.43	0.52
4:4:358:ARG:HB3	29:Y:255:ARG:HG2	1.92	0.51
5:A:1239:C:H2'	5:A:1240:A:C8	2.46	0.51
10:F:237:ALA:HB3	31:a:190:LEU:HD13	1.92	0.51
12:H:71:ILE:O	12:H:150:GLY:N	2.42	0.51
13:I:136:ALA:HB3	13:I:168:GLY:HA3	1.91	0.51
11:G:285:VAL:HG22	11:G:328:VAL:HG22	1.92	0.51
28:X:67:HIS:HB3	28:X:98:CYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:110:THR:OG1	31:a:112:GLU:OE1	2.28	0.51
4:4:573:ALA:O	4:4:577:ASN:ND2	2.43	0.51
21:Q:77:ARG:NH2	27:W:166:ASN:OD1	2.44	0.51
23:S:63:ILE:HD13	27:W:84:LEU:HD21	1.91	0.51
26:V:156:ASN:ND2	26:V:159:ASP:OD2	2.43	0.51
5:A:1057:G:H4'	5:A:1578:A:H4'	1.92	0.51
5:A:1398:U:OP1	30:Z:29:LYS:NZ	2.35	0.51
6:B:165:TYR:HE2	11:G:146:PRO:HD2	1.76	0.51
20:P:57:PRO:HG3	23:S:68:ASP:HB3	1.93	0.51
4:4:154:GLU:OE2	4:4:184:SER:N	2.34	0.51
4:4:308:LYS:HE3	4:4:310:GLU:HB3	1.93	0.51
5:A:1014:A:O3'	13:I:184:ASN:ND2	2.44	0.51
9:E:31:ASP:OD1	25:U:170:ARG:NH2	2.31	0.51
22:R:294:ILE:HG13	22:R:349:TYR:CZ	2.46	0.51
25:U:77:GLU:OE1	25:U:80:ARG:NH2	2.33	0.51
8:D:148:LEU:HD23	8:D:149:MET:HE2	1.92	0.51
11:G:198:ARG:N	11:G:246:ARG:O	2.36	0.51
1:0:91:GLU:OE1	1:0:91:GLU:N	2.42	0.51
7:C:40:ALA:HB3	7:C:59:PRO:HG3	1.92	0.51
8:D:380:LEU:HD12	8:D:381:PRO:HD2	1.92	0.51
11:G:281:ALA:HB2	11:G:332:VAL:HG23	1.93	0.51
5:A:752:C:O2'	5:A:793:C:N4	2.42	0.50
5:A:1387:A:H61	5:A:1419:G:H1	1.59	0.50
26:V:43:ARG:NH2	26:V:77:ASP:OD1	2.44	0.50
5:A:1237:A:OP1	15:K:36:ARG:NH2	2.44	0.50
7:C:152:ARG:HG3	29:Y:304:TRP:HH2	1.76	0.50
16:L:175:TYR:HB2	18:N:89:GLY:HA3	1.93	0.50
4:4:260:CYS:SG	4:4:293:THR:OG1	2.69	0.50
5:A:1547:U:O2'	5:A:1548:A:O5'	2.29	0.50
19:O:91:ARG:NH1	19:O:103:ASN:O	2.42	0.50
26:V:197:SER:OG	26:V:199:GLU:OE1	2.29	0.50
2:1:155:ASP:OD1	2:1:215:ARG:NH1	2.44	0.50
5:A:845:A:OP1	25:U:64:ARG:NH2	2.43	0.50
23:S:99:PHE:HA	23:S:125:LEU:HD11	1.92	0.50
28:X:129:GLU:O	28:X:134:LYS:NZ	2.45	0.50
4:4:245:GLU:HG2	4:4:262:MET:HE1	1.94	0.50
22:R:224:HIS:NE2	22:R:252:ASP:OD2	2.33	0.50
24:T:44:ALA:O	24:T:47:PHE:HB3	2.12	0.50
5:A:741:A:OP1	25:U:86:ARG:NH2	2.38	0.50
5:A:992:U:O2'	5:A:994:A:N7	2.35	0.50
5:A:1402:A:OP1	15:K:51:ARG:NH2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:197:HIS:NE2	6:B:240:ASP:O	2.42	0.50
5:A:1265:C:OP1	15:K:112:ARG:NH2	2.44	0.50
6:B:167:HIS:CD2	11:G:153:THR:HA	2.46	0.50
1:0:41:LEU:HD13	1:0:55:TRP:CG	2.47	0.49
9:E:102:LEU:HD11	20:P:71:HIS:HB2	1.94	0.49
11:G:291:GLY:HA3	11:G:324:GLY:HA2	1.94	0.49
16:L:92:LEU:HD13	25:U:160:LEU:HD11	1.94	0.49
23:S:85:PHE:HB2	27:W:100:VAL:HG12	1.93	0.49
5:A:1205:U:H2'	5:A:1206:G:H8	1.77	0.49
5:A:1282:G:N2	5:A:1286:A:OP2	2.34	0.49
5:A:1497:C:H2'	5:A:1498:C:C6	2.48	0.49
22:R:209:ILE:HD11	22:R:218:MET:HG3	1.95	0.49
1:0:178:ARG:NH1	1:0:187:GLU:O	2.43	0.49
5:A:1089:U:H2'	5:A:1090:A:H8	1.78	0.49
5:A:1567:A:H5'	5:A:1569:G:N7	2.27	0.49
28:X:203:LYS:O	28:X:250:GLN:NE2	2.45	0.49
21:Q:83:PRO:HG2	21:Q:84:TRP:CD1	2.48	0.49
32:b:321:PHE:N	32:b:325:GLU:OE2	2.44	0.49
8:D:141:TRP:CD1	30:Z:70:LEU:HD21	2.48	0.49
25:U:160:LEU:O	25:U:164:VAL:HG23	2.13	0.49
26:V:226:TYR:HE1	26:V:282:VAL:HG21	1.77	0.49
5:A:1452:U:OP2	11:G:380:LYS:NZ	2.37	0.49
5:A:1488:C:H2'	5:A:1489:G:C8	2.48	0.49
5:A:738:A:H2'	5:A:740:G:C5	2.47	0.49
12:H:181:PRO:HD2	12:H:184:ILE:HD12	1.95	0.49
22:R:162:SER:O	22:R:170:ARG:NH1	2.35	0.49
1:0:43:ARG:NE	5:A:706:C:OP1	2.35	0.48
22:R:155:LYS:HB3	22:R:177:PRO:HD3	1.94	0.48
32:b:75:VAL:HG21	32:b:396:GLY:HA3	1.95	0.48
5:A:1376:C:H4'	5:A:1377:C:H5'	1.95	0.48
21:Q:28:ARG:HH22	31:a:121:ASN:HD21	1.61	0.48
28:X:349:ASN:ND2	28:X:352:GLU:OE1	2.46	0.48
4:4:318:GLU:OE2	4:4:322:HIS:NE2	2.46	0.48
4:4:197:TYR:CZ	29:Y:281:GLU:HG3	2.49	0.48
5:A:1104:A:OP1	5:A:1591:C:O2'	2.28	0.48
17:M:67:ALA:HB2	22:R:196:TYR:CZ	2.48	0.48
5:A:900:C:N4	14:J:74:ASN:OD1	2.34	0.48
5:A:702:C:OP1	5:A:848:U:O2'	2.30	0.48
5:A:993:A:H1'	32:b:353:THR:HG21	1.95	0.48
6:B:165:TYR:OH	11:G:146:PRO:O	2.27	0.48
32:b:322:HIS:CE1	32:b:325:GLU:H	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:43:ARG:NH2	5:A:705:C:O2'	2.47	0.48
5:A:769:G:OP2	18:N:73:ARG:NH2	2.47	0.48
5:A:1431:G:O2'	5:A:1457:G:O6	2.27	0.48
11:G:275:LYS:HG2	11:G:280:LYS:HG3	1.96	0.48
14:J:127:ARG:NE	14:J:132:CYS:SG	2.87	0.48
32:b:83:CYS:SG	32:b:379:HIS:NE2	2.80	0.48
3:3:139:ASN:ND2	5:A:1141:C:OP1	2.34	0.48
5:A:743:C:O2'	17:M:38:HIS:NE2	2.45	0.48
5:A:1426:U:H2'	5:A:1427:A:H8	1.78	0.48
28:X:276:ARG:NH1	28:X:281:PRO:O	2.46	0.48
2:1:151:ILE:HD11	2:1:173:LEU:HD12	1.95	0.48
4:4:548:PHE:HB3	4:4:582:LEU:HD22	1.96	0.48
5:A:1542:U:H2'	5:A:1543:U:C6	2.48	0.48
5:A:1577:U:H2'	5:A:1578:A:C8	2.49	0.48
6:B:172:ARG:O	6:B:175:MET:HG2	2.14	0.48
13:I:98:GLN:HB2	13:I:109:PHE:HD1	1.79	0.48
22:R:168:ARG:NH1	22:R:238:ASP:OD2	2.35	0.48
22:R:336:ALA:HB1	22:R:342:ILE:HD12	1.96	0.48
18:N:8:VAL:HB	18:N:68:ALA:HB1	1.96	0.47
22:R:161:ILE:O	24:T:125:HIS:NE2	2.43	0.47
5:A:713:C:O2'	5:A:852:A:O2'	2.25	0.47
32:b:86:PRO:HB3	32:b:113:ILE:HD12	1.95	0.47
4:4:256:GLU:HG2	4:4:287:LEU:HB3	1.96	0.47
22:R:231:CYS:SG	22:R:242:TYR:HA	2.54	0.47
31:a:239:ILE:HD13	32:b:226:TYR:HE2	1.79	0.47
6:B:239:ASN:HD21	27:W:119:LYS:HG3	1.79	0.47
26:V:212:GLY:O	26:V:224:GLN:NE2	2.43	0.47
4:4:281:GLU:O	4:4:285:ASN:ND2	2.40	0.47
12:H:104:ILE:HG21	12:H:145:LEU:HD23	1.95	0.47
20:P:124:TYR:HB3	21:Q:9:ALA:HB2	1.95	0.47
7:C:88:GLU:HG2	7:C:147:TYR:CE1	2.49	0.47
1:0:37:ASP:O	1:0:41:LEU:N	2.45	0.47
2:1:65:ASP:OD2	2:1:68:SER:OG	2.27	0.47
4:4:161:ILE:HA	4:4:194:LEU:HD22	1.96	0.47
6:B:165:TYR:CD1	11:G:149:TYR:HA	2.50	0.47
15:K:120:LEU:HB3	15:K:123:ILE:HD12	1.97	0.47
24:T:48:VAL:HA	24:T:52:ILE:HG12	1.95	0.47
24:T:80:LEU:HD12	24:T:84:GLU:HB2	1.95	0.47
3:3:174:ARG:HA	3:3:177:TRP:CE2	2.49	0.47
5:A:1366:C:H3'	5:A:1367:A:H5'	1.96	0.47
8:D:132:ILE:HG22	8:D:144:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:336:ASN:ND2	4:4:409:ASP:OD2	2.48	0.47
5:A:845:A:H4'	25:U:60:TYR:CE2	2.50	0.47
6:B:66:PRO:HB2	6:B:134:HIS:HE1	1.79	0.47
21:Q:28:ARG:HH22	31:a:121:ASN:ND2	2.13	0.47
5:A:957:C:H3'	5:A:958:C:H2'	1.97	0.47
15:K:34:MET:HE3	15:K:95:SER:HB2	1.97	0.47
28:X:163:LYS:NZ	28:X:314:GLY:O	2.44	0.47
1:0:163:SER:HB2	1:0:190:MET:HB3	1.96	0.46
5:A:948:U:OP2	5:A:1045:G:N1	2.48	0.46
5:A:1443:U:O2'	5:A:1445:G:N7	2.41	0.46
6:B:149:ARG:NH2	21:Q:82:ASP:OD1	2.35	0.46
2:1:86:ARG:NH1	2:1:96:PRO:O	2.43	0.46
6:B:141:ILE:HB	6:B:190:PRO:HA	1.97	0.46
11:G:318:HIS:NE2	28:X:379:GLU:OE2	2.49	0.46
12:H:70:ASP:OD1	12:H:71:ILE:N	2.48	0.46
4:4:626:GLN:O	4:4:630:VAL:HG23	2.15	0.46
5:A:663:A:H2'	5:A:664:G:C8	2.49	0.46
2:1:114:LEU:O	11:G:110:TYR:OH	2.22	0.46
2:1:266:LEU:HD11	2:1:289:ILE:HD11	1.97	0.46
5:A:1000:U:H5"	5:A:1001:C:H5'	1.98	0.46
6:B:118:LEU:HA	6:B:121:THR:HB	1.97	0.46
6:B:146:SER:OG	6:B:197:HIS:ND1	2.37	0.46
12:H:57:ASP:OD1	12:H:58:LEU:N	2.48	0.46
27:W:152:ARG:NE	27:W:159:ASP:OD1	2.39	0.46
28:X:162:VAL:HB	28:X:272:THR:HG22	1.97	0.46
31:a:183:GLN:HG2	31:a:185:LYS:HG3	1.97	0.46
6:B:124:HIS:CE1	23:S:41:LEU:HD12	2.51	0.46
6:B:230:CYS:SG	6:B:231:LEU:N	2.89	0.46
14:J:109:LEU:HD13	14:J:130:TYR:HE2	1.80	0.46
32:b:96:THR:HG21	32:b:169:ASP:O	2.16	0.46
4:4:446:LYS:HA	29:Y:292:GLN:HG3	1.98	0.46
5:A:732:A:O2'	17:M:15:GLY:O	2.30	0.46
26:V:149:ASP:HA	26:V:152:ILE:HB	1.98	0.46
6:B:66:PRO:HB2	6:B:134:HIS:CE1	2.50	0.46
6:B:165:TYR:CE2	11:G:146:PRO:HD2	2.51	0.46
23:S:106:LEU:HB3	23:S:117:LEU:HD11	1.98	0.46
24:T:75:PHE:HA	24:T:90:VAL:HG22	1.97	0.46
5:A:1225:C:H5	5:A:1361:G:H21	1.64	0.46
26:V:250:ILE:HG23	26:V:252:LYS:H	1.81	0.46
32:b:383:LEU:HD12	32:b:401:LEU:HD22	1.97	0.46
4:4:400:LEU:HD22	4:4:405:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1035:U:OP1	9:E:4:TYR:OH	2.31	0.46
7:C:92:LEU:HD22	7:C:119:ILE:HD11	1.98	0.46
28:X:210:TRP:CE2	28:X:228:GLN:HG2	2.51	0.45
1:0:29:ARG:HE	1:0:105:THR:HG21	1.81	0.45
4:4:309:PHE:CZ	4:4:352:PRO:HG2	2.52	0.45
4:4:567:THR:HG22	4:4:568:ALA:H	1.82	0.45
5:A:1210:U:H1'	5:A:1356:A:H62	1.82	0.45
19:O:127:VAL:HG22	19:O:134:ILE:HG12	1.98	0.45
28:X:273:THR:HG23	28:X:316:LEU:HD13	1.98	0.45
2:1:312:TYR:OH	28:X:338:ASP:OD1	2.21	0.45
15:K:64:PRO:HG3	29:Y:392:ILE:HD12	1.99	0.45
16:L:143:LEU:HD11	16:L:153:LYS:HA	1.97	0.45
32:b:214:LEU:O	32:b:243:ARG:NH1	2.46	0.45
4:4:373:HIS:HB2	4:4:415:PHE:HA	1.98	0.45
4:4:450:PRO:HD2	4:4:453:HIS:ND1	2.31	0.45
5:A:942:A:C6	5:A:1047:A:H5'	2.52	0.45
5:A:1368:U:O4	5:A:1383:A:O2'	2.28	0.45
7:C:42:VAL:HG11	7:C:51:VAL:HG11	1.97	0.45
7:C:89:ASP:OD1	7:C:112:ARG:NH2	2.43	0.45
8:D:282:ILE:HG23	8:D:353:LEU:HB3	1.98	0.45
16:L:79:VAL:HG23	16:L:82:ILE:HB	1.99	0.45
26:V:58:ASP:OD2	26:V:91:TYR:OH	2.21	0.45
4:4:272:TYR:CD1	4:4:300:ALA:HA	2.51	0.45
7:C:92:LEU:HD11	7:C:117:LEU:HD21	1.99	0.45
9:E:44:GLU:OE2	9:E:60:ARG:NE	2.43	0.45
11:G:88:LEU:HD21	11:G:107:ALA:HB3	1.98	0.45
13:I:94:ASN:OD1	13:I:95:THR:N	2.47	0.45
27:W:110:ASN:O	27:W:126:ARG:N	2.47	0.45
5:A:1089:U:H2'	5:A:1090:A:C8	2.52	0.45
7:C:96:MET:HB2	7:C:108:LEU:HD11	1.99	0.45
11:G:197:SER:HB2	11:G:245:ARG:HB3	1.99	0.45
22:R:282:ASP:HB3	22:R:342:ILE:HD11	1.99	0.45
29:Y:323:ASP:OD1	29:Y:323:ASP:N	2.50	0.45
4:4:372:TYR:CD2	4:4:400:LEU:HD11	2.51	0.45
5:A:1545:U:H2'	5:A:1546:A:C8	2.51	0.45
8:D:285:TYR:OH	8:D:372:GLU:OE1	2.24	0.45
10:F:116:GLU:OE2	10:F:120:ARG:NH2	2.46	0.45
26:V:30:LEU:HD13	26:V:34:TYR:CD1	2.51	0.45
26:V:95:PHE:O	26:V:98:SER:OG	2.33	0.45
27:W:162:VAL:HG23	27:W:164:GLU:HG2	1.98	0.45
28:X:206:GLU:OE2	28:X:249:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:316:ASN:HB3	29:Y:319:ALA:HB2	1.98	0.45
4:4:531:ILE:HG22	4:4:535:MET:HE2	1.99	0.45
5:A:1279:C:O2'	6:B:177:THR:OG1	2.28	0.45
8:D:285:TYR:N	8:D:289:THR:O	2.47	0.45
17:M:100:HIS:H	17:M:103:MET:HE3	1.81	0.45
26:V:40:TRP:O	26:V:43:ARG:NH1	2.38	0.45
28:X:268:LEU:HD21	28:X:293:LEU:HD23	1.98	0.45
5:A:1307:G:O2'	11:G:118:GLU:OE1	2.35	0.45
10:F:170:VAL:HG21	10:F:239:TYR:HB2	1.98	0.45
11:G:196:GLY:HA2	11:G:248:VAL:HG12	1.98	0.45
2:1:49:ARG:HH22	7:C:126:GLN:HA	1.81	0.45
2:1:159:SER:HB2	7:C:112:ARG:HB3	1.98	0.45
13:I:81:GLU:OE1	13:I:81:GLU:N	2.47	0.45
26:V:123:ASP:OD1	26:V:123:ASP:N	2.49	0.45
1:0:95:TRP:CE2	1:0:131:ILE:HG23	2.52	0.44
23:S:89:ASN:HB3	23:S:92:PHE:HB2	1.99	0.44
4:4:73:ALA:HB2	12:H:61:PRO:HG3	1.99	0.44
4:4:593:TRP:CH2	4:4:626:GLN:HB3	2.52	0.44
30:Z:4:LEU:HB3	30:Z:8:ALA:HB3	1.99	0.44
32:b:212:ASN:HA	32:b:243:ARG:HD2	1.99	0.44
3:3:173:LEU:HB3	16:L:209:LEU:HD22	1.98	0.44
5:A:1503:G:O6	5:A:1547:U:O2	2.35	0.44
6:B:239:ASN:ND2	27:W:119:LYS:HG3	2.33	0.44
8:D:243:VAL:HG11	8:D:268:PHE:CD1	2.52	0.44
9:E:37:ARG:HG3	25:U:167:PHE:CE1	2.52	0.44
17:M:64:LYS:HE3	22:R:154:THR:HB	1.98	0.44
28:X:56:PRO:HB2	28:X:144:PHE:HD1	1.82	0.44
28:X:211:ASN:ND2	28:X:214:GLU:OE1	2.51	0.44
5:A:931:C:H2'	14:J:42:PRO:HG2	2.00	0.44
32:b:322:HIS:CE1	32:b:324:LEU:HB2	2.53	0.44
4:4:345:PHE:HB3	4:4:348:PHE:HB2	1.99	0.44
7:C:77:ASP:OD2	12:H:114:LYS:HD3	2.17	0.44
8:D:296:LEU:HD11	8:D:348:GLY:O	2.18	0.44
10:F:84:SER:OG	28:X:379:GLU:OE1	2.31	0.44
22:R:142:LEU:HD21	22:R:183:LYS:HE3	1.99	0.44
26:V:128:THR:HB	26:V:137:ILE:HG13	1.99	0.44
26:V:205:GLY:HA2	26:V:227:GLY:HA2	1.99	0.44
31:a:138:ALA:O	31:a:182:VAL:N	2.43	0.44
5:A:1003:A:H2'	5:A:1004:G:C8	2.53	0.44
5:A:1225:C:O2'	5:A:1449:G:O2'	2.33	0.44
7:C:115:ASN:ND2	29:Y:309:LYS:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:112:MET:HE3	16:L:119:PRO:HA	2.00	0.44
5:A:1389:G:O6	5:A:1415:G:O2'	2.29	0.44
11:G:73:PHE:O	11:G:77:GLN:HG2	2.17	0.44
26:V:270:PRO:HD2	26:V:273:ILE:HD12	1.99	0.44
28:X:109:LEU:HD22	28:X:144:PHE:CD2	2.53	0.44
32:b:330:LYS:HB2	32:b:402:ARG:CZ	2.47	0.44
4:4:66:ASP:OD1	4:4:67:LYS:N	2.49	0.44
5:A:702:C:OP1	25:U:41:ARG:NH2	2.44	0.44
6:B:192:LEU:HD11	6:B:220:VAL:HG23	1.99	0.44
7:C:110:LEU:HD22	7:C:119:ILE:HG12	1.99	0.44
4:4:278:LEU:HD12	4:4:278:LEU:HA	1.86	0.43
4:4:405:PHE:HZ	4:4:438:LEU:HD21	1.82	0.43
5:A:890:C:H4'	5:A:891:C:H5"	1.99	0.43
19:O:91:ARG:HD2	19:O:94:CYS:SG	2.58	0.43
28:X:55:ASP:HB3	28:X:58:LYS:HB2	2.00	0.43
2:1:133:TRP:CD2	2:1:134:PRO:HD2	2.53	0.43
4:4:567:THR:HG22	4:4:568:ALA:N	2.33	0.43
8:D:235:GLU:OE1	8:D:235:GLU:N	2.48	0.43
28:X:159:HIS:ND1	28:X:267:ALA:HB2	2.33	0.43
32:b:74:PRO:HB2	32:b:77:VAL:HB	1.99	0.43
4:4:75:ALA:HB2	29:Y:298:PHE:HB3	2.01	0.43
5:A:1150:C:H2'	5:A:1152:A:C8	2.53	0.43
27:W:97:ASP:N	27:W:144:LEU:O	2.50	0.43
30:Z:61:LEU:O	30:Z:65:LEU:HG	2.18	0.43
32:b:270:ARG:HD2	32:b:280:ILE:HG13	2.00	0.43
32:b:334:LEU:HD21	32:b:377:LEU:HD11	1.99	0.43
5:A:738:A:H5'	5:A:739:C:O4'	2.17	0.43
5:A:1048:C:C4	35:A:1710:NAD:H52A	2.53	0.43
17:M:101:PRO:HB3	25:U:59:ARG:HB3	1.99	0.43
28:X:70:ILE:HB	28:X:97:ALA:HB3	2.00	0.43
4:4:267:VAL:HG22	4:4:300:ALA:HB2	2.01	0.43
19:O:55:PRO:HB3	19:O:114:HIS:HB2	2.00	0.43
22:R:191:ARG:HG3	22:R:204:ILE:HG23	2.01	0.43
26:V:241:ARG:HA	26:V:244:TYR:CE2	2.54	0.43
4:4:332:LEU:HD21	4:4:368:SER:HB3	2.01	0.43
5:A:993:A:OP1	13:I:192:ARG:NH1	2.45	0.43
5:A:845:A:H2'	5:A:846:A:C8	2.53	0.43
5:A:994:A:N1	5:A:1075:A:O2'	2.51	0.43
5:A:1422:G:H2'	5:A:1423:A:C8	2.54	0.43
6:B:222:ILE:HD13	6:B:236:VAL:HB	2.01	0.43
4:4:152:ILE:HA	4:4:172:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:875:U:O2'	5:A:882:A:N1	2.43	0.43
5:A:1119:U:H5'	23:S:50:ARG:HH12	1.83	0.43
28:X:192:LYS:HB2	28:X:226:VAL:HG11	2.01	0.43
31:a:125:SER:N	31:a:139:TYR:O	2.49	0.43
1:0:35:ALA:O	1:0:44:PRO:HD2	2.19	0.43
4:4:148:GLN:N	4:4:159:GLU:OE2	2.39	0.43
5:A:890:C:H2'	5:A:902:G:C8	2.54	0.43
26:V:177:SER:HB2	26:V:367:CYS:HB3	2.00	0.43
1:0:100:VAL:HG12	1:0:102:PRO:HD3	2.00	0.43
9:E:26:ILE:HD11	9:E:39:LEU:HD22	2.00	0.43
28:X:50:ARG:NE	28:X:362:GLU:OE2	2.52	0.43
28:X:109:LEU:HD21	28:X:141:VAL:HA	2.01	0.43
28:X:368:HIS:N	28:X:398:LEU:OXT	2.52	0.43
2:1:152:ASP:HB2	2:1:172:VAL:HB	2.00	0.42
5:A:743:C:HO2'	17:M:38:HIS:HE2	1.66	0.42
5:A:1195:U:H2'	5:A:1196:A:C8	2.54	0.42
23:S:117:LEU:HD12	23:S:117:LEU:HA	1.86	0.42
24:T:48:VAL:HA	24:T:52:ILE:CG1	2.49	0.42
27:W:150:THR:HG22	27:W:161:THR:HB	2.01	0.42
5:A:1180:U:H2'	5:A:1181:G:H8	1.84	0.42
5:A:1344:U:OP1	30:Z:101:ARG:NH1	2.52	0.42
27:W:104:ILE:HD12	27:W:138:THR:HB	2.01	0.42
5:A:1401:G:N2	5:A:1404:A:O5'	2.44	0.42
20:P:126:ASP:HB3	20:P:129:TYR:CD2	2.55	0.42
22:R:254:ASP:HB2	22:R:275:PHE:CZ	2.53	0.42
27:W:144:LEU:HD23	27:W:167:ALA:HB2	2.02	0.42
4:4:372:TYR:CE2	4:4:400:LEU:HD21	2.54	0.42
5:A:871:A:OP1	19:O:97:ARG:NH1	2.52	0.42
8:D:244:LEU:HD11	8:D:256:PHE:HD2	1.85	0.42
8:D:316:CYS:HB3	8:D:334:ALA:HB3	2.00	0.42
28:X:117:PHE:HB3	28:X:303:GLY:HA2	2.01	0.42
32:b:177:LEU:HD23	32:b:395:ARG:NH1	2.33	0.42
5:A:1142:A:N1	5:A:1160:A:H5"	2.34	0.42
5:A:1271:C:HO2'	5:A:1272:A:P	2.42	0.42
5:A:1497:C:H2'	5:A:1498:C:H6	1.83	0.42
6:B:157:ASN:OD1	6:B:160:ARG:NH2	2.52	0.42
12:H:108:VAL:HG13	12:H:143:LEU:HD23	2.02	0.42
17:M:105:THR:OG1	25:U:56:LEU:HD13	2.19	0.42
20:P:65:CYS:SG	20:P:68:CYS:HB2	2.60	0.42
22:R:195:VAL:HG13	24:T:143:VAL:HG11	2.01	0.42
5:A:1341:C:OP1	30:Z:100:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1377:C:H5”	28:X:320:ARG:HD3	2.02	0.42
8:D:209:GLY:N	8:D:213:GLU:O	2.33	0.42
9:E:17:GLU:OE1	9:E:17:GLU:N	2.51	0.42
28:X:153:LEU:HD21	28:X:244:LEU:HD23	2.01	0.42
40:b:501:SAH:H4’	40:b:501:SAH:HG1	1.56	0.42
7:C:58:ALA:HB3	7:C:60:HIS:CE1	2.55	0.42
11:G:229:LEU:HD11	11:G:241:VAL:HG11	2.01	0.42
4:4:266:MET:O	4:4:271:ALA:N	2.45	0.42
5:A:758:U:O4	5:A:1159:A:H1’	2.19	0.42
5:A:1347:G:H2’	5:A:1348:G:H8	1.85	0.42
8:D:412:LYS:HG3	8:D:417:MET:HB2	2.02	0.42
11:G:200:LEU:HD22	11:G:244:PHE:HB3	2.01	0.42
2:1:304:GLU:HB3	28:X:324:LEU:HD13	2.02	0.42
5:A:1066:C:O2’	13:I:187:ARG:O	2.36	0.42
7:C:95:PHE:HD2	30:Z:62:MET:HE1	1.84	0.42
11:G:115:GLY:N	12:H:84:ASP:OD2	2.50	0.42
26:V:44:GLU:HB2	26:V:383:HIS:NE2	2.34	0.42
2:1:254:GLU:OE1	2:1:254:GLU:N	2.51	0.41
28:X:81:HIS:CD2	28:X:154:HIS:HD2	2.38	0.41
2:1:133:TRP:CE2	12:H:147:HIS:HB3	2.56	0.41
5:A:821:U:H2’	5:A:822:G:H8	1.85	0.41
5:A:955:A:H3’	5:A:956:C:H5”	2.02	0.41
5:A:1379:A:H2’	5:A:1380:G:C8	2.55	0.41
14:J:114:ARG:HA	14:J:122:LYS:HA	2.01	0.41
19:O:110:ASP:HB3	19:O:113:LEU:HD12	2.02	0.41
23:S:102:LYS:HB3	23:S:121:THR:HG23	2.02	0.41
31:a:130:THR:HG22	31:a:137:ARG:NH2	2.35	0.41
4:4:470:GLN:NE2	4:4:472:ASP:OD2	2.45	0.41
5:A:1322:C:H2’	5:A:1323:G:O4’	2.19	0.41
10:F:61:GLU:O	10:F:65:VAL:HG23	2.20	0.41
22:R:272:VAL:HG22	22:R:284:LEU:HD21	2.03	0.41
4:4:279:TYR:HB2	4:4:297:LEU:HD21	2.01	0.41
4:4:376:ILE:HG23	4:4:422:ILE:HD12	2.02	0.41
5:A:1003:A:H2’	5:A:1004:G:H8	1.86	0.41
5:A:1053:A:N1	5:A:1100:C:O2’	2.38	0.41
5:A:1103:A:N7	5:A:1574:G:O2’	2.46	0.41
2:1:284:LEU:HA	2:1:289:ILE:HG21	2.03	0.41
5:A:1266:A:OP2	7:C:36:LYS:N	2.54	0.41
5:A:1430:A:N1	5:A:1458:A:H5”	2.35	0.41
8:D:241:ILE:HG21	8:D:264:ARG:HG3	2.02	0.41
8:D:254:ALA:O	8:D:280:HIS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:175:ILE:HD11	21:Q:19:VAL:HG13	2.01	0.41
2:1:237:GLU:HB2	2:1:240:GLU:HG3	2.01	0.41
5:A:965:C:C4	5:A:1022:A:H4'	2.56	0.41
5:A:1426:U:H2'	5:A:1427:A:C8	2.56	0.41
5:A:1541:U:H2'	5:A:1542:U:C2	2.55	0.41
16:L:115:ILE:HD11	16:L:184:GLY:HA3	2.02	0.41
18:N:51:ALA:HB2	18:N:66:LEU:HD13	2.02	0.41
28:X:61:ASP:HA	28:X:64:GLU:HB2	2.02	0.41
4:4:128:PHE:HB2	4:4:142:PRO:HG3	2.02	0.41
5:A:845:A:P	25:U:64:ARG:HH22	2.43	0.41
5:A:881:A:H1'	19:O:80:ASN:HB3	2.03	0.41
5:A:904:C:H42	8:D:117:ARG:HA	1.84	0.41
5:A:1295:A:C5	6:B:202:ILE:HG21	2.55	0.41
8:D:160:ARG:HB3	8:D:164:GLU:HG3	2.02	0.41
18:N:17:VAL:HG22	18:N:28:VAL:HG22	2.02	0.41
19:O:74:TRP:CD2	19:O:140:THR:HG22	2.55	0.41
1:0:90:ASP:CG	19:O:215:ARG:HH22	2.29	0.41
2:1:129:PHE:HB3	12:H:155:VAL:HG21	2.02	0.41
4:4:376:ILE:HG23	4:4:422:ILE:CD1	2.51	0.41
10:F:88:ASP:HB3	10:F:91:ILE:HB	2.01	0.41
17:M:108:GLU:OE2	25:U:59:ARG:NH2	2.36	0.41
17:M:111:ARG:NH2	22:R:146:LYS:O	2.53	0.41
20:P:49:ASP:HA	27:W:85:ARG:HH11	1.85	0.41
20:P:73:ASP:OD1	20:P:74:TYR:N	2.54	0.41
28:X:269:TRP:HA	28:X:294:ARG:HH21	1.86	0.41
32:b:76:MET:HE2	32:b:79:GLU:HG3	2.03	0.41
32:b:85:SER:HB2	32:b:315:ARG:HH12	1.84	0.41
4:4:299:GLU:HA	4:4:341:CYS:SG	2.61	0.41
5:A:672:A:H2'	5:A:673:U:C6	2.56	0.41
5:A:768:A:H4'	18:N:24:LYS:HB2	2.02	0.41
5:A:1471:A:H2'	5:A:1472:G:C8	2.56	0.41
7:C:38:ARG:HD2	7:C:43:ARG:NH1	2.35	0.41
7:C:115:ASN:O	7:C:149:CYS:HB2	2.21	0.41
12:H:91:TYR:OH	12:H:160:ILE:O	2.28	0.41
17:M:89:LYS:HA	17:M:103:MET:HE2	2.03	0.41
19:O:202:TRP:CD1	19:O:202:TRP:H	2.38	0.41
28:X:132:THR:HA	28:X:388:PRO:HD2	2.03	0.41
29:Y:286:LEU:O	29:Y:289:VAL:HG22	2.21	0.41
30:Z:58:TYR:O	30:Z:62:MET:HG2	2.21	0.41
31:a:111:PRO:HA	31:a:118:TYR:HB2	2.03	0.41
4:4:369:LEU:HD22	4:4:415:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:470:GLN:HG2	4:4:472:ASP:H	1.86	0.41
5:A:867:C:H1'	5:A:870:C:H41	1.85	0.41
12:H:113:ARG:HB3	12:H:139:LEU:HD23	2.02	0.41
16:L:112:MET:O	16:L:116:VAL:HG22	2.20	0.41
1:0:11:ILE:HB	5:A:806:C:C2	2.56	0.40
8:D:412:LYS:HE3	8:D:418:LYS:HD3	2.02	0.40
2:1:231:HIS:O	12:H:189:TRP:NE1	2.54	0.40
4:4:108:LEU:HD22	8:D:154:VAL:HG21	2.03	0.40
4:4:188:THR:HB	4:4:251:MET:HE3	2.02	0.40
5:A:1007:G:H2'	5:A:1008:A:C8	2.57	0.40
5:A:1221:A:OP1	5:A:1223:C:H5'	2.20	0.40
6:B:167:HIS:HE1	6:B:171:PHE:HA	1.85	0.40
5:A:845:A:H4'	25:U:60:TYR:CZ	2.56	0.40
5:A:1452:U:H2'	5:A:1453:A:C8	2.55	0.40
17:M:52:GLY:HA3	17:M:67:ALA:O	2.21	0.40
4:4:388:ARG:O	4:4:392:ILE:HG12	2.22	0.40
5:A:740:G:H2'	5:A:741:A:H8	1.86	0.40
5:A:1124:A:N6	5:A:1127:A:OP1	2.53	0.40
22:R:279:LYS:HA	22:R:304:TYR:HE2	1.87	0.40
32:b:229:GLU:OE2	32:b:270:ARG:NH1	2.41	0.40
2:1:86:ARG:HB3	2:1:96:PRO:HB2	2.02	0.40
4:4:197:TYR:CE2	29:Y:281:GLU:HG3	2.57	0.40
4:4:346:HIS:HA	4:4:378:LEU:HD12	2.04	0.40
4:4:359:GLU:OE1	29:Y:257:ASN:N	2.47	0.40
4:4:360:MET:HE1	4:4:371:THR:HG21	2.03	0.40
5:A:894:C:H41	14:J:78:ARG:NH2	2.14	0.40
5:A:1374:A:H2'	5:A:1375:C:O4'	2.22	0.40
8:D:306:LYS:HB2	8:D:333:TYR:HB3	2.04	0.40
17:M:78:GLY:O	25:U:75:VAL:HG22	2.20	0.40
22:R:218:MET:SD	22:R:223:ARG:NH1	2.95	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	213/218 (98%)	211 (99%)	2 (1%)	0	100	100
2	1	276/323 (85%)	271 (98%)	5 (2%)	0	100	100
3	3	69/199 (35%)	68 (99%)	1 (1%)	0	100	100
4	4	586/689 (85%)	574 (98%)	12 (2%)	0	100	100
6	B	223/296 (75%)	219 (98%)	4 (2%)	0	100	100
7	C	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
8	D	341/430 (79%)	334 (98%)	7 (2%)	0	100	100
9	E	116/125 (93%)	114 (98%)	2 (2%)	0	100	100
10	F	191/242 (79%)	190 (100%)	1 (0%)	0	100	100
11	G	298/396 (75%)	290 (97%)	8 (3%)	0	100	100
12	H	138/201 (69%)	135 (98%)	2 (1%)	1 (1%)	18	53
13	I	135/194 (70%)	132 (98%)	3 (2%)	0	100	100
14	J	106/138 (77%)	100 (94%)	6 (6%)	0	100	100
15	K	99/128 (77%)	99 (100%)	0	0	100	100
16	L	172/257 (67%)	170 (99%)	2 (1%)	0	100	100
17	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
18	N	108/130 (83%)	105 (97%)	3 (3%)	0	100	100
19	O	191/258 (74%)	188 (98%)	3 (2%)	0	100	100
20	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
21	Q	83/87 (95%)	83 (100%)	0	0	100	100
22	R	293/360 (81%)	284 (97%)	9 (3%)	0	100	100
23	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
24	T	166/173 (96%)	163 (98%)	3 (2%)	0	100	100
25	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
26	V	358/414 (86%)	352 (98%)	6 (2%)	0	100	100
27	W	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
28	X	350/398 (88%)	341 (97%)	9 (3%)	0	100	100
29	Y	147/395 (37%)	142 (97%)	5 (3%)	0	100	100
30	Z	98/106 (92%)	97 (99%)	1 (1%)	0	100	100
31	a	138/343 (40%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	b	322/407 (79%)	317 (98%)	5 (2%)	0	100	100
All	All	5964/7935 (75%)	5853 (98%)	110 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	H	126	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	188/190 (99%)	188 (100%)	0	100	100
2	1	256/291 (88%)	256 (100%)	0	100	100
3	3	65/166 (39%)	65 (100%)	0	100	100
4	4	527/609 (86%)	527 (100%)	0	100	100
6	B	198/249 (80%)	198 (100%)	0	100	100
7	C	115/143 (80%)	115 (100%)	0	100	100
8	D	286/357 (80%)	286 (100%)	0	100	100
9	E	100/107 (94%)	100 (100%)	0	100	100
10	F	174/209 (83%)	174 (100%)	0	100	100
11	G	263/342 (77%)	263 (100%)	0	100	100
12	H	130/180 (72%)	130 (100%)	0	100	100
13	I	105/147 (71%)	105 (100%)	0	100	100
14	J	93/118 (79%)	93 (100%)	0	100	100
15	K	91/113 (80%)	91 (100%)	0	100	100
16	L	158/226 (70%)	158 (100%)	0	100	100
17	M	97/113 (86%)	97 (100%)	0	100	100
18	N	96/115 (84%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	O	174/230 (76%)	174 (100%)	0	100	100
20	P	88/123 (72%)	88 (100%)	0	100	100
21	Q	78/79 (99%)	78 (100%)	0	100	100
22	R	264/318 (83%)	264 (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	87/158 (55%)	87 (100%)	0	100	100
28	X	311/351 (89%)	311 (100%)	0	100	100
29	Y	137/357 (38%)	137 (100%)	0	100	100
30	Z	90/95 (95%)	90 (100%)	0	100	100
31	a	127/288 (44%)	127 (100%)	0	100	100
32	b	275/350 (79%)	274 (100%)	1 (0%)	84	90
All	All	5319/6883 (77%)	5318 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	b	294	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	207	GLN
4	4	545	GLN
6	B	74	ASN
6	B	167	HIS
6	B	201	ASN
7	C	60	HIS
8	D	175	GLN
9	E	59	ASN
10	F	147	GLN
10	F	207	HIS
11	G	288	HIS
19	O	204	ASN

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Mol	Chain	Res	Type
20	P	71	HIS
20	P	78	GLN
21	Q	53	GLN
22	R	139	ASN
22	R	278	ASN
25	U	43	ASN
25	U	147	GLN
27	W	91	GLN
28	X	154	HIS
28	X	347	ASN
29	Y	295	GLN
31	a	115	GLN
31	a	187	ASN
32	b	102	HIS
32	b	294	ASN
32	b	297	ASN
32	b	343	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	914/955 (95%)	113 (12%)	1 (0%)

All (113) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	649	A
5	A	651	A
5	A	680	U
5	A	688	A
5	A	704	U
5	A	721	U
5	A	738	A
5	A	739	C
5	A	753	A
5	A	761	A
5	A	766	G
5	A	773	U
5	A	791	G
5	A	796	G
5	A	808	C

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Mol	Chain	Res	Type
5	A	829	C
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	868	C
5	A	871	A
5	A	890	C
5	A	902	G
5	A	904	C
5	A	919	A
5	A	923	A
5	A	929	A
5	A	931	C
5	A	932	C
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	956	C
5	A	958	C
5	A	959	C
5	A	960	C
5	A	961	U
5	A	962	C
5	A	964	C
5	A	965	C
5	A	967	A
5	A	993	A
5	A	1001	C
5	A	1011	C
5	A	1015	A
5	A	1030	G
5	A	1031	G
5	A	1042	U
5	A	1065	C
5	A	1075	A
5	A	1103	A

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Mol	Chain	Res	Type
5	A	1105	C
5	A	1106	C
5	A	1107	U
5	A	1116	A
5	A	1118	A
5	A	1121	A
5	A	1126	A
5	A	1151	C
5	A	1152	A
5	A	1155	G
5	A	1167	A
5	A	1223	C
5	A	1230	C
5	A	1247	G
5	A	1248	C
5	A	1250	C
5	A	1251	A
5	A	1271	C
5	A	1272	A
5	A	1273	G
5	A	1284	U
5	A	1285	G
5	A	1290	C
5	A	1291	U
5	A	1294	A
5	A	1326	A
5	A	1327	G
5	A	1343	A
5	A	1356	A
5	A	1365	A
5	A	1378	C
5	A	1390	A
5	A	1405	C
5	A	1406	U
5	A	1422	G
5	A	1447	G
5	A	1466	C
5	A	1474	G
5	A	1478	A
5	A	1481	C
5	A	1493	C
5	A	1494	C

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Mol	Chain	Res	Type
5	A	1502	A
5	A	1506	U
5	A	1508	C
5	A	1546	A
5	A	1547	U
5	A	1548	A
5	A	1549	G
5	A	1557	A
5	A	1558	A
5	A	1559	G
5	A	1568	U
5	A	1585	A
5	A	1594	G
5	A	1595	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	1271	C

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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	$\#\|Z\|>2$
38	GDP	X	401	-	28,30,30	1.15	3 (10%)	44,47,47	1.87	8 (18%)
37	FES	P	201	20,9	0,4,4	-	-	-		
39	ATP	X	402	-	29,33,33	0.33	0	44,52,52	0.54	0
37	FES	T	201	24,17	0,4,4	-	-	-		
35	NAD	A	1710	-	45,48,48	0.79	1 (2%)	63,73,73	0.77	3 (4%)
40	SAH	b	501	-	27,28,28	0.61	0	38,40,40	0.55	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
38	GDP	X	401	-	-	7/16/32/32	0/3/3/3
37	FES	P	201	20,9	-	-	0/1/1/1
39	ATP	X	402	-	-	3/22/38/38	0/3/3/3
37	FES	T	201	24,17	-	-	0/1/1/1
35	NAD	A	1710	-	-	6/30/62/62	0/5/5/5
40	SAH	b	501	-	-	8/15/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	401	GDP	C5-C4	3.05	1.47	1.38
38	X	401	GDP	C6-N1	-2.50	1.34	1.38
35	A	1710	NAD	O4D-C1D	-2.46	1.37	1.41
38	X	401	GDP	C5-N7	-2.27	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	X	401	GDP	C5-C4-N3	-6.05	118.64	128.46
38	X	401	GDP	C2-N3-C4	4.84	120.92	112.30
38	X	401	GDP	N9-C4-N3	4.58	135.14	125.94
38	X	401	GDP	PA-O3A-PB	-4.17	118.51	132.83
38	X	401	GDP	C6-C5-N7	2.99	135.82	130.25
38	X	401	GDP	C4-C5-N7	-2.43	106.87	110.72
38	X	401	GDP	C3'-C2'-C1'	2.39	105.97	101.43
35	A	1710	NAD	PN-O3-PA	-2.33	124.85	132.83
35	A	1710	NAD	O2A-PA-O1A	2.14	122.81	112.24
38	X	401	GDP	O6-C6-C5	-2.12	120.97	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	1710	NAD	O7N-C7N-N7N	2.02	125.44	122.58

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	1710	NAD	C5B-O5B-PA-O1A
35	A	1710	NAD	O4B-C4B-C5B-O5B
35	A	1710	NAD	C3B-C4B-C5B-O5B
35	A	1710	NAD	C5D-O5D-PN-O3
38	X	401	GDP	C5'-O5'-PA-O3A
38	X	401	GDP	C5'-O5'-PA-O2A
38	X	401	GDP	C3'-C4'-C5'-O5'
39	X	402	ATP	O4'-C4'-C5'-O5'
39	X	402	ATP	C3'-C4'-C5'-O5'
40	b	501	SAH	N-CA-CB-CG
40	b	501	SAH	C-CA-CB-CG
40	b	501	SAH	C4'-C5'-SD-CG
40	b	501	SAH	OXT-C-CA-N
38	X	401	GDP	O4'-C4'-C5'-O5'
40	b	501	SAH	O-C-CA-CB
40	b	501	SAH	OXT-C-CA-CB
40	b	501	SAH	O-C-CA-N
39	X	402	ATP	PB-O3A-PA-O1A
35	A	1710	NAD	C5D-O5D-PN-O1N
35	A	1710	NAD	C5D-O5D-PN-O2N
38	X	401	GDP	C5'-O5'-PA-O1A
40	b	501	SAH	CB-CG-SD-C5'
38	X	401	GDP	PB-O3A-PA-O1A
38	X	401	GDP	PB-O3A-PA-O2A

There are no ring outliers.

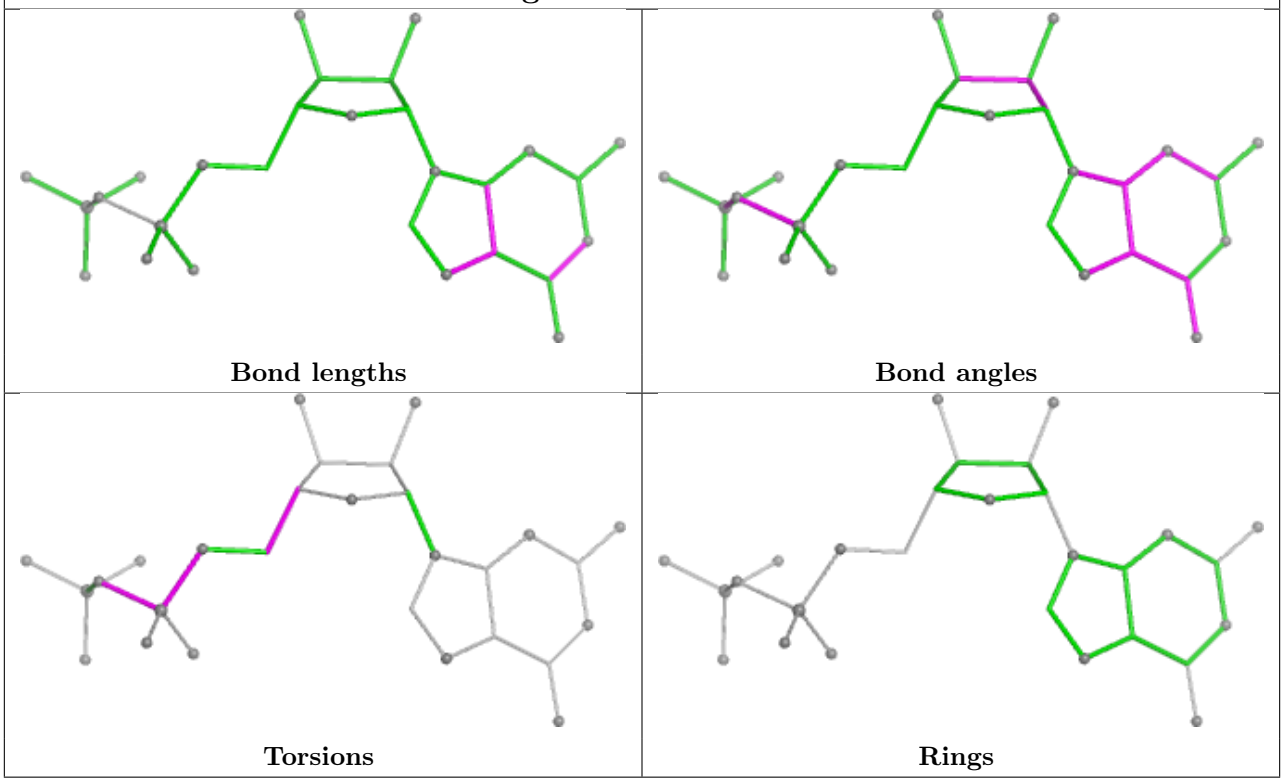
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	1710	NAD	1	0
40	b	501	SAH	1	0

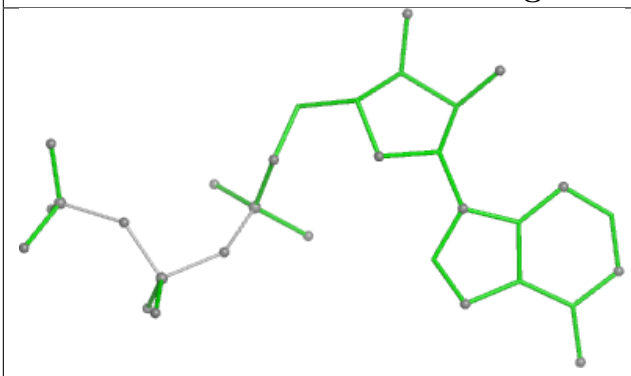
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

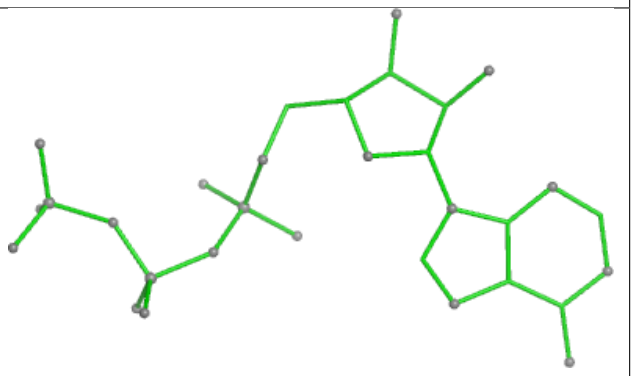
Ligand GDP X 401



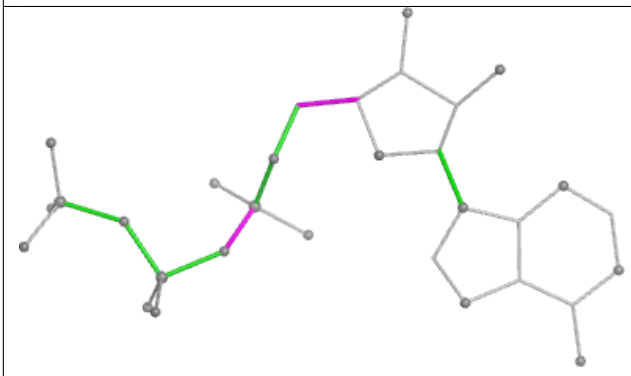
Ligand ATP X 402



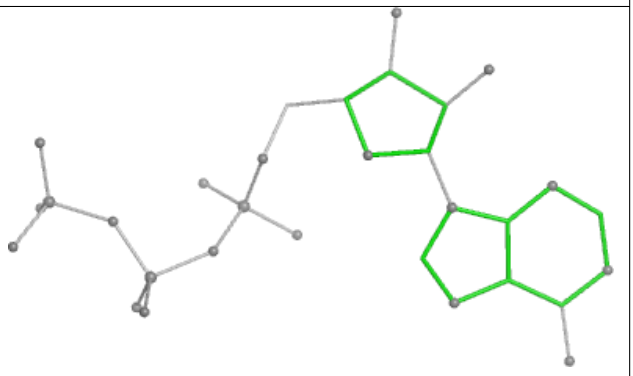
Bond lengths



Bond angles

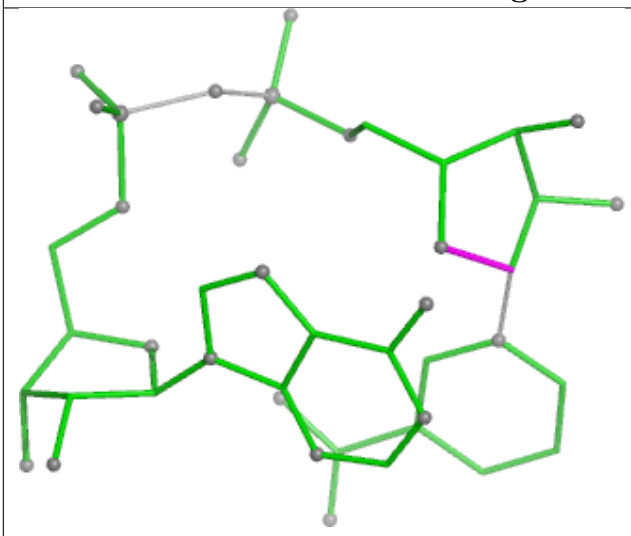


Torsions

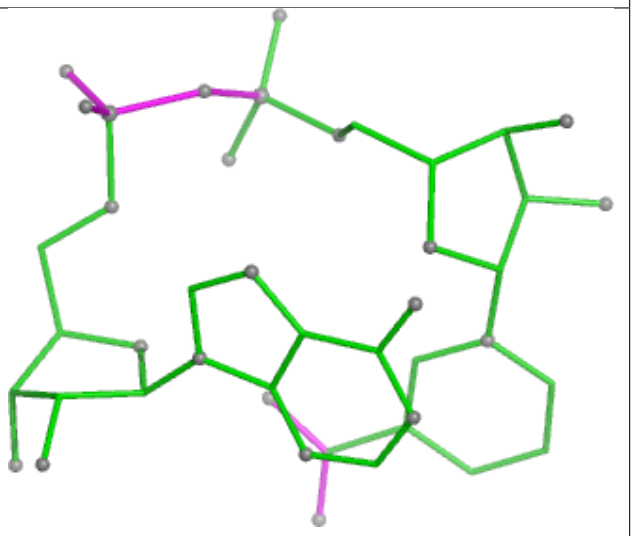


Rings

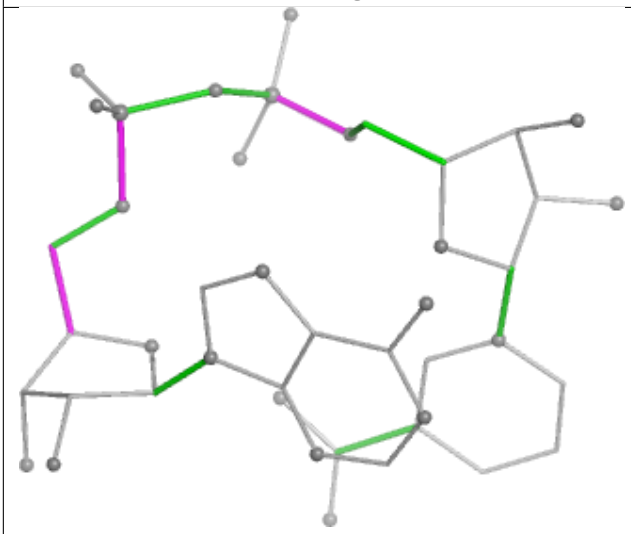
Ligand NAD A 1710



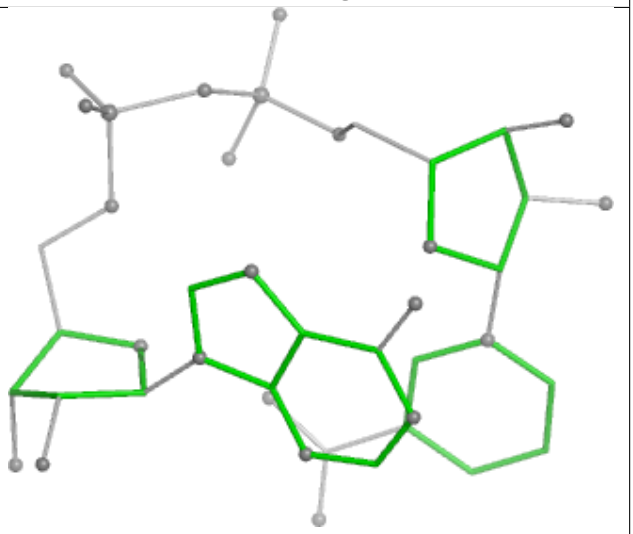
Bond lengths



Bond angles

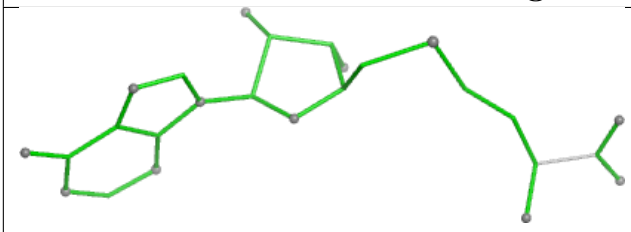


Torsions

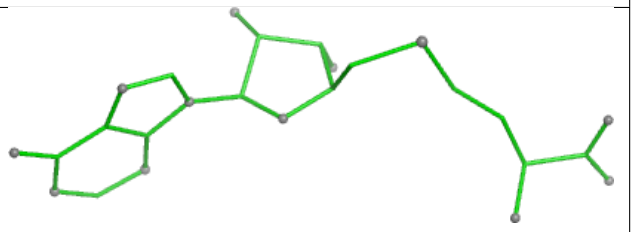


Rings

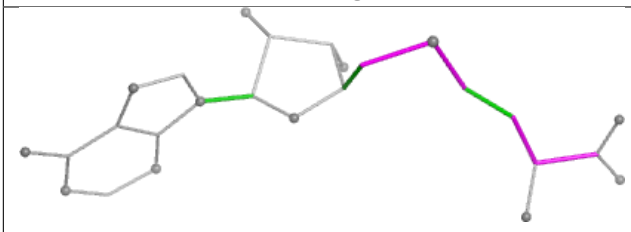
Ligand SAH b 501



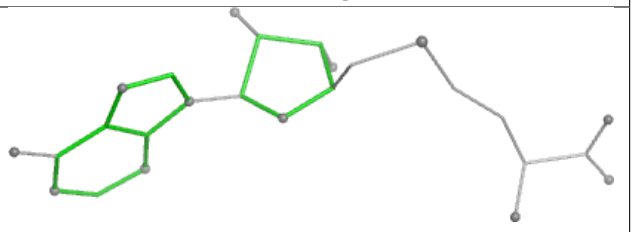
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

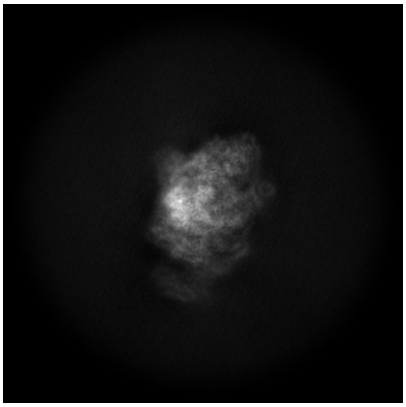
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51085. These allow visual inspection of the internal detail of the map and identification of artifacts.

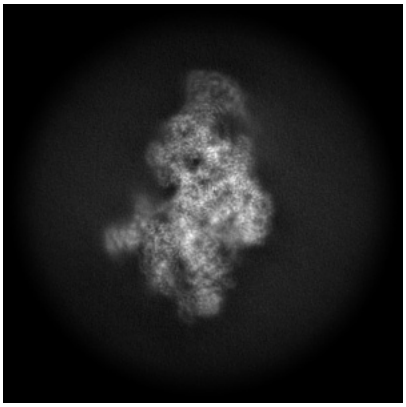
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

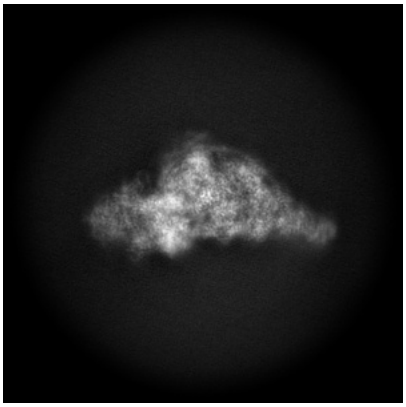
6.1.1 Primary map



X



Y

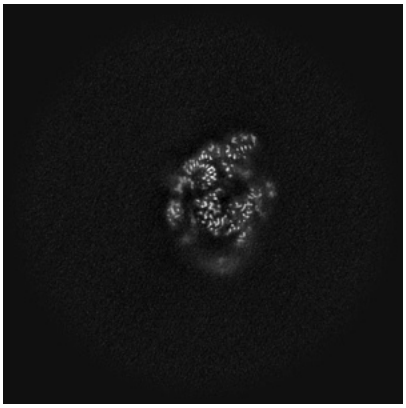


Z

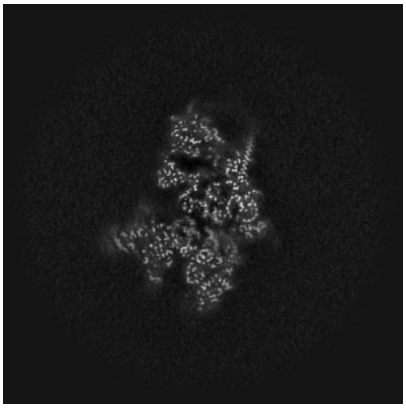
The images above show the map projected in three orthogonal directions.

6.2 Central slices

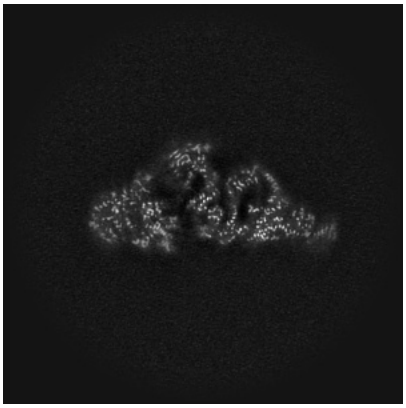
6.2.1 Primary map



X Index: 220



Y Index: 220

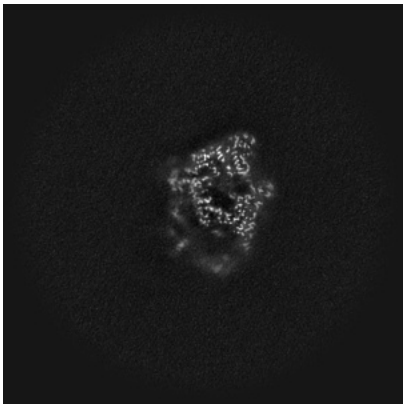


Z Index: 220

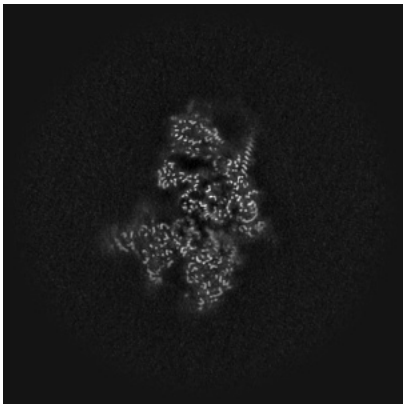
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

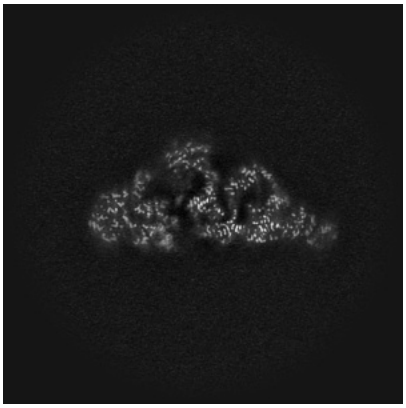
6.3.1 Primary map



X Index: 214



Y Index: 219

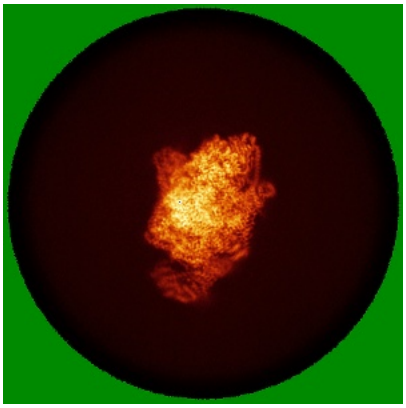


Z Index: 222

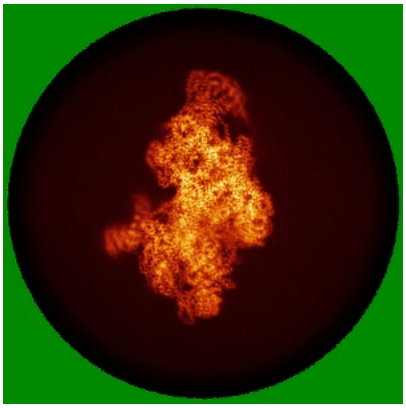
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

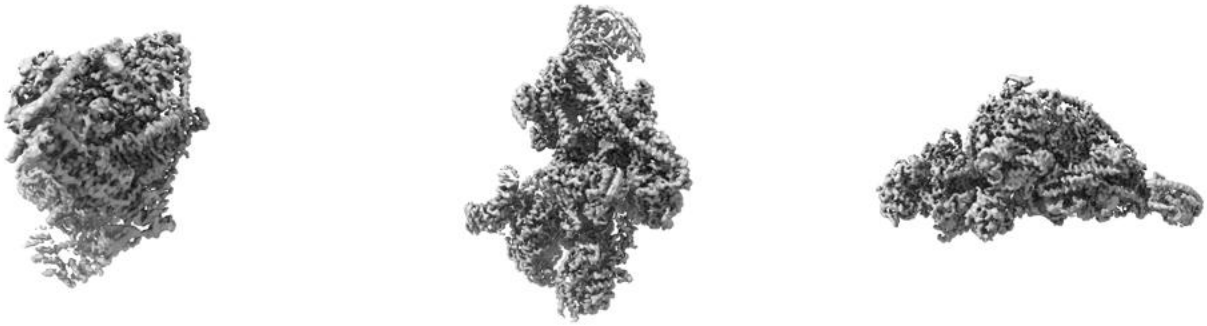


Z

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 0.39. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

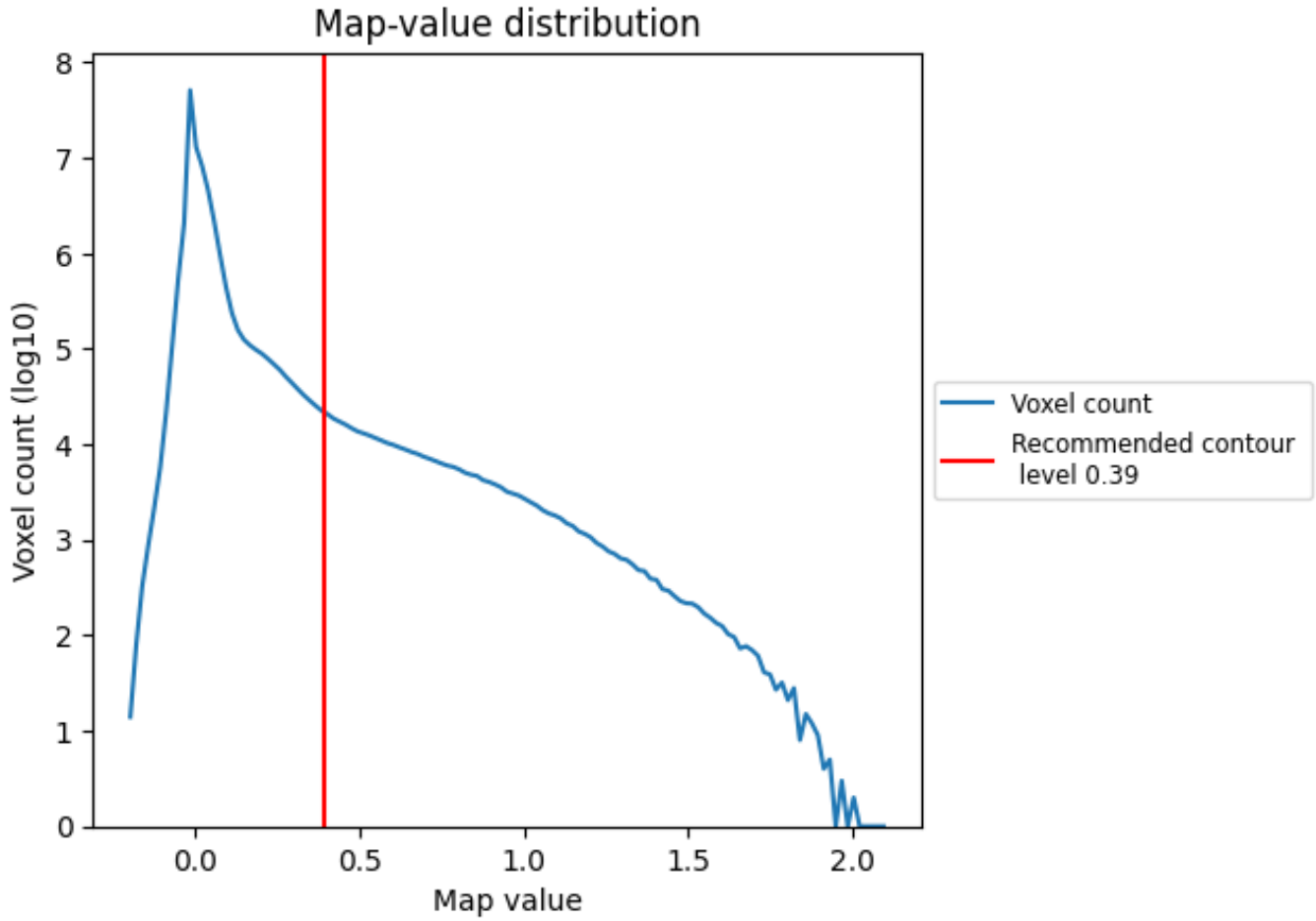
6.6 Mask visualisation (i)

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

7 Map analysis

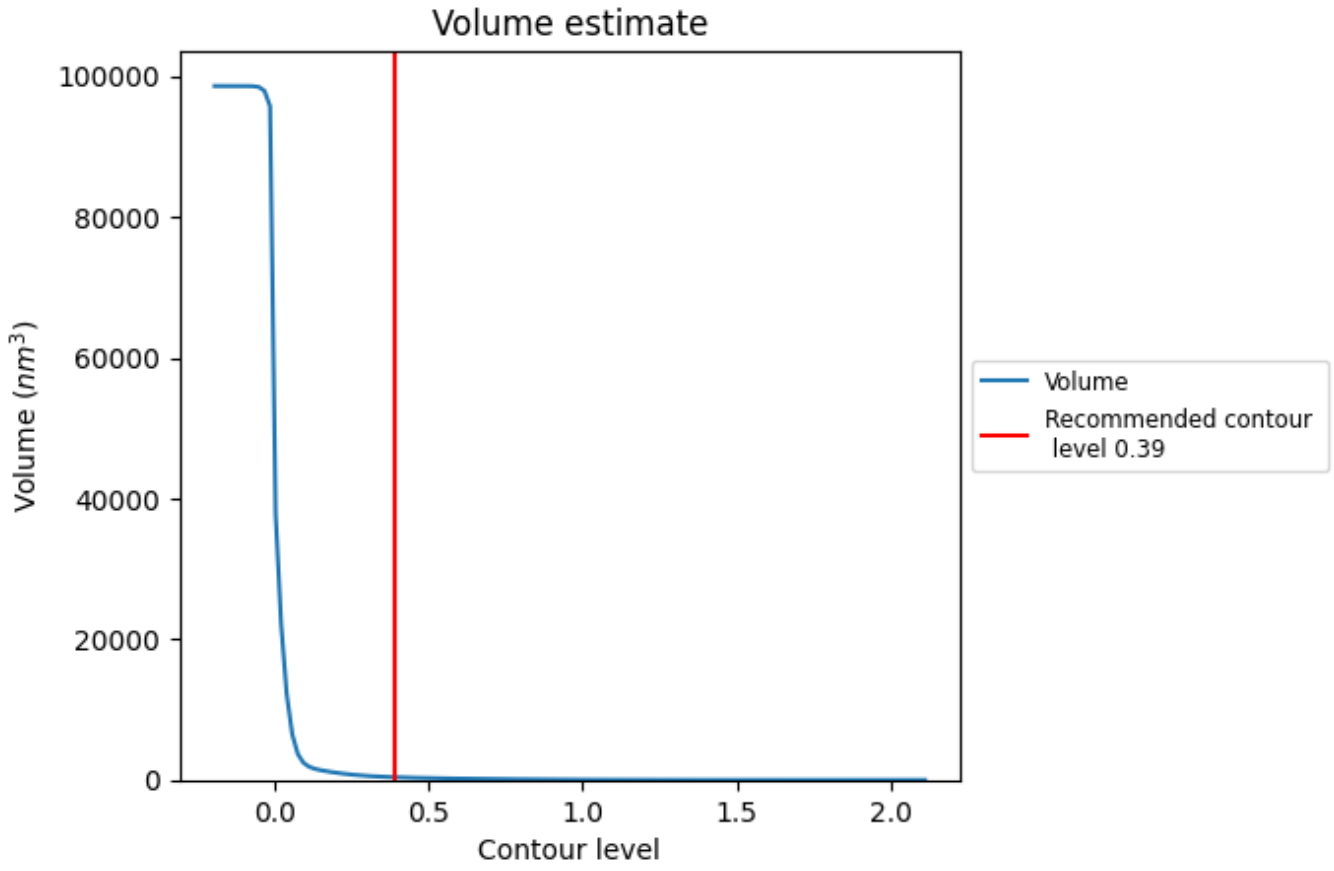
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

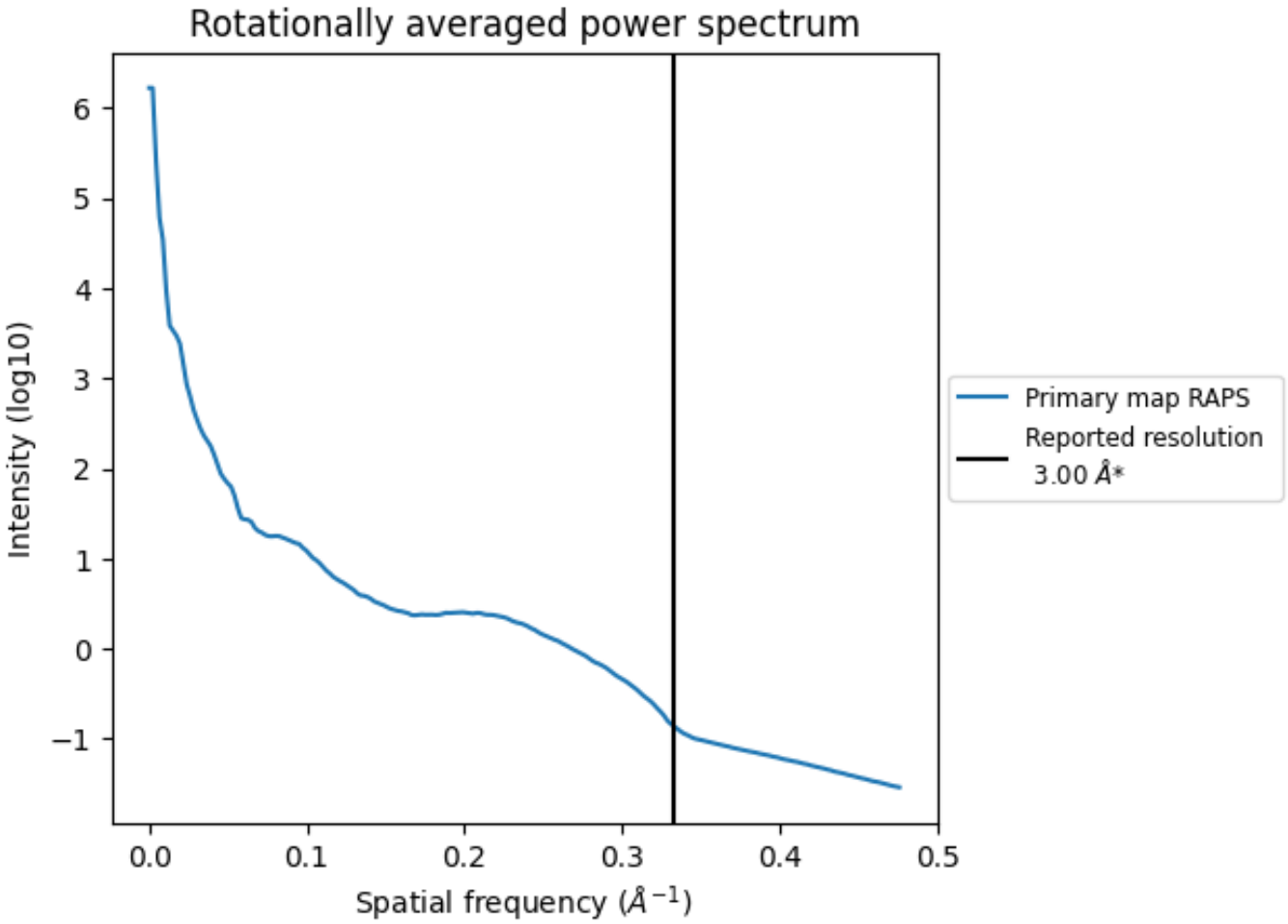
7.2 Volume estimate



The volume at the recommended contour level is 390 nm^3; this corresponds to an approximate mass of 352 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

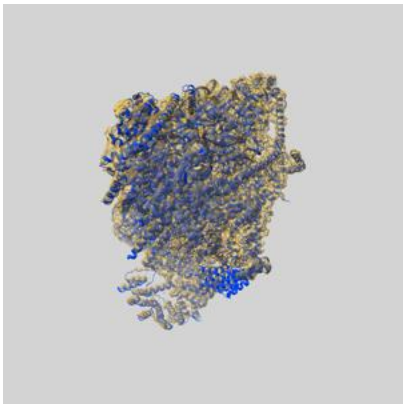
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

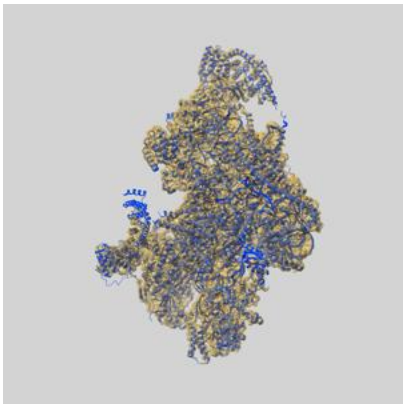
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51085 and PDB model 9G5D. Per-residue inclusion information can be found in section 3 on page 13.

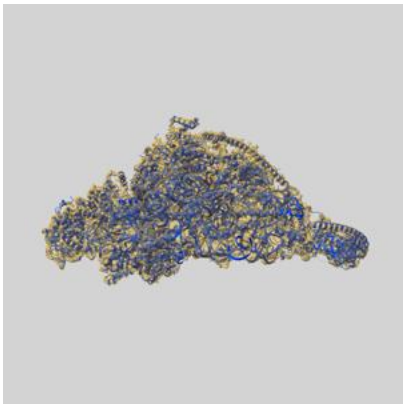
9.1 Map-model overlay



X



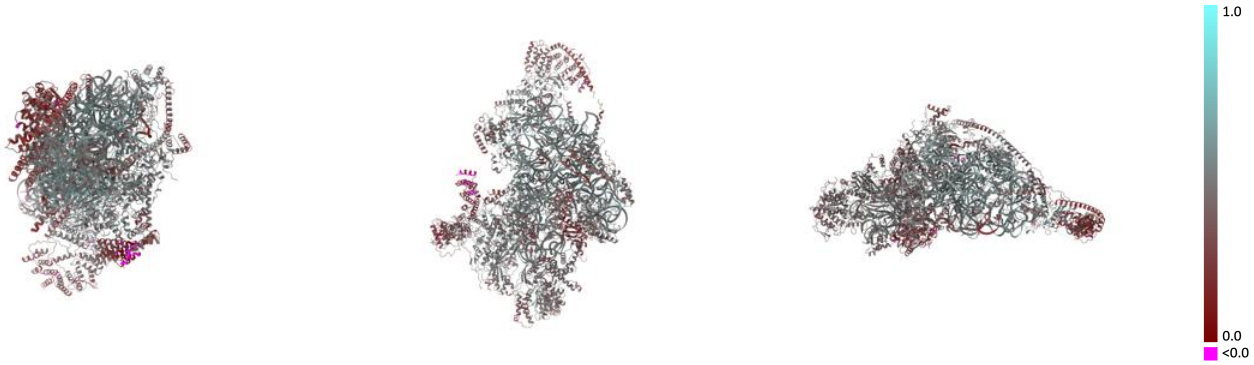
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.39 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

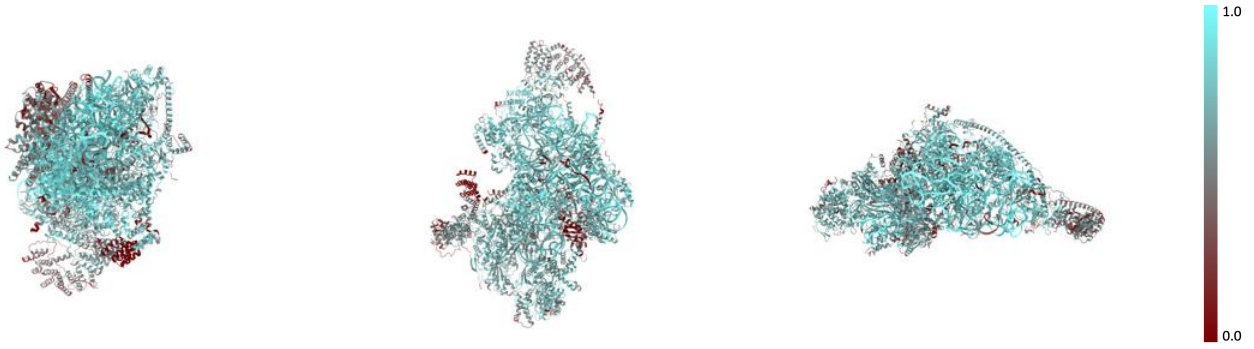
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

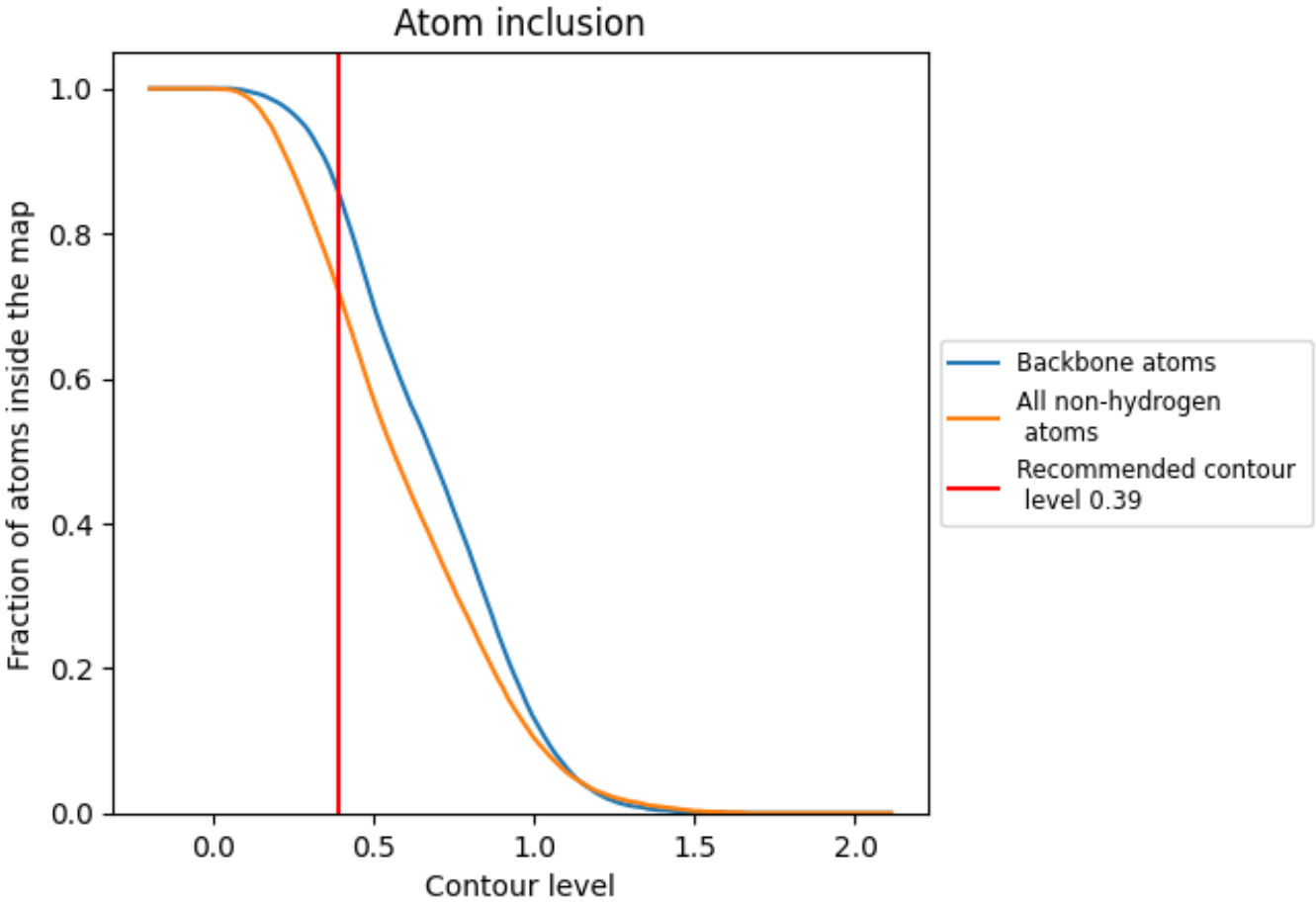
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.39).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.39) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.4400
0	0.6720	0.4550
1	0.6760	0.4240
3	0.6920	0.4670
4	0.4150	0.2790
A	0.8970	0.4970
B	0.8040	0.4900
C	0.7380	0.5020
D	0.6780	0.4670
E	0.6860	0.4510
F	0.6660	0.4270
G	0.6780	0.4240
H	0.6840	0.4650
I	0.7500	0.4600
J	0.7370	0.4880
K	0.8030	0.4850
L	0.7270	0.4690
M	0.8100	0.5080
N	0.8270	0.5200
O	0.8220	0.5140
P	0.7590	0.4810
Q	0.7040	0.4590
R	0.7720	0.4650
S	0.6700	0.4300
T	0.7890	0.5060
U	0.7160	0.4380
V	0.4580	0.2890
W	0.7100	0.4710
X	0.6820	0.4280
Y	0.5800	0.3840
Z	0.6210	0.3920
a	0.1880	0.2600
b	0.5470	0.3140

