Full wwPDB EM Validation Report ⓘ

Sep 15, 2026 – 04:04 pm BST

PDB ID	:	9RU6 / pdb_00009ru6
EMDB ID	:	EMD-54264
Title	:	Human mitoribosome bound to TACO1 (Translational activator of COX1), mRNA, A/A-, P/P- and (partial) E/E-tRNAs
Authors	:	Singh, V.; Khawaja, A.; Rorbach, J.
Deposited on	:	2025-07-03
Resolution	:	2.64 Å(reported)

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:

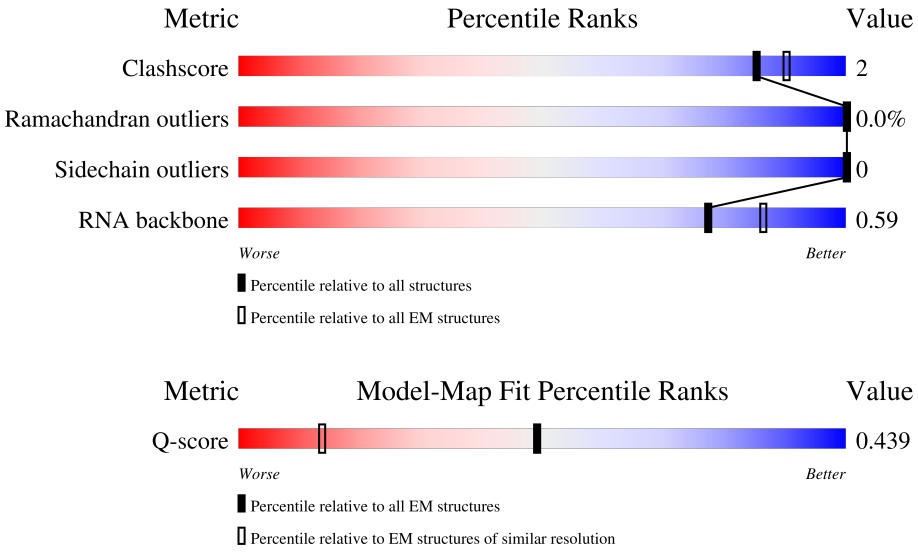
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.64 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	8968 (2.14 - 3.14)

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	A5	297	7% 44% 11% 45%
2	AA	954	76% 21%
3	AB	296	72% 24%

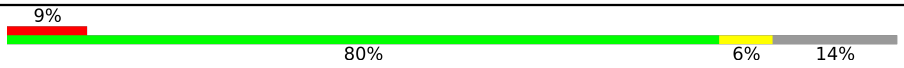
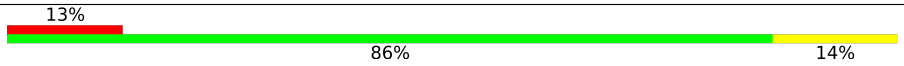
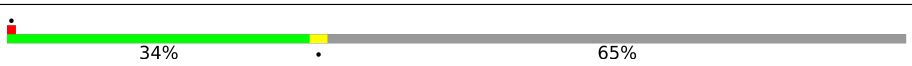
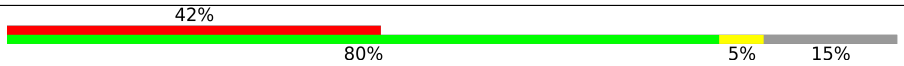
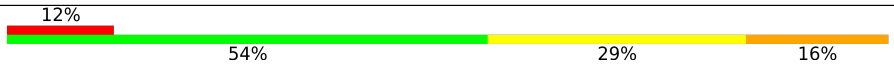
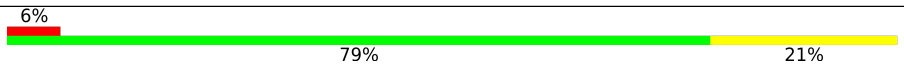
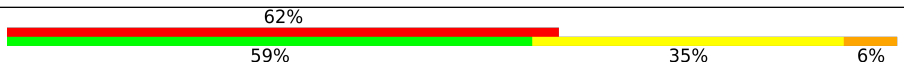
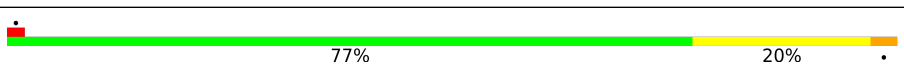
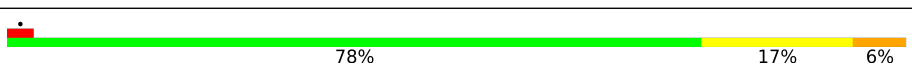
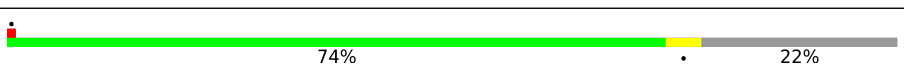
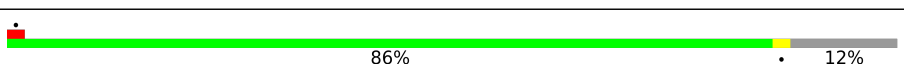
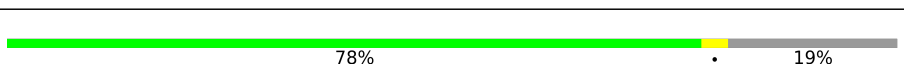
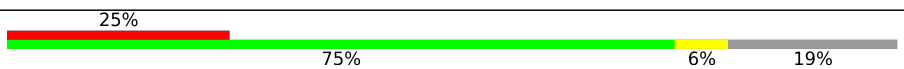
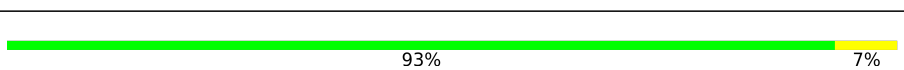
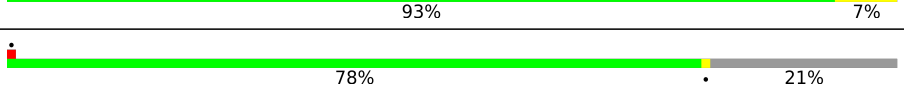
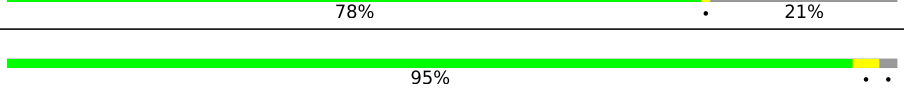
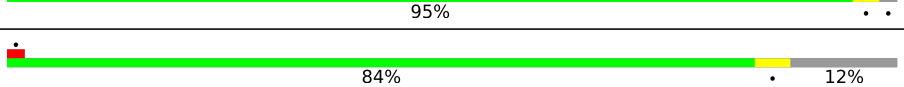
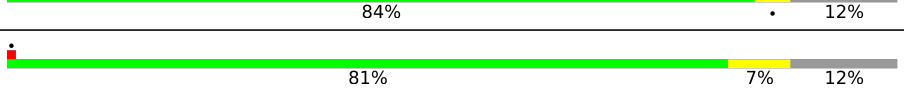
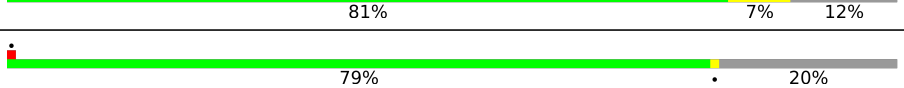
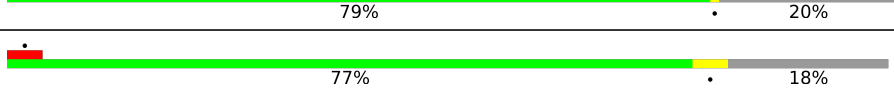
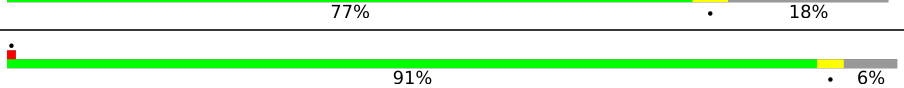
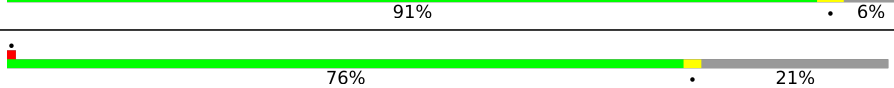
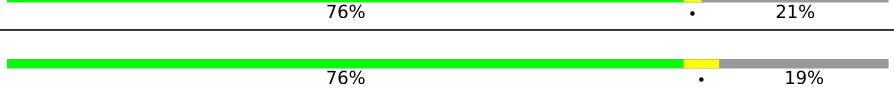
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Mol	Chain	Length	Quality of chain
4	AC	167	76% 21%
5	AD	430	7% 75% 5% 20%
6	AE	125	90% 8%
7	AF	242	7% 83% 14%
8	AG	396	7% 79% 17%
9	AH	201	7% 65% 5% 30%
10	AI	193	68% 30%
11	AJ	138	62% 15% 22%
12	AK	128	78% 21%
13	AL	257	6% 65% 32%
14	AM	137	12% 78% 9% 13%
15	AN	130	75% 10% 15%
16	AO	258	14% 68% 7% 25%
17	AP	142	63% 6% 32%
18	AQ	87	92% 8%
19	AR	360	13% 79% 18%
20	AS	190	11% 64% 7% 29%
21	AT	173	7% 92% 5%
22	AU	205	7% 82% 14%
23	AV	414	46% 81% 6% 13%
24	AW	187	45% 8% 47%
25	AX	398	6% 85% 12%
26	AY	395	11% 36% 62%
27	AZ	106	10% 90% 5% 6%
28	A0	217	36% 89% 10%

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Mol	Chain	Length	Quality of chain
29	A1	323	
30	A2	118	
31	A3	199	
32	A4	689	
33	Aw	68	
34	Ax	70	
35	Ay	70	
36	Az	34	
37	A	1558	
38	B	72	
39	D	305	
40	E	348	
41	F	311	
42	I	261	
43	J	192	
44	K	178	
45	L	145	
46	M	296	
47	N	251	
48	O	175	
49	P	180	
50	Q	292	
51	R	149	
52	S	205	
53	T	206	

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Mol	Chain	Length	Quality of chain
54	U	153	9% 95% 5%
55	V	216	91% 5%
56	W	148	76% 22%
57	X	256	92% 5%
58	Y	250	70% 28%
59	Z	161	71% 5% 24%
60	0	188	55% 41%
61	1	65	5% 83% 14%
62	2	92	49% 50%
63	3	188	49% 49%
64	4	103	37% 63%
65	5	423	90% 7%
66	6	380	89% 7%
67	7	338	84% 13%
68	8	206	9% 71% 5% 24%
69	9	137	88% 9%
70	a	142	6% 69% 30%
71	b	215	64% 6% 30%
72	c	332	82% 5% 14%
73	d	306	8% 70% 8% 23%
74	e	279	13% 80% 5% 15%
75	f	212	8% 71% 26%
76	g	166	77% 19%
77	h	158	65% 5% 30%
78	i	128	74% 24%

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Mol	Chain	Length	Quality of chain
79	j	123	5% 68% 8% 24%
80	k	112	88% 9%
81	l	138	52% 7% 41%
82	m	128	12% 69% 28%
83	o	102	87% 5% 8%
84	p	206	8% 67% 29%
85	q	222	17% 71% 26%
86	r	196	82% 17%
87	s	439	86% 12%
88	t	198	20% 20% 77%
88	t1	198	16% 35% 64%
88	u	198	16% 13% 84%
88	v	198	16% 16% 84%
88	w	198	16% 15% 84%
88	x	198	16% 16% 84%
88	y	198	16% 15% 84%
89	H	267	40% 69% 7% 24%
90	z	325	74% 72% 5% 22%

2 Entry composition

There are 100 unique types of molecules in this entry. The entry contains 338524 atoms, of which 155317 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 Translational activator of cytochrome c oxidase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A5	164	2521	786	1253	223	253	6	0	0

- Molecule 2 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	AA	954	30518	9088	10258	3647	6571	954	0	0

- Molecule 3 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	AB	225	3643	1164	1815	331	323	10	0	0

- Molecule 4 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	AC	132	2171	699	1088	195	185	4	0	0

- Molecule 5 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	AD	343	5535	1713	2804	518	487	13	0	0

- Molecule 6 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	AE	122	1972	614	1000	177	177	4	0	0

- Molecule 7 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	AF	208	Total	C	H	N	O	S	0	0
			3494	1104	1769	312	298	11		

- Molecule 8 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	AG	327	Total	C	H	N	O	S	0	0
			5375	1710	2687	477	487	14		

- Molecule 9 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AH	140	Total	C	H	N	O	S	0	0
			2335	745	1183	194	210	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AI	136	Total	C	H	N	O	S	0	0
			2063	637	1052	191	179	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	?	-	ASN	deletion	UNP P82912

- Molecule 11 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AJ	108	Total	C	H	N	O	S	0	0
			1724	521	885	169	143	6		

- Molecule 12 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AK	101	Total	C	H	N	O	S	0	0
			1747	537	885	179	141	5		

- Molecule 13 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AL	174	Total	C	H	N	O	S	0	0
			2993	925	1540	270	251	7		

- Molecule 14 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AM	119	Total	C	H	N	O	S	0	0
			1907	594	965	185	157	6		

- Molecule 15 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AN	110	Total	C	H	N	O	S	0	0
			1796	562	928	156	147	3		

- Molecule 16 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AO	193	Total	C	H	N	O	S	0	0
			3149	1014	1557	294	277	7		

- Molecule 17 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AP	97	Total	C	H	N	O	S	0	0
			1587	501	806	134	138	8		

- Molecule 18 is a protein called MRPS21 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AQ	87	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	1	ACE	-	acetylation	UNP A0A2J8VEN6

- Molecule 19 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AR	295	Total	C	H	N	O	S	0	0
			4837	1533	2428	413	455	8		

- Molecule 20 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AS	135	Total	C	H	N	O	S	0	0
			2226	716	1115	198	196	1		

- Molecule 21 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AT	168	Total	C	H	N	O	S	0	0
			2764	877	1393	239	244	11		

- Molecule 22 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AU	176	Total	C	H	N	O	S	0	0
			2987	916	1499	301	267	4		

- Molecule 23 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AV	362	Total	C	H	N	O	S	0	0
			5930	1904	2961	495	558	12		

- Molecule 24 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AW	100	Total	C	H	N	O	S	0	0
			1591	498	802	141	146	4		

- Molecule 25 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AX	352	Total	C	H	N	O	S	0	0
			5692	1822	2843	499	517	11		

- Molecule 26 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AY	149	Total	C	H	N	O	S	0	0
			2443	801	1197	207	234	4		

- Molecule 27 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AZ	100	Total	C	H	N	O	S	0	0
			1697	534	858	153	148	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	A0	215	Total	C	H	N	O	S	0	0
			3583	1130	1796	339	313	5		

- Molecule 29 is a protein called Small ribosomal subunit protein mS35.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	A1	279	Total	C	H	N	O	S	0	0
			4556	1434	2292	387	432	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	45	ASP	GLU	conflict	UNP P82673

- Molecule 30 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	A2	118	Total	C	H	N	O	S	0	0
			1906	579	971	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 31 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	A3	70	Total	C	H	N	O	S	0	0
			1324	401	699	134	89	1		

- Molecule 32 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	A4	588	Total	C	H	N	O	S	0	0
			9534	3053	4766	808	879	28		

- Molecule 33 is a RNA chain called A-site tRNA (68-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Aw	68	Total	C	H	N	O	P	0	0
			2147	643	720	237	479	68		

- Molecule 34 is a RNA chain called P-site RNA (70-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Ax	70	Total	C	H	N	O	P	0	0
			2232	665	750	259	488	70		

- Molecule 35 is a RNA chain called E-site tRNA (70-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
35	Ay	55	Total	C	H	N	O	P	0	0
			1761	524	592	209	381	55		

- Molecule 36 is a RNA chain called mRNA (34-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
36	Az	34	Total	C	H	N	O	P	0	0
			1079	324	361	124	236	34		

- Molecule 37 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	A	1557	Total	C	H	N	O	P	0	0
			49813	14833	16765	5958	10700	1557		

- Molecule 38 is a RNA chain called tRNA-Val (73-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
38	B	72	Total	C	H	N	O	P	0	0
			2295	685	771	269	498	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	74	C	G	conflict	GB NC_012920.1
B	76	A	U	conflict	GB NC_012920.1

- Molecule 39 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	D	238	Total	C	H	N	O	S	0	0
			3779	1157	1920	376	317	9		

- Molecule 40 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	E	305	Total	C	H	N	O	S	0	0
			4821	1545	2415	418	432	11		

- Molecule 41 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	F	252	Total	C	H	N	O	S	0	0
			4096	1305	2065	370	350	6		

- Molecule 42 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	I	212	Total	C	H	N	O	S	0	0
			3480	1088	1785	304	292	11		

- Molecule 43 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	J	175	Total	C	H	N	O	S	0	0
			2737	847	1407	237	244	2		

- Molecule 44 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	K	178	Total	C	H	N	O	S	0	0
			2907	936	1452	259	253	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP Q9BYD1

- Molecule 45 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	L	115	Total	C	H	N	O	S	0	0
			1832	559	942	171	155	5		

- Molecule 46 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	M	289	Total	C	H	N	O	S	0	0
			4698	1476	2384	427	405	6		

- Molecule 47 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	N	222	Total	C	H	N	O	S	0	0
			3603	1143	1817	326	307	10		

- Molecule 48 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	O	154	Total	C	H	N	O	S	0	0
			2553	792	1294	241	219	7		

- Molecule 49 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	P	144	Total	C	H	N	O	S	0	0
			2338	733	1165	224	211	5		

- Molecule 50 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	Q	238	Total	C	H	N	O	S	0	0
			4001	1268	2022	352	350	9		

- Molecule 51 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	R	140	Total	C	H	N	O	S	0	0
			2368	732	1214	231	187	4		

- Molecule 52 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	S	161	Total	C	H	N	O	S	0	0
			2658	835	1365	227	227	4		

- Molecule 53 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	T	166	Total	C	H	N	O	S	0	0
			2779	875	1410	254	233	7		

- Molecule 54 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	U	153	Total	C	H	N	O	S	0	0
			2483	788	1232	234	226	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	1	ACE	-	acetylation	UNP Q16540

- Molecule 55 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	V	205	Total	C	H	N	O	S	0	0
			3363	1068	1687	298	302	8		

- Molecule 56 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	W	116	Total	C	H	N	O	S	0	0
			1839	577	935	171	153	3		

- Molecule 57 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	X	244	Total	C	H	N	O	S	0	0
			4104	1322	2060	352	365	5		

- Molecule 58 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Y	181	Total	C	H	N	O	S	0	0
			3153	995	1597	298	259	4		

- Molecule 59 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	Z	122	Total	C	H	N	O	S	0	0
			2040	636	1044	186	171	3		

- Molecule 60 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	0	110	Total	C	H	N	O	S	0	0
			1814	554	916	176	162	6		

- Molecule 61 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	1	56	Total	C	H	N	O	S	0	0
			975	296	511	89	77	2		

- Molecule 62 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	2	46	Total	C	H	N	O	S	0	0
			783	233	406	83	60	1		

- Molecule 63 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	3	95	Total	C	H	N	O	S	0	0
			1715	539	883	162	128	3		

- Molecule 64 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	4	38	Total	C	H	N	O	S	0	0
			703	217	361	72	49	4		

- Molecule 65 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	5	394	Total	C	H	N	O	S	0	0
			6416	2073	3206	560	566	11		

- Molecule 66 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	6	354	Total	C	H	N	O	S	0	0
			5789	1881	2841	525	533	9		

- Molecule 67 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	7	294	Total	C	H	N	O	S	0	0
			4787	1529	2397	405	438	18		

- Molecule 68 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	8	157	Total	C	H	N	O	S	0	0
			2695	844	1368	235	246	2		

- Molecule 69 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	9	124	Total	C	H	N	O	S	0	0
			1984	644	987	170	181	2		

- Molecule 70 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	a	100	Total	C	H	N	O	S	0	0
			1650	529	810	152	154	5		

- Molecule 71 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	b	150	Total	C	H	N	O	S	0	0
			2391	744	1195	231	218	3		

- Molecule 72 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	c	286	Total	C	H	N	O	S	0	0
			4619	1470	2320	397	423	9		

- Molecule 73 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	d	237	Total	C	H	N	O	S	0	0
			3879	1251	1930	331	354	13		

- Molecule 74 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	e	238	Total	C	H	N	O	S	0	0
			3847	1222	1916	339	364	6		

- Molecule 75 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	f	157	Total	C	H	N	O	S	0	0
			2521	799	1269	207	242	4		

- Molecule 76 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	g	134	Total	C	H	N	O	S	0	0
			2210	719	1097	193	199	2		

- Molecule 77 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	h	110	Total	C	H	N	O	S	0	0
			1776	568	881	156	168	3		

- Molecule 78 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	i	97	Total	C	H	N	O	S	0	0
			1685	532	857	165	127	4		

- Molecule 79 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	j	94	Total	C	H	N	O	S	0	0
			1491	463	746	144	136	2		

- Molecule 80 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	k	102	Total	C	H	N	O	S	0	0
			1558	479	784	148	142	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	1	ACE	-	acetylation	UNP Q96EL3

- Molecule 81 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	l	82	Total	C	H	N	O	S	0	0
			1362	437	674	120	128	3		

- Molecule 82 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	m	92	Total	C	H	N	O	S	0	0
			1588	488	797	159	142	2		

- Molecule 83 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	o	94	Total	C	H	N	O	S	0	0
			1602	501	804	165	129	3		

- Molecule 84 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	p	147	Total	C	H	N	O	S	0	0
			2428	748	1223	228	225	4		

- Molecule 85 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	q	165	Total	C	H	N	O	S	0	0
			2763	865	1374	270	249	5		

- Molecule 86 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	r	162	Total	C	H	N	O	S	0	0
			2670	839	1348	252	223	8		

- Molecule 87 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	s	386	Total	C	H	N	O	S	0	0
			6294	2023	3139	559	559	14		

- Molecule 88 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	t	46	Total	C	H	N	O	0	0
			731	228	377	56	70		
88	u	32	Total	C	H	N	O	0	0
			540	168	283	40	49		
88	v	32	Total	C	H	N	O	0	0
			540	168	283	40	49		
88	w	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
88	x	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
88	y	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
88	t1	71	Total	C	H	N	O	0	0
			1145	352	599	93	101		

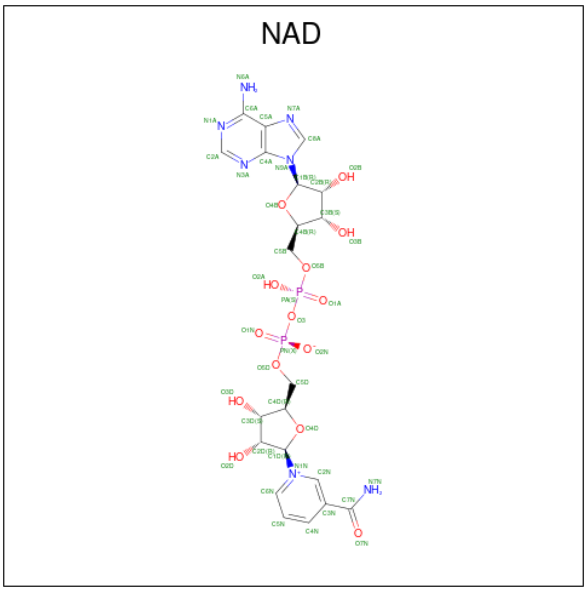
- Molecule 89 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	H	202	Total	C	H	N	O	S	0	0
			3395	1067	1734	304	286	4		

- Molecule 90 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
90	z	252	Total	C	H	N	O	S	0	0
			4103	1304	2076	336	381	6		

- Molecule 91 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
91	AA	1	Total	C	H	N	O	P	0
			69	21	25	7	14	2	

- Molecule 92 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
92	AA	55	Total	Mg	0
			55	55	
92	AB	1	Total	Mg	0
			1	1	
92	AX	1	Total	Mg	0
			1	1	
92	Az	1	Total	Mg	0
			1	1	

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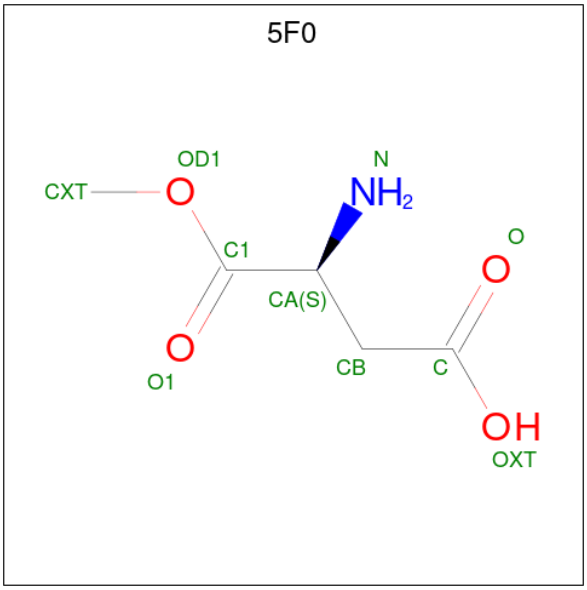
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Mol	Chain	Residues	Atoms	AltConf
92	A	136	Total Mg 136 136	0
92	D	1	Total Mg 1 1	0

- Molecule 93 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
93	AA	13	Total K 13 13	0
93	A	24	Total K 24 24	0
93	D	1	Total K 1 1	0
93	M	1	Total K 1 1	0

- Molecule 94 is (3 {S})-3-azanyl-4-methoxy-4-oxidanylidene-butanoic acid (CCD ID: 5F0) (formula: $C_5H_9NO_4$).

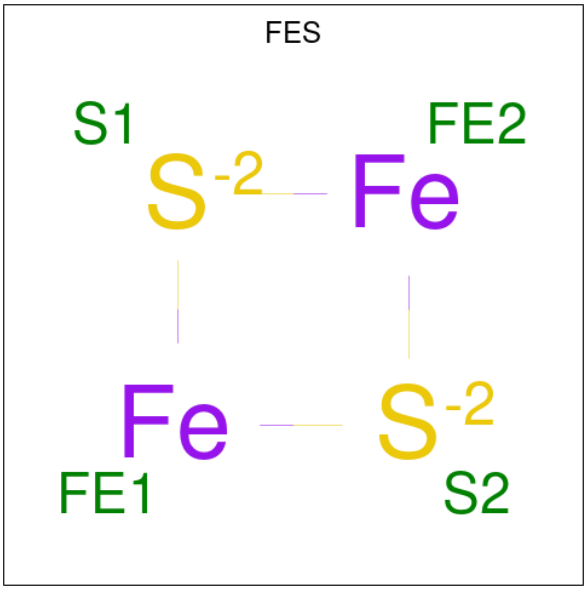


Mol	Chain	Residues	Atoms	AltConf
94	AI	1	Total C N O 9 5 1 3	0

- Molecule 95 is ZINC ION (CCD ID: ZN) (formula: Zn).

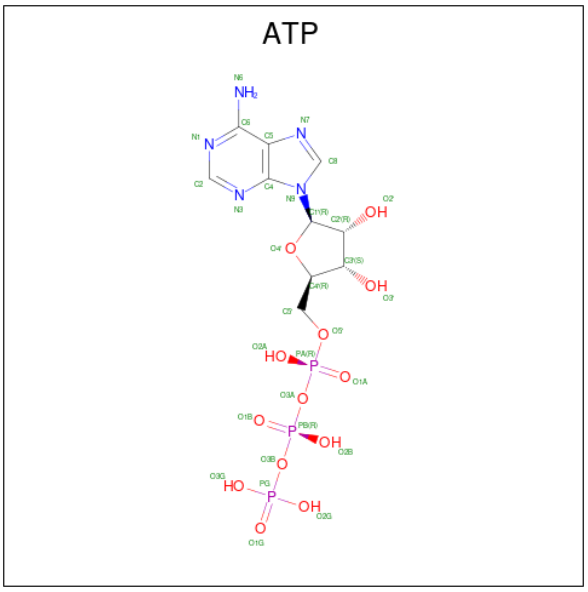
Mol	Chain	Residues	Atoms	AltConf
95	AO	1	Total Zn 1 1	0
95	0	1	Total Zn 1 1	0
95	4	1	Total Zn 1 1	0

- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



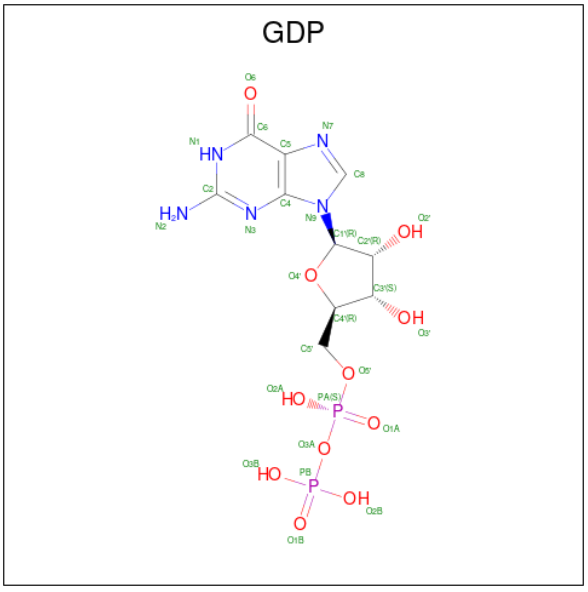
Mol	Chain	Residues	Atoms	AltConf
96	AP	1	Total Fe S 4 2 2	0
96	AT	1	Total Fe S 4 2 2	0
96	r	1	Total Fe S 4 2 2	0

- Molecule 97 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



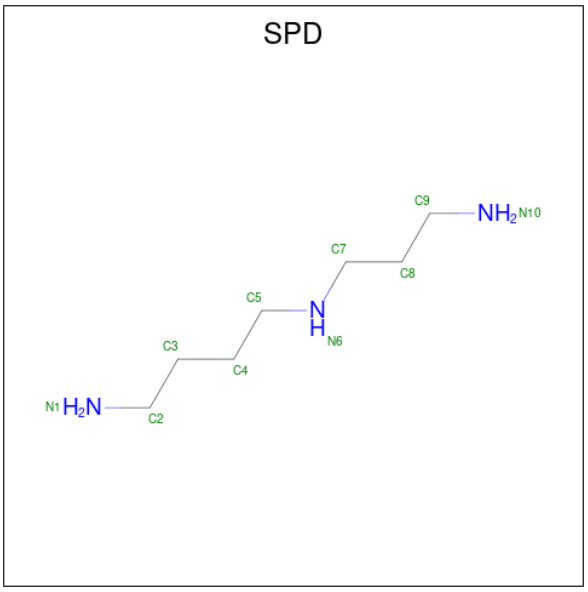
Mol	Chain	Residues	Atoms						AltConf
97	AX	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 98 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



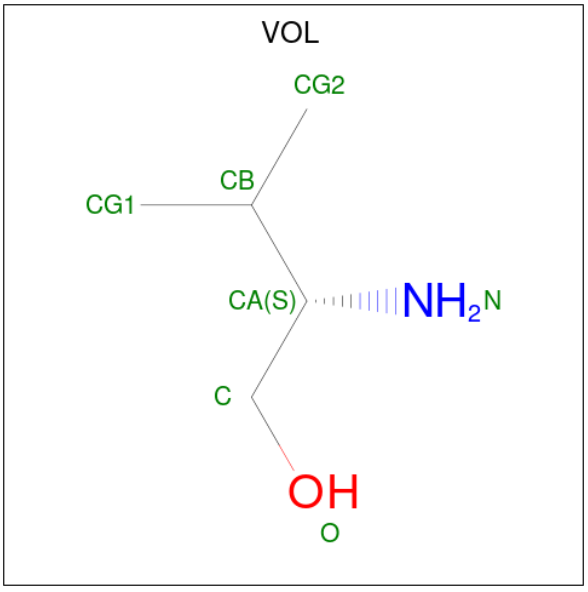
Mol	Chain	Residues	Atoms						AltConf
98	AX	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

- Molecule 99 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms				AltConf
99	A	1	Total	C	H	N	0
			31	7	21	3	

- Molecule 100 is L-VALINOL (CCD ID: VOL) (formula: $C_5H_{13}NO$).



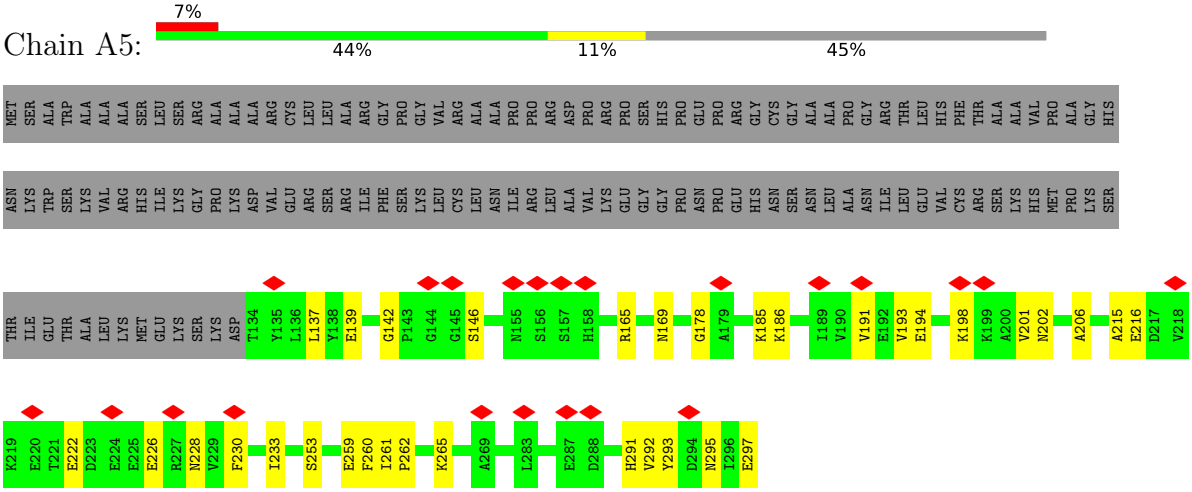
Mol	Chain	Residues	Atoms					AltConf
100	e	1	Total	C	H	N	O	0
			15	5	8	1	1	

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.

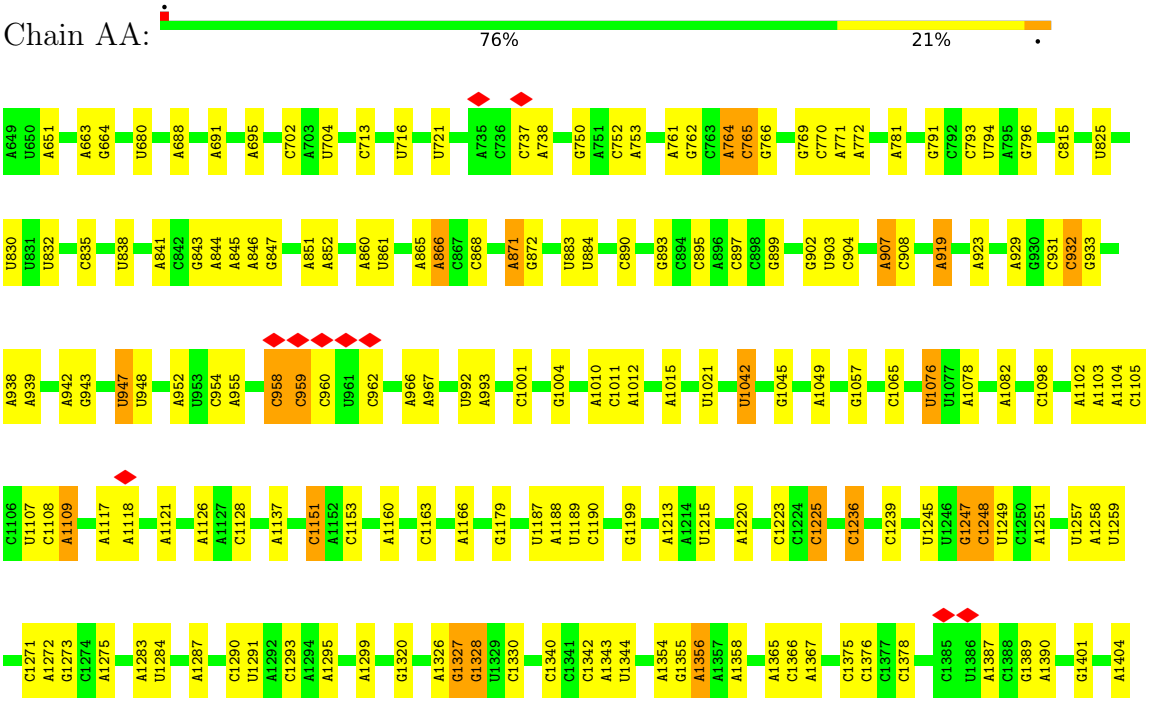
• Molecule 1: Translational activator of cytochrome c oxidase 1

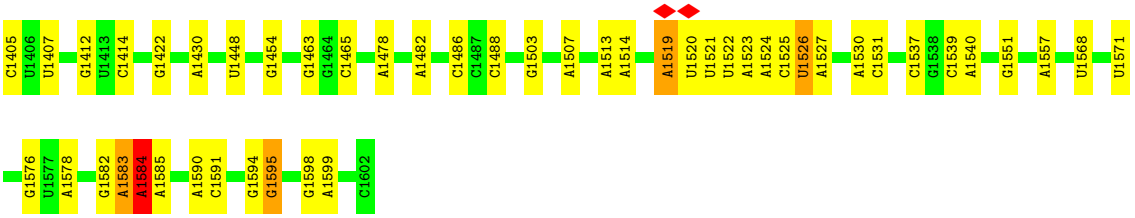
Chain A5:



• Molecule 2: 12S mitochondrial rRNA

Chain AA:

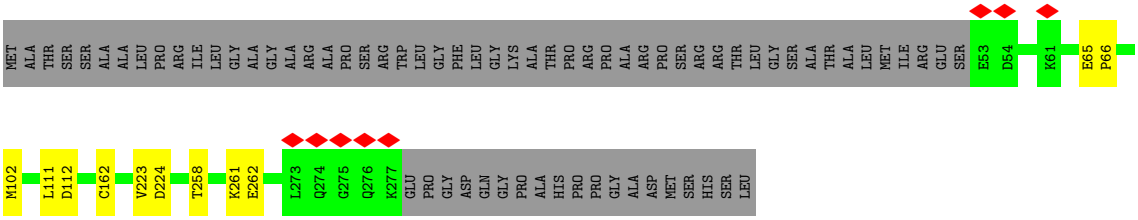




• Molecule 3: 28S ribosomal protein S2, mitochondrial

Chain AB:

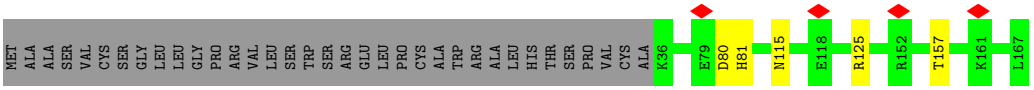




• Molecule 4: 28S ribosomal protein S24, mitochondrial

Chain AC:

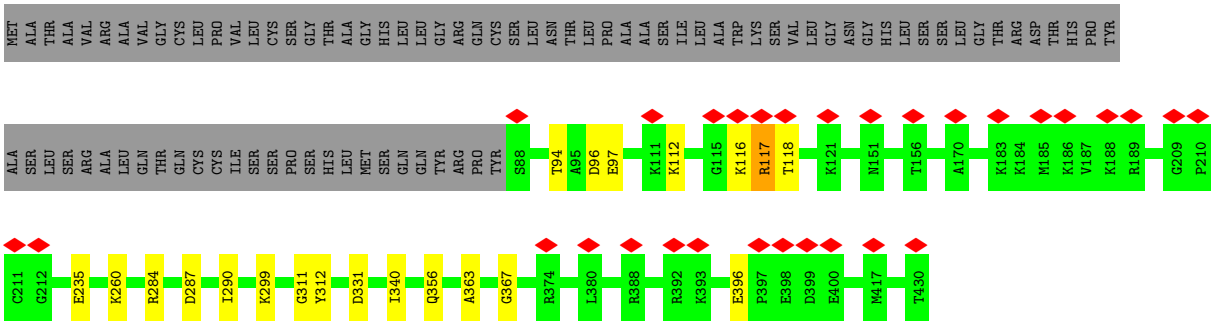




• Molecule 5: 28S ribosomal protein S5, mitochondrial

Chain AD:

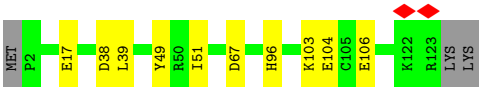




• Molecule 6: 28S ribosomal protein S6, mitochondrial

Chain AE:

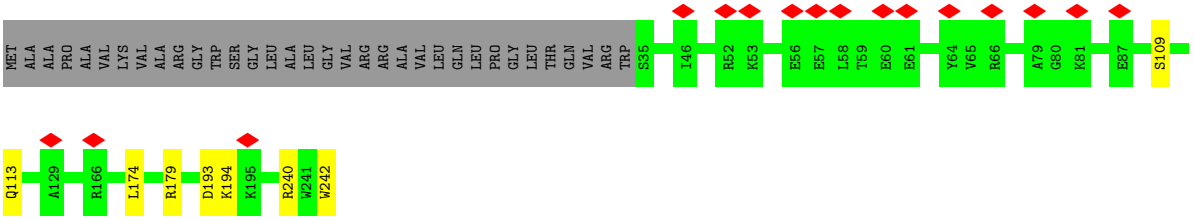




• Molecule 7: 28S ribosomal protein S7, mitochondrial

Chain AF:

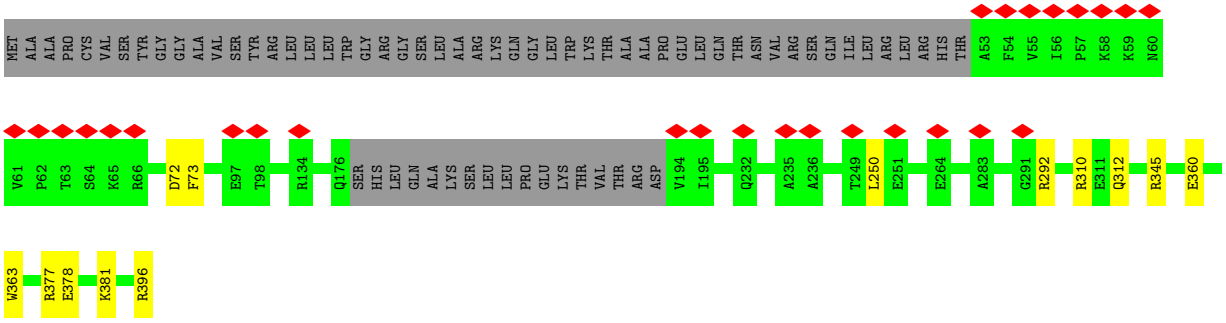




• Molecule 8: 28S ribosomal protein S9, mitochondrial

Chain AG:

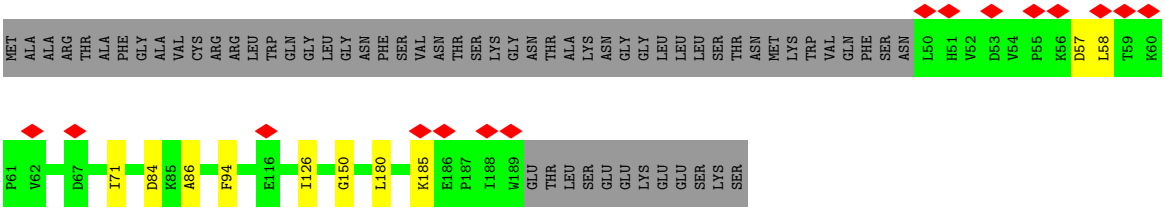




• Molecule 9: 28S ribosomal protein S10, mitochondrial

Chain AH:

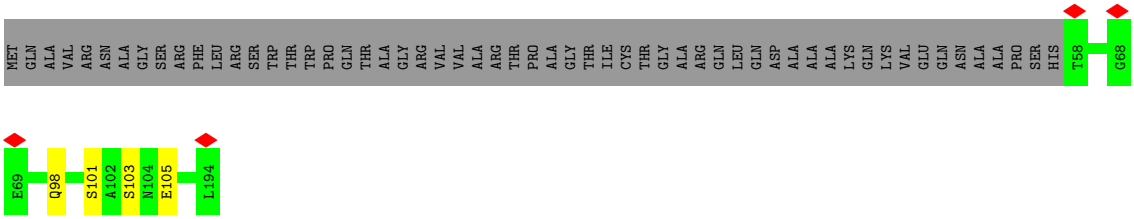




• Molecule 10: Small ribosomal subunit protein uS11m

Chain AI:

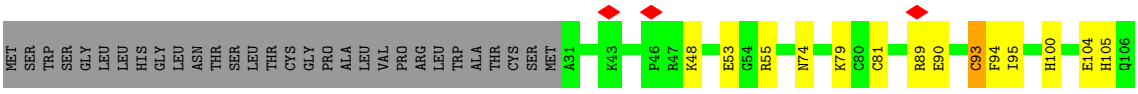




• Molecule 11: 28S ribosomal protein S12, mitochondrial

Chain AJ:



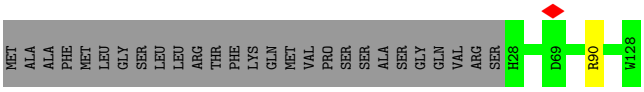




• Molecule 12: 28S ribosomal protein S14, mitochondrial

Chain AK:



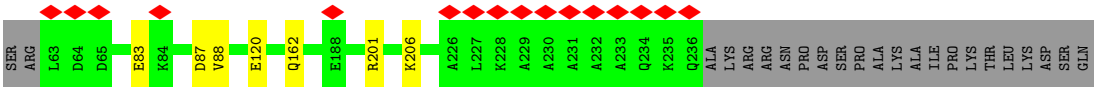


• Molecule 13: 28S ribosomal protein S15, mitochondrial

Chain AL:



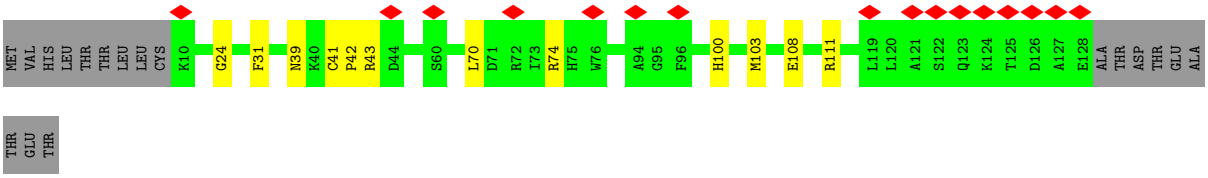




• Molecule 14: 28S ribosomal protein S16, mitochondrial

Chain AM:

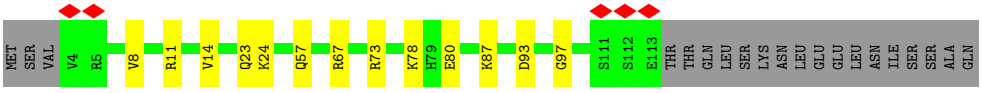




• Molecule 15: 28S ribosomal protein S17, mitochondrial

Chain AN:



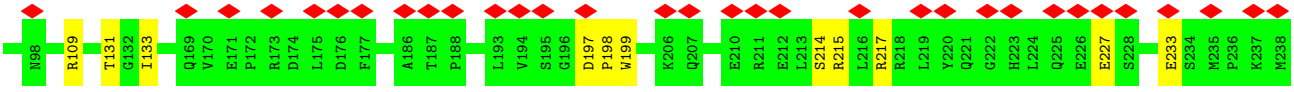


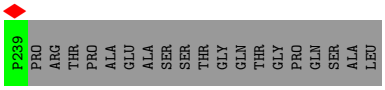
• Molecule 16: 28S ribosomal protein S18b, mitochondrial

Chain AO:





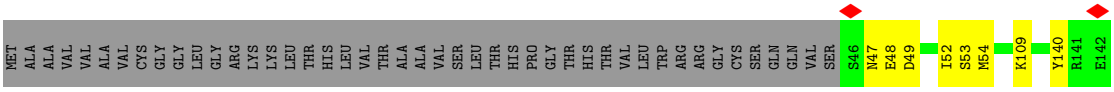




• Molecule 17: 28S ribosomal protein S18c, mitochondrial

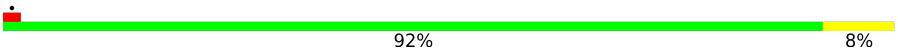
Chain AP:





• Molecule 18: MRPS21 isoform 1

Chain AQ:



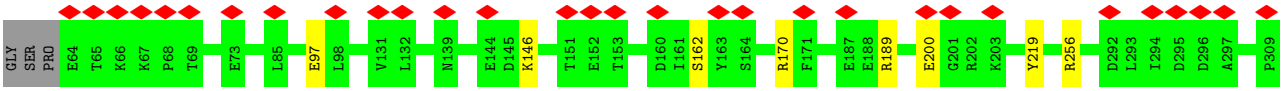


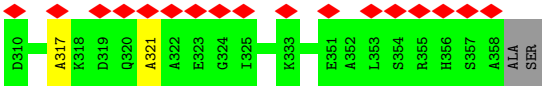
• Molecule 19: 28S ribosomal protein S22, mitochondrial

Chain AR:





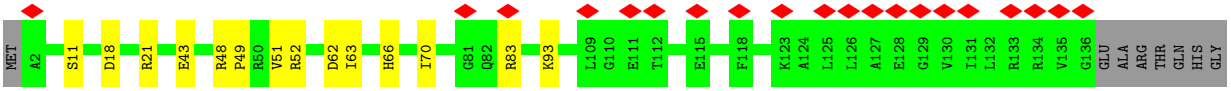


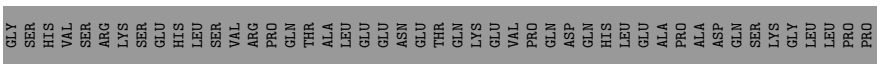


• Molecule 20: 28S ribosomal protein S23, mitochondrial

Chain AS:

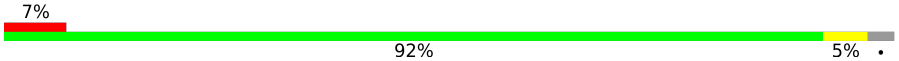


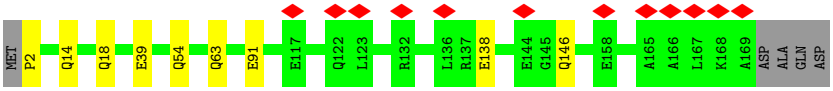




• Molecule 21: 28S ribosomal protein S25, mitochondrial

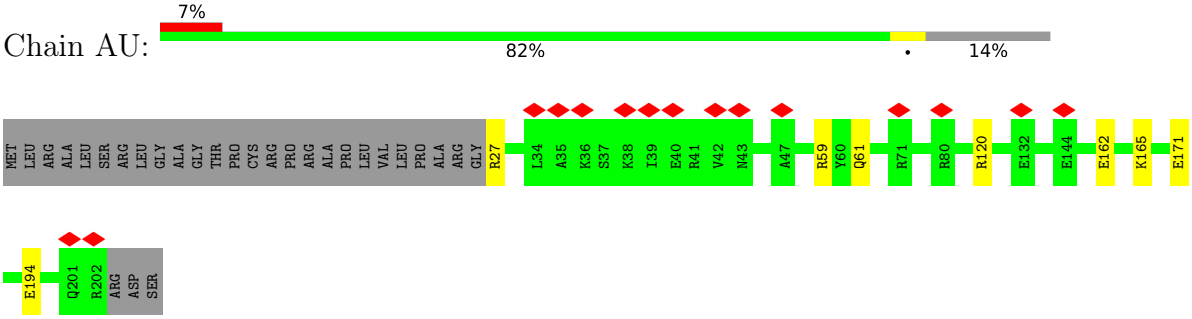
Chain AT:





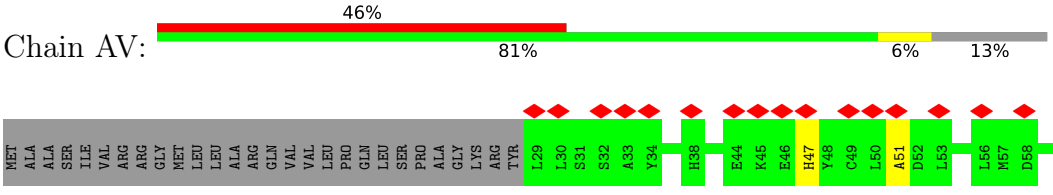
• Molecule 22: 28S ribosomal protein S26, mitochondrial

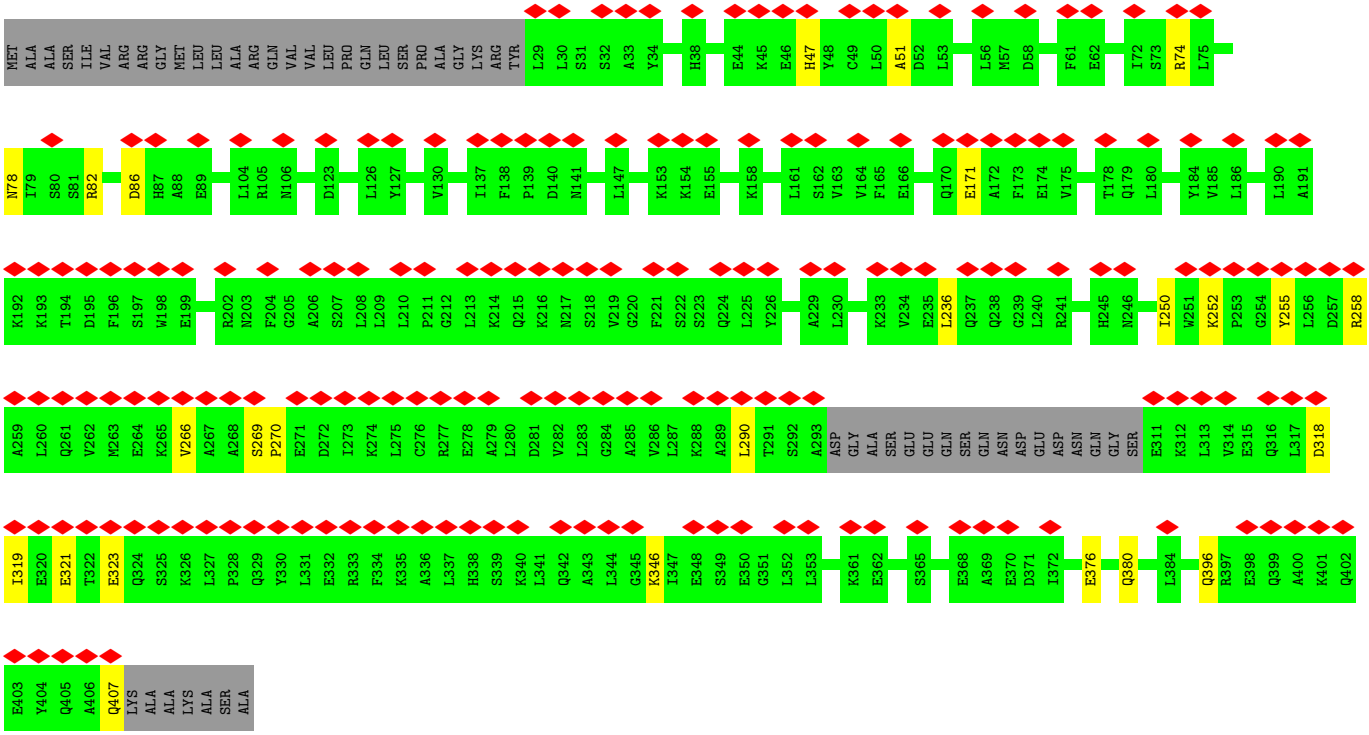
Chain AU:



• Molecule 23: 28S ribosomal protein S27, mitochondrial

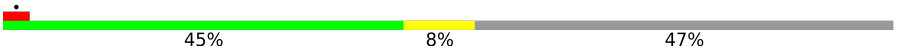
Chain AV:

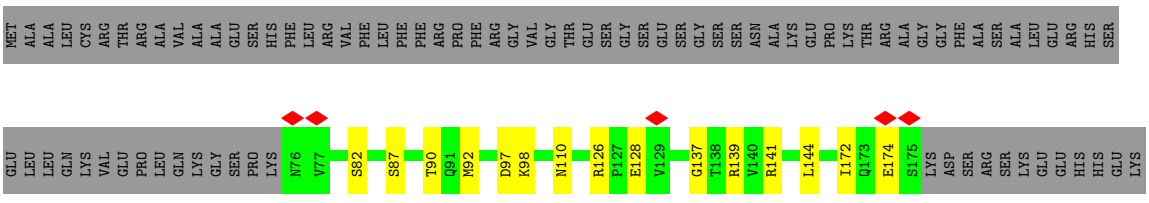




• Molecule 24: 28S ribosomal protein S28, mitochondrial

Chain AW:

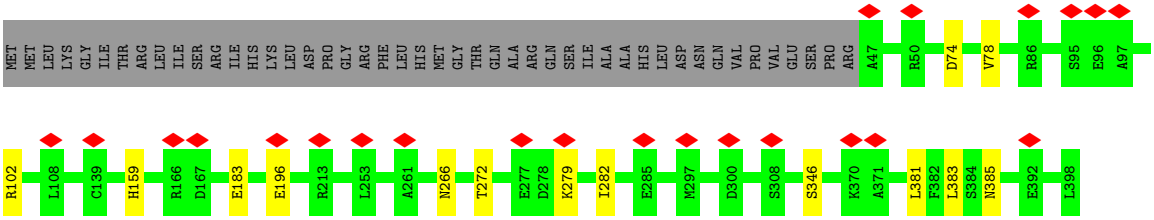




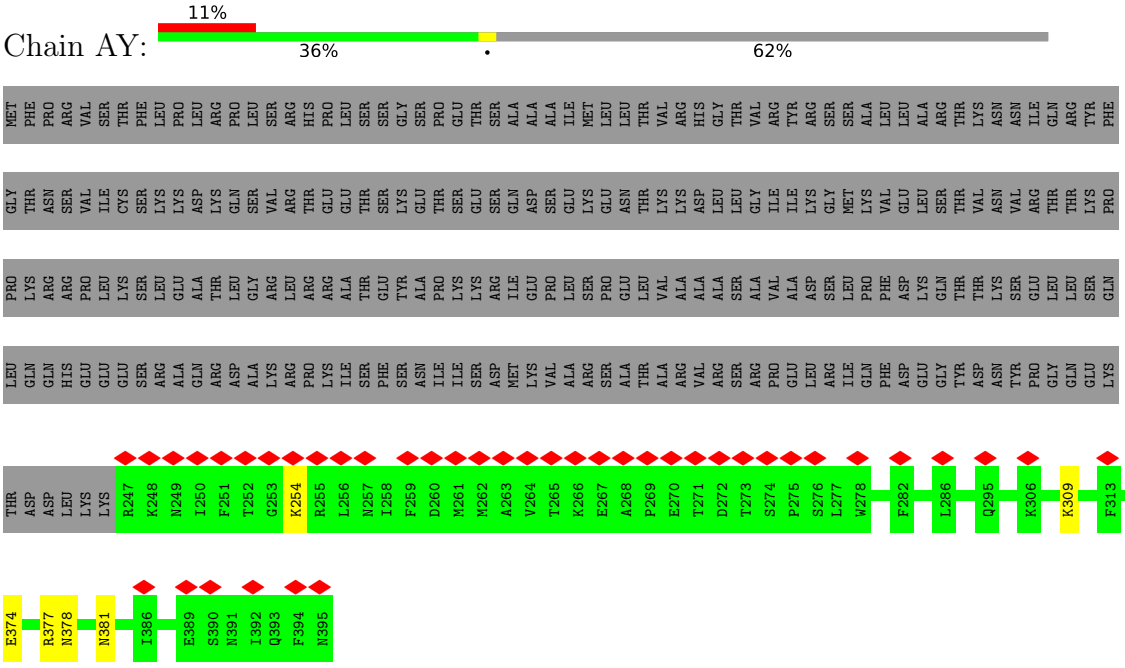
• Molecule 25: 28S ribosomal protein S29, mitochondrial

Chain AX:

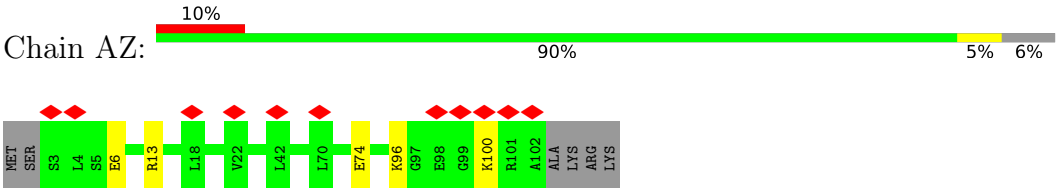




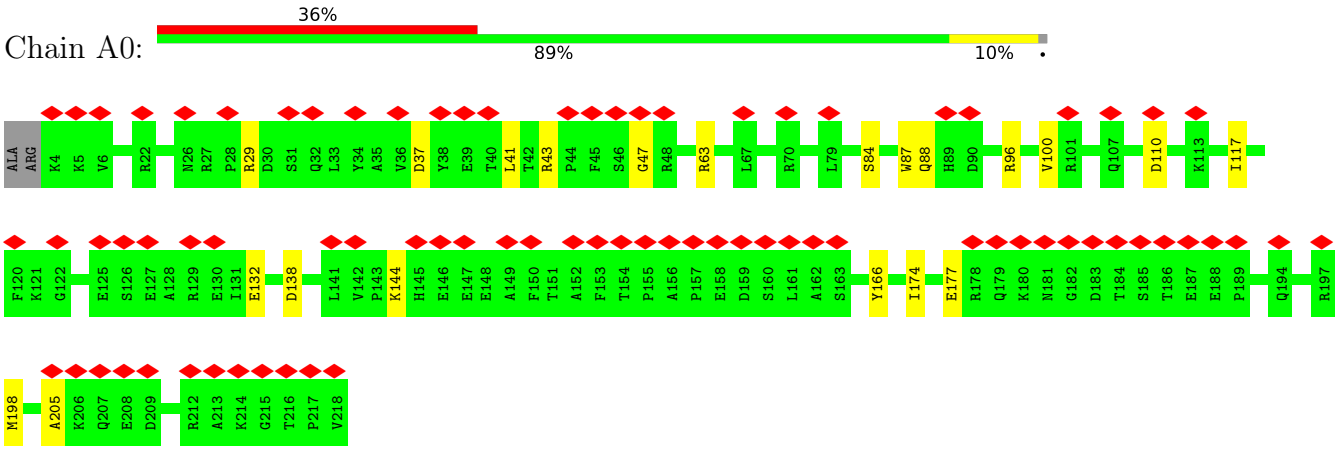
• Molecule 26: 28S ribosomal protein S31, mitochondrial



• Molecule 27: 28S ribosomal protein S33, mitochondrial

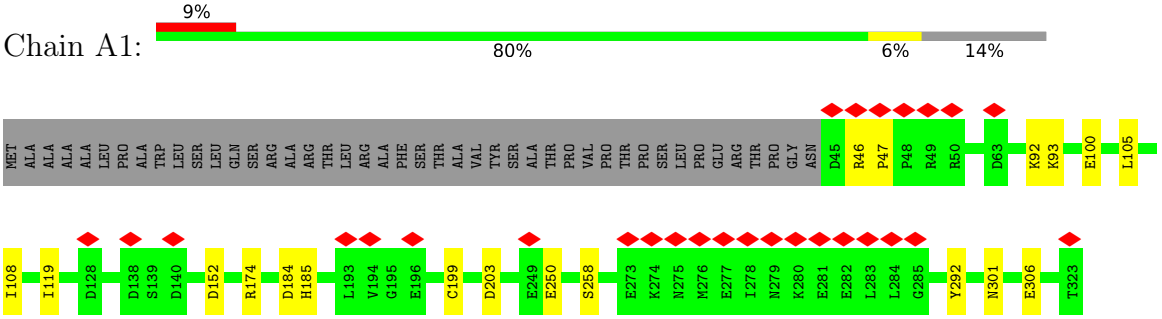


• Molecule 28: 28S ribosomal protein S34, mitochondrial



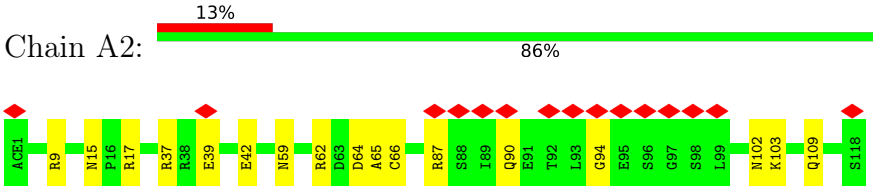
• Molecule 29: Small ribosomal subunit protein mS35

Chain A1:



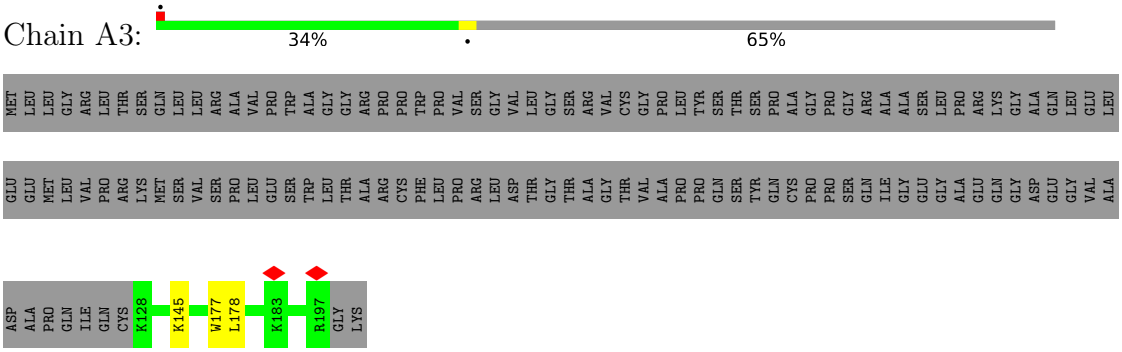
• Molecule 30: Small ribosomal subunit protein mS37

Chain A2:



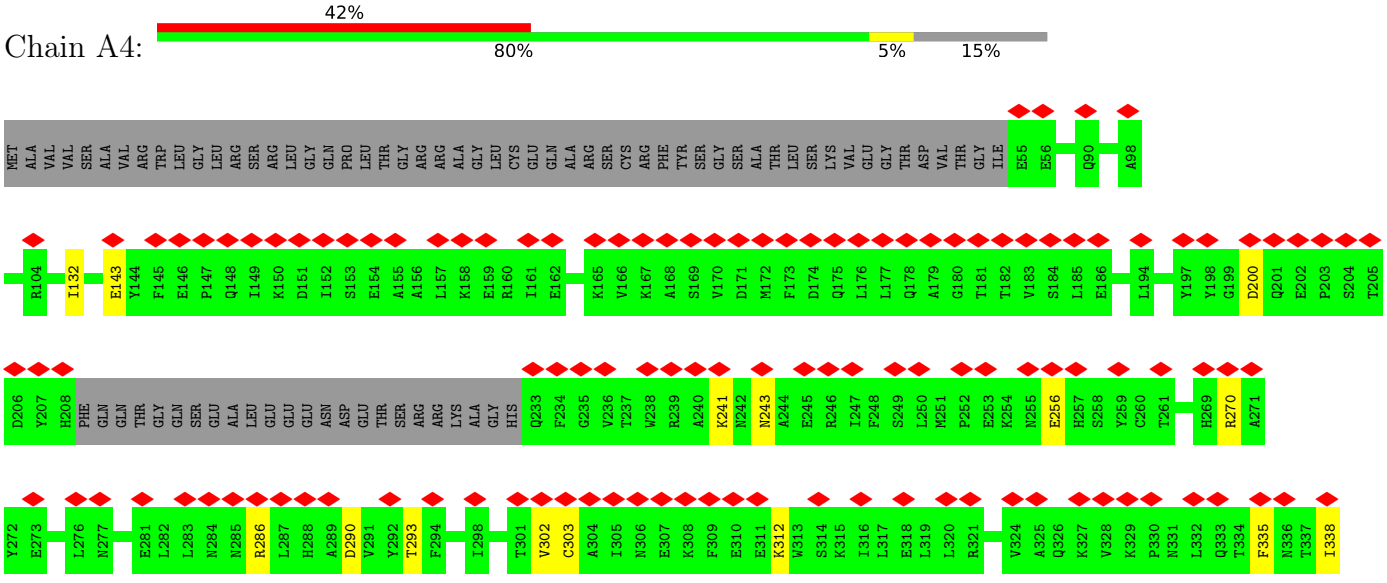
• Molecule 31: Aurora kinase A-interacting protein

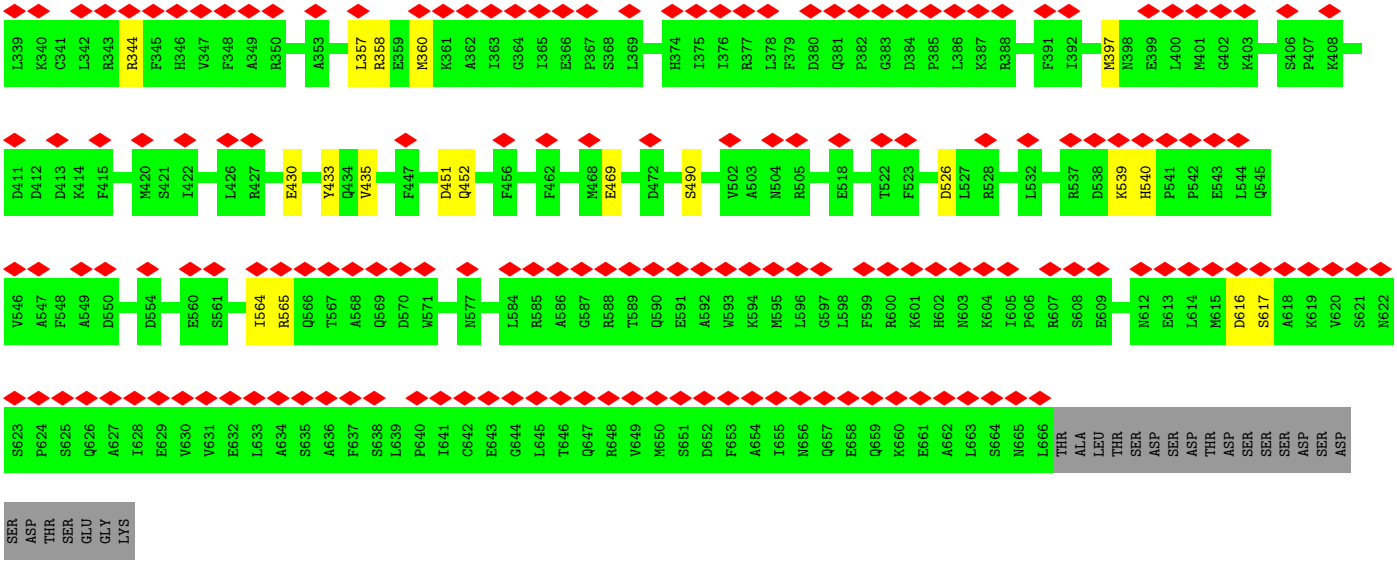
Chain A3:



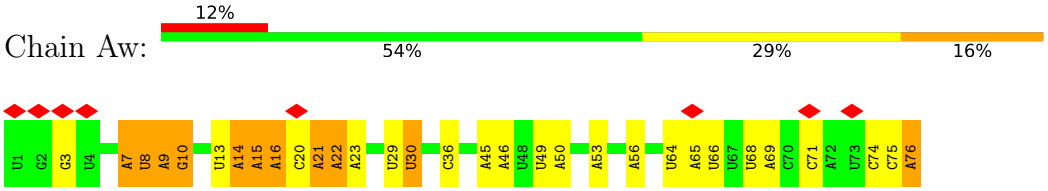
• Molecule 32: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4:

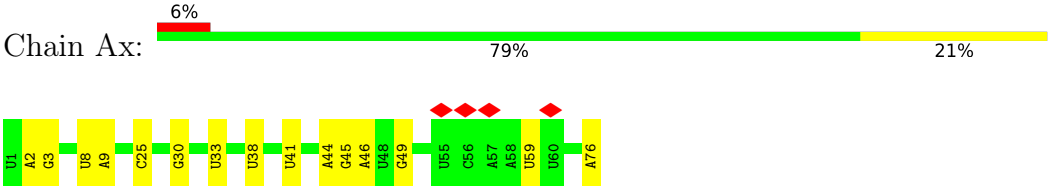




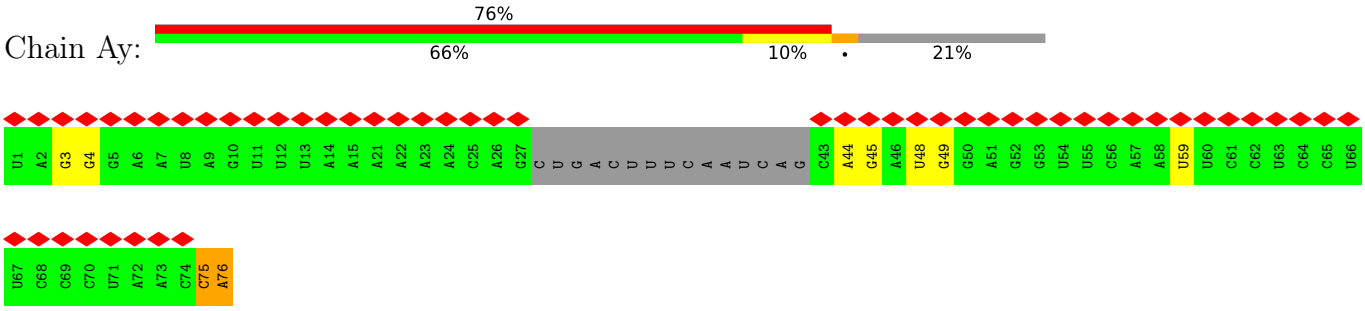
• Molecule 33: A-site tRNA (68-MER)



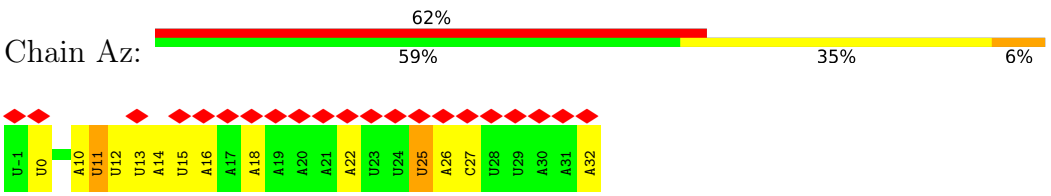
• Molecule 34: P-site RNA (70-MER)



• Molecule 35: E-site tRNA (70-MER)

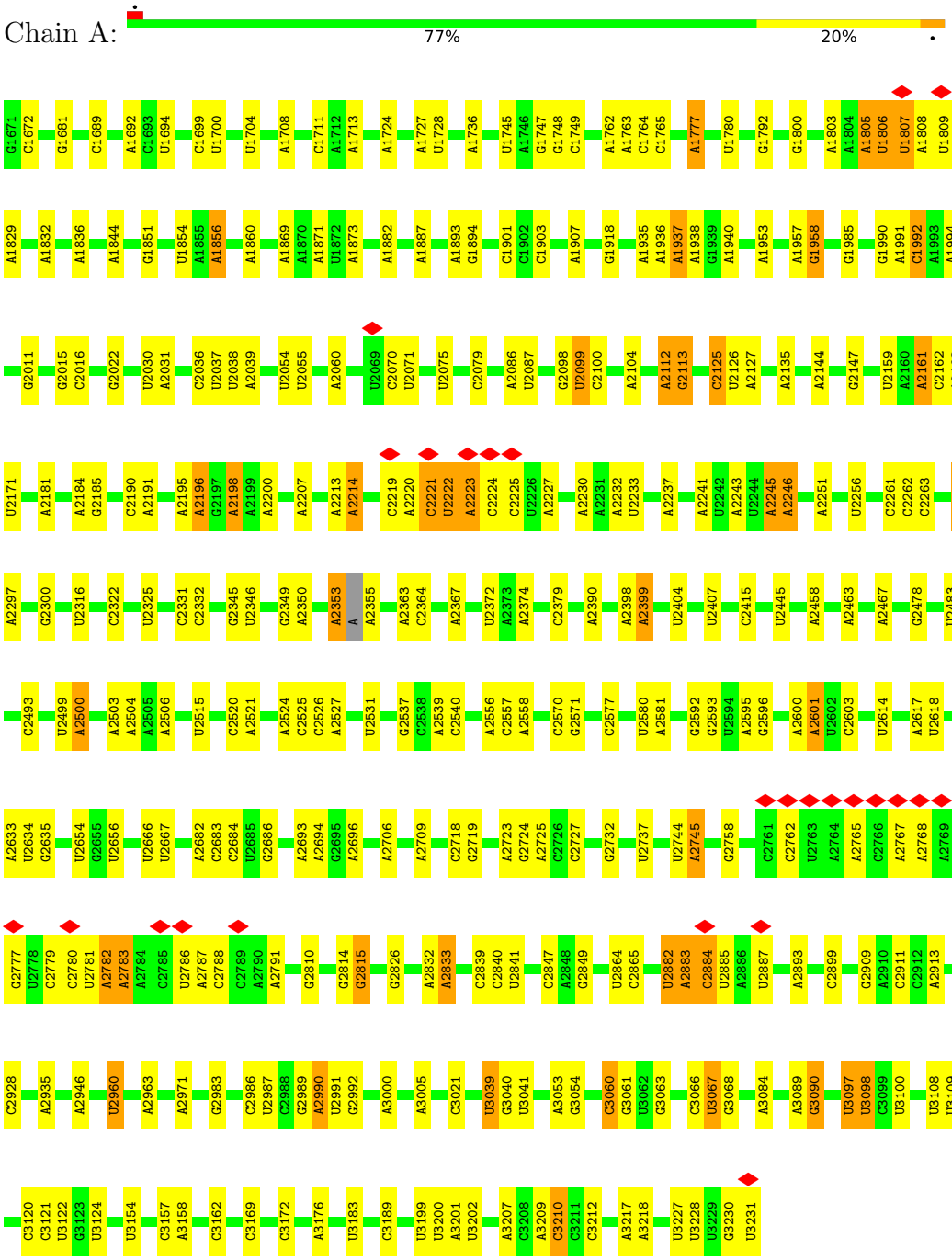


• Molecule 36: mRNA (34-MER)



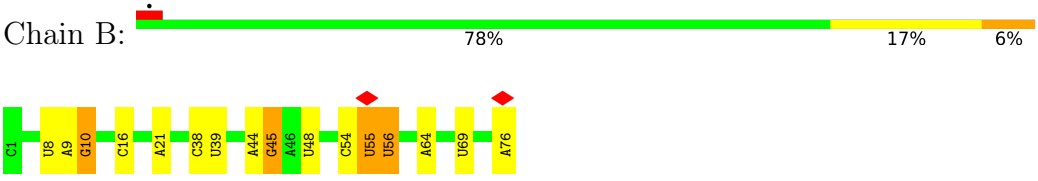
• Molecule 37: 16S mitochondrial rRNA

Chain A:



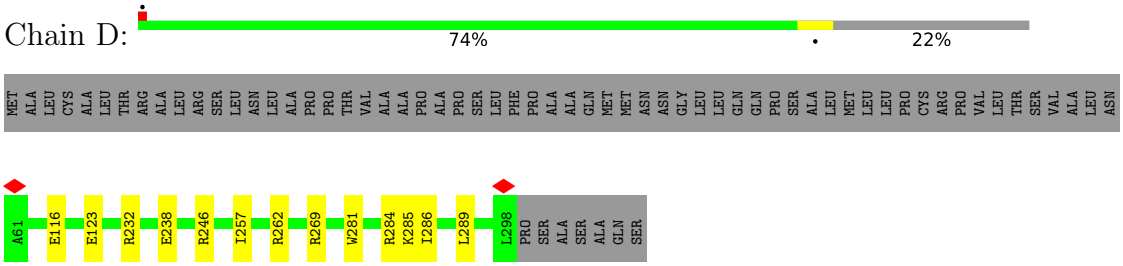
• Molecule 38: tRNA-Val (73-MER)

Chain B:



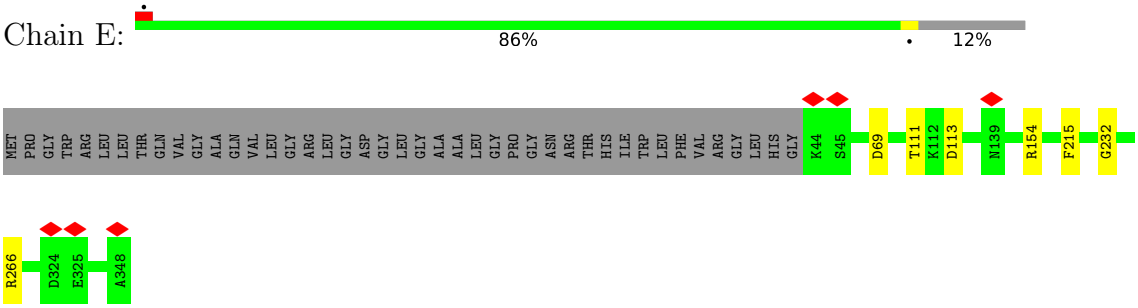
• Molecule 39: 39S ribosomal protein L2, mitochondrial

Chain D:



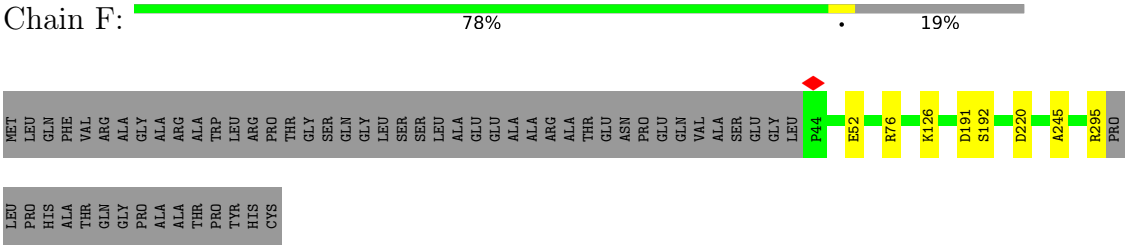
• Molecule 40: 39S ribosomal protein L3, mitochondrial

Chain E:



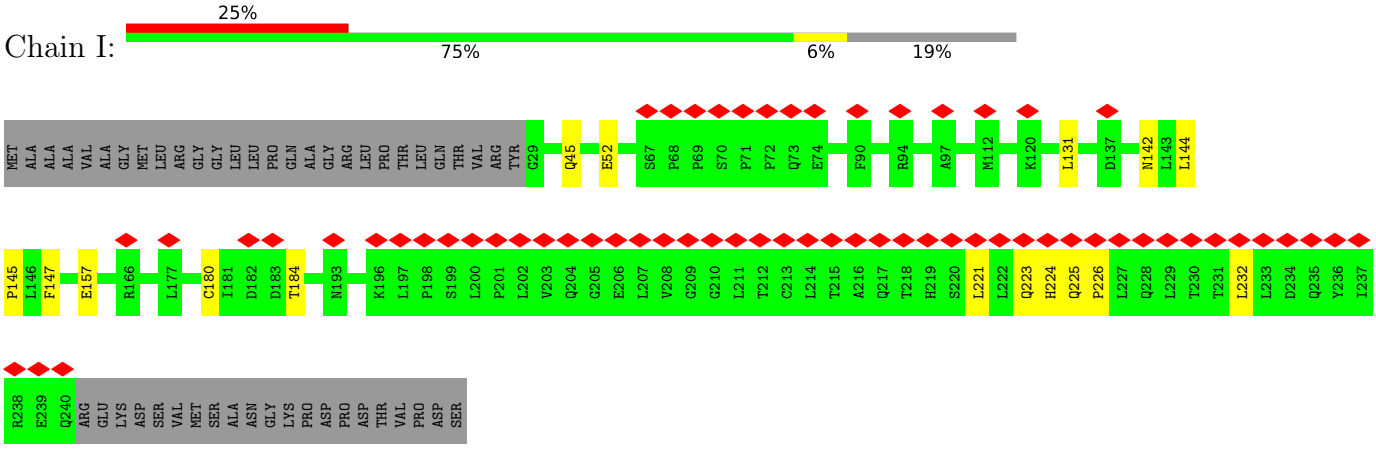
• Molecule 41: 39S ribosomal protein L4, mitochondrial

Chain F:



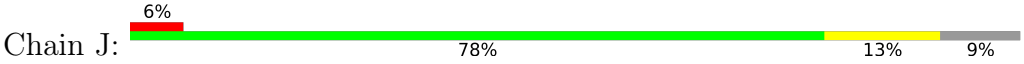
• Molecule 42: 39S ribosomal protein L10, mitochondrial

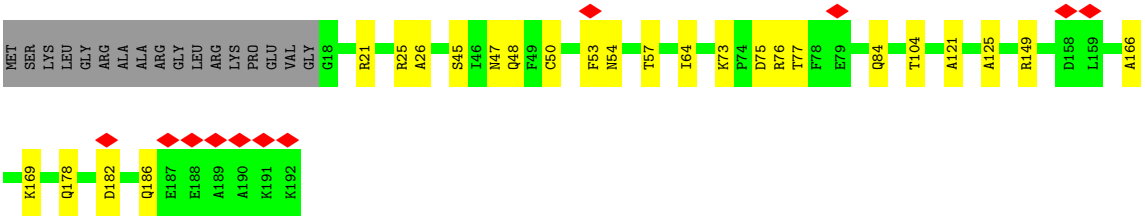
Chain I:



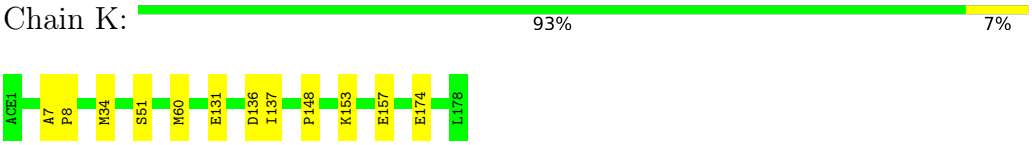
• Molecule 43: 39S ribosomal protein L11, mitochondrial

Chain J:

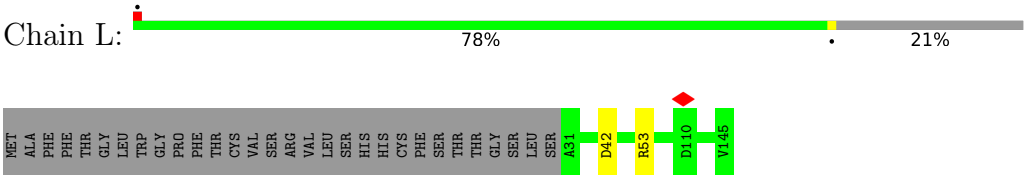




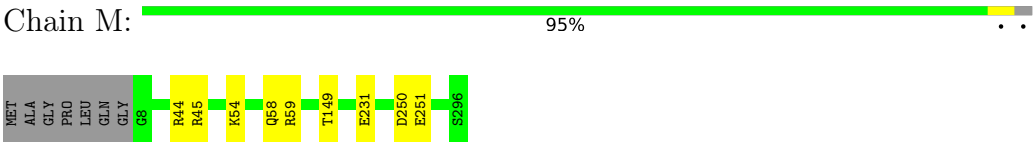
• Molecule 44: Large ribosomal subunit protein uL13m



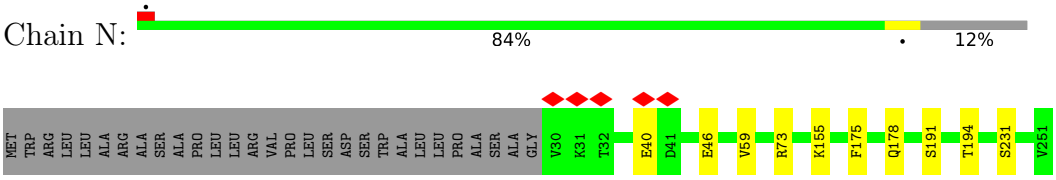
• Molecule 45: 39S ribosomal protein L14, mitochondrial



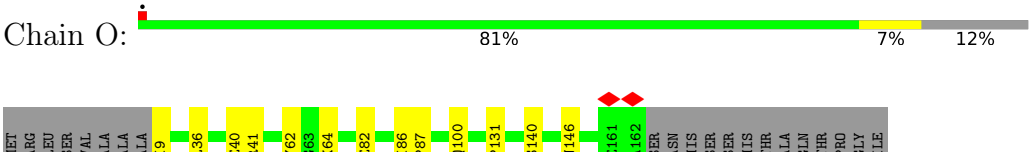
• Molecule 46: 39S ribosomal protein L15, mitochondrial



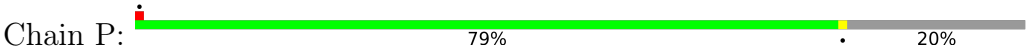
• Molecule 47: 39S ribosomal protein L16, mitochondrial

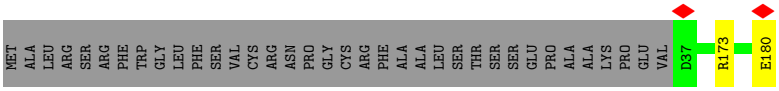


• Molecule 48: 39S ribosomal protein L17, mitochondrial

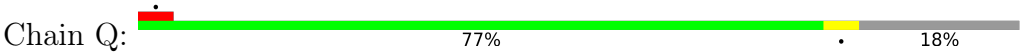


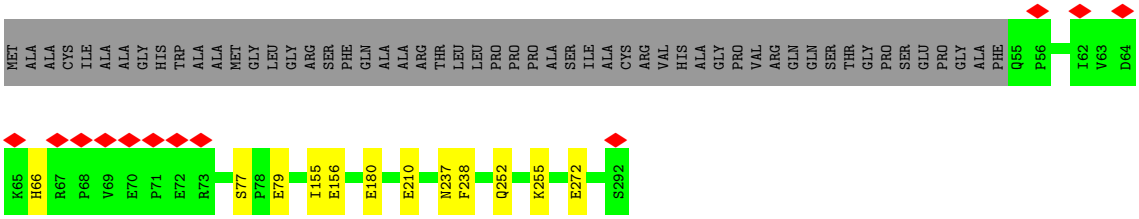
• Molecule 49: 39S ribosomal protein L18, mitochondrial



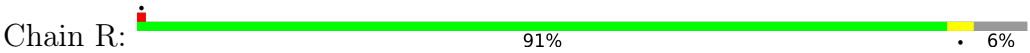


• Molecule 50: 39S ribosomal protein L19, mitochondrial



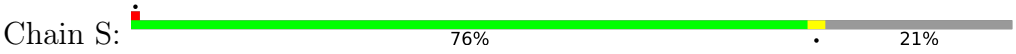


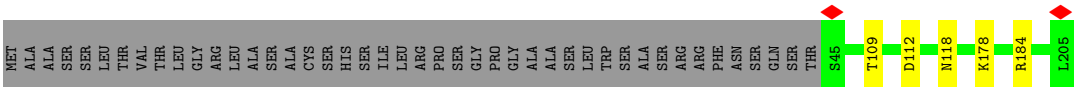
• Molecule 51: 39S ribosomal protein L20, mitochondrial



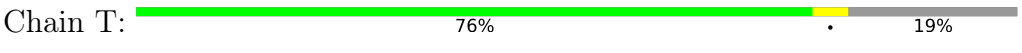


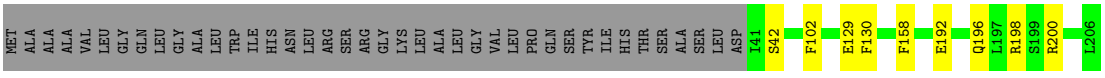
• Molecule 52: 39S ribosomal protein L21, mitochondrial



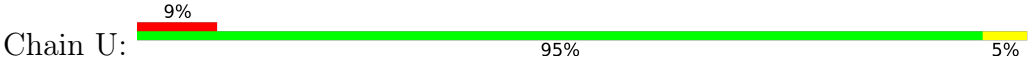


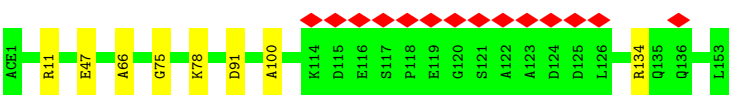
• Molecule 53: 39S ribosomal protein L22, mitochondrial



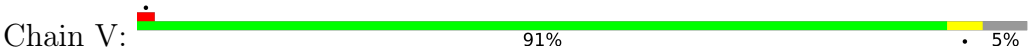


• Molecule 54: Large ribosomal subunit protein uL23m





• Molecule 55: 39S ribosomal protein L24, mitochondrial

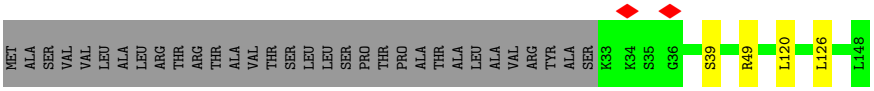




• Molecule 56: 39S ribosomal protein L27, mitochondrial

Chain W:

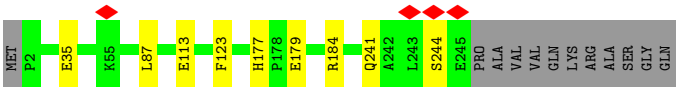




• Molecule 57: 39S ribosomal protein L28, mitochondrial

Chain X:





• Molecule 58: 39S ribosomal protein L47, mitochondrial

Chain Y:



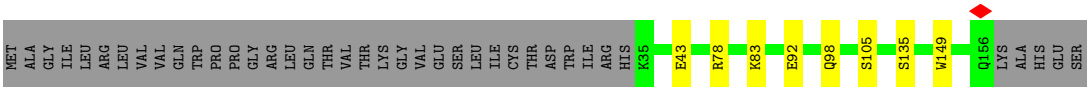




• Molecule 59: 39S ribosomal protein L30, mitochondrial

Chain Z:



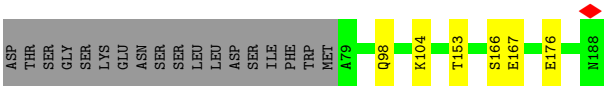


• Molecule 60: 39S ribosomal protein L32, mitochondrial

Chain 0:



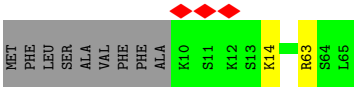




• Molecule 61: 39S ribosomal protein L33, mitochondrial

Chain 1:

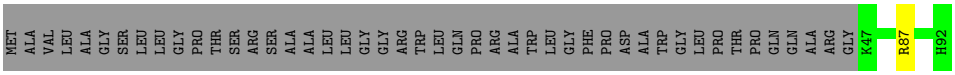




• Molecule 62: 39S ribosomal protein L34, mitochondrial

Chain 2:

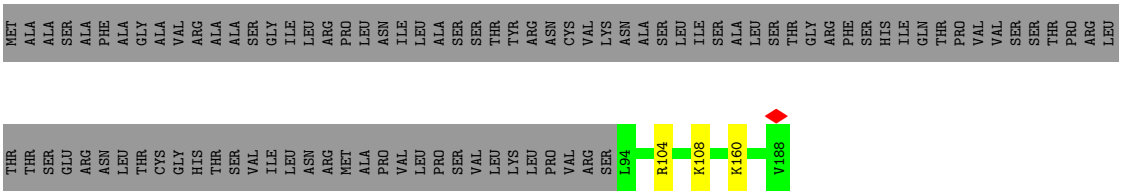




• Molecule 63: 39S ribosomal protein L35, mitochondrial

Chain 3:

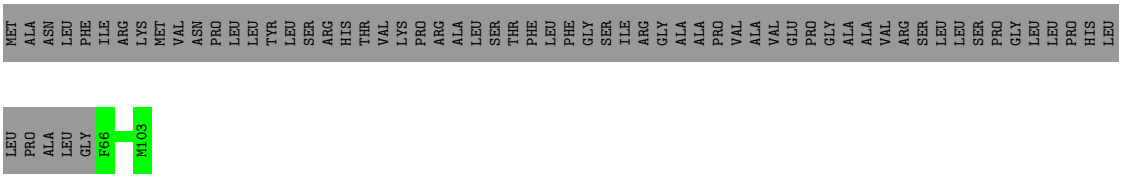




• Molecule 64: 39S ribosomal protein L36, mitochondrial

Chain 4:

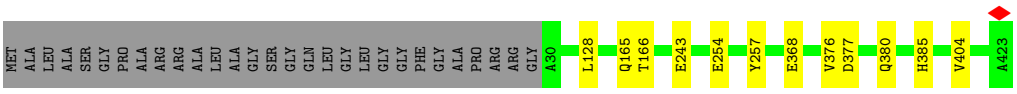




• Molecule 65: 39S ribosomal protein L37, mitochondrial

Chain 5:

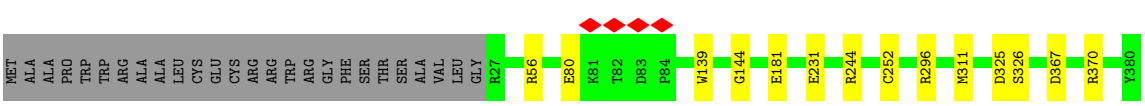




• Molecule 66: 39S ribosomal protein L38, mitochondrial

Chain 6:

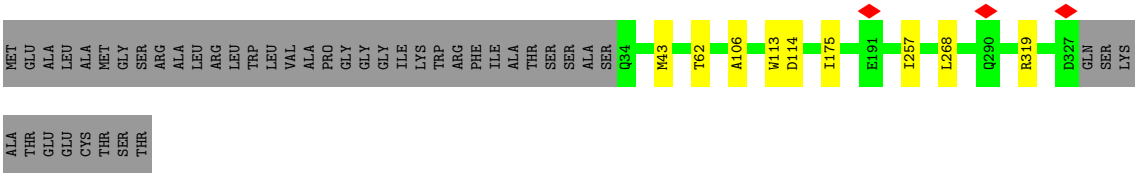




• Molecule 67: 39S ribosomal protein L39, mitochondrial

Chain 7:

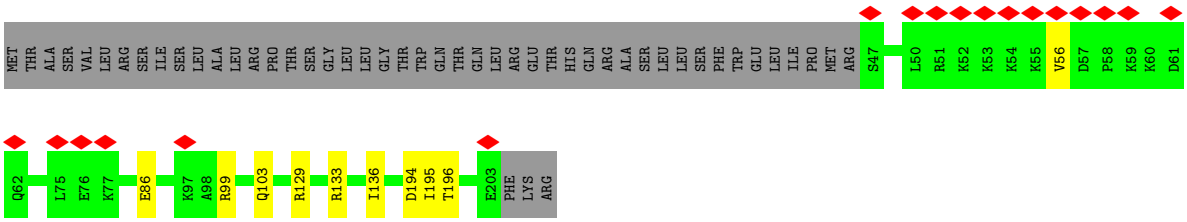




• Molecule 68: 39S ribosomal protein L40, mitochondrial

Chain 8:

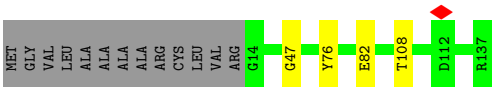




• Molecule 69: 39S ribosomal protein L41, mitochondrial

Chain 9:

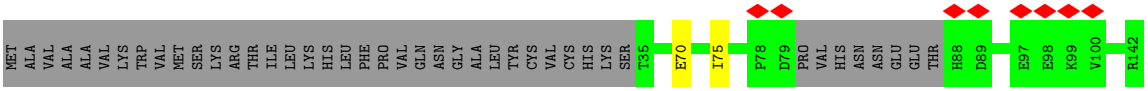




• Molecule 70: 39S ribosomal protein L42, mitochondrial

Chain a:

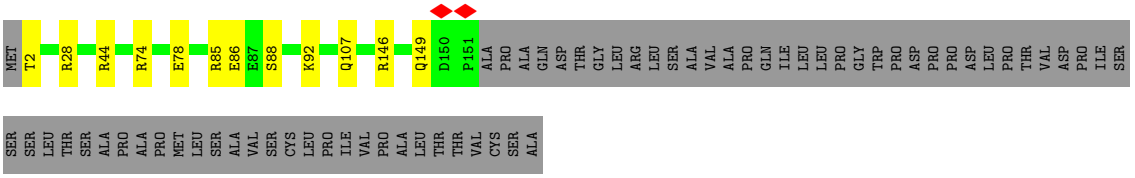




• Molecule 71: 39S ribosomal protein L43, mitochondrial

Chain b:

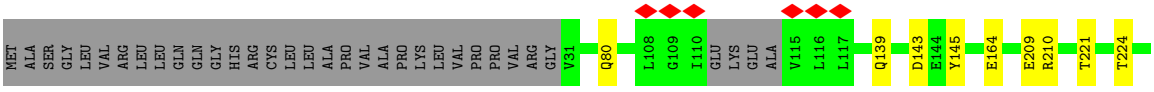


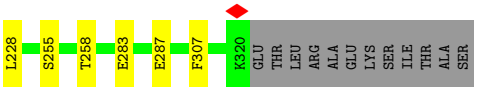


• Molecule 72: 39S ribosomal protein L44, mitochondrial

Chain c:



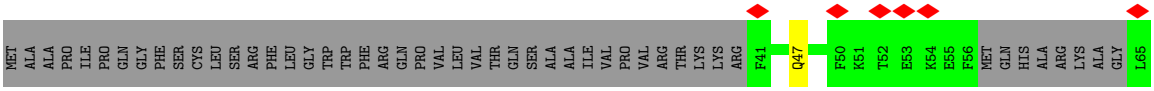


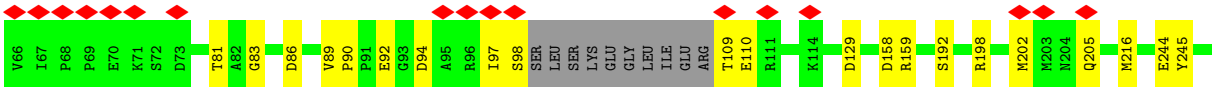


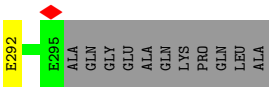
• Molecule 73: 39S ribosomal protein L45, mitochondrial

Chain d:





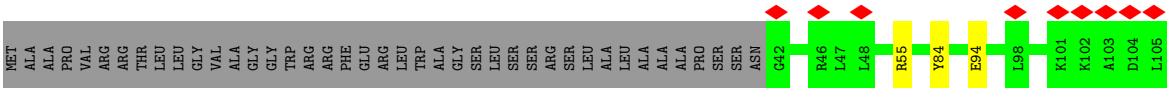


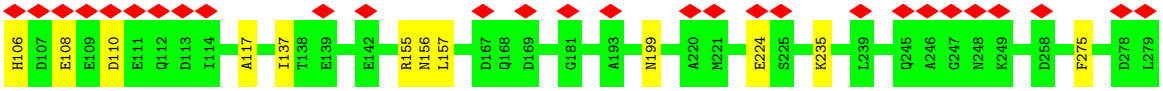


• Molecule 74: 39S ribosomal protein L46, mitochondrial

Chain e:



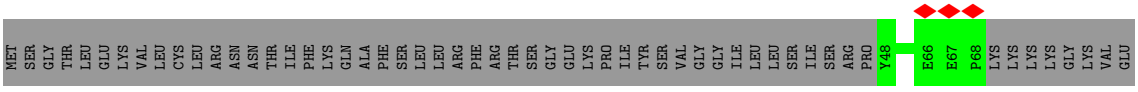


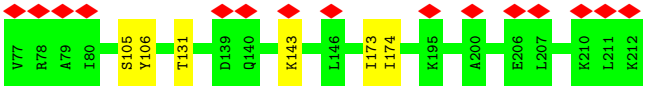


• Molecule 75: 39S ribosomal protein L48, mitochondrial

Chain f:



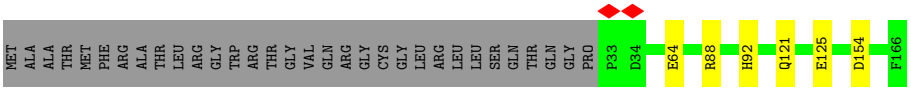




• Molecule 76: 39S ribosomal protein L49, mitochondrial

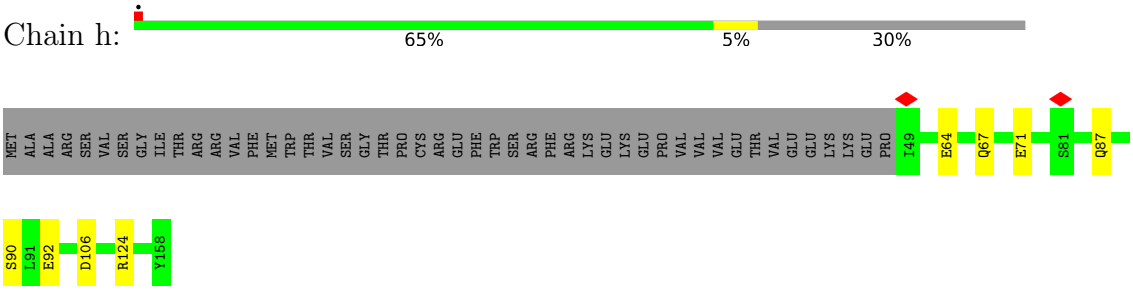
Chain g:





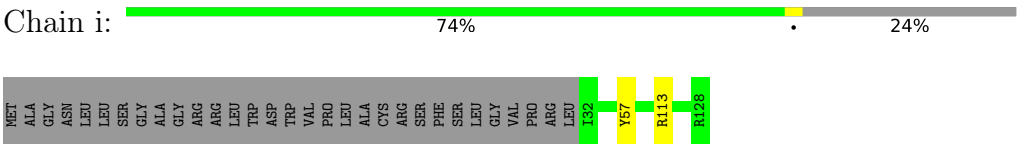
• Molecule 77: 39S ribosomal protein L50, mitochondrial

Chain h:



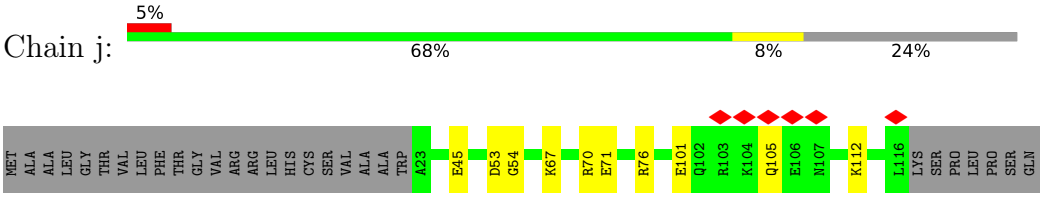
• Molecule 78: 39S ribosomal protein L51, mitochondrial

Chain i:



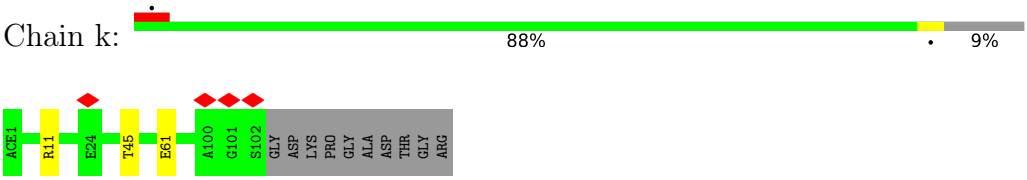
• Molecule 79: 39S ribosomal protein L52, mitochondrial

Chain j:



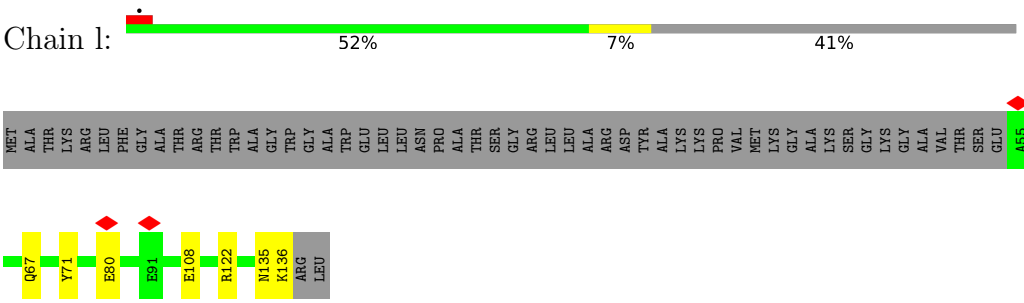
• Molecule 80: Large ribosomal subunit protein mL53

Chain k:



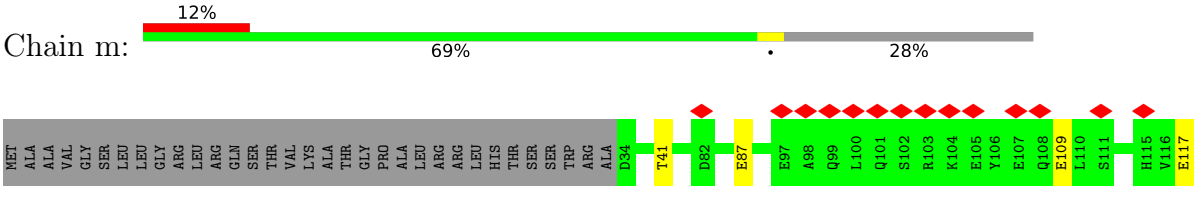
• Molecule 81: 39S ribosomal protein L54, mitochondrial

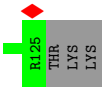
Chain l:



• Molecule 82: 39S ribosomal protein L55, mitochondrial

Chain m:





• Molecule 83: Ribosomal protein 63, mitochondrial

Chain o:

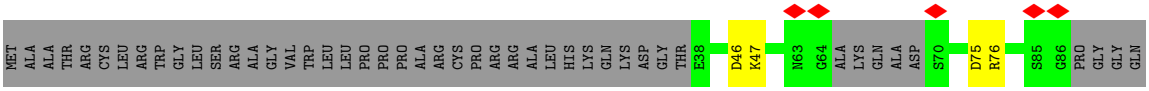


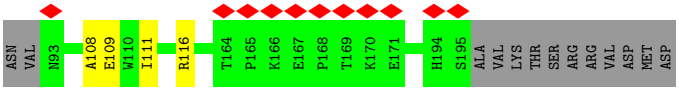


• Molecule 84: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:



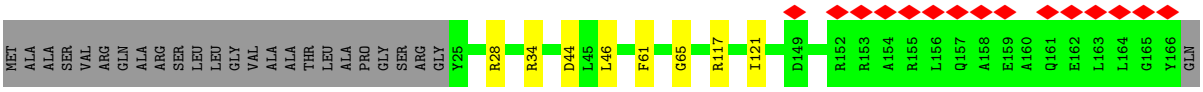


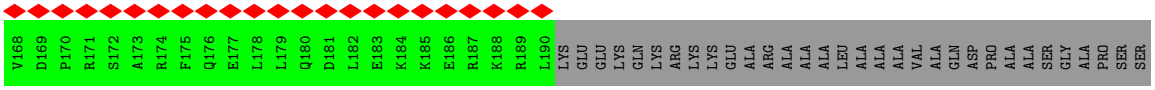


• Molecule 85: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



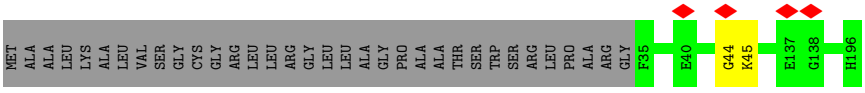




• Molecule 86: 39S ribosomal protein S18a, mitochondrial

Chain r:

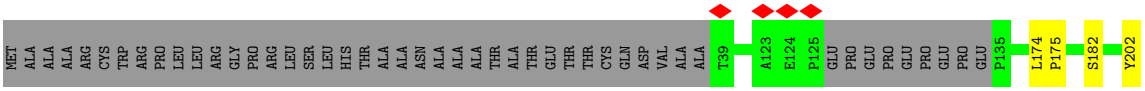


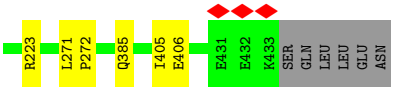


• Molecule 87: 39S ribosomal protein S30, mitochondrial

Chain s:



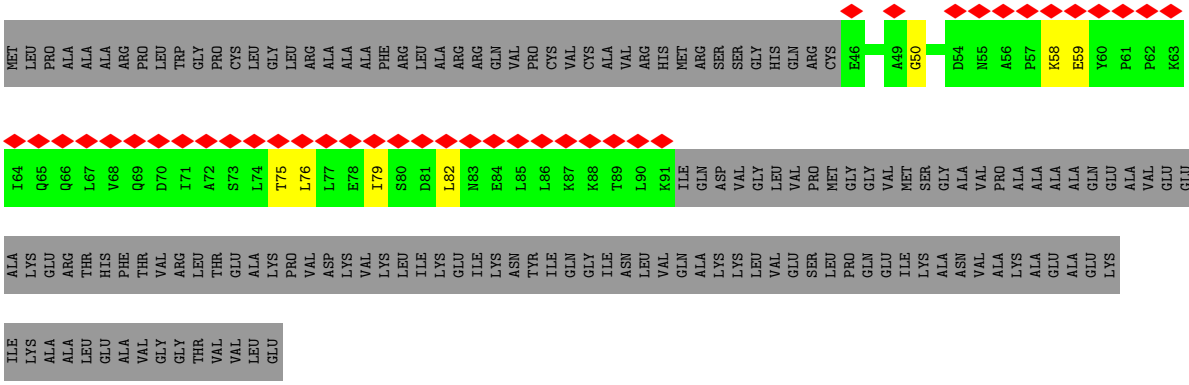




• Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain t:

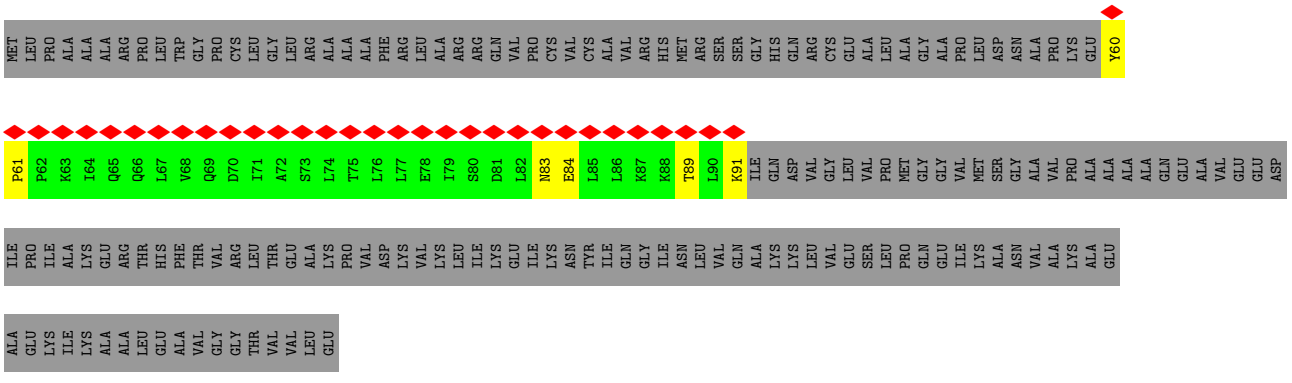




• Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain u:

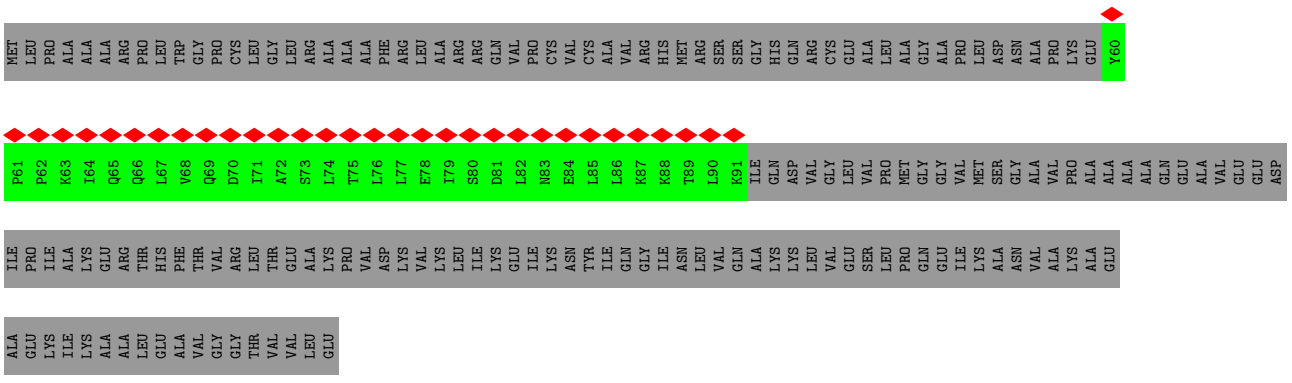




• Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain v:





• Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain w:



• Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain x:



• Molecule 88: 39S ribosomal protein L12, mitochondrial

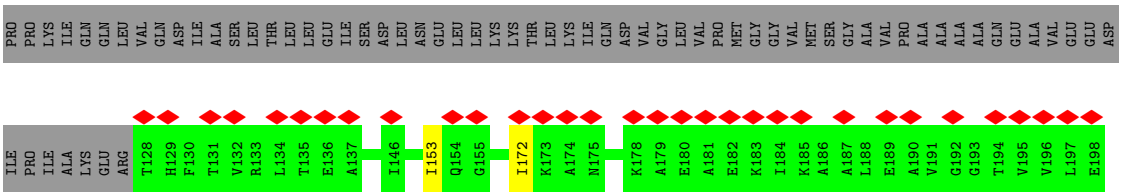
Chain y:



• Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain t1:

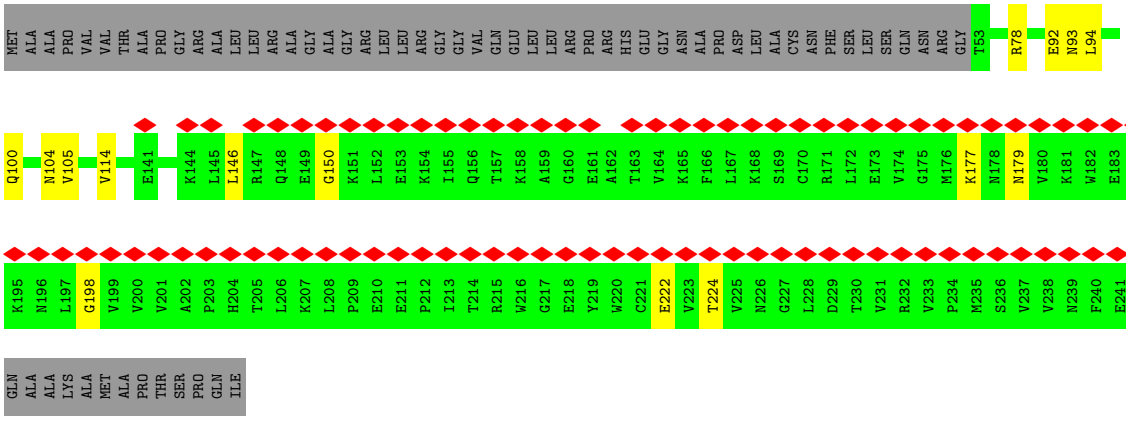




• Molecule 89: 39S ribosomal protein L9, mitochondrial

Chain H:

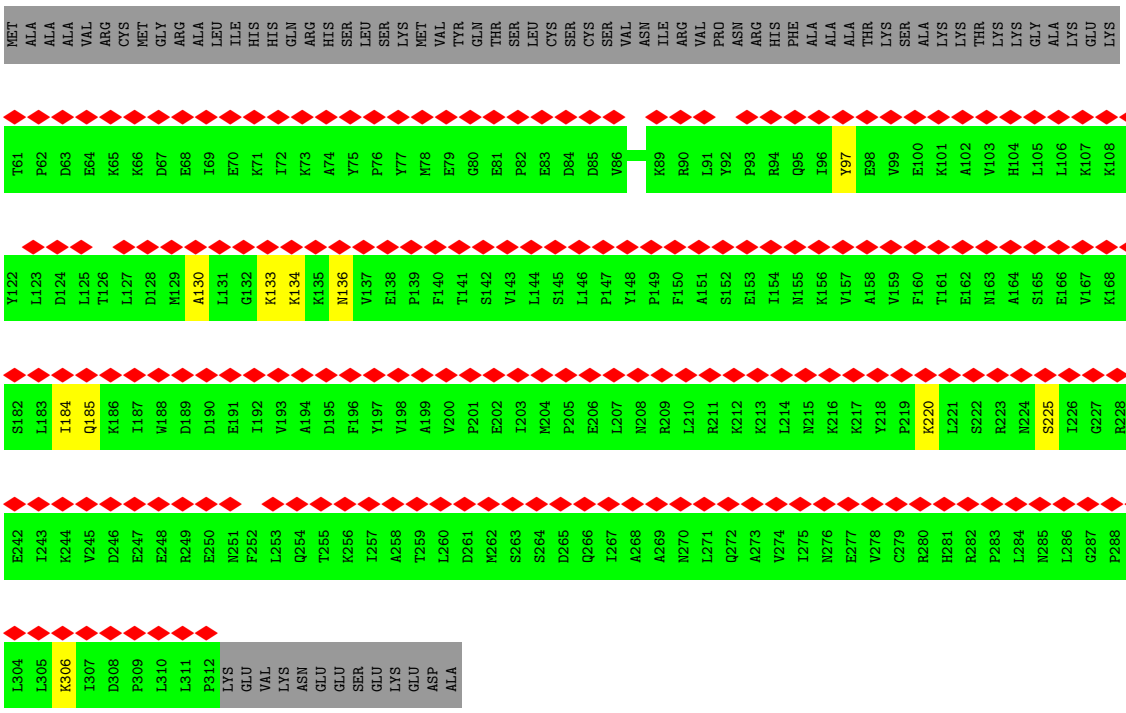




• Molecule 90: 39S ribosomal protein L1, mitochondrial

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61682	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.402	Depositor
Minimum map value	-0.416	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.24	Depositor
Map size (Å)	528.128, 528.128, 528.128	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82519996, 0.82519996, 0.82519996	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, OMU, 2MG, FES, K, MA6, ZN, GDP, ACE, 5MU, ATP, 5F0, 1MA, PSU, B8T, VOL, 5MC, NAD, THC, OMG, 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	A5	0.12	0/1284	0.32	0/1729
2	AA	0.10	0/22537	0.19	0/35085
3	AB	0.08	0/1871	0.22	0/2531
4	AC	0.09	0/1113	0.24	0/1505
5	AD	0.10	0/2783	0.23	0/3724
6	AE	0.10	0/989	0.23	0/1335
7	AF	0.08	0/1767	0.21	0/2373
8	AG	0.08	0/2746	0.21	0/3681
9	AH	0.09	0/1178	0.23	0/1598
10	AI	0.08	0/1030	0.21	0/1386
11	AJ	0.19	0/855	0.40	1/1148 (0.1%)
12	AK	0.07	0/880	0.20	0/1182
13	AL	0.10	0/1477	0.20	0/1974
14	AM	0.08	0/963	0.24	0/1295
15	AN	0.08	0/886	0.23	0/1199
16	AO	0.08	0/1648	0.23	0/2243
17	AP	0.10	0/798	0.25	0/1070
18	AQ	0.14	0/754	0.25	0/1003
19	AR	0.07	0/2456	0.20	0/3317
20	AS	0.10	0/1138	0.23	0/1533
21	AT	0.09	0/1402	0.22	0/1883
22	AU	0.07	0/1510	0.19	0/2025
23	AV	0.10	0/3030	0.22	0/4093
24	AW	0.09	0/801	0.23	0/1079
25	AX	0.07	0/2921	0.21	0/3954
26	AY	0.08	0/1280	0.20	0/1725
27	AZ	0.08	0/857	0.22	0/1141
28	A0	0.08	0/1834	0.23	0/2484
29	A1	0.08	0/2312	0.22	0/3128
30	A2	0.15	0/947	0.27	0/1266
31	A3	0.10	0/636	0.26	0/839

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	A4	0.08	0/4877	0.22	0/6598
33	Aw	0.11	0/1590	0.23	0/2459
34	Ax	0.07	0/1654	0.14	0/2565
35	Ay	0.06	0/1305	0.16	0/2023
36	Az	0.08	0/803	0.19	0/1246
37	A	0.15	0/36850	0.25	0/57359
38	B	0.07	0/1626	0.15	0/2523
39	D	0.11	0/1896	0.25	0/2549
40	E	0.11	0/2475	0.25	0/3355
41	F	0.12	0/2090	0.25	0/2842
42	I	0.10	0/1731	0.26	0/2345
43	J	0.11	0/1348	0.28	0/1813
44	K	0.15	0/1497	0.26	0/2031
45	L	0.11	0/905	0.26	0/1218
46	M	0.12	0/2368	0.25	0/3195
47	N	0.11	0/1833	0.24	0/2468
48	O	0.10	0/1283	0.22	0/1727
49	P	0.09	0/1199	0.22	0/1623
50	Q	0.10	0/2027	0.23	0/2734
51	R	0.12	0/1175	0.21	0/1572
52	S	0.12	0/1320	0.25	0/1789
53	T	0.12	0/1403	0.25	0/1886
54	U	0.13	0/1280	0.24	0/1732
55	V	0.10	0/1721	0.23	0/2333
56	W	0.13	0/926	0.24	0/1244
57	X	0.10	0/2099	0.21	0/2837
58	Y	0.11	0/1593	0.21	0/2136
59	Z	0.12	0/1021	0.26	0/1378
60	0	0.11	0/913	0.24	0/1224
61	1	0.09	0/469	0.23	0/621
62	2	0.13	0/383	0.26	0/507
63	3	0.12	0/853	0.25	0/1136
64	4	0.11	0/350	0.25	0/461
65	5	0.10	0/3305	0.23	0/4502
66	6	0.11	0/3043	0.23	0/4140
67	7	0.09	0/2447	0.23	0/3310
68	8	0.09	0/1354	0.26	0/1819
69	9	0.10	0/1025	0.23	0/1379
70	a	0.11	0/866	0.26	0/1174
71	b	0.13	0/1211	0.24	0/1639
72	c	0.12	0/2347	0.25	0/3171
73	d	0.10	0/2003	0.24	0/2713
74	e	0.07	0/1970	0.21	0/2658

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	f	0.09	0/1273	0.21	0/1716
76	g	0.12	0/1151	0.24	0/1569
77	h	0.09	0/918	0.21	0/1249
78	i	0.13	0/850	0.26	0/1135
79	j	0.12	0/760	0.23	0/1023
80	k	0.14	0/783	0.24	0/1057
81	l	0.10	0/707	0.25	0/960
82	m	0.07	0/805	0.21	0/1081
83	o	0.15	0/819	0.30	0/1097
84	p	0.08	0/1223	0.21	0/1641
85	q	0.09	0/1422	0.19	0/1916
86	r	0.11	0/1362	0.26	0/1846
87	s	0.10	0/3239	0.24	0/4400
88	t	0.10	0/358	0.30	0/486
88	t1	0.10	0/550	0.27	0/740
88	u	0.10	0/259	0.23	0/350
88	v	0.06	0/259	0.16	0/350
88	w	0.08	0/246	0.22	0/331
88	x	0.07	0/246	0.18	0/331
88	y	0.09	0/246	0.20	0/331
89	H	0.09	0/1698	0.25	0/2292
90	z	0.09	0/2067	0.27	0/2793
All	All	0.11	0/192358	0.23	1/273256 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AJ	93	CYS	CA-CB-SG	5.85	127.86	114.40

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	A5	1268	1253	1253	20	0
2	AA	20260	10258	10287	85	0
3	AB	1828	1815	1815	6	0
4	AC	1083	1088	1088	4	0
5	AD	2731	2804	2804	14	0
6	AE	972	1000	1000	6	0
7	AF	1725	1769	1769	4	0
8	AG	2688	2687	2687	9	0
9	AH	1152	1183	1183	5	0
10	AI	1011	1052	1052	3	0
11	AJ	839	885	885	21	0
12	AK	862	885	885	1	0
13	AL	1453	1540	1540	6	0
14	AM	942	965	965	9	0
15	AN	868	928	928	9	0
16	AO	1592	1557	1557	12	0
17	AP	781	806	806	8	0
18	AQ	744	758	758	6	0
19	AR	2409	2428	2428	7	0
20	AS	1111	1115	1115	9	0
21	AT	1371	1393	1393	8	0
22	AU	1488	1499	1499	7	0
23	AV	2969	2961	2961	16	0
24	AW	789	802	802	9	0
25	AX	2849	2843	2843	9	0
26	AY	1246	1197	1197	5	0
27	AZ	839	858	858	6	0
28	A0	1787	1796	1796	14	0
29	A1	2264	2292	2292	11	0
30	A2	935	971	971	11	0
31	A3	625	699	699	2	0
32	A4	4768	4766	4766	24	0
33	Aw	1427	720	723	13	0
34	Ax	1482	750	752	4	0
35	Ay	1169	592	594	4	0
36	Az	718	361	360	4	0
37	A	33048	16765	16786	114	0
38	B	1524	771	780	3	0
39	D	1859	1920	1920	10	0
40	E	2406	2415	2415	5	0
41	F	2031	2065	2065	6	0
42	I	1695	1785	1785	15	0
43	J	1330	1407	1407	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	K	1455	1452	1452	8	0
45	L	890	942	941	2	0
46	M	2314	2384	2384	6	0
47	N	1786	1817	1817	7	0
48	O	1259	1294	1294	8	0
49	P	1173	1165	1165	2	0
50	Q	1979	2022	2022	8	0
51	R	1154	1214	1214	3	0
52	S	1293	1365	1365	4	0
53	T	1369	1410	1410	7	0
54	U	1251	1232	1232	6	0
55	V	1676	1687	1687	8	0
56	W	904	935	935	4	0
57	X	2044	2060	2060	7	0
58	Y	1556	1597	1597	5	0
59	Z	996	1044	1044	7	0
60	0	898	916	916	5	0
61	1	464	511	511	2	0
62	2	377	406	406	1	0
63	3	832	883	883	2	0
64	4	342	361	361	0	0
65	5	3210	3206	3206	8	0
66	6	2948	2841	2841	10	0
67	7	2390	2397	2397	6	0
68	8	1327	1368	1368	8	0
69	9	997	987	987	4	0
70	a	840	810	810	2	0
71	b	1196	1195	1190	9	0
72	c	2299	2320	2320	12	0
73	d	1949	1930	1930	16	0
74	e	1931	1916	1916	10	0
75	f	1252	1269	1269	5	0
76	g	1113	1097	1097	4	0
77	h	895	881	881	6	0
78	i	828	857	857	2	0
79	j	745	746	746	8	0
80	k	774	784	784	2	0
81	l	688	674	674	8	0
82	m	791	797	796	4	0
83	o	798	804	804	4	0
84	p	1205	1223	1223	6	0
85	q	1389	1374	1374	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	r	1322	1348	1348	1	0
87	s	3155	3139	3139	7	0
88	t	354	377	377	8	0
88	t1	546	599	599	1	0
88	u	257	283	283	4	0
88	v	257	283	283	0	0
88	w	245	275	275	5	0
88	x	245	275	275	0	0
88	y	245	275	275	3	0
89	H	1661	1734	1734	15	0
90	z	2027	2076	2076	12	0
91	AA	44	25	25	1	0
92	A	136	0	0	0	0
92	AA	55	0	0	0	0
92	AB	1	0	0	0	0
92	AX	1	0	0	0	0
92	Az	1	0	0	0	0
92	D	1	0	0	0	0
93	A	24	0	0	0	0
93	AA	13	0	0	0	0
93	D	1	0	0	0	0
93	M	1	0	0	0	0
94	AI	9	0	0	0	0
95	0	1	0	0	0	0
95	4	1	0	0	0	0
95	AO	1	0	0	0	0
96	AP	4	0	0	0	0
96	AT	4	0	0	0	0
96	r	4	0	0	0	0
97	AX	31	12	12	0	0
98	AX	28	10	12	0	0
99	A	10	21	19	0	0
100	e	7	8	9	0	0
All	All	183207	155317	155376	713	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 2.

All (713) 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)
2:AA:1076:5MU:C4	2:AA:1076:5MU:C5	1.80	1.68
54:U:11:ARG:NH1	55:V:212:LYS:O	2.05	0.88
59:Z:105:SER:OG	83:o:59:GLU:OE2	1.96	0.84
71:b:28:ARG:NH1	71:b:78:GLU:OE1	2.11	0.83
37:A:2325:U:O2'	48:O:82:GLU:OE2	1.96	0.83
66:6:367:ASP:OD1	66:6:370:ARG:NH1	2.15	0.80
37:A:2125:C:OP2	52:S:178:LYS:NZ	2.16	0.78
37:A:1777:A:N6	37:A:1780:U:OP2	2.17	0.77
43:J:25:ARG:NH1	81:l:58:ASP:OD1	2.17	0.77
65:5:243:GLU:N	65:5:243:GLU:OE1	2.18	0.77
73:d:244:GLU:N	73:d:244:GLU:OE1	2.18	0.77
53:T:102:PHE:O	60:0:104:LYS:NZ	2.18	0.76
88:u:83:ASN:OD1	88:u:84:GLU:N	2.19	0.76
11:AJ:74:ASN:ND2	11:AJ:117:ASP:OD1	2.18	0.76
79:j:101:GLU:OE2	79:j:105:GLN:NE2	2.19	0.75
32:A4:433:TYR:OH	32:A4:469:GLU:OE1	2.04	0.75
5:AD:284:ARG:NH1	5:AD:287:ASP:OD1	2.20	0.74
73:d:86:ASP:OD2	73:d:198:ARG:NH2	2.21	0.74
11:AJ:81:CYS:O	11:AJ:93:CYS:HB3	1.87	0.74
74:e:235:LYS:NZ	74:e:275:PHE:O	2.18	0.74
2:AA:1166:A:OP2	11:AJ:114:ARG:NH2	2.20	0.73
9:AH:180:LEU:O	9:AH:185:LYS:NZ	2.22	0.73
41:F:76:ARG:NH2	77:h:106:ASP:OD1	2.22	0.73
66:6:80:GLU:OE1	66:6:80:GLU:N	2.22	0.73
89:H:104:ASN:OD1	89:H:105:VAL:N	2.20	0.73
32:A4:200:ASP:OD2	32:A4:243:ASN:N	2.21	0.72
28:A0:88:GLN:OE1	28:A0:88:GLN:N	2.22	0.72
75:f:106:TYR:OH	75:f:174:ILE:O	2.07	0.72
37:A:2709:A:N3	60:0:98:GLN:NE2	2.37	0.71
42:I:52:GLU:N	42:I:52:GLU:OE1	2.22	0.71
21:AT:14:GLN:N	21:AT:14:GLN:OE1	2.24	0.71
11:AJ:53:GLU:OE2	11:AJ:89:ARG:NH2	2.24	0.71
73:d:292:GLU:N	73:d:292:GLU:OE1	2.23	0.71
37:A:1990:G:OP1	39:D:269:ARG:NH2	2.23	0.71
44:K:136:ASP:OD1	44:K:137:ILE:N	2.24	0.70
17:AP:140:TYR:OH	18:AQ:33:ASP:OD1	2.10	0.70
32:A4:430:GLU:N	32:A4:430:GLU:OE1	2.24	0.70
43:J:84:GLN:OE1	43:J:84:GLN:N	2.25	0.70
21:AT:39:GLU:N	21:AT:39:GLU:OE1	2.24	0.70
32:A4:616:ASP:OD1	32:A4:617:SER:N	2.25	0.70
57:X:177:HIS:O	57:X:184:ARG:NH1	2.24	0.70
21:AT:138:GLU:OE1	21:AT:138:GLU:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:h:87:GLN:OE1	77:h:124:ARG:NH1	2.24	0.70
24:AW:110:ASN:OD1	24:AW:126:ARG:N	2.24	0.69
81:l:135:ASN:OD1	81:l:136:LYS:N	2.25	0.69
2:AA:1358:A:O2'	34:Ax:30:G:OP1	2.10	0.69
54:U:134:ARG:O	54:U:134:ARG:NH1	2.25	0.69
23:AV:252:LYS:O	23:AV:258:ARG:NH2	2.26	0.69
24:AW:137:GLY:O	24:AW:139:ARG:NH1	2.25	0.69
50:Q:155:ILE:HG22	50:Q:156:GLU:OE1	1.92	0.69
37:A:2016:C:OP2	46:M:59:ARG:NH1	2.26	0.69
82:m:87:GLU:OE1	82:m:87:GLU:N	2.25	0.69
67:7:175:ILE:O	67:7:319:ARG:NH2	2.26	0.68
37:A:2256:U:O2'	52:S:118:ASN:ND2	2.26	0.68
2:AA:1520:U:OP2	23:AV:407:GLN:NE2	2.25	0.68
2:AA:1199:G:N1	2:AA:1422:G:OP2	2.27	0.68
7:AF:174:LEU:O	7:AF:179:ARG:NH1	2.27	0.68
87:s:385:GLN:N	87:s:385:GLN:OE1	2.27	0.68
29:A1:100:GLU:N	29:A1:100:GLU:OE1	2.26	0.67
23:AV:321:GLU:OE1	23:AV:321:GLU:N	2.26	0.67
25:AX:272:THR:OG1	25:AX:282:ILE:O	2.11	0.67
68:8:136:ILE:HG22	75:f:173:ILE:HD11	1.75	0.67
10:AI:103:SER:OG	10:AI:105:GLU:OE1	2.11	0.67
26:AY:374:GLU:OE2	26:AY:378:ASN:ND2	2.27	0.67
32:A4:451:ASP:OD1	32:A4:452:GLN:N	2.27	0.67
55:V:139:GLU:N	55:V:139:GLU:OE1	2.28	0.67
49:P:180:GLU:N	49:P:180:GLU:OE1	2.28	0.67
59:Z:78:ARG:O	59:Z:83:LYS:NZ	2.27	0.66
88:t:76:LEU:HA	88:t:79:ILE:HG22	1.77	0.66
4:AC:125:ARG:NH2	4:AC:157:THR:O	2.29	0.66
32:A4:241:LYS:HD2	32:A4:241:LYS:O	1.95	0.66
19:AR:200:GLU:N	19:AR:200:GLU:OE1	2.26	0.66
27:AZ:6:GLU:N	27:AZ:6:GLU:OE1	2.29	0.66
39:D:116:GLU:OE1	39:D:116:GLU:N	2.28	0.65
6:AE:38:ASP:OD1	6:AE:39:LEU:N	2.29	0.65
8:AG:72:ASP:OD1	8:AG:73:PHE:N	2.29	0.65
21:AT:91:GLU:OE1	22:AU:120:ARG:NH2	2.29	0.65
21:AT:146:GLN:N	21:AT:146:GLN:OE1	2.28	0.65
43:J:178:GLN:O	43:J:182:ASP:N	2.28	0.65
2:AA:1530:A:OP1	28:A0:29:ARG:NH2	2.30	0.65
2:AA:952:A:N3	2:AA:954:C:N4	2.46	0.64
37:A:2169:A:OP1	43:J:21:ARG:NH1	2.30	0.64
33:Aw:9:A:OP1	33:Aw:21:A:N6	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:3067:PSU:H5'	40:E:232:GLY:O	1.98	0.64
28:A0:63:ARG:NH2	28:A0:110:ASP:OD2	2.31	0.63
2:AA:897:C:OP2	11:AJ:116:GLN:NE2	2.31	0.63
13:AL:120:GLU:N	13:AL:120:GLU:OE1	2.31	0.63
21:AT:18:GLN:NE2	21:AT:54:GLN:OE1	2.29	0.63
11:AJ:107:ILE:N	11:AJ:131:ASP:OD2	2.31	0.63
77:h:64:GLU:OE1	77:h:64:GLU:N	2.31	0.63
22:AU:194:GLU:N	22:AU:194:GLU:OE1	2.32	0.62
11:AJ:90:GLU:N	11:AJ:90:GLU:OE1	2.32	0.62
2:AA:713:C:O2	22:AU:27:ARG:N	2.33	0.62
65:5:254:GLU:OE1	65:5:254:GLU:N	2.31	0.62
16:AO:199:TRP:NE1	28:A0:166:TYR:O	2.30	0.62
76:g:64:GLU:N	76:g:64:GLU:OE1	2.32	0.62
88:t:75:THR:HA	88:w:68:VAL:HG11	1.81	0.62
37:A:3063:G:O2'	37:A:3066:C:OP2	2.17	0.62
23:AV:171:GLU:O	28:A0:144:LYS:NZ	2.32	0.62
29:A1:184:ASP:OD1	29:A1:185:HIS:N	2.32	0.61
37:A:2364:C:OP2	54:U:78:LYS:NZ	2.34	0.61
88:u:89:THR:O	88:w:76:LEU:HD13	2.01	0.61
13:AL:87:ASP:OD1	13:AL:88:VAL:N	2.34	0.61
24:AW:87:SER:HG	24:AW:90:THR:HG1	1.47	0.61
68:8:99:ARG:NH1	74:e:84:TYR:O	2.34	0.61
73:d:158:ASP:OD1	73:d:159:ARG:N	2.33	0.61
2:AA:1287:A:OP2	5:AD:260:LYS:NZ	2.32	0.61
2:AA:1526:U:N3	28:A0:100:VAL:O	2.34	0.61
32:A4:303:CYS:SG	32:A4:344:ARG:NH2	2.74	0.61
37:A:2499:U:O2'	37:A:2500:A:OP1	2.19	0.61
15:AN:57:GLN:N	15:AN:57:GLN:OE1	2.33	0.60
73:d:192:SER:OG	73:d:216:MET:SD	2.50	0.60
81:l:108:GLU:N	81:l:108:GLU:OE1	2.32	0.60
1:A5:139:GLU:OE1	1:A5:178:GLY:N	2.34	0.60
16:AO:73:VAL:O	16:AO:109:ARG:NH2	2.34	0.60
37:A:1672:C:OP2	53:T:42:SER:OG	2.13	0.60
2:AA:947:U:OP1	13:AL:162:GLN:NE2	2.32	0.60
41:F:52:GLU:N	41:F:52:GLU:OE1	2.35	0.60
58:Y:134:LYS:NZ	69:9:76:TYR:OH	2.33	0.60
37:A:1747:G:OP2	37:A:1749:C:N4	2.35	0.59
9:AH:94:PHE:CE1	29:A1:119:ILE:HD13	2.36	0.59
84:p:111:ILE:O	84:p:116:ARG:NH1	2.35	0.59
2:AA:1454:G:OP2	8:AG:377:ARG:NH1	2.34	0.59
26:AY:335:GLU:OE1	26:AY:348:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:5:368:GLU:OE1	65:5:368:GLU:N	2.35	0.59
32:A4:143:GLU:N	32:A4:143:GLU:OE1	2.36	0.59
43:J:182:ASP:O	43:J:186:GLN:N	2.35	0.59
14:AM:108:GLU:OE2	22:AU:59:ARG:NH2	2.35	0.59
24:AW:174:GLU:OE1	24:AW:174:GLU:N	2.35	0.59
59:Z:135:SER:HA	79:j:71:GLU:OE2	2.03	0.59
11:AJ:81:CYS:C	11:AJ:93:CYS:HB3	2.28	0.59
43:J:45:SER:OG	43:J:47:ASN:OD1	2.20	0.59
2:AA:1583:MA6:OP1	31:A3:145:LYS:NZ	2.36	0.58
28:A0:132:GLU:OE2	28:A0:205:ALA:N	2.35	0.58
58:Y:77:GLU:OE1	58:Y:77:GLU:N	2.35	0.58
41:F:191:ASP:OD1	41:F:192:SER:N	2.36	0.58
5:AD:94:THR:OG1	5:AD:96:ASP:OD1	2.22	0.58
37:A:1953:A:O2'	37:A:2463:A:OP1	2.20	0.58
4:AC:80:ASP:OD1	4:AC:81:HIS:ND1	2.36	0.58
5:AD:117:ARG:NH2	36:Az:14:A:O5'	2.37	0.58
30:A2:102:ASN:OD1	30:A2:103:LYS:N	2.35	0.58
37:A:2346:U:OP1	87:s:223:ARG:NH2	2.37	0.58
54:U:75:GLY:N	54:U:91:ASP:OD1	2.34	0.58
25:AX:196:GLU:OE1	25:AX:196:GLU:N	2.33	0.58
33:Aw:8:U:HO2'	33:Aw:13:U:H3	1.50	0.58
42:I:157:GLU:OE1	42:I:157:GLU:N	2.34	0.58
81:l:67:GLN:O	81:l:71:TYR:N	2.32	0.58
85:q:117:ARG:O	85:q:121:ILE:HD12	2.04	0.58
14:AM:111:ARG:NH1	16:AO:233:GLU:O	2.37	0.57
9:AH:71:ILE:O	9:AH:150:GLY:N	2.35	0.57
84:p:109:GLU:OE1	84:p:109:GLU:N	2.33	0.57
23:AV:250:ILE:O	23:AV:255:TYR:OH	2.22	0.57
30:A2:15:ASN:OD1	30:A2:17:ARG:NH1	2.37	0.57
66:6:311:MET:O	79:j:112:LYS:NZ	2.37	0.57
89:H:146:LEU:O	89:H:150:GLY:N	2.37	0.57
3:AB:102:MET:HE1	3:AB:223:VAL:HG23	1.87	0.57
32:A4:256:GLU:OE1	32:A4:256:GLU:N	2.35	0.57
68:8:103:GLN:OE1	68:8:103:GLN:N	2.37	0.57
1:A5:216:GLU:N	1:A5:233:ILE:O	2.27	0.57
37:A:2499:U:OP2	37:A:2504:A:N6	2.35	0.57
60:0:176:GLU:OE1	60:0:176:GLU:N	2.32	0.57
27:AZ:74:GLU:OE1	27:AZ:74:GLU:N	2.37	0.57
30:A2:64:ASP:OD1	30:A2:65:ALA:N	2.37	0.57
80:k:11:ARG:NH1	80:k:45:THR:O	2.37	0.57
42:I:225:GLN:CG	42:I:226:PRO:HD3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:948:U:OP2	2:AA:1045:G:N2	2.33	0.56
40:E:69:ASP:OD1	40:E:154:ARG:NH1	2.38	0.56
1:A5:142:GLY:N	1:A5:146:SER:O	2.36	0.56
2:AA:1583:MA6:H93	2:AA:1584:MA6:H92	1.86	0.56
8:AG:312:GLN:OE1	8:AG:345:ARG:NH1	2.38	0.56
88:u:91:LYS:C	88:w:76:LEU:HD11	2.29	0.56
48:O:64:LYS:NZ	48:O:100:GLN:O	2.39	0.56
6:AE:106:GLU:OE1	6:AE:106:GLU:N	2.33	0.56
19:AR:97:GLU:OE1	19:AR:97:GLU:N	2.39	0.56
9:AH:57:ASP:OD1	9:AH:58:LEU:N	2.39	0.55
71:b:149:GLN:OE1	71:b:149:GLN:N	2.39	0.55
84:p:75:ASP:OD1	84:p:76:ARG:N	2.39	0.55
2:AA:843:G:N2	2:AA:846:A:OP2	2.38	0.55
35:Ay:75:C:O2'	35:Ay:76:A:OP1	2.21	0.55
47:N:40:GLU:OE1	47:N:40:GLU:N	2.36	0.55
88:t:76:LEU:HD13	88:w:68:VAL:HG13	1.89	0.55
37:A:2220:A:H3'	37:A:2221:C:H4'	1.88	0.55
15:AN:8:VAL:O	15:AN:11:ARG:NH1	2.39	0.55
48:O:62:TYR:OH	50:Q:272:GLU:OE2	2.25	0.55
59:Z:92:GLU:OE1	59:Z:92:GLU:N	2.32	0.55
19:AR:317:ALA:O	19:AR:321:ALA:N	2.40	0.55
46:M:231:GLU:N	46:M:231:GLU:OE1	2.37	0.55
72:c:228:LEU:HD13	72:c:307:PHE:CD2	2.41	0.55
2:AA:1590:A:OP2	18:AQ:47:LYS:NZ	2.39	0.55
37:A:2284:C:OP2	71:b:74:ARG:NH2	2.37	0.55
2:AA:1524:A:N6	23:AV:396:GLN:OE1	2.39	0.55
50:Q:77:SER:OG	50:Q:79:GLU:OE1	2.25	0.55
57:X:35:GLU:N	57:X:35:GLU:OE1	2.40	0.55
6:AE:103:LYS:NZ	6:AE:104:GLU:OE2	2.40	0.54
17:AP:47:ASN:ND2	17:AP:49:ASP:OD1	2.39	0.54
37:A:3210:C:N4	37:A:3227:U:O4	2.35	0.54
57:X:35:GLU:O	57:X:35:GLU:HG2	2.08	0.54
8:AG:378:GLU:OE2	8:AG:381:LYS:NZ	2.40	0.54
24:AW:128:GLU:OE1	24:AW:128:GLU:N	2.39	0.54
42:I:225:GLN:HE22	88:y:68:VAL:HG13	1.73	0.54
33:Aw:14:A:H3'	33:Aw:15:A:O4'	2.07	0.54
47:N:46:GLU:OE1	47:N:46:GLU:N	2.37	0.54
10:AI:101:SER:OG	10:AI:105:GLU:OE1	2.26	0.54
37:A:1856:A:OP2	37:A:2986:C:O2'	2.25	0.54
50:Q:210:GLU:N	50:Q:210:GLU:OE1	2.39	0.54
33:Aw:9:A:H1'	33:Aw:45:A:H2'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:2499:U:O2	37:A:2503:A:N6	2.41	0.54
42:I:45:GLN:NE2	83:o:25:ARG:O	2.35	0.54
69:9:82:GLU:OE1	69:9:82:GLU:N	2.37	0.54
37:A:2882:U:O2	49:P:173:ARG:NH2	2.40	0.54
41:F:295:ARG:NE	41:F:295:ARG:O	2.41	0.54
43:J:50:CYS:O	43:J:54:ASN:ND2	2.41	0.54
11:AJ:104:GLU:OE1	11:AJ:105:HIS:ND1	2.42	0.53
18:AQ:69:ALA:O	18:AQ:73:ASN:ND2	2.36	0.53
5:AD:312:TYR:N	5:AD:331:ASP:OD2	2.41	0.53
20:AS:18:ASP:OD1	20:AS:21:ARG:NH2	2.41	0.53
33:Aw:15:A:H2'	33:Aw:16:A:H4'	1.90	0.53
2:AA:765:C:O2	2:AA:765:C:O2'	2.25	0.53
37:A:2398:A:H2'	37:A:2399:A:O4'	2.09	0.53
43:J:47:ASN:OD1	43:J:48:GLN:N	2.41	0.53
3:AB:102:MET:HE2	3:AB:224:ASP:O	2.08	0.53
37:A:2098:G:O2'	37:A:2099:U:OP2	2.21	0.53
89:H:93:ASN:OD1	89:H:94:LEU:N	2.42	0.53
90:z:230:ILE:N	90:z:231:PRO:CD	2.72	0.53
2:AA:781:A:O2'	91:AA:1701:NAD:N7N	2.42	0.53
2:AA:893:G:OP2	11:AJ:79:LYS:NZ	2.41	0.53
37:A:2161:A:H5'	37:A:2162:C:OP2	2.08	0.53
3:AB:258:THR:O	3:AB:262:GLU:OE1	2.27	0.53
37:A:2011:G:O6	78:i:113:ARG:NH1	2.41	0.52
2:AA:752:C:O2'	2:AA:793:C:N4	2.42	0.52
2:AA:1595:G:O6	18:AQ:50:ARG:NH2	2.43	0.52
18:AQ:77:ARG:O	18:AQ:80:ARG:NH1	2.42	0.52
37:A:2531:U:O4	39:D:246:ARG:NH2	2.43	0.52
2:AA:838:U:O2	14:AM:43:ARG:NH1	2.42	0.52
37:A:2776:G:N2	89:H:179:ASN:OD1	2.42	0.52
74:e:106:HIS:NE2	74:e:108:GLU:OE1	2.42	0.52
29:A1:152:ASP:OD2	29:A1:174:ARG:NH1	2.41	0.52
2:AA:702:C:O3'	2:AA:847:G:N2	2.42	0.52
38:B:38:C:OP1	66:6:56:ARG:NH2	2.41	0.52
72:c:209:GLU:OE1	72:c:209:GLU:N	2.38	0.52
88:t:58:LYS:NZ	88:t:59:GLU:O	2.42	0.52
5:AD:396:GLU:N	5:AD:396:GLU:OE1	2.40	0.52
37:A:3060:C:OP1	37:A:3061:G:OP1	2.28	0.52
59:Z:43:GLU:OE1	59:Z:43:GLU:N	2.33	0.52
57:X:87:LEU:O	89:H:78:ARG:NH1	2.42	0.52
30:A2:90:GLN:O	30:A2:94:GLY:N	2.38	0.52
68:8:86:GLU:OE1	68:8:86:GLU:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:s:405:ILE:HG23	87:s:405:ILE:O	2.10	0.52
15:AN:93:ASP:O	15:AN:97:GLY:N	2.38	0.51
37:A:2883:A:H4'	37:A:2884:C:OP2	2.10	0.51
70:a:70:GLU:OE1	70:a:70:GLU:N	2.39	0.51
37:A:1745:U:O4	63:3:108:LYS:NZ	2.43	0.51
2:AA:691:A:N7	2:AA:716:U:O2'	2.43	0.51
2:AA:764:A:H4'	2:AA:765:C:O5'	2.09	0.51
44:K:174:GLU:N	44:K:174:GLU:OE1	2.39	0.51
1:A5:137:LEU:N	37:A:2960:U:O4	2.44	0.51
22:AU:171:GLU:OE1	22:AU:171:GLU:N	2.41	0.51
68:8:194:ASP:OD1	68:8:196:THR:HG23	2.11	0.51
74:e:55:ARG:NH2	74:e:155:ARG:O	2.44	0.51
89:H:222:GLU:OE2	89:H:224:THR:OG1	2.28	0.51
16:AO:62:GLU:N	16:AO:62:GLU:OE1	2.42	0.51
5:AD:116:LYS:O	5:AD:118:THR:N	2.43	0.51
13:AL:83:GLU:OE1	13:AL:83:GLU:N	2.41	0.51
37:A:2196:A:OP1	81:l:122:ARG:NH1	2.44	0.51
72:c:164:GLU:OE1	72:c:164:GLU:N	2.42	0.51
89:H:177:LYS:NZ	90:z:114:PHE:O	2.36	0.51
2:AA:1583:MA6:O5'	2:AA:1583:MA6:H8	2.10	0.51
6:AE:49:TYR:O	6:AE:51:ILE:HD12	2.11	0.51
25:AX:183:GLU:OE1	25:AX:183:GLU:N	2.42	0.51
65:5:128:LEU:HD11	65:5:376:VAL:HG12	1.93	0.51
66:6:181:GLU:OE1	66:6:181:GLU:N	2.42	0.51
41:F:220:ASP:O	41:F:245:ALA:N	2.44	0.51
43:J:25:ARG:NE	81:l:56:LEU:O	2.41	0.51
47:N:175:PHE:O	47:N:178:GLN:HG2	2.10	0.51
63:3:104:ARG:NH1	63:3:160:LYS:O	2.44	0.51
2:AA:762:G:OP1	13:AL:206:LYS:NZ	2.43	0.51
2:AA:1414:C:OP2	75:f:143:LYS:NZ	2.43	0.51
15:AN:67:ARG:NH2	15:AN:80:GLU:OE2	2.44	0.51
65:5:377:ASP:OD1	65:5:380:GLN:NE2	2.43	0.51
74:e:224:GLU:OE1	74:e:224:GLU:N	2.44	0.51
23:AV:82:ARG:NH1	23:AV:86:ASP:OD1	2.44	0.50
37:A:2245:A:H4'	37:A:2246:A:OP1	2.09	0.50
56:W:120:LEU:HD11	56:W:126:LEU:CD1	2.41	0.50
71:b:44:ARG:NH2	83:o:99:LYS:O	2.44	0.50
2:AA:932:C:O2'	21:AT:2:PRO:O	2.26	0.50
33:Aw:20:C:OP1	33:Aw:21:A:O2'	2.30	0.50
73:d:90:PRO:HB3	73:d:245:TYR:HE2	1.77	0.50
84:p:76:ARG:NH1	84:p:109:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Ay:75:C:N4	37:A:2909:G:O2'	2.44	0.50
68:8:56:VAL:HG23	68:8:56:VAL:O	2.12	0.50
2:AA:1163:C:OP2	11:AJ:48:LYS:NZ	2.45	0.50
7:AF:193:ASP:OD1	7:AF:194:LYS:N	2.45	0.50
20:AS:48:ARG:HD2	20:AS:49:PRO:O	2.11	0.50
37:A:1749:C:OP2	37:A:2899:C:O2'	2.29	0.50
37:A:2580:U:O4	37:A:2581:A:N6	2.44	0.50
35:Ay:75:C:HO2'	35:Ay:76:A:P	2.33	0.50
90:z:130:ALA:HB1	90:z:136:ASN:HB2	1.94	0.50
14:AM:111:ARG:NH2	19:AR:146:LYS:O	2.45	0.50
37:A:1805:A:OP2	55:V:94:HIS:NE2	2.37	0.50
90:z:239:ASN:OD1	90:z:240:GLY:N	2.44	0.50
1:A5:194:GLU:HB2	1:A5:198:LYS:HA	1.94	0.49
37:A:2099:U:H2'	37:A:2100:C:C6	2.47	0.49
3:AB:162:CYS:O	3:AB:261:LYS:NZ	2.45	0.49
23:AV:376:GLU:OE2	23:AV:380:GLN:NE2	2.45	0.49
60:0:153:THR:HG22	60:0:153:THR:O	2.13	0.49
73:d:202:MET:N	73:d:202:MET:SD	2.84	0.49
9:AH:84:ASP:OD1	9:AH:86:ALA:N	2.45	0.49
43:J:73:LYS:N	43:J:77:THR:O	2.45	0.49
5:AD:96:ASP:OD1	5:AD:97:GLU:N	2.45	0.49
55:V:112:GLU:N	55:V:112:GLU:OE1	2.42	0.49
11:AJ:81:CYS:O	11:AJ:93:CYS:CB	2.60	0.49
6:AE:17:GLU:N	6:AE:17:GLU:OE1	2.46	0.49
42:I:225:GLN:HG2	42:I:226:PRO:HD3	1.95	0.49
77:h:67:GLN:NE2	77:h:71:GLU:OE2	2.45	0.49
79:j:53:ASP:OD1	79:j:54:GLY:N	2.45	0.49
15:AN:23:GLN:NE2	15:AN:24:LYS:HG3	2.28	0.49
37:A:2484:C:H5"	37:A:2485:U:OP1	2.13	0.49
37:A:3201:A:H2'	37:A:3202:U:O4'	2.13	0.49
89:H:193:PHE:O	89:H:198:GLY:N	2.46	0.49
5:AD:290:ILE:HB	5:AD:356:GLN:HE22	1.78	0.49
2:AA:1259:U:OP2	2:AA:1327:G:P	2.71	0.48
37:A:1800:G:N1	37:A:1803:A:OP2	2.46	0.48
22:AU:61:GLN:O	28:A0:198:MET:HE2	2.13	0.48
39:D:257:ILE:O	39:D:262:ARG:NH1	2.39	0.48
37:A:2826:G:OP1	56:W:49:ARG:NH1	2.45	0.48
55:V:133:ILE:HG21	55:V:145:ARG:HB3	1.94	0.48
74:e:108:GLU:O	74:e:110:ASP:N	2.46	0.48
17:AP:48:GLU:OE1	17:AP:48:GLU:N	2.46	0.48
37:A:2779:C:OP1	90:z:119:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:2783:A:O4'	90:z:296:ARG:NH1	2.46	0.48
16:AO:215:ARG:NH1	28:A0:87:TRP:O	2.41	0.48
71:b:74:ARG:HD3	71:b:86:GLU:OE2	2.13	0.48
87:s:406:GLU:N	87:s:406:GLU:OE1	2.47	0.48
37:A:2191:A:N6	37:A:2198:A:OP2	2.43	0.48
67:7:106:ALA:O	67:7:113:TRP:N	2.44	0.48
89:H:92:GLU:N	89:H:92:GLU:OE1	2.47	0.48
2:AA:1583:MA6:H102	2:AA:1584:MA6:H103	1.96	0.48
19:AR:170:ARG:O	19:AR:189:ARG:NH1	2.44	0.48
90:z:133:LYS:HG2	90:z:134:LYS:H	1.78	0.48
8:AG:310:ARG:NE	25:AX:383:LEU:O	2.46	0.48
16:AO:197:ASP:OD1	16:AO:198:PRO:HD2	2.13	0.48
2:AA:1401:G:N1	2:AA:1404:A:OP2	2.47	0.48
24:AW:141:ARG:NH1	24:AW:172:ILE:O	2.47	0.48
37:A:2499:U:HO2'	37:A:2500:A:P	2.36	0.48
1:A5:291:HIS:ND1	1:A5:293:TYR:CE2	2.82	0.48
5:AD:112:LYS:NZ	5:AD:235:GLU:O	2.47	0.48
66:6:231:GLU:N	66:6:231:GLU:OE1	2.47	0.48
46:M:54:LYS:N	46:M:58:GLN:OE1	2.36	0.47
2:AA:1057:G:H4'	2:AA:1578:A:H4'	1.95	0.47
32:A4:539:LYS:NZ	32:A4:540:HIS:O	2.47	0.47
50:Q:237:ASN:OD1	50:Q:238:PHE:N	2.47	0.47
71:b:85:ARG:NH1	71:b:107:GLN:OE1	2.47	0.47
32:A4:490:SER:OG	36:Az:25:U:N3	2.38	0.47
2:AA:844:A:H2'	2:AA:845:A:O4'	2.15	0.47
37:A:2127:A:H4'	37:A:2251:A:C5	2.48	0.47
37:A:2909:G:OP1	61:1:63:ARG:NH1	2.43	0.47
42:I:223:GLN:C	42:I:226:PRO:HD2	2.40	0.47
74:e:156:ASN:OD1	74:e:157:LEU:N	2.46	0.47
2:AA:1004:G:O2'	10:AI:98:GLN:NE2	2.47	0.47
55:V:188:VAL:O	55:V:188:VAL:HG23	2.14	0.47
85:q:44:ASP:OD1	85:q:46:LEU:N	2.44	0.47
33:Aw:9:A:O2'	33:Aw:10:G:N7	2.48	0.47
30:A2:39:GLU:OE2	30:A2:87:ARG:NE	2.48	0.47
6:AE:67:ASP:OD2	6:AE:96:HIS:NE2	2.48	0.47
14:AM:100:HIS:O	14:AM:103:MET:HG2	2.15	0.47
23:AV:236:LEU:HD12	23:AV:290:LEU:HD13	1.97	0.47
33:Aw:7:A:O2'	33:Aw:8:U:OP1	2.31	0.47
65:5:165:GLN:HG2	65:5:166:THR:HG23	1.97	0.47
4:AC:115:ASN:ND2	26:AY:309:LYS:O	2.48	0.46
29:A1:250:GLU:OE2	29:A1:301:ASN:ND2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:2379:C:O2	69:9:47:GLY:N	2.49	0.46
50:Q:180:GLU:OE1	50:Q:180:GLU:N	2.48	0.46
71:b:88:SER:O	71:b:92:LYS:NZ	2.48	0.46
2:AA:1272:A:N6	2:AA:1320:G:O2'	2.44	0.46
42:I:142:ASN:OD1	88:t:50:GLY:N	2.48	0.46
43:J:26:ALA:N	43:J:64:ILE:O	2.43	0.46
90:z:220:LYS:N	90:z:225:SER:OG	2.46	0.46
37:A:1991:A:H5"	37:A:1992:C:OP1	2.15	0.46
39:D:123:GLU:OE1	65:5:257:TYR:OH	2.31	0.46
86:r:44:GLY:O	86:r:45:LYS:HG2	2.15	0.46
28:A0:84:SER:OG	28:A0:138:ASP:OD2	2.28	0.46
37:A:1764:C:OP1	85:q:34:ARG:NH1	2.49	0.46
73:d:81:THR:HG22	73:d:83:GLY:H	1.80	0.46
2:AA:1078:A:OP1	34:Ax:38:U:O2'	2.31	0.46
68:8:129:ARG:O	68:8:133:ARG:N	2.43	0.46
1:A5:185:LYS:HA	1:A5:260:PHE:HA	1.98	0.46
23:AV:270:PRO:O	23:AV:346:LYS:NZ	2.48	0.46
23:AV:318:ASP:OD1	23:AV:319:ILE:N	2.49	0.46
66:6:325:ASP:OD1	66:6:326:SER:N	2.49	0.46
2:AA:1236:C:OP2	12:AK:90:ARG:NH2	2.47	0.46
37:A:2539:A:H4'	37:A:2540:C:OP1	2.16	0.46
84:p:108:ALA:O	84:p:116:ARG:NH1	2.49	0.46
2:AA:1257:U:O4	2:AA:1330:C:O2'	2.30	0.46
37:A:2213:A:H3'	37:A:2214:A:H5"	1.97	0.46
37:A:2261:C:O2'	52:S:184:ARG:NH1	2.47	0.46
37:A:2882:U:H4'	37:A:2883:A:H5"	1.97	0.46
43:J:121:ALA:O	43:J:125:ALA:N	2.34	0.46
88:t:76:LEU:CD1	88:w:68:VAL:HG13	2.46	0.46
2:AA:1293:C:N4	18:AQ:80:ARG:O	2.49	0.46
29:A1:46:ARG:HB2	29:A1:47:PRO:HD3	1.97	0.46
37:A:2458:A:OP2	48:O:9:ILE:N	2.49	0.46
75:f:105:SER:CB	82:m:41:THR:HG21	2.45	0.46
37:A:2849:G:OP1	61:1:14:LYS:NZ	2.49	0.46
42:I:225:GLN:HG3	42:I:226:PRO:HD3	1.98	0.46
84:p:46:ASP:OD1	84:p:47:LYS:N	2.49	0.46
2:AA:958:C:H4'	2:AA:959:C:O4'	2.15	0.45
2:AA:1342:C:OP2	27:AZ:96:LYS:NZ	2.48	0.45
28:A0:37:ASP:O	28:A0:41:LEU:N	2.45	0.45
72:c:221:THR:O	72:c:224:THR:OG1	2.31	0.45
88:u:60:TYR:HB2	88:u:61:PRO:HD3	1.97	0.45
2:AA:1340:C:OP2	27:AZ:100:LYS:NZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AX:102:ARG:NH2	25:AX:346:SER:O	2.42	0.45
37:A:1851:G:H2'	37:A:2693:A:N7	2.32	0.45
42:I:180:CYS:SG	42:I:184:THR:N	2.89	0.45
56:W:120:LEU:HD11	56:W:126:LEU:HD12	1.99	0.45
14:AM:70:LEU:O	14:AM:74:ARG:HD2	2.17	0.45
17:AP:53:SER:O	17:AP:54:MET:HG3	2.16	0.45
23:AV:51:ALA:HB3	50:Q:66:HIS:HB2	1.99	0.45
37:A:2458:A:O2'	40:E:215:PHE:O	2.27	0.45
39:D:286:ILE:HG13	39:D:286:ILE:O	2.16	0.45
42:I:225:GLN:NE2	88:y:68:VAL:HG13	2.30	0.45
77:h:90:SER:OG	77:h:92:GLU:OE1	2.20	0.45
37:A:2774:C:H2'	37:A:2775:A:C8	2.51	0.45
73:d:97:ILE:O	73:d:98:SER:C	2.58	0.45
81:l:80:GLU:OE1	81:l:80:GLU:N	2.42	0.45
37:A:1806:U:H4'	37:A:1807:U:H5'	1.99	0.45
43:J:104:THR:OG1	43:J:149:ARG:O	2.33	0.45
50:Q:252:GLN:O	50:Q:255:LYS:HG2	2.17	0.45
1:A5:191:VAL:O	1:A5:230:PHE:N	2.50	0.45
11:AJ:81:CYS:H	11:AJ:93:CYS:HB3	1.81	0.45
14:AM:41:CYS:SG	14:AM:42:PRO:HD2	2.57	0.45
33:Aw:29:U:H3'	33:Aw:30:U:H5"	1.98	0.45
39:D:238:GLU:OE1	39:D:238:GLU:N	2.49	0.45
70:a:75:ILE:HD13	72:c:255:SER:HB2	1.99	0.45
72:c:139:GLN:NE2	72:c:143:ASP:OD2	2.50	0.45
89:H:177:LYS:HD2	90:z:114:PHE:O	2.17	0.45
23:AV:47:HIS:O	23:AV:47:HIS:ND1	2.50	0.45
29:A1:258:SER:HG	29:A1:292:TYR:HH	1.62	0.45
69:9:108:THR:HG23	69:9:108:THR:O	2.16	0.45
37:A:2515:U:OP1	39:D:284:ARG:NH2	2.50	0.45
42:I:221:LEU:O	42:I:224:HIS:ND1	2.44	0.45
23:AV:74:ARG:O	23:AV:78:ASN:ND2	2.50	0.45
23:AV:236:LEU:HD21	23:AV:323:GLU:HB2	1.99	0.45
31:A3:177:TRP:CD1	31:A3:178:LEU:HD12	2.52	0.45
37:A:1907:A:OP1	41:F:126:LYS:NZ	2.48	0.45
37:A:2777:G:OP1	89:H:245:THR:OG1	2.33	0.45
57:X:113:GLU:OE2	57:X:123:PHE:N	2.50	0.45
2:AA:1366:C:H3'	2:AA:1367:A:H5'	1.98	0.44
16:AO:214:SER:OG	16:AO:217:ARG:NH2	2.51	0.44
17:AP:49:ASP:OD2	24:AW:82:SER:N	2.50	0.44
37:A:2144:A:OP1	51:R:57:ARG:NH1	2.46	0.44
51:R:85:ALA:O	51:R:89:ASN:ND2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AF:109:SER:O	7:AF:113:GLN:HG3	2.16	0.44
26:AY:254:LYS:O	32:A4:358:ARG:NH1	2.50	0.44
37:A:2135:A:N3	37:A:2135:A:H2'	2.31	0.44
59:Z:98:GLN:OE1	79:j:76:ARG:NE	2.50	0.44
2:AA:1021:U:OP2	30:A2:9:ARG:NH2	2.51	0.44
32:A4:132:ILE:O	32:A4:132:ILE:HG22	2.16	0.44
32:A4:270:ARG:O	32:A4:270:ARG:HG2	2.18	0.44
37:A:2744:U:H4'	37:A:2745:A:H5'	2.00	0.44
37:A:3039:OMU:O5'	37:A:3039:OMU:H6	2.18	0.44
28:A0:96:ARG:HB3	28:A0:117:ILE:HG22	1.99	0.44
2:AA:769:G:OP2	15:AN:73:ARG:NH2	2.51	0.44
20:AS:62:ASP:OD1	20:AS:63:ILE:N	2.51	0.44
25:AX:159:HIS:NE2	25:AX:266:ASN:OD1	2.51	0.44
29:A1:92:LYS:O	29:A1:93:LYS:HG2	2.18	0.44
32:A4:132:ILE:O	32:A4:132:ILE:CG2	2.66	0.44
37:A:2814:G:O2'	37:A:2983:G:OP1	2.36	0.44
37:A:3068:G:OP2	37:A:3068:G:N2	2.50	0.44
46:M:44:ARG:HG3	46:M:45:ARG:HG3	1.99	0.44
47:N:73:ARG:O	47:N:155:LYS:NZ	2.51	0.44
73:d:89:VAL:HG23	73:d:89:VAL:O	2.18	0.44
11:AJ:110:VAL:HG12	11:AJ:125:VAL:HG12	2.00	0.44
26:AY:377:ARG:O	26:AY:381:ASN:ND2	2.50	0.44
29:A1:306:GLU:OE1	29:A1:306:GLU:N	2.48	0.44
32:A4:290:ASP:OD1	32:A4:293:THR:OG1	2.29	0.44
43:J:166:ALA:O	43:J:169:LYS:HG2	2.17	0.44
73:d:129:ASP:OD1	73:d:129:ASP:O	2.36	0.44
74:e:137:ILE:HG23	74:e:137:ILE:O	2.18	0.44
17:AP:52:ILE:CD1	20:AS:66:HIS:CD2	3.01	0.44
30:A2:42:GLU:OE1	30:A2:42:GLU:HA	2.18	0.44
33:Aw:8:U:O2'	33:Aw:13:U:N3	2.42	0.44
37:A:2883:A:N3	37:A:2883:A:H2'	2.33	0.44
1:A5:201:VAL:HG12	1:A5:202:ASN:N	2.33	0.43
2:AA:1412:G:OP1	25:AX:279:LYS:NZ	2.45	0.43
47:N:59:VAL:O	47:N:59:VAL:HG13	2.18	0.43
54:U:47:GLU:OE1	54:U:47:GLU:N	2.47	0.43
83:o:93:ASP:OD1	83:o:96:ASN:ND2	2.48	0.43
89:H:100:GLN:OE1	89:H:100:GLN:N	2.51	0.43
2:AA:899:G:O2'	2:AA:907:A:N1	2.42	0.43
2:AA:1104:A:OP1	2:AA:1591:C:O2'	2.35	0.43
2:AA:1151:C:OP2	13:AL:201:ARG:NH1	2.46	0.43
8:AG:396:ARG:NH1	34:Ax:33:U:OP2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A4:526:ASP:OD1	32:A4:526:ASP:N	2.51	0.43
37:A:2777:G:O3'	89:H:177:LYS:HE3	2.18	0.43
48:O:140:SER:O	48:O:146:ASN:ND2	2.49	0.43
72:c:228:LEU:HD13	72:c:307:PHE:CE2	2.53	0.43
72:c:258:THR:OG1	72:c:283:GLU:OE2	2.31	0.43
80:k:61:GLU:OE1	80:k:61:GLU:N	2.34	0.43
87:s:271:LEU:N	87:s:272:PRO:HA	2.34	0.43
37:A:2001:C:H4'	37:A:2002:G:OP1	2.19	0.43
55:V:122:LEU:HB2	55:V:133:ILE:HD12	2.01	0.43
60:0:166:SER:OG	60:0:167:GLU:N	2.52	0.43
11:AJ:94:PHE:HB2	11:AJ:121:VAL:HG11	2.00	0.43
33:Aw:64:U:H2'	33:Aw:65:A:O4'	2.18	0.43
38:B:44:A:H2'	38:B:45:G:O4'	2.18	0.43
48:O:41:ARG:NH2	48:O:131:PRO:O	2.43	0.43
57:X:179:GLU:OE1	57:X:179:GLU:N	2.48	0.43
87:s:174:LEU:HB3	87:s:175:PRO:HD3	2.01	0.43
1:A5:259:GLU:HB3	1:A5:293:TYR:OH	2.18	0.43
2:AA:1365:A:H4'	2:AA:1389:G:H4'	2.00	0.43
8:AG:250:LEU:HD12	8:AG:250:LEU:O	2.18	0.43
73:d:109:THR:OG1	73:d:110:GLU:N	2.51	0.43
77:h:92:GLU:OE1	77:h:92:GLU:N	2.41	0.43
2:AA:919:A:OP2	16:AO:92:LYS:HD3	2.19	0.43
37:A:2987:U:O2'	37:A:2991:U:OP1	2.35	0.43
53:T:158:PHE:CZ	73:d:47:GLN:HG2	2.53	0.43
53:T:198:ARG:NH2	72:c:287:GLU:OE1	2.51	0.43
76:g:121:GLN:O	76:g:125:GLU:HG3	2.18	0.43
2:AA:1247:G:H4'	2:AA:1248:C:OP2	2.19	0.43
5:AD:363:ALA:O	5:AD:367:GLY:N	2.51	0.43
37:A:2506:A:H1'	37:A:2601:A:N6	2.33	0.43
46:M:250:ASP:OD1	46:M:251:GLU:N	2.52	0.43
58:Y:171:ASP:C	58:Y:171:ASP:OD1	2.62	0.43
2:AA:1327:G:O2'	2:AA:1328:G:OP1	2.34	0.43
32:A4:286:ARG:O	32:A4:286:ARG:NE	2.52	0.43
37:A:3089:A:H3'	37:A:3090:G:H5"	2.01	0.43
1:A5:262:PRO:HB3	1:A5:295:ASN:HA	2.01	0.43
7:AF:240:ARG:NH2	7:AF:242:TRP:OXT	2.52	0.43
28:A0:43:ARG:O	28:A0:47:GLY:N	2.45	0.43
37:A:2537:G:O2'	37:A:2634:U:OP2	2.33	0.43
37:A:3110:C:O2'	40:E:266:ARG:NH1	2.52	0.43
1:A5:265:LYS:HB3	1:A5:297:GLU:HG2	2.00	0.43
37:A:3110:C:OP2	37:A:3110:C:H3'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:180:GLU:OE1	55:V:180:GLU:N	2.41	0.43
66:6:139:TRP:O	66:6:144:GLY:N	2.51	0.43
79:j:45:GLU:OE2	79:j:70:ARG:NH2	2.47	0.43
2:AA:1247:G:H3'	2:AA:1249:U:OP2	2.19	0.42
30:A2:62:ARG:NH1	30:A2:64:ASP:OD1	2.52	0.42
35:Ay:75:C:O2'	35:Ay:76:A:P	2.77	0.42
37:A:2556:A:H2'	37:A:2557:C:O4'	2.19	0.42
1:A5:222:GLU:HB3	1:A5:226:GLU:HA	2.01	0.42
2:AA:883:U:H4'	2:AA:884:U:OP1	2.19	0.42
16:AO:95:ILE:HG13	16:AO:95:ILE:O	2.19	0.42
25:AX:381:LEU:O	25:AX:385:ASN:N	2.48	0.42
27:AZ:13:ARG:NH1	82:m:109:GLU:O	2.52	0.42
44:K:131:GLU:OE1	44:K:131:GLU:N	2.45	0.42
72:c:80:GLN:O	72:c:210:ARG:NH2	2.52	0.42
76:g:154:ASP:OD1	76:g:154:ASP:N	2.51	0.42
90:z:184:ILE:HG13	90:z:185:GLN:N	2.34	0.42
2:AA:895:C:N4	11:AJ:117:ASP:OD2	2.52	0.42
36:Az:15:U:O4	36:Az:16:A:N6	2.52	0.42
43:J:75:ASP:O	43:J:76:ARG:HB2	2.20	0.42
72:c:228:LEU:HD13	72:c:307:PHE:HD2	1.82	0.42
1:A5:215:ALA:HB1	1:A5:233:ILE:O	2.19	0.42
14:AM:24:GLY:N	14:AM:31:PHE:O	2.41	0.42
16:AO:217:ARG:NH1	16:AO:227:GLU:OE2	2.52	0.42
19:AR:219:TYR:O	19:AR:256:ARG:NH2	2.52	0.42
37:A:1860:A:O2'	37:A:2682:A:OP1	2.29	0.42
37:A:1957:A:H3'	37:A:1958:G:H5'	2.02	0.42
37:A:2525:C:OP2	37:A:2526:C:O2'	2.35	0.42
85:q:61:PHE:O	85:q:65:GLY:N	2.43	0.42
2:AA:1519:A:H2'	2:AA:1519:A:N3	2.35	0.42
15:AN:14:VAL:O	21:AT:63:GLN:NE2	2.51	0.42
37:A:2595:A:H2'	37:A:2596:G:O4'	2.19	0.42
37:A:2727:C:O2'	37:A:2815:OMG:N2	2.51	0.42
4:AC:80:ASP:OD1	4:AC:81:HIS:N	2.52	0.42
5:AD:311:GLY:N	5:AD:331:ASP:OD2	2.53	0.42
19:AR:162:SER:O	19:AR:170:ARG:NH1	2.52	0.42
37:A:1935:A:C2	37:A:1936:A:H1'	2.54	0.42
57:X:241:GLN:OE1	57:X:244:SER:OG	2.35	0.42
45:L:42:ASP:OD1	45:L:42:ASP:C	2.62	0.42
68:8:195:ILE:HG13	75:f:131:THR:HG23	2.01	0.42
2:AA:750:G:OP1	15:AN:78:LYS:NZ	2.50	0.42
20:AS:11:SER:OG	20:AS:43:GLU:OE2	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:3120:C:H2'	37:A:3121:C:O4'	2.20	0.42
1:A5:292:VAL:HG12	1:A5:293:TYR:N	2.34	0.42
2:AA:1295:A:N6	30:A2:109:GLN:O	2.53	0.42
2:AA:1422:G:N3	34:Ax:41:U:O2'	2.52	0.42
11:AJ:81:CYS:N	11:AJ:93:CYS:HB3	2.35	0.42
16:AO:131:THR:HG22	16:AO:133:ILE:HG12	2.02	0.42
17:AP:52:ILE:HD11	20:AS:66:HIS:CD2	2.54	0.42
29:A1:199:CYS:O	29:A1:203:ASP:N	2.51	0.42
33:Aw:22:A:H2'	33:Aw:23:A:O4'	2.19	0.42
37:A:1828:A:O2'	37:A:2684:C:H5	2.03	0.42
38:B:55:U:H3'	38:B:56:U:H5"	2.02	0.42
39:D:232:ARG:HA	39:D:289:LEU:HD21	2.01	0.42
44:K:34:MET:HE1	44:K:148:PRO:HD3	2.01	0.42
67:7:62:THR:O	67:7:62:THR:HG23	2.20	0.42
87:s:182:SER:OG	87:s:202:TYR:OH	2.37	0.42
5:AD:340:ILE:HG22	5:AD:340:ILE:O	2.19	0.42
11:AJ:81:CYS:O	11:AJ:93:CYS:N	2.52	0.42
24:AW:97:ASP:N	24:AW:144:LEU:O	2.52	0.42
79:j:67:LYS:O	79:j:71:GLU:HG2	2.19	0.42
2:AA:1225:C:N4	2:AA:1448:U:O2'	2.53	0.41
20:AS:70:ILE:HD12	20:AS:70:ILE:H	1.84	0.41
37:A:3097:U:H4'	37:A:3098:U:O5'	2.20	0.41
48:O:86:ILE:HB	48:O:87:PRO:HD3	2.00	0.41
52:S:109:THR:N	52:S:112:ASP:OD2	2.52	0.41
66:6:252:CYS:SG	66:6:296:ARG:NH1	2.93	0.41
74:e:199:ASN:OD1	74:e:199:ASN:O	2.38	0.41
1:A5:165:ARG:O	1:A5:169:ASN:ND2	2.53	0.41
2:AA:770:C:H2'	2:AA:771:A:O4'	2.20	0.41
2:AA:865:A:H2'	2:AA:866:A:O4'	2.20	0.41
25:AX:74:ASP:O	25:AX:78:VAL:N	2.45	0.41
30:A2:59:ASN:ND2	30:A2:66:CYS:SG	2.83	0.41
37:A:2367:A:N3	58:Y:123:ARG:NH2	2.68	0.41
37:A:2614:U:H5"	45:L:53:ARG:HE	1.85	0.41
37:A:2776:G:H5'	89:H:249:LYS:HE3	2.02	0.41
48:O:36:LEU:O	48:O:40:GLU:N	2.49	0.41
73:d:205:GLN:O	73:d:205:GLN:CD	2.63	0.41
2:AA:1245:U:O2'	27:AZ:96:LYS:NZ	2.47	0.41
20:AS:83:ARG:NH1	20:AS:93:LYS:O	2.52	0.41
37:A:2841:U:OP2	56:W:39:SER:OG	2.37	0.41
66:6:244:ARG:NE	66:6:244:ARG:HA	2.35	0.41
74:e:94:GLU:OE1	74:e:117:ALA:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:l:60:ASP:OD1	81:l:60:ASP:O	2.38	0.41
82:m:117:GLU:N	82:m:117:GLU:OE1	2.54	0.41
88:t:79:ILE:HD12	88:t:82:LEU:HD23	2.02	0.41
1:A5:206:ALA:HB2	1:A5:230:PHE:CE2	2.55	0.41
2:AA:769:G:N2	2:AA:772:A:OP2	2.43	0.41
2:AA:825:U:O2'	11:AJ:55:ARG:NH2	2.54	0.41
2:AA:1522:U:H2'	2:AA:1523:A:O4'	2.20	0.41
5:AD:116:LYS:O	5:AD:117:ARG:C	2.64	0.41
37:A:2990:A:H4'	37:A:2991:U:OP1	2.20	0.41
43:J:53:PHE:O	43:J:57:THR:HG22	2.21	0.41
44:K:60:MET:HE1	71:b:146:ARG:HE	1.85	0.41
1:A5:191:VAL:HA	1:A5:253:SER:HA	2.02	0.41
36:Az:10:A:H5'	36:Az:11:U:P	2.61	0.41
37:A:2075:U:O2'	37:A:2833:A:N7	2.49	0.41
37:A:2483:U:H2'	37:A:2484:C:O4'	2.21	0.41
39:D:281:TRP:O	39:D:285:LYS:NZ	2.50	0.41
44:K:153:LYS:HG2	44:K:157:GLU:HB2	2.03	0.41
53:T:192:GLU:O	53:T:196:GLN:HG3	2.21	0.41
67:7:43:MET:SD	67:7:43:MET:C	3.03	0.41
1:A5:186:LYS:HB2	1:A5:261:ILE:HG12	2.02	0.41
37:A:2086:A:H2'	37:A:2087:U:C6	2.56	0.41
2:AA:1098:C:OP1	2:AA:1151:C:N4	2.53	0.41
2:AA:1598:G:O2'	30:A2:37:ARG:NH2	2.54	0.41
37:A:2112:A:H4'	37:A:2113:G:OP1	2.20	0.41
37:A:2666:U:H2'	37:A:2667:U:O4'	2.21	0.41
42:I:131:LEU:HD23	42:I:147:PHE:CE2	2.55	0.41
44:K:51:SER:O	53:T:200:ARG:HD2	2.20	0.41
59:Z:149:TRP:NE1	79:j:45:GLU:OE1	2.54	0.41
67:7:114:ASP:OD1	67:7:268:LEU:N	2.53	0.41
73:d:92:GLU:OE1	73:d:92:GLU:HA	2.21	0.41
89:H:93:ASN:OD1	89:H:114:VAL:O	2.38	0.41
2:AA:663:A:H2'	2:AA:664:G:C8	2.55	0.41
2:AA:955:A:O4'	2:AA:1042:U:H1'	2.21	0.41
2:AA:966:A:OP2	17:AP:109:LYS:NZ	2.48	0.41
8:AG:292:ARG:HA	8:AG:292:ARG:CZ	2.51	0.41
16:AO:90:THR:HG22	16:AO:91:ARG:N	2.36	0.41
37:A:2781:U:O3'	37:A:2782:A:H2'	2.21	0.41
47:N:191:SER:H	47:N:194:THR:HG1	1.66	0.41
78:i:57:TYR:OH	85:q:28:ARG:O	2.38	0.41
88:t:75:THR:O	88:t:79:ILE:N	2.46	0.41
2:AA:871:A:N6	2:AA:919:A:O5'	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:1102:A:H5'	2:AA:1576:G:H4'	2.03	0.41
2:AA:1375:C:H2'	2:AA:1376:C:O4'	2.21	0.41
3:AB:111:LEU:O	3:AB:112:ASP:HB2	2.20	0.41
23:AV:266:VAL:O	23:AV:269:SER:OG	2.33	0.41
32:A4:302:VAL:O	32:A4:312:LYS:NZ	2.53	0.41
32:A4:397:MET:HE1	32:A4:435:VAL:HG23	2.02	0.41
33:Aw:75:C:H2'	33:Aw:76:A:C4	2.56	0.41
37:A:1792:G:N7	62:2:87:ARG:NH2	2.57	0.41
37:A:2190:C:O4'	43:J:149:ARG:NH1	2.53	0.41
37:A:2467:A:O2'	37:A:3154:U:H4'	2.20	0.41
37:A:2737:U:O2'	37:A:3084:A:N3	2.51	0.41
37:A:3111:A:H2'	37:A:3112:A:H5"	2.03	0.41
46:M:149:THR:O	46:M:149:THR:HG22	2.21	0.41
65:5:385:HIS:O	65:5:404:VAL:N	2.50	0.41
90:z:220:LYS:N	90:z:225:SER:HG	2.19	0.41
11:AJ:95:ILE:HG21	11:AJ:100:HIS:HB3	2.03	0.41
32:A4:565:ARG:HD2	32:A4:565:ARG:C	2.45	0.41
37:A:2104:A:OP1	47:N:231:SER:OG	2.35	0.41
37:A:2284:C:OP2	71:b:74:ARG:NH1	2.51	0.41
37:A:2353:A:H2'	37:A:2355:A:OP1	2.21	0.41
42:I:232:LEU:HD21	88:y:86:LEU:HD22	2.02	0.41
67:7:257:ILE:O	67:7:257:ILE:HG13	2.21	0.41
73:d:94:ASP:OD2	73:d:245:TYR:OH	2.35	0.41
2:AA:1355:G:N2	2:AA:1356:A:N7	2.58	0.40
15:AN:57:GLN:O	15:AN:87:LYS:NZ	2.53	0.40
29:A1:105:LEU:O	29:A1:108:ILE:HG22	2.21	0.40
32:A4:335:PHE:O	32:A4:338:ILE:HG22	2.21	0.40
32:A4:564:ILE:O	32:A4:564:ILE:HG13	2.21	0.40
58:Y:171:ASP:OD1	58:Y:173:PHE:N	2.54	0.40
3:AB:65:GLU:N	3:AB:66:PRO:HD2	2.37	0.40
32:A4:357:LEU:HA	32:A4:360:MET:HE3	2.03	0.40
40:E:111:THR:OG1	40:E:113:ASP:OD1	2.34	0.40
51:R:65:ARG:HA	51:R:68:TRP:CE3	2.57	0.40
53:T:129:GLU:HG2	53:T:130:PHE:N	2.36	0.40
2:AA:841:A:OP1	14:AM:39:ASN:ND2	2.52	0.40
2:AA:1108:C:H4'	2:AA:1109:A:OP2	2.21	0.40
42:I:144:LEU:N	42:I:145:PRO:HD2	2.36	0.40
90:z:97:TYR:HB3	90:z:306:LYS:HB2	2.03	0.40
1:A5:193:VAL:CG2	1:A5:228:ASN:HB3	2.51	0.40
11:AJ:104:GLU:O	11:AJ:105:HIS:HB2	2.22	0.40
20:AS:51:VAL:HG12	20:AS:52:ARG:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AU:162:GLU:O	22:AU:165:LYS:HG2	2.22	0.40
24:AW:92:MET:O	24:AW:98:LYS:NZ	2.55	0.40
28:A0:174:ILE:O	28:A0:177:GLU:HG2	2.22	0.40
37:A:1762:A:H2'	37:A:1763:A:O4'	2.22	0.40
37:A:1937:A:N6	37:A:1938:A:N1	2.70	0.40
72:c:145:TYR:CZ	72:c:307:PHE:HE1	2.38	0.40
88:t1:153:ILE:HD11	88:t1:172:ILE:HG23	2.03	0.40
2:AA:1213:A:N3	2:AA:1239:C:O2'	2.50	0.40
2:AA:1327:G:HO2'	2:AA:1328:G:P	2.44	0.40
8:AG:360:GLU:HA	8:AG:363:TRP:HD1	1.87	0.40
37:A:2195:A:H5"	37:A:2196:A:OP1	2.22	0.40
37:A:2222:U:C1'	37:A:2223:A:OP1	2.69	0.40
44:K:7:ALA:HB3	44:K:8:PRO:HD3	2.02	0.40
54:U:66:ALA:HB2	54:U:100:ALA:HA	2.04	0.40
76:g:88:ARG:NH1	76:g:92:HIS:O	2.52	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	A5	162/297 (54%)	151 (93%)	11 (7%)	0	100	100
3	AB	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
4	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
5	AD	341/430 (79%)	330 (97%)	9 (3%)	2 (1%)	21	31
6	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
7	AF	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
8	AG	323/396 (82%)	320 (99%)	3 (1%)	0	100	100
9	AH	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AI	132/193 (68%)	130 (98%)	2 (2%)	0	100	100
11	AJ	106/138 (77%)	97 (92%)	9 (8%)	0	100	100
12	AK	99/128 (77%)	99 (100%)	0	0	100	100
13	AL	172/257 (67%)	172 (100%)	0	0	100	100
14	AM	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
15	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
16	AO	191/258 (74%)	190 (100%)	1 (0%)	0	100	100
17	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
18	AQ	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
19	AR	293/360 (81%)	286 (98%)	7 (2%)	0	100	100
20	AS	133/190 (70%)	127 (96%)	6 (4%)	0	100	100
21	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
22	AU	174/205 (85%)	174 (100%)	0	0	100	100
23	AV	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
24	AW	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
25	AX	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
26	AY	147/395 (37%)	147 (100%)	0	0	100	100
27	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
28	A0	213/217 (98%)	210 (99%)	3 (1%)	0	100	100
29	A1	277/323 (86%)	274 (99%)	3 (1%)	0	100	100
30	A2	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
31	A3	68/199 (34%)	68 (100%)	0	0	100	100
32	A4	584/689 (85%)	579 (99%)	5 (1%)	0	100	100
39	D	236/305 (77%)	233 (99%)	3 (1%)	0	100	100
40	E	303/348 (87%)	296 (98%)	7 (2%)	0	100	100
41	F	250/311 (80%)	248 (99%)	2 (1%)	0	100	100
42	I	210/261 (80%)	203 (97%)	7 (3%)	0	100	100
43	J	173/192 (90%)	164 (95%)	9 (5%)	0	100	100
44	K	176/178 (99%)	174 (99%)	2 (1%)	0	100	100
45	L	113/145 (78%)	113 (100%)	0	0	100	100
46	M	287/296 (97%)	284 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
48	O	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
49	P	142/180 (79%)	142 (100%)	0	0	100	100
50	Q	236/292 (81%)	235 (100%)	1 (0%)	0	100	100
51	R	138/149 (93%)	138 (100%)	0	0	100	100
52	S	159/205 (78%)	157 (99%)	2 (1%)	0	100	100
53	T	164/206 (80%)	164 (100%)	0	0	100	100
54	U	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
55	V	203/216 (94%)	200 (98%)	3 (2%)	0	100	100
56	W	114/148 (77%)	114 (100%)	0	0	100	100
57	X	242/256 (94%)	242 (100%)	0	0	100	100
58	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
59	Z	120/161 (74%)	120 (100%)	0	0	100	100
60	0	108/188 (57%)	108 (100%)	0	0	100	100
61	1	54/65 (83%)	54 (100%)	0	0	100	100
62	2	44/92 (48%)	44 (100%)	0	0	100	100
63	3	93/188 (50%)	93 (100%)	0	0	100	100
64	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
65	5	392/423 (93%)	390 (100%)	2 (0%)	0	100	100
66	6	352/380 (93%)	345 (98%)	7 (2%)	0	100	100
67	7	292/338 (86%)	286 (98%)	6 (2%)	0	100	100
68	8	155/206 (75%)	153 (99%)	2 (1%)	0	100	100
69	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
70	a	96/142 (68%)	96 (100%)	0	0	100	100
71	b	148/215 (69%)	147 (99%)	1 (1%)	0	100	100
72	c	282/332 (85%)	280 (99%)	2 (1%)	0	100	100
73	d	231/306 (76%)	228 (99%)	3 (1%)	0	100	100
74	e	236/279 (85%)	225 (95%)	11 (5%)	0	100	100
75	f	153/212 (72%)	152 (99%)	1 (1%)	0	100	100
76	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
77	h	108/158 (68%)	108 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	i	95/128 (74%)	95 (100%)	0	0	100	100
79	j	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
80	k	100/112 (89%)	100 (100%)	0	0	100	100
81	l	80/138 (58%)	77 (96%)	3 (4%)	0	100	100
82	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
83	o	92/102 (90%)	92 (100%)	0	0	100	100
84	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
85	q	161/222 (72%)	160 (99%)	1 (1%)	0	100	100
86	r	160/196 (82%)	160 (100%)	0	0	100	100
87	s	382/439 (87%)	379 (99%)	3 (1%)	0	100	100
88	t	44/198 (22%)	44 (100%)	0	0	100	100
88	t1	69/198 (35%)	68 (99%)	1 (1%)	0	100	100
88	u	30/198 (15%)	30 (100%)	0	0	100	100
88	v	30/198 (15%)	30 (100%)	0	0	100	100
88	w	29/198 (15%)	29 (100%)	0	0	100	100
88	x	29/198 (15%)	29 (100%)	0	0	100	100
88	y	29/198 (15%)	29 (100%)	0	0	100	100
89	H	200/267 (75%)	198 (99%)	2 (1%)	0	100	100
90	z	250/325 (77%)	245 (98%)	5 (2%)	0	100	100
All	All	14928/19978 (75%)	14736 (99%)	189 (1%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	AH	126	ILE
5	AD	117	ARG
5	AD	299	LYS

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	A5	139/245 (57%)	139 (100%)	0	100	100
3	AB	198/249 (80%)	198 (100%)	0	100	100
4	AC	115/143 (80%)	115 (100%)	0	100	100
5	AD	286/357 (80%)	286 (100%)	0	100	100
6	AE	104/107 (97%)	104 (100%)	0	100	100
7	AF	185/209 (88%)	185 (100%)	0	100	100
8	AG	285/342 (83%)	285 (100%)	0	100	100
9	AH	130/180 (72%)	130 (100%)	0	100	100
10	AI	104/146 (71%)	104 (100%)	0	100	100
11	AJ	93/118 (79%)	93 (100%)	0	100	100
12	AK	91/113 (80%)	91 (100%)	0	100	100
13	AL	158/226 (70%)	158 (100%)	0	100	100
14	AM	97/113 (86%)	97 (100%)	0	100	100
15	AN	96/115 (84%)	96 (100%)	0	100	100
16	AO	174/230 (76%)	174 (100%)	0	100	100
17	AP	88/123 (72%)	88 (100%)	0	100	100
18	AQ	78/78 (100%)	78 (100%)	0	100	100
19	AR	264/318 (83%)	264 (100%)	0	100	100
20	AS	116/164 (71%)	116 (100%)	0	100	100
21	AT	153/157 (98%)	153 (100%)	0	100	100
22	AU	152/174 (87%)	152 (100%)	0	100	100
23	AV	325/364 (89%)	325 (100%)	0	100	100
24	AW	87/158 (55%)	87 (100%)	0	100	100
25	AX	311/351 (89%)	311 (100%)	0	100	100
26	AY	137/357 (38%)	137 (100%)	0	100	100
27	AZ	90/95 (95%)	90 (100%)	0	100	100
28	A0	188/189 (100%)	188 (100%)	0	100	100
29	A1	257/291 (88%)	257 (100%)	0	100	100
30	A2	100/100 (100%)	100 (100%)	0	100	100
31	A3	65/166 (39%)	65 (100%)	0	100	100
32	A4	526/609 (86%)	526 (100%)	0	100	100
39	D	192/245 (78%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	E	260/290 (90%)	260 (100%)	0	100	100
41	F	219/262 (84%)	219 (100%)	0	100	100
42	I	194/232 (84%)	194 (100%)	0	100	100
43	J	138/150 (92%)	138 (100%)	0	100	100
44	K	155/155 (100%)	155 (100%)	0	100	100
45	L	98/124 (79%)	98 (100%)	0	100	100
46	M	245/249 (98%)	245 (100%)	0	100	100
47	N	189/211 (90%)	189 (100%)	0	100	100
48	O	134/150 (89%)	134 (100%)	0	100	100
49	P	126/155 (81%)	126 (100%)	0	100	100
50	Q	220/256 (86%)	220 (100%)	0	100	100
51	R	118/126 (94%)	118 (100%)	0	100	100
52	S	146/180 (81%)	146 (100%)	0	100	100
53	T	146/176 (83%)	146 (100%)	0	100	100
54	U	134/134 (100%)	134 (100%)	0	100	100
55	V	183/191 (96%)	183 (100%)	0	100	100
56	W	94/119 (79%)	94 (100%)	0	100	100
57	X	220/229 (96%)	220 (100%)	0	100	100
58	Y	163/223 (73%)	163 (100%)	0	100	100
59	Z	113/147 (77%)	113 (100%)	0	100	100
60	0	99/164 (60%)	99 (100%)	0	100	100
61	1	53/60 (88%)	53 (100%)	0	100	100
62	2	40/72 (56%)	40 (100%)	0	100	100
63	3	88/166 (53%)	88 (100%)	0	100	100
64	4	37/89 (42%)	37 (100%)	0	100	100
65	5	353/368 (96%)	353 (100%)	0	100	100
66	6	313/332 (94%)	313 (100%)	0	100	100
67	7	270/303 (89%)	270 (100%)	0	100	100
68	8	146/190 (77%)	146 (100%)	0	100	100
69	9	104/112 (93%)	104 (100%)	0	100	100
70	a	96/133 (72%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	b	131/185 (71%)	131 (100%)	0	100	100
72	c	251/288 (87%)	251 (100%)	0	100	100
73	d	219/274 (80%)	219 (100%)	0	100	100
74	e	207/236 (88%)	207 (100%)	0	100	100
75	f	139/188 (74%)	139 (100%)	0	100	100
76	g	124/148 (84%)	124 (100%)	0	100	100
77	h	104/148 (70%)	104 (100%)	0	100	100
78	i	86/110 (78%)	86 (100%)	0	100	100
79	j	74/97 (76%)	74 (100%)	0	100	100
80	k	83/89 (93%)	83 (100%)	0	100	100
81	l	76/116 (66%)	76 (100%)	0	100	100
82	m	85/113 (75%)	85 (100%)	0	100	100
83	o	80/87 (92%)	80 (100%)	0	100	100
84	p	135/181 (75%)	135 (100%)	0	100	100
85	q	142/178 (80%)	142 (100%)	0	100	100
86	r	147/169 (87%)	147 (100%)	0	100	100
87	s	340/381 (89%)	340 (100%)	0	100	100
88	t	40/158 (25%)	40 (100%)	0	100	100
88	t1	59/158 (37%)	59 (100%)	0	100	100
88	u	31/158 (20%)	31 (100%)	0	100	100
88	v	31/158 (20%)	31 (100%)	0	100	100
88	w	30/158 (19%)	30 (100%)	0	100	100
88	x	30/158 (19%)	30 (100%)	0	100	100
88	y	30/158 (19%)	30 (100%)	0	100	100
89	H	182/228 (80%)	182 (100%)	0	100	100
90	z	226/287 (79%)	226 (100%)	0	100	100
All	All	13360/17189 (78%)	13360 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A5	169	ASN
4	AC	126	GLN
5	AD	130	GLN
5	AD	356	GLN
5	AD	359	HIS
5	AD	361	GLN
7	AF	146	HIS
7	AF	147	GLN
8	AG	77	GLN
8	AG	82	ASN
8	AG	163	HIS
8	AG	288	HIS
9	AH	183	HIS
10	AI	87	HIS
11	AJ	134	HIS
13	AL	146	HIS
14	AM	50	GLN
16	AO	103	ASN
16	AO	169	GLN
17	AP	78	GLN
18	AQ	85	GLN
20	AS	66	HIS
20	AS	97	GLN
22	AU	109	ASN
23	AV	87	HIS
23	AV	383	HIS
23	AV	388	GLN
23	AV	391	GLN
24	AW	91	GLN
25	AX	69	ASN
25	AX	148	GLN
25	AX	385	ASN
26	AY	381	ASN
28	A0	145	HIS
29	A1	235	ASN
30	A2	113	ASN
32	A4	322	HIS
32	A4	355	GLN
32	A4	590	GLN
32	A4	626	GLN
39	D	195	ASN
40	E	202	GLN
41	F	188	HIS

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Mol	Chain	Res	Type
41	F	223	HIS
42	I	43	GLN
42	I	151	ASN
42	I	225	GLN
43	J	116	HIS
44	K	89	GLN
44	K	117	HIS
45	L	48	ASN
49	P	79	HIS
49	P	115	HIS
50	Q	253	GLN
52	S	118	ASN
53	T	126	HIS
53	T	204	HIS
56	W	62	HIS
57	X	27	HIS
57	X	172	GLN
58	Y	88	GLN
58	Y	99	HIS
58	Y	179	HIS
61	1	31	ASN
63	3	170	ASN
65	5	160	HIS
65	5	275	ASN
65	5	384	GLN
66	6	69	HIS
66	6	292	GLN
66	6	332	HIS
67	7	34	GLN
68	8	177	HIS
68	8	186	GLN
71	b	27	GLN
71	b	120	HIS
71	b	129	GLN
71	b	135	ASN
72	c	42	GLN
72	c	77	HIS
72	c	107	GLN
72	c	168	HIS
72	c	177	GLN
74	e	67	GLN
74	e	248	ASN

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Mol	Chain	Res	Type
74	e	251	HIS
75	f	158	GLN
78	i	120	HIS
78	i	124	HIS
79	j	30	GLN
81	l	67	GLN
84	p	152	GLN
85	q	180	GLN
86	r	79	HIS
86	r	109	GLN
86	r	123	HIS
87	s	107	GLN
87	s	423	HIS
89	H	156	GLN
90	z	276	ASN
88	t1	129	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	AA	953/954 (99%)	135 (14%)	4 (0%)
33	Aw	65/68 (95%)	23 (35%)	0
34	Ax	67/70 (95%)	11 (16%)	0
35	Ay	52/70 (74%)	9 (17%)	0
36	Az	33/34 (97%)	10 (30%)	0
37	A	1554/1558 (99%)	233 (14%)	8 (0%)
38	B	70/72 (97%)	12 (17%)	0
All	All	2794/2826 (98%)	433 (15%)	12 (0%)

All (433) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	AA	651	A
2	AA	680	U
2	AA	688	A
2	AA	695	A
2	AA	704	U
2	AA	721	U
2	AA	737	C
2	AA	738	A
2	AA	753	A

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Mol	Chain	Res	Type
2	AA	761	A
2	AA	764	A
2	AA	765	C
2	AA	766	G
2	AA	791	G
2	AA	794	U
2	AA	796	G
2	AA	815	C
2	AA	830	U
2	AA	832	U
2	AA	835	C
2	AA	851	A
2	AA	852	A
2	AA	860	A
2	AA	861	U
2	AA	866	A
2	AA	868	C
2	AA	871	A
2	AA	872	G
2	AA	890	C
2	AA	902	G
2	AA	903	U
2	AA	904	C
2	AA	907	A
2	AA	908	C
2	AA	919	A
2	AA	923	A
2	AA	929	A
2	AA	931	C
2	AA	932	C
2	AA	933	G
2	AA	938	A
2	AA	939	A
2	AA	942	A
2	AA	943	G
2	AA	947	U
2	AA	958	C
2	AA	959	C
2	AA	960	C
2	AA	962	C
2	AA	967	A
2	AA	992	U

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Mol	Chain	Res	Type
2	AA	993	A
2	AA	1001	C
2	AA	1010	A
2	AA	1011	C
2	AA	1012	A
2	AA	1015	A
2	AA	1042	U
2	AA	1049	A
2	AA	1065	C
2	AA	1082	A
2	AA	1103	A
2	AA	1105	C
2	AA	1107	U
2	AA	1109	A
2	AA	1117	A
2	AA	1118	A
2	AA	1121	A
2	AA	1126	A
2	AA	1128	C
2	AA	1137	A
2	AA	1151	C
2	AA	1153	C
2	AA	1160	A
2	AA	1179	G
2	AA	1187	U
2	AA	1188	A
2	AA	1189	U
2	AA	1190	C
2	AA	1215	U
2	AA	1220	A
2	AA	1223	C
2	AA	1225	C
2	AA	1236	C
2	AA	1247	G
2	AA	1248	C
2	AA	1251	A
2	AA	1258	A
2	AA	1271	C
2	AA	1273	G
2	AA	1275	A
2	AA	1283	A
2	AA	1284	U

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Mol	Chain	Res	Type
2	AA	1290	C
2	AA	1291	U
2	AA	1299	A
2	AA	1326	A
2	AA	1327	G
2	AA	1328	G
2	AA	1343	A
2	AA	1344	U
2	AA	1354	A
2	AA	1356	A
2	AA	1378	C
2	AA	1387	A
2	AA	1390	A
2	AA	1405	C
2	AA	1407	U
2	AA	1430	A
2	AA	1463	G
2	AA	1478	A
2	AA	1482	A
2	AA	1503	G
2	AA	1507	A
2	AA	1513	A
2	AA	1514	A
2	AA	1519	A
2	AA	1521	U
2	AA	1525	C
2	AA	1526	U
2	AA	1527	A
2	AA	1531	C
2	AA	1537	C
2	AA	1539	C
2	AA	1540	A
2	AA	1551	G
2	AA	1557	A
2	AA	1568	U
2	AA	1571	U
2	AA	1582	G
2	AA	1584	MA6
2	AA	1585	A
2	AA	1594	G
2	AA	1595	G
2	AA	1599	A

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Mol	Chain	Res	Type
33	Aw	3	G
33	Aw	7	A
33	Aw	8	U
33	Aw	9	A
33	Aw	10	G
33	Aw	14	A
33	Aw	15	A
33	Aw	16	A
33	Aw	21	A
33	Aw	22	A
33	Aw	30	U
33	Aw	36	C
33	Aw	46	A
33	Aw	49	U
33	Aw	50	A
33	Aw	53	A
33	Aw	56	A
33	Aw	66	U
33	Aw	68	U
33	Aw	69	A
33	Aw	71	C
33	Aw	74	C
33	Aw	76	A
34	Ax	2	A
34	Ax	3	G
34	Ax	8	U
34	Ax	9	A
34	Ax	25	C
34	Ax	44	A
34	Ax	45	G
34	Ax	46	A
34	Ax	49	G
34	Ax	59	U
34	Ax	76	A
35	Ay	3	G
35	Ay	4	G
35	Ay	44	A
35	Ay	45	G
35	Ay	48	U
35	Ay	49	G
35	Ay	59	U
35	Ay	75	C

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Mol	Chain	Res	Type
35	Ay	76	A
36	Az	0	U
36	Az	11	U
36	Az	12	U
36	Az	13	U
36	Az	18	A
36	Az	22	A
36	Az	25	U
36	Az	26	A
36	Az	27	C
36	Az	32	A
37	A	1681	G
37	A	1689	C
37	A	1692	A
37	A	1694	U
37	A	1699	C
37	A	1700	U
37	A	1704	U
37	A	1708	A
37	A	1711	C
37	A	1713	A
37	A	1724	A
37	A	1727	A
37	A	1728	U
37	A	1736	A
37	A	1748	G
37	A	1765	C
37	A	1777	A
37	A	1805	A
37	A	1806	U
37	A	1807	U
37	A	1808	A
37	A	1809	U
37	A	1821	A
37	A	1827	C
37	A	1828	A
37	A	1829	A
37	A	1832	A
37	A	1836	A
37	A	1844	A
37	A	1854	U
37	A	1856	A

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Mol	Chain	Res	Type
37	A	1869	A
37	A	1871	A
37	A	1873	A
37	A	1882	A
37	A	1887	A
37	A	1893	A
37	A	1894	G
37	A	1901	C
37	A	1903	C
37	A	1918	G
37	A	1937	A
37	A	1940	A
37	A	1958	G
37	A	1985	G
37	A	1992	C
37	A	1994	A
37	A	2003	A
37	A	2015	G
37	A	2022	G
37	A	2030	U
37	A	2031	A
37	A	2036	C
37	A	2037	U
37	A	2038	U
37	A	2039	A
37	A	2054	U
37	A	2055	U
37	A	2060	A
37	A	2070	C
37	A	2071	U
37	A	2079	C
37	A	2099	U
37	A	2113	G
37	A	2125	C
37	A	2126	U
37	A	2147	G
37	A	2159	U
37	A	2161	A
37	A	2163	A
37	A	2168	U
37	A	2171	U
37	A	2181	A

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Mol	Chain	Res	Type
37	A	2184	A
37	A	2185	G
37	A	2196	A
37	A	2198	A
37	A	2200	A
37	A	2207	A
37	A	2214	A
37	A	2219	C
37	A	2221	C
37	A	2222	U
37	A	2223	A
37	A	2224	C
37	A	2225	C
37	A	2227	A
37	A	2230	A
37	A	2232	A
37	A	2233	U
37	A	2237	A
37	A	2241	A
37	A	2243	A
37	A	2245	A
37	A	2246	A
37	A	2262	C
37	A	2263	C
37	A	2284	C
37	A	2285	U
37	A	2294	A
37	A	2296	U
37	A	2297	A
37	A	2300	G
37	A	2316	U
37	A	2322	C
37	A	2331	C
37	A	2332	C
37	A	2345	G
37	A	2349	G
37	A	2350	A
37	A	2353	A
37	A	2363	A
37	A	2372	U
37	A	2374	A
37	A	2390	A

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Mol	Chain	Res	Type
37	A	2399	A
37	A	2404	U
37	A	2407	U
37	A	2415	C
37	A	2445	U
37	A	2478	G
37	A	2488	C
37	A	2493	C
37	A	2500	A
37	A	2520	C
37	A	2521	A
37	A	2524	A
37	A	2527	A
37	A	2558	A
37	A	2570	C
37	A	2571	G
37	A	2577	C
37	A	2592	G
37	A	2593	G
37	A	2600	A
37	A	2601	A
37	A	2603	C
37	A	2618	U
37	A	2627	G
37	A	2630	U
37	A	2633	A
37	A	2635	G
37	A	2654	U
37	A	2656	U
37	A	2683	C
37	A	2686	G
37	A	2694	A
37	A	2696	A
37	A	2706	A
37	A	2718	C
37	A	2719	G
37	A	2723	A
37	A	2724	G
37	A	2725	A
37	A	2732	G
37	A	2745	A
37	A	2758	G

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Mol	Chain	Res	Type
37	A	2762	C
37	A	2765	A
37	A	2767	A
37	A	2768	A
37	A	2774	C
37	A	2775	A
37	A	2780	C
37	A	2782	A
37	A	2783	A
37	A	2786	U
37	A	2787	A
37	A	2788	C
37	A	2791	A
37	A	2810	G
37	A	2832	A
37	A	2833	A
37	A	2840	C
37	A	2847	C
37	A	2864	U
37	A	2865	C
37	A	2882	U
37	A	2883	A
37	A	2884	C
37	A	2885	U
37	A	2887	U
37	A	2893	A
37	A	2911	C
37	A	2913	A
37	A	2917	G
37	A	2919	A
37	A	2922	A
37	A	2928	C
37	A	2935	A
37	A	2946	A
37	A	2960	U
37	A	2963	A
37	A	2971	A
37	A	2989	G
37	A	2990	A
37	A	2992	G
37	A	3000	A
37	A	3005	A

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Mol	Chain	Res	Type
37	A	3021	C
37	A	3041	U
37	A	3053	A
37	A	3054	G
37	A	3060	C
37	A	3090	G
37	A	3098	U
37	A	3100	U
37	A	3108	U
37	A	3109	U
37	A	3110	C
37	A	3111	A
37	A	3113	A
37	A	3122	U
37	A	3124	U
37	A	3157	C
37	A	3158	A
37	A	3162	C
37	A	3169	C
37	A	3172	C
37	A	3176	A
37	A	3183	U
37	A	3189	C
37	A	3199	U
37	A	3200	U
37	A	3207	A
37	A	3209	A
37	A	3210	C
37	A	3212	C
37	A	3217	A
37	A	3218	A
37	A	3228	U
37	A	3230	G
37	A	3231	U
38	B	8	U
38	B	10	2MG
38	B	16	C
38	B	21	A
38	B	45	G
38	B	48	U
38	B	54	C
38	B	55	U

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Mol	Chain	Res	Type
38	B	56	U
38	B	64	A
38	B	69	U
38	B	76	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AA	907	A
2	AA	1117	A
2	AA	1327	G
2	AA	1465	C
37	A	2030	U
37	A	2112	A
37	A	2222	U
37	A	2224	C
37	A	2245	A
37	A	2839	C
37	A	2883	A
37	A	3097	U

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

14 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	$\#\|Z\| > 2$
37	OMG	A	3040	93,33,37	23,26,27	2.42	8 (34%)	33,38,41	2.27	10 (30%)
37	PSU	A	3067	37	18,21,22	1.10	2 (11%)	22,30,33	1.90	6 (27%)
2	5MU	AA	1076	2	19,22,23	7.27	8 (42%)	28,32,35	3.28	10 (35%)
37	OMU	A	3039	93,37	19,22,23	2.99	8 (42%)	26,31,34	1.72	5 (19%)
2	B8T	AA	1486	92,2	19,22,23	3.31	8 (42%)	26,31,34	0.83	1 (3%)
71	THC	b	2	71	8,9,10	1.10	1 (12%)	9,11,13	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	OMG	A	2815	34,93,37	23,26,27	2.43	8 (34%)	33,38,41	2.22	10 (30%)
38	PSU	B	39	38	18,21,22	1.06	1 (5%)	22,30,33	1.82	5 (22%)
2	5MC	AA	1488	2	18,22,23	3.55	7 (38%)	26,32,35	0.97	1 (3%)
2	MA6	AA	1584	2	23,26,27	1.45	4 (17%)	34,38,41	3.48	12 (35%)
38	1MA	B	9	38	21,25,26	2.87	5 (23%)	31,37,40	1.68	5 (16%)
2	MA6	AA	1583	2	23,26,27	1.45	4 (17%)	34,38,41	3.41	11 (32%)
37	1MA	A	2617	37	21,25,26	2.89	5 (23%)	31,37,40	1.68	5 (16%)
38	2MG	B	10	38	23,26,27	2.96	9 (39%)	32,38,41	2.82	11 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OMG	A	3040	93,33,37	-	0/9/27/28	0/3/3/3
37	PSU	A	3067	37	-	0/7/25/26	0/2/2/2
2	5MU	AA	1076	2	-	0/7/25/26	0/2/2/2
37	OMU	A	3039	93,37	-	0/9/27/28	0/2/2/2
2	B8T	AA	1486	92,2	-	0/7/27/28	0/2/2/2
71	THC	b	2	71	-	0/8/10/12	-
37	OMG	A	2815	34,93,37	-	1/9/27/28	0/3/3/3
38	PSU	B	39	38	-	0/7/25/26	0/2/2/2
2	5MC	AA	1488	2	-	0/7/25/26	0/2/2/2
2	MA6	AA	1584	2	-	1/11/29/30	0/3/3/3
38	1MA	B	9	38	-	0/7/25/26	0/3/3/3
2	MA6	AA	1583	2	-	0/11/29/30	0/3/3/3
37	1MA	A	2617	37	-	0/7/25/26	0/3/3/3
38	2MG	B	10	38	-	1/9/27/28	0/3/3/3

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	1076	5MU	C4-C5	21.19	1.80	1.44
2	AA	1076	5MU	C6-N1	15.42	1.64	1.38
2	AA	1076	5MU	C6-C5	-11.93	1.15	1.34
2	AA	1076	5MU	C4-N3	-11.38	1.17	1.38
2	AA	1488	5MC	C6-C5	9.08	1.49	1.34
38	B	9	1MA	C2-N3	8.68	1.46	1.30
37	A	2617	1MA	C2-N3	8.65	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	B	10	2MG	C2-N3	7.76	1.46	1.31
2	AA	1486	B8T	C4-N3	6.97	1.44	1.32
37	A	3039	OMU	C2-N1	6.93	1.49	1.38
37	A	2617	1MA	C4-N3	6.82	1.49	1.35
38	B	9	1MA	C4-N3	6.74	1.49	1.35
37	A	3039	OMU	C2-N3	6.68	1.49	1.38
2	AA	1486	B8T	C2-N3	6.56	1.49	1.36
38	B	10	2MG	C4-N3	6.52	1.49	1.34
2	AA	1488	5MC	C4-N3	6.49	1.45	1.34
37	A	2815	OMG	C4-N3	6.42	1.49	1.34
37	A	3040	OMG	C4-N3	6.36	1.49	1.34
2	AA	1486	B8T	C6-C5	6.12	1.49	1.35
2	AA	1488	5MC	C2-N3	6.07	1.48	1.36
38	B	10	2MG	C2-N2	5.77	1.46	1.33
38	B	10	2MG	C2-N1	5.71	1.45	1.36
37	A	3039	OMU	C6-C5	5.59	1.48	1.35
37	A	2815	OMG	C2-N3	5.57	1.46	1.33
37	A	3040	OMG	C2-N3	5.46	1.46	1.33
2	AA	1486	B8T	C4-N4	5.13	1.46	1.35
37	A	2617	1MA	C2-N1	4.76	1.44	1.35
37	A	3040	OMG	C2-N2	4.73	1.45	1.34
38	B	9	1MA	C2-N1	4.66	1.44	1.35
37	A	2815	OMG	C2-N2	4.65	1.45	1.34
2	AA	1584	MA6	C6-N6	4.58	1.50	1.36
2	AA	1583	MA6	C6-N6	4.56	1.50	1.36
2	AA	1488	5MC	C6-N1	4.47	1.45	1.38
2	AA	1488	5MC	C4-N4	4.40	1.45	1.34
2	AA	1486	B8T	C2-N1	4.15	1.49	1.40
2	AA	1076	5MU	C2-N3	4.08	1.45	1.38
2	AA	1488	5MC	C2-N1	4.08	1.48	1.40
37	A	3039	OMU	C4-N3	4.00	1.45	1.38
38	B	9	1MA	C5-C6	3.78	1.53	1.43
2	AA	1486	B8T	C5-C4	3.77	1.48	1.40
37	A	2617	1MA	C5-C6	3.60	1.53	1.43
2	AA	1076	5MU	C2-N1	3.55	1.44	1.38
2	AA	1486	B8T	C6-N1	3.49	1.46	1.38
37	A	2815	OMG	C5-N7	-3.41	1.32	1.39
38	B	39	PSU	C6-C5	3.37	1.39	1.35
37	A	3067	PSU	C6-C5	3.34	1.39	1.35
37	A	3040	OMG	C5-N7	-3.07	1.33	1.39
37	A	2617	1MA	C5-N7	-2.97	1.33	1.39
37	A	3039	OMU	O4-C4	-2.97	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	B	9	1MA	C5-N7	-2.89	1.33	1.39
38	B	10	2MG	C5-C6	2.84	1.54	1.44
37	A	3039	OMU	C6-N1	2.82	1.44	1.38
38	B	10	2MG	C6-N1	2.82	1.44	1.38
2	AA	1486	B8T	O2-C2	-2.80	1.18	1.23
2	AA	1583	MA6	C5-C4	-2.75	1.33	1.39
2	AA	1584	MA6	C5-C4	-2.65	1.34	1.39
2	AA	1488	5MC	O2-C2	-2.64	1.18	1.23
37	A	3040	OMG	C2-N1	2.60	1.44	1.37
2	AA	1076	5MU	O4-C4	-2.59	1.18	1.23
37	A	2815	OMG	O6-C6	-2.57	1.18	1.23
37	A	3040	OMG	O6-C6	-2.52	1.18	1.23
37	A	2815	OMG	C2-N1	2.49	1.43	1.37
37	A	3040	OMG	C5-C6	2.48	1.53	1.44
37	A	2815	OMG	C5-C6	2.42	1.53	1.44
2	AA	1076	5MU	O2-C2	-2.41	1.18	1.23
37	A	3039	OMU	C5-C4	2.36	1.48	1.43
38	B	10	2MG	O6-C6	-2.32	1.19	1.23
71	b	2	THC	CA-N1	-2.32	1.43	1.46
37	A	3040	OMG	C6-N1	2.30	1.43	1.38
37	A	3039	OMU	O2-C2	-2.27	1.18	1.23
2	AA	1584	MA6	C5-N7	-2.21	1.34	1.39
38	B	10	2MG	C5-N7	-2.20	1.34	1.39
37	A	2815	OMG	C6-N1	2.18	1.42	1.38
2	AA	1583	MA6	C5-N7	-2.13	1.35	1.39
37	A	3067	PSU	O4'-C1'	-2.10	1.40	1.43
2	AA	1584	MA6	C8-N9	-2.08	1.33	1.37
2	AA	1583	MA6	C8-N9	-2.06	1.33	1.37
38	B	10	2MG	C8-N7	2.04	1.38	1.32

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	1584	MA6	N1-C6-N6	-14.18	101.58	117.08
2	AA	1583	MA6	N1-C6-N6	-13.82	101.98	117.08
2	AA	1076	5MU	C5-C4-N3	10.34	124.14	115.31
38	B	10	2MG	C1'-N9-C8	-7.91	104.19	126.70
2	AA	1076	5MU	C5-C6-N1	-7.53	115.59	123.34
2	AA	1584	MA6	C5-C6-N6	7.50	138.37	125.30
2	AA	1583	MA6	C5-C6-N6	7.28	137.98	125.30
38	B	10	2MG	C1'-N9-C4	6.88	146.93	126.50
2	AA	1076	5MU	C4-N3-C2	-6.81	118.53	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	B	10	2MG	C2-N3-C4	6.43	120.02	112.04
37	A	3040	OMG	C1'-N9-C4	-5.85	109.14	126.50
37	A	2815	OMG	C5-C4-N3	-5.71	119.19	128.46
37	A	3040	OMG	C1'-N9-C8	5.60	142.63	126.70
2	AA	1583	MA6	N1-C2-N3	-5.43	120.11	128.60
2	AA	1584	MA6	N1-C2-N3	-5.33	120.26	128.60
37	A	2617	1MA	N1-C2-N3	-5.29	119.71	126.00
37	A	3039	OMU	C4-N3-C2	-5.29	119.60	126.58
2	AA	1584	MA6	C5-C4-N3	-5.25	119.90	126.75
38	B	9	1MA	N1-C2-N3	-5.06	119.99	126.00
37	A	3040	OMG	C5-C4-N3	-5.03	120.30	128.46
2	AA	1583	MA6	C5-C4-N3	-5.02	120.20	126.75
37	A	2815	OMG	C1'-N9-C4	-4.94	111.82	126.50
37	A	2815	OMG	C1'-N9-C8	4.82	140.43	126.70
38	B	10	2MG	C5-C4-N3	-4.79	120.69	128.46
37	A	3067	PSU	N1-C2-N3	4.75	120.51	115.13
38	B	9	1MA	C5-C4-N3	-4.74	120.19	127.26
37	A	3067	PSU	C4-N3-C2	-4.68	119.59	126.34
38	B	39	PSU	C4-N3-C2	-4.60	119.72	126.34
37	A	2617	1MA	C5-C4-N3	-4.58	120.43	127.26
38	B	39	PSU	N1-C2-N3	4.56	120.30	115.13
37	A	2815	OMG	C2-N3-C4	4.53	120.37	112.30
2	AA	1583	MA6	N9-C8-N7	-4.52	107.72	113.91
2	AA	1076	5MU	N3-C2-N1	4.46	120.81	114.89
2	AA	1584	MA6	N9-C8-N7	-4.45	107.83	113.91
37	A	3040	OMG	C2-N3-C4	4.42	120.18	112.30
2	AA	1076	5MU	C5M-C5-C6	-4.39	116.98	122.85
38	B	10	2MG	C2-N1-C6	-4.15	119.71	124.48
38	B	9	1MA	C2-N3-C4	3.94	120.16	112.41
2	AA	1076	5MU	C5M-C5-C4	3.88	123.03	118.77
37	A	2617	1MA	C2-N3-C4	3.87	120.01	112.41
2	AA	1076	5MU	O4-C4-C5	-3.78	120.52	124.90
37	A	3039	OMU	N3-C2-N1	3.77	119.89	114.89
38	B	10	2MG	N9-C8-N7	-3.61	106.60	113.39
37	A	2815	OMG	N9-C4-N3	3.59	133.15	125.94
2	AA	1584	MA6	C4-C5-C6	3.59	119.90	115.88
2	AA	1584	MA6	C2-N3-C4	3.51	120.04	111.75
2	AA	1583	MA6	C2-N1-C6	3.49	119.99	111.75
2	AA	1583	MA6	C4-C5-C6	3.47	119.77	115.88
2	AA	1583	MA6	C2-N3-C4	3.45	119.90	111.75
2	AA	1584	MA6	C2-N1-C6	3.43	119.85	111.75
37	A	3039	OMU	C5-C4-N3	3.43	119.97	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	1584	MA6	N3-C4-N9	3.22	132.40	127.08
2	AA	1488	5MC	C5-C6-N1	-3.20	120.05	123.34
2	AA	1584	MA6	C5-N7-C8	3.15	107.99	103.51
2	AA	1583	MA6	N3-C4-N9	3.12	132.22	127.08
37	A	2815	OMG	C2-N1-C6	-3.09	119.46	125.10
2	AA	1583	MA6	C5-N7-C8	3.08	107.88	103.51
37	A	3040	OMG	N9-C4-N3	2.99	131.95	125.94
37	A	3040	OMG	N9-C8-N7	-2.90	107.93	113.39
37	A	3039	OMU	O4-C4-C5	-2.89	120.08	125.16
37	A	3040	OMG	C2-N1-C6	-2.81	119.97	125.10
37	A	3067	PSU	O2-C2-N1	-2.78	119.73	122.79
38	B	10	2MG	N9-C4-N3	2.67	131.30	125.94
37	A	2815	OMG	C5-C6-N1	2.67	119.97	113.19
37	A	3040	OMG	C5-C6-N1	2.67	119.96	113.19
38	B	39	PSU	O2-C2-N1	-2.66	119.87	122.79
2	AA	1583	MA6	C4-N9-C8	2.65	108.60	105.73
37	A	2815	OMG	N9-C8-N7	-2.64	108.42	113.39
38	B	10	2MG	C5-C6-N1	2.61	119.82	113.19
37	A	2617	1MA	N9-C8-N7	-2.57	108.56	113.39
38	B	9	1MA	N9-C8-N7	-2.56	108.57	113.39
38	B	10	2MG	N1-C2-N3	-2.51	120.07	123.95
37	A	2815	OMG	O6-C6-C5	-2.50	119.97	126.60
38	B	10	2MG	C8-N7-C5	2.50	108.76	104.24
2	AA	1076	5MU	O4-C4-N3	-2.49	115.34	120.12
2	AA	1076	5MU	O2-C2-N1	-2.47	119.50	122.79
37	A	3067	PSU	O4'-C1'-C2'	2.46	108.62	105.14
2	AA	1584	MA6	C4-N9-C8	2.44	108.38	105.73
38	B	10	2MG	O6-C6-C5	-2.44	120.14	126.60
37	A	3040	OMG	O6-C6-C5	-2.42	120.18	126.60
2	AA	1486	B8T	C6-C5-C4	2.41	119.91	116.96
38	B	39	PSU	C6-C5-C4	2.38	119.86	118.20
2	AA	1076	5MU	C6-C5-C4	2.33	119.98	118.03
37	A	3067	PSU	C6-N1-C2	-2.33	120.30	122.68
37	A	3067	PSU	C6-C5-C4	2.25	119.77	118.20
37	A	2617	1MA	N9-C4-N3	2.20	132.08	126.94
38	B	39	PSU	C6-N1-C2	-2.19	120.45	122.68
37	A	3039	OMU	O2-C2-N1	-2.11	119.98	122.79
38	B	9	1MA	N9-C4-N3	2.11	131.85	126.94
37	A	2815	OMG	C8-N7-C5	2.09	108.02	104.24
2	AA	1584	MA6	C4-C5-N7	-2.08	108.09	110.62
37	A	3040	OMG	C8-N7-C5	2.05	107.95	104.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AA	1584	MA6	C4'-C5'-O5'-P
37	A	2815	OMG	C4'-C5'-O5'-P
38	B	10	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	A	3067	PSU	1	0
2	AA	1076	5MU	1	0
37	A	3039	OMU	1	0
37	A	2815	OMG	1	0
2	AA	1584	MA6	2	0
2	AA	1583	MA6	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 246 ligands modelled in this entry, 237 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
98	GDP	AX	503	-	28,30,30	1.15	3 (10%)	44,47,47	1.84	7 (15%)
100	VOL	e	301	-	6,6,6	1.86	1 (16%)	4,7,7	2.27	1 (25%)
97	ATP	AX	501	92	29,33,33	3.10	10 (34%)	44,52,52	2.89	15 (34%)
96	FES	r	201	86,42	0,4,4	-	-	-		
96	FES	AT	201	14,21	0,4,4	-	-	-		
99	SPD	A	3301	-	9,9,9	0.31	0	8,8,8	0.86	0
94	5F0	AI	201	-	8,8,9	2.19	3 (37%)	7,9,11	2.52	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
91	NAD	AA	1701	92	45,48,48	3.58	19 (42%)	63,73,73	1.75	14 (22%)
96	FES	AP	201	6,17	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
100	VOL	e	301	-	-	2/6/6/6	-
97	ATP	AX	501	92	-	1/22/38/38	0/3/3/3
96	FES	r	201	86,42	-	-	0/1/1/1
96	FES	AT	201	14,21	-	-	0/1/1/1
99	SPD	A	3301	-	-	0/7/7/7	-
94	5F0	AI	201	-	-	0/9/9/10	-
91	NAD	AA	1701	92	-	3/30/62/62	0/5/5/5
98	GDP	AX	503	-	-	0/16/32/32	0/3/3/3
96	FES	AP	201	6,17	-	-	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AX	501	ATP	C2'-C3'	-10.67	1.24	1.53
91	AA	1701	NAD	C7N-N7N	9.62	1.51	1.33
91	AA	1701	NAD	C3D-C4D	-8.43	1.31	1.53
91	AA	1701	NAD	O4B-C1B	8.40	1.61	1.42
91	AA	1701	NAD	O4D-C4D	7.37	1.61	1.45
91	AA	1701	NAD	C2B-C1B	-7.15	1.30	1.53
91	AA	1701	NAD	O4D-C1D	-6.67	1.31	1.41
97	AX	501	ATP	C6-N6	6.39	1.50	1.34
91	AA	1701	NAD	O4B-C4B	-6.33	1.30	1.45
91	AA	1701	NAD	C3N-C7N	5.60	1.59	1.50
97	AX	501	ATP	O4'-C1'	-4.83	1.30	1.42
94	AI	201	5F0	O-C	4.79	1.47	1.19
100	e	301	VOL	O-C	-4.48	1.23	1.42
97	AX	501	ATP	C2'-C1'	4.36	1.67	1.53
91	AA	1701	NAD	O7N-C7N	-4.19	1.16	1.24
97	AX	501	ATP	C5'-C4'	-3.99	1.39	1.51
91	AA	1701	NAD	C5A-C4A	-3.82	1.31	1.39
97	AX	501	ATP	O3'-C3'	3.74	1.51	1.43
91	AA	1701	NAD	C8A-N9A	-3.53	1.31	1.37
91	AA	1701	NAD	O3D-C3D	3.20	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	AA	1701	NAD	O3B-C3B	-3.11	1.35	1.43
98	AX	503	GDP	C5-C4	3.07	1.47	1.38
97	AX	501	ATP	O4'-C4'	3.00	1.51	1.45
97	AX	501	ATP	C3'-C4'	2.97	1.60	1.53
91	AA	1701	NAD	O2B-C2B	2.79	1.49	1.43
94	AI	201	5F0	OD1-C1	2.61	1.39	1.33
97	AX	501	ATP	C5-C4	-2.61	1.34	1.39
91	AA	1701	NAD	C5N-C4N	-2.60	1.33	1.38
98	AX	503	GDP	C6-N1	-2.45	1.34	1.38
91	AA	1701	NAD	C5A-N7A	-2.34	1.34	1.39
97	AX	501	ATP	O2'-C2'	2.32	1.48	1.43
91	AA	1701	NAD	C6A-N6A	2.24	1.39	1.34
94	AI	201	5F0	CB-C	2.18	1.55	1.49
98	AX	503	GDP	C5-N7	-2.18	1.34	1.39
91	AA	1701	NAD	C4N-C3N	-2.15	1.35	1.39
91	AA	1701	NAD	C8A-N7A	2.03	1.35	1.31

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
97	AX	501	ATP	C1'-N9-C8	-8.41	108.15	127.14
97	AX	501	ATP	N9-C8-N7	-6.30	105.30	113.91
98	AX	503	GDP	C5-C4-N3	-6.13	118.51	128.46
97	AX	501	ATP	C4-N9-C1'	5.79	140.40	126.59
97	AX	501	ATP	N6-C6-N1	-5.79	105.67	118.35
97	AX	501	ATP	N3-C2-N1	-5.49	120.01	128.60
91	AA	1701	NAD	N3A-C2A-N1A	-5.45	120.08	128.60
94	AI	201	5F0	O-C-CB	-5.38	109.76	125.43
97	AX	501	ATP	C4-N9-C8	5.28	111.45	105.73
91	AA	1701	NAD	C5A-C4A-N3A	-5.25	119.90	126.75
97	AX	501	ATP	C5-C6-N6	5.04	134.41	123.43
98	AX	503	GDP	C2-N3-C4	4.86	120.97	112.30
98	AX	503	GDP	N9-C4-N3	4.71	135.39	125.94
91	AA	1701	NAD	N9A-C8A-N7A	-4.65	107.55	113.91
97	AX	501	ATP	C5-C4-N3	-4.59	120.76	126.75
100	e	301	VOL	O-C-CA	4.51	120.91	111.43
97	AX	501	ATP	N3-C4-N9	3.85	133.42	127.08
98	AX	503	GDP	PA-O3A-PB	-3.82	119.71	132.83
97	AX	501	ATP	C5-N7-C8	3.82	108.93	103.51
91	AA	1701	NAD	C2A-N3A-C4A	3.69	120.46	111.75
91	AA	1701	NAD	C1B-N9A-C8A	-3.61	118.99	127.14
91	AA	1701	NAD	N3A-C4A-N9A	3.51	132.87	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
97	AX	501	ATP	C2-N3-C4	3.28	119.51	111.75
94	AI	201	5F0	OD1-C1-CA	3.28	119.92	111.52
91	AA	1701	NAD	C5A-N7A-C8A	3.20	108.05	103.51
98	AX	503	GDP	C6-C5-N7	3.13	136.08	130.25
91	AA	1701	NAD	C4A-N9A-C8A	2.78	108.74	105.73
97	AX	501	ATP	PB-O3B-PG	-2.68	123.62	132.83
98	AX	503	GDP	C4-C5-N7	-2.59	106.62	110.72
97	AX	501	ATP	C3'-C2'-C1'	2.51	106.20	101.43
97	AX	501	ATP	PA-O3A-PB	-2.50	124.23	132.83
91	AA	1701	NAD	C4A-N9A-C1B	2.38	132.26	126.59
91	AA	1701	NAD	C3N-C7N-N7N	2.32	120.53	117.75
91	AA	1701	NAD	C6N-N1N-C2N	-2.24	119.93	121.97
98	AX	503	GDP	O6-C6-C5	-2.17	120.86	126.60
91	AA	1701	NAD	O7N-C7N-N7N	-2.16	119.51	122.58
91	AA	1701	NAD	PN-O3-PA	-2.13	125.51	132.83
97	AX	501	ATP	O4'-C1'-N9	2.12	112.24	108.06
91	AA	1701	NAD	C5A-C6A-N1A	2.01	121.70	117.39

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
100	e	301	VOL	O-C-CA-N
100	e	301	VOL	O-C-CA-CB
91	AA	1701	NAD	O4D-C4D-C5D-O5D
91	AA	1701	NAD	C3D-C4D-C5D-O5D
91	AA	1701	NAD	C4B-C5B-O5B-PA
97	AX	501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

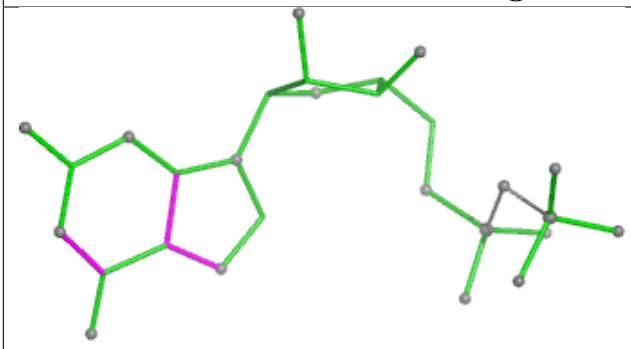
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	AA	1701	NAD	1	0

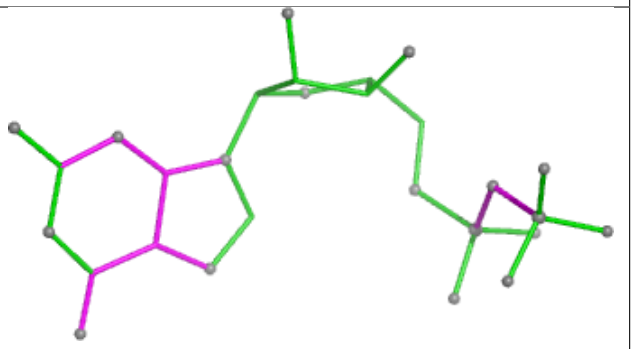
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

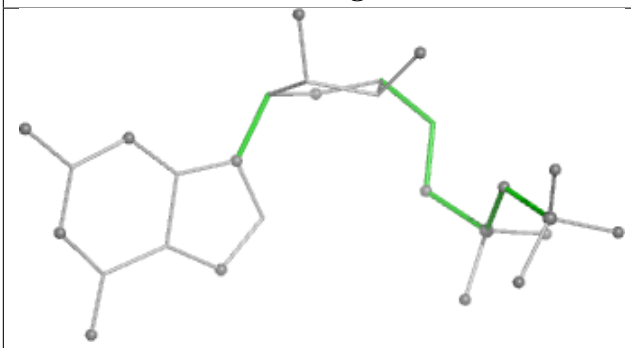
Ligand GDP AX 503



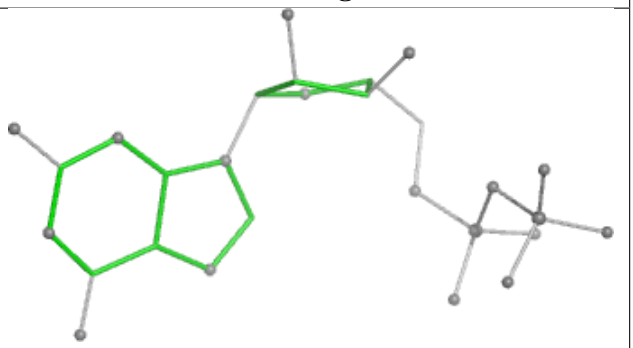
Bond lengths



Bond angles

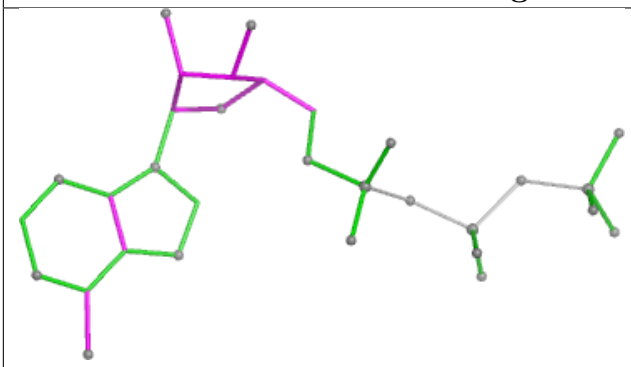


Torsions

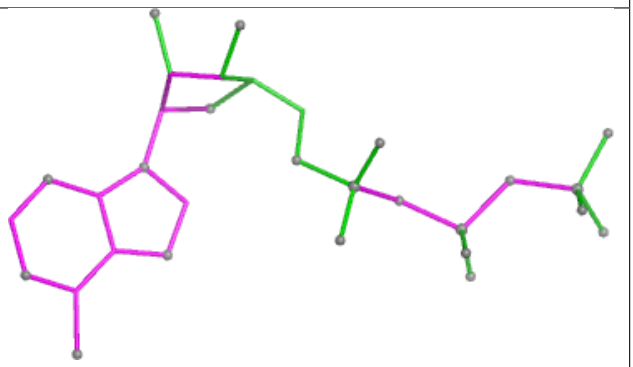


Rings

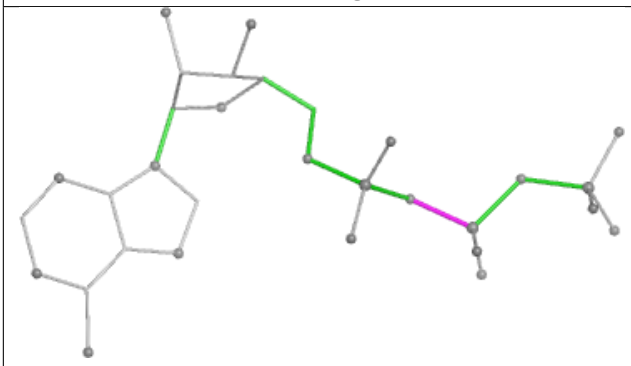
Ligand ATP AX 501



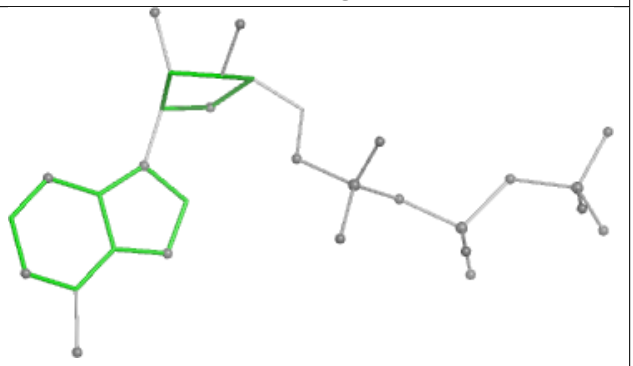
Bond lengths



Bond angles

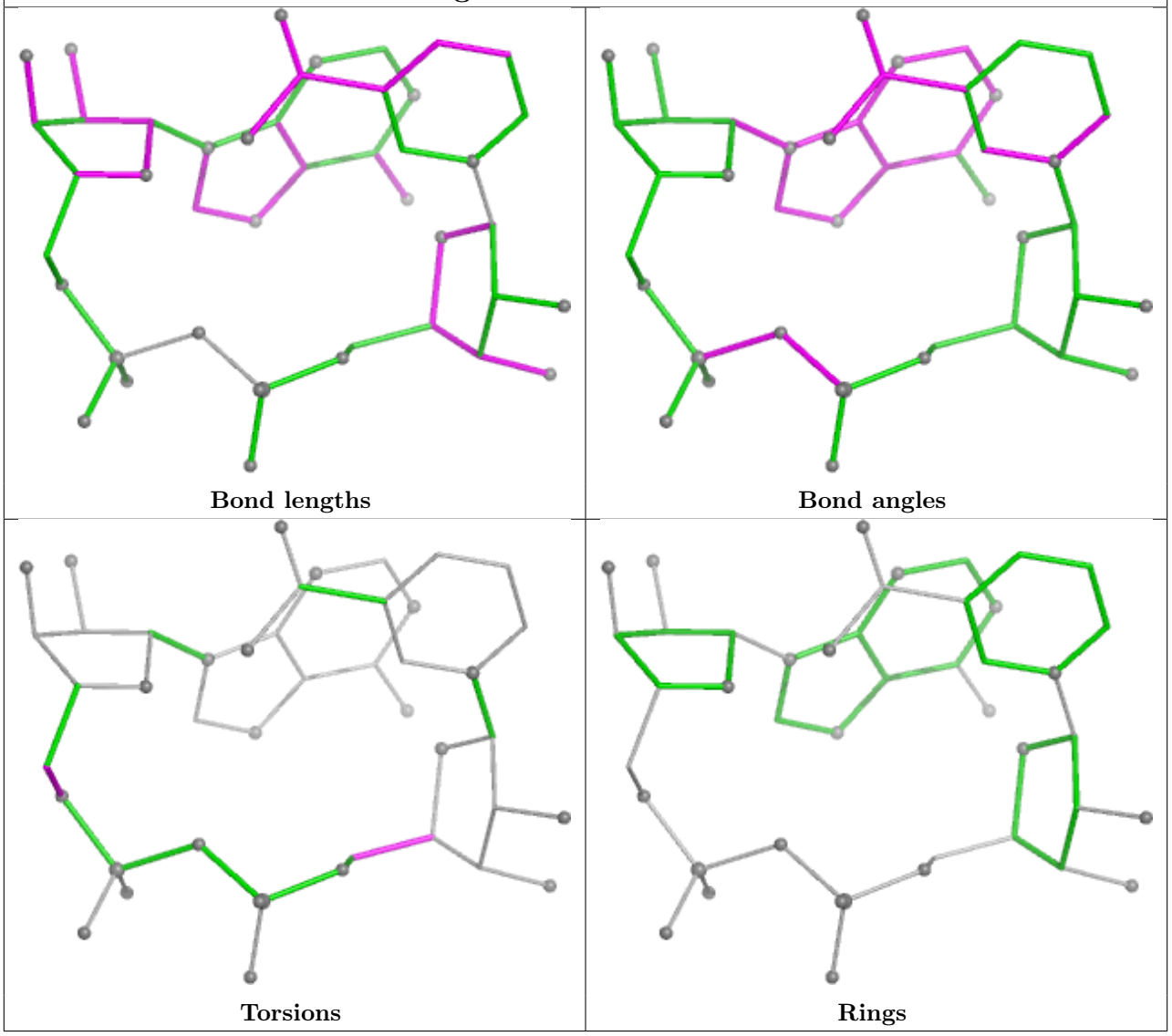


Torsions



Rings

Ligand NAD AA 1701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	Aw	3
34	Ax	2
35	Ay	1
37	A	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
10	AI	1
38	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ay	15:A	O3'	21:A	P	9.66
1	A	2357:C	O3'	2361:G	P	9.59
1	Ax	15:A	O3'	21:A	P	8.45
1	AI	183:HIS	C	185:GLY	N	4.99
1	B	56:U	O3'	58:A	P	4.53
1	Aw	56:A	O3'	61:U	P	4.02
1	Ax	46:A	O3'	48:U	P	3.84
1	Aw	46:A	O3'	48:U	P	3.74
1	Aw	16:A	O3'	20:C	P	3.14

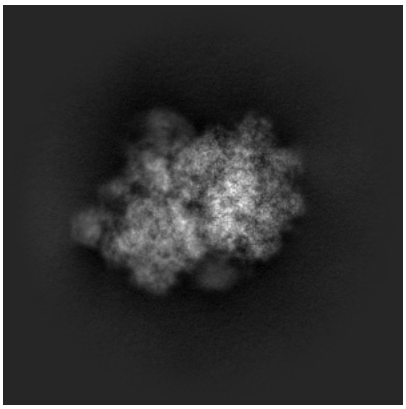
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54264. These allow visual inspection of the internal detail of the map and identification of artifacts.

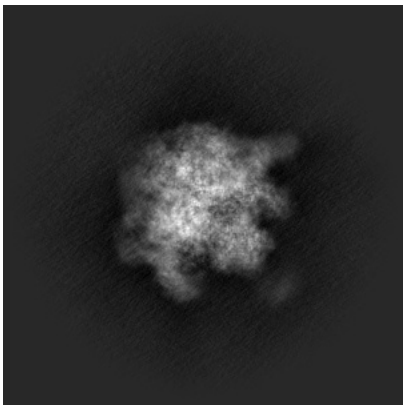
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

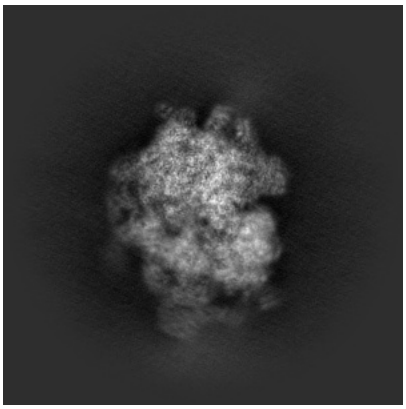
6.1.1 Primary map



X

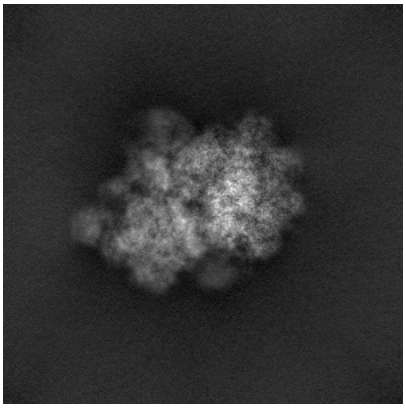


Y

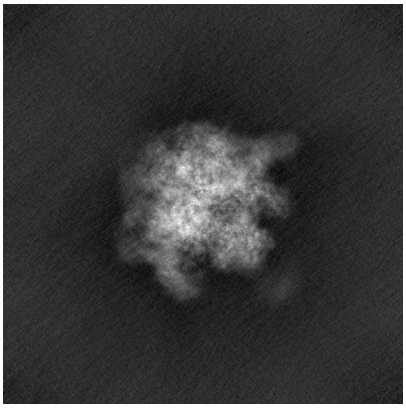


Z

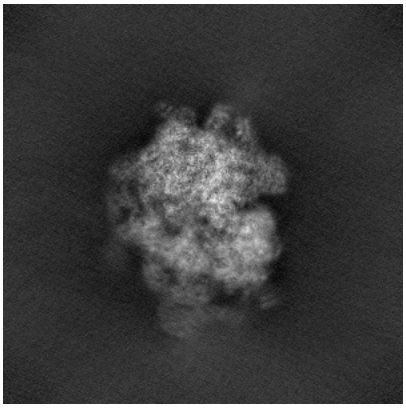
6.1.2 Raw map



X



Y

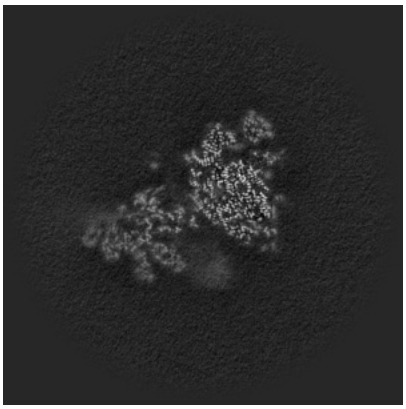


Z

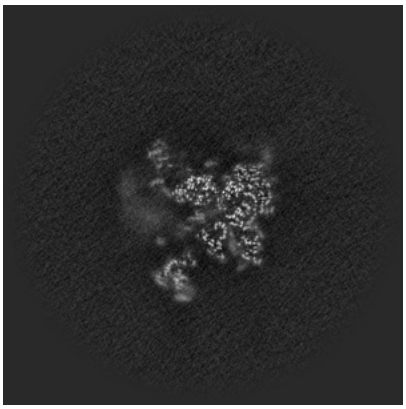
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

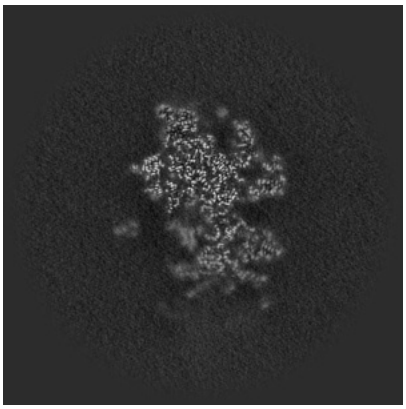
6.2.1 Primary map



X Index: 320

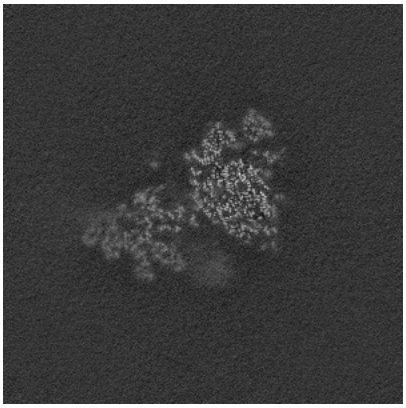


Y Index: 320

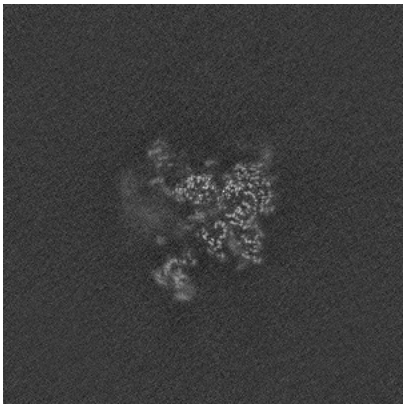


Z Index: 320

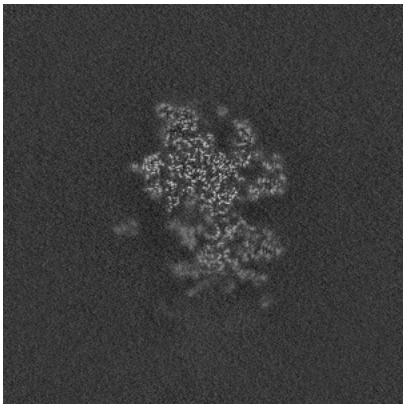
6.2.2 Raw map



X Index: 320



Y Index: 320

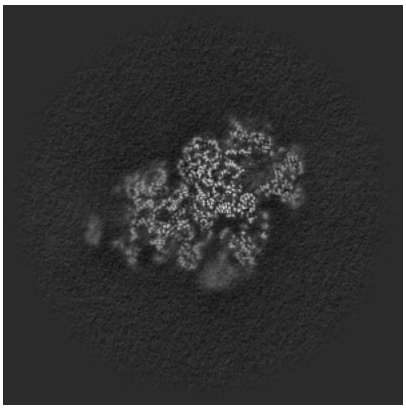


Z Index: 320

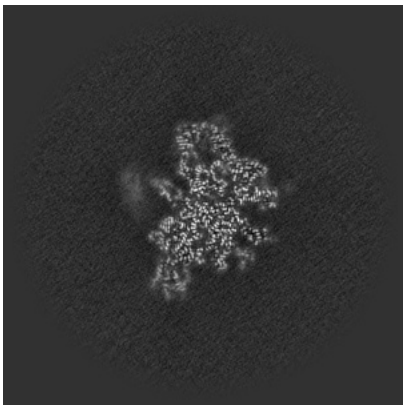
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

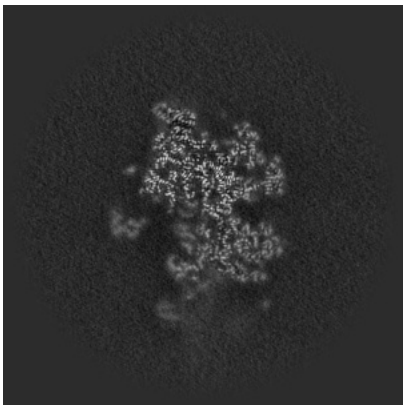
6.3.1 Primary map



X Index: 346

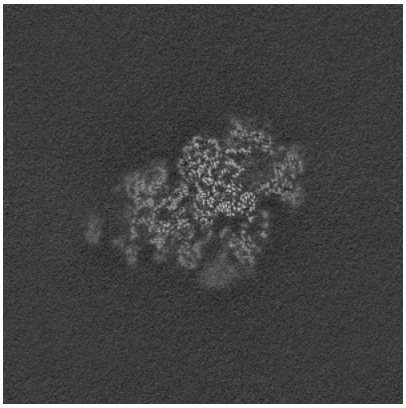


Y Index: 362

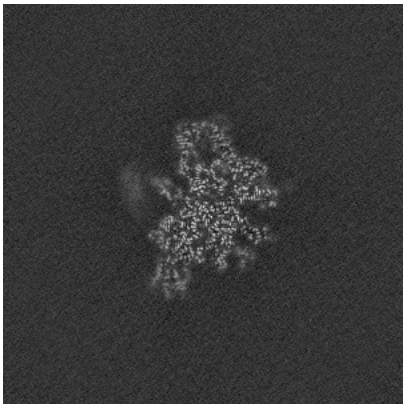


Z Index: 311

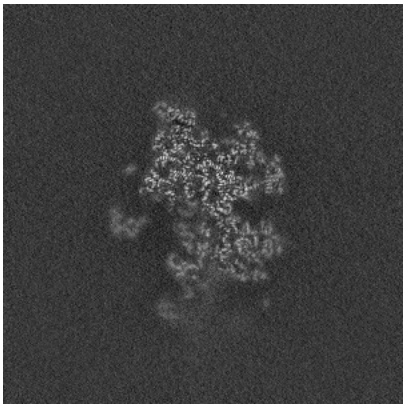
6.3.2 Raw map



X Index: 346



Y Index: 362

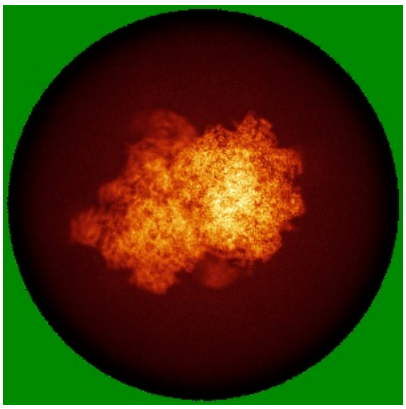


Z Index: 310

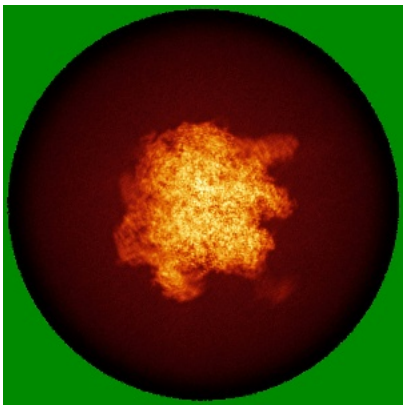
The images above show the largest variance slices of the map in three orthogonal directions.

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

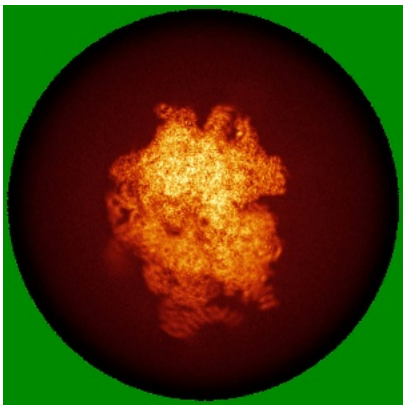
6.4.1 Primary map



X

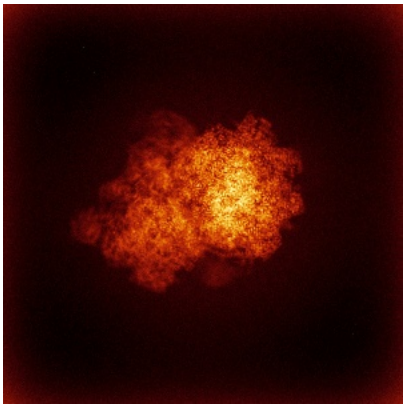


Y

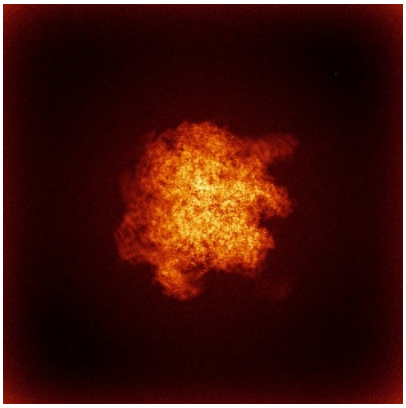


Z

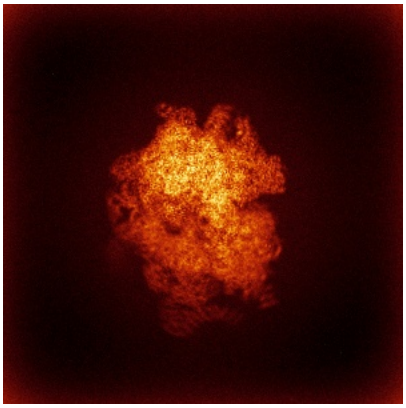
6.4.2 Raw map



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)

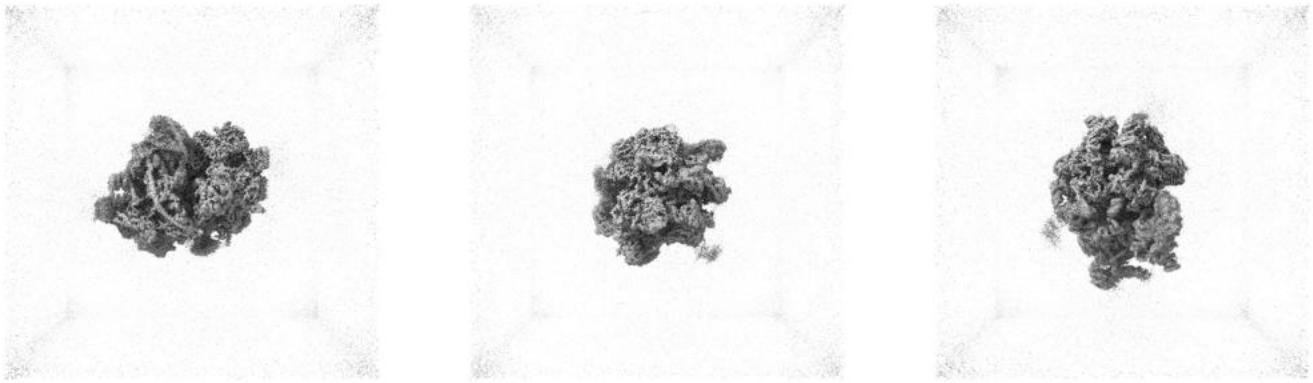
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

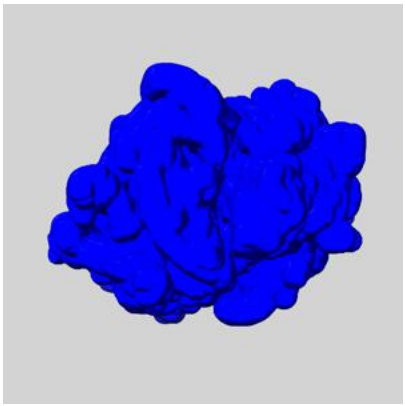
6.6 Mask visualisation

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

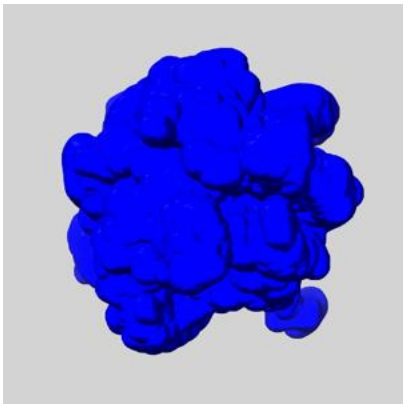
A mask typically either:

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

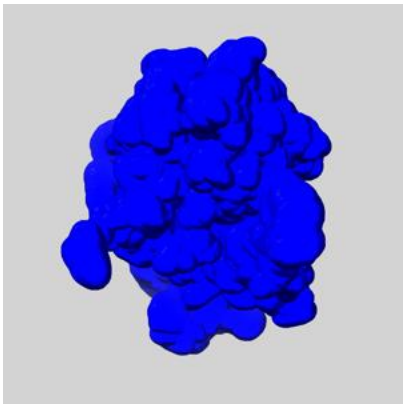
6.6.1 emd_54264_msk_1.map



X



Y

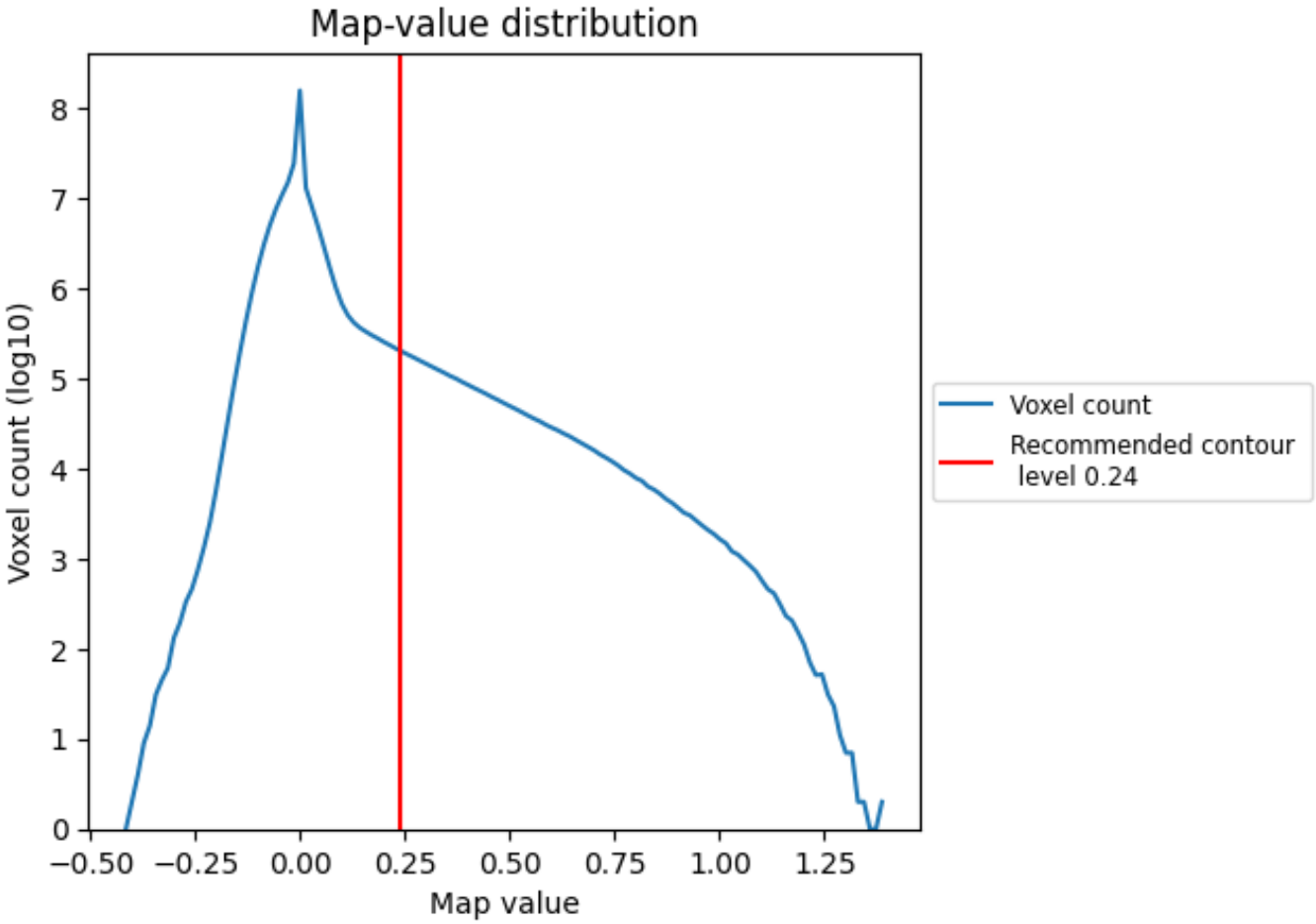


Z

7 Map analysis

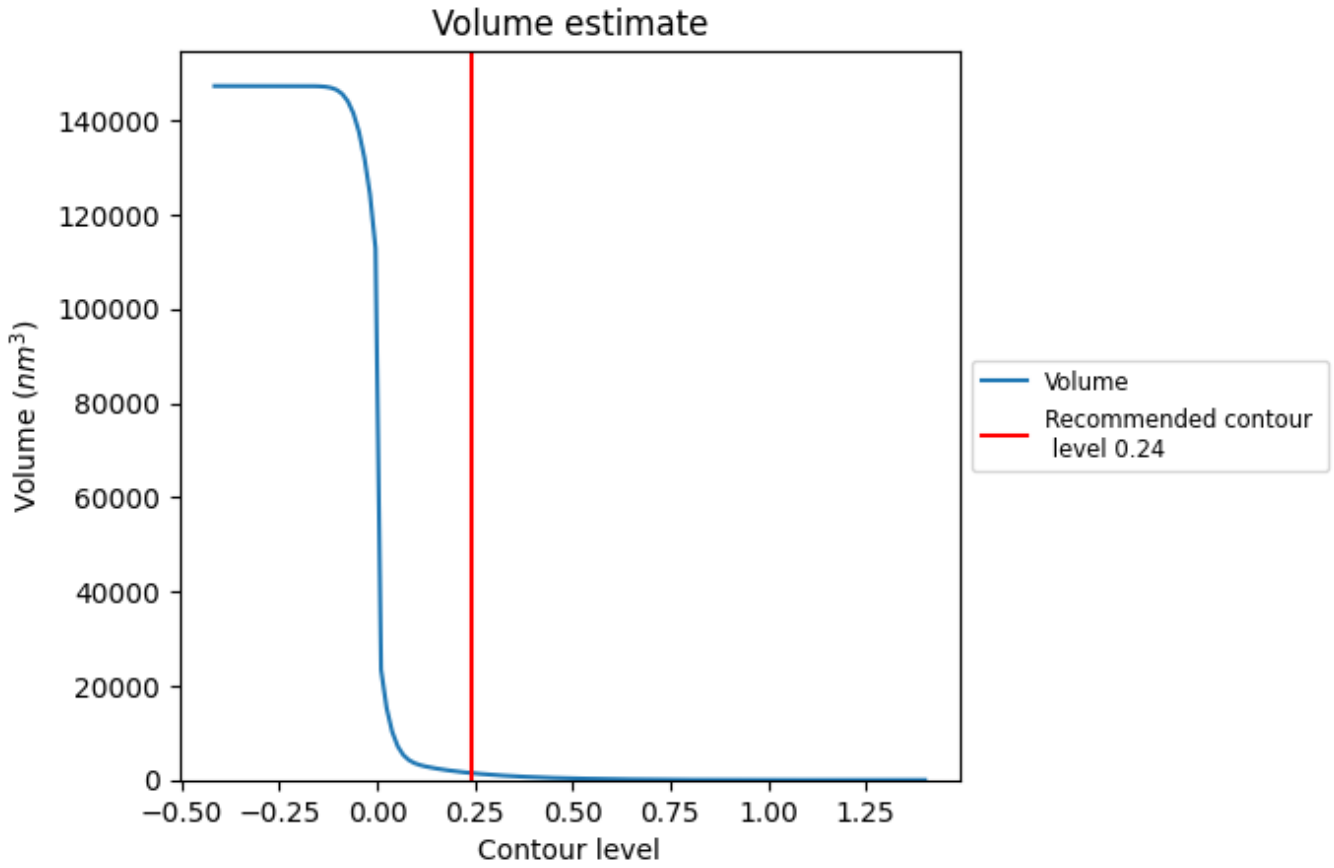
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

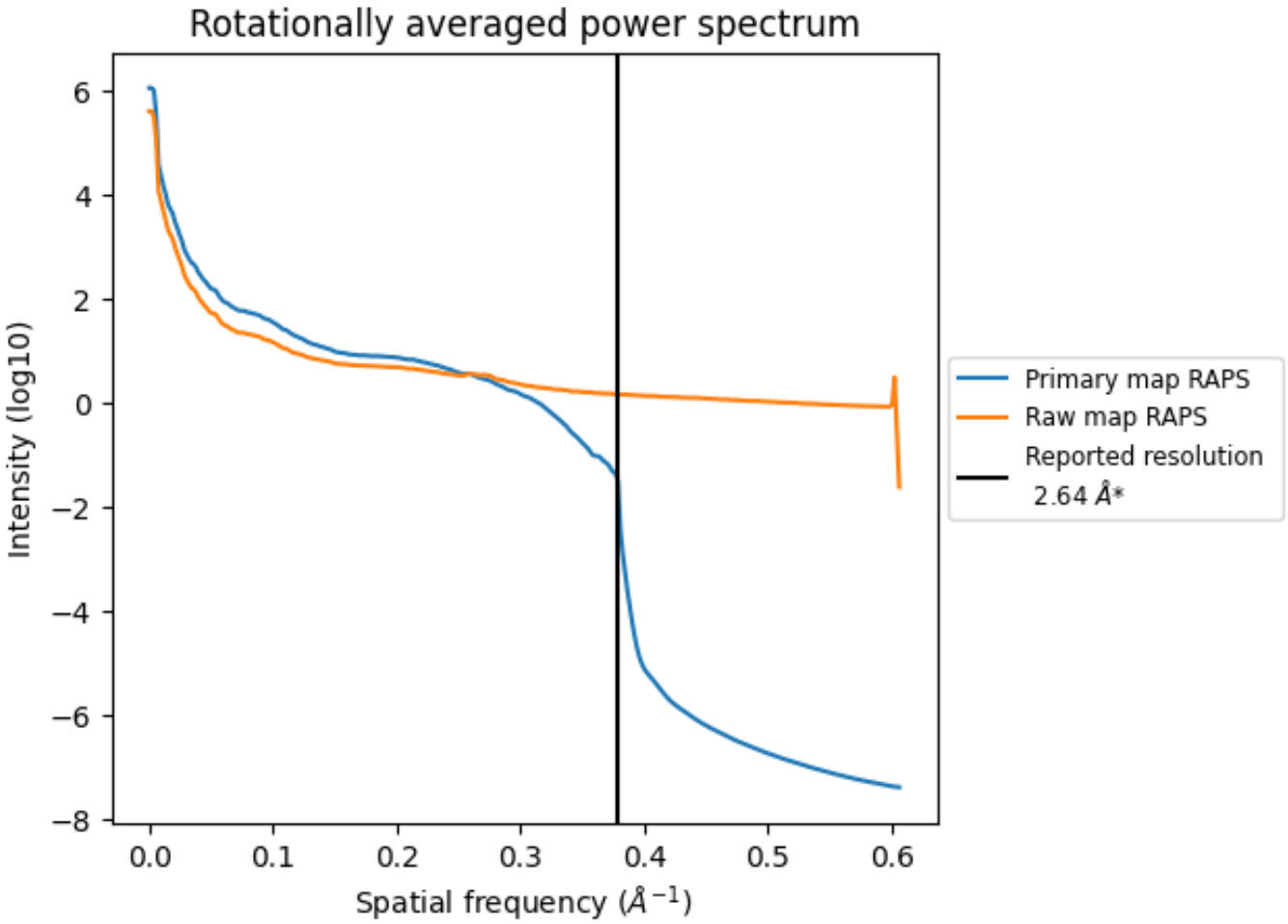
7.2 Volume estimate



The volume at the recommended contour level is 1476 nm^3; this corresponds to an approximate mass of 1333 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)

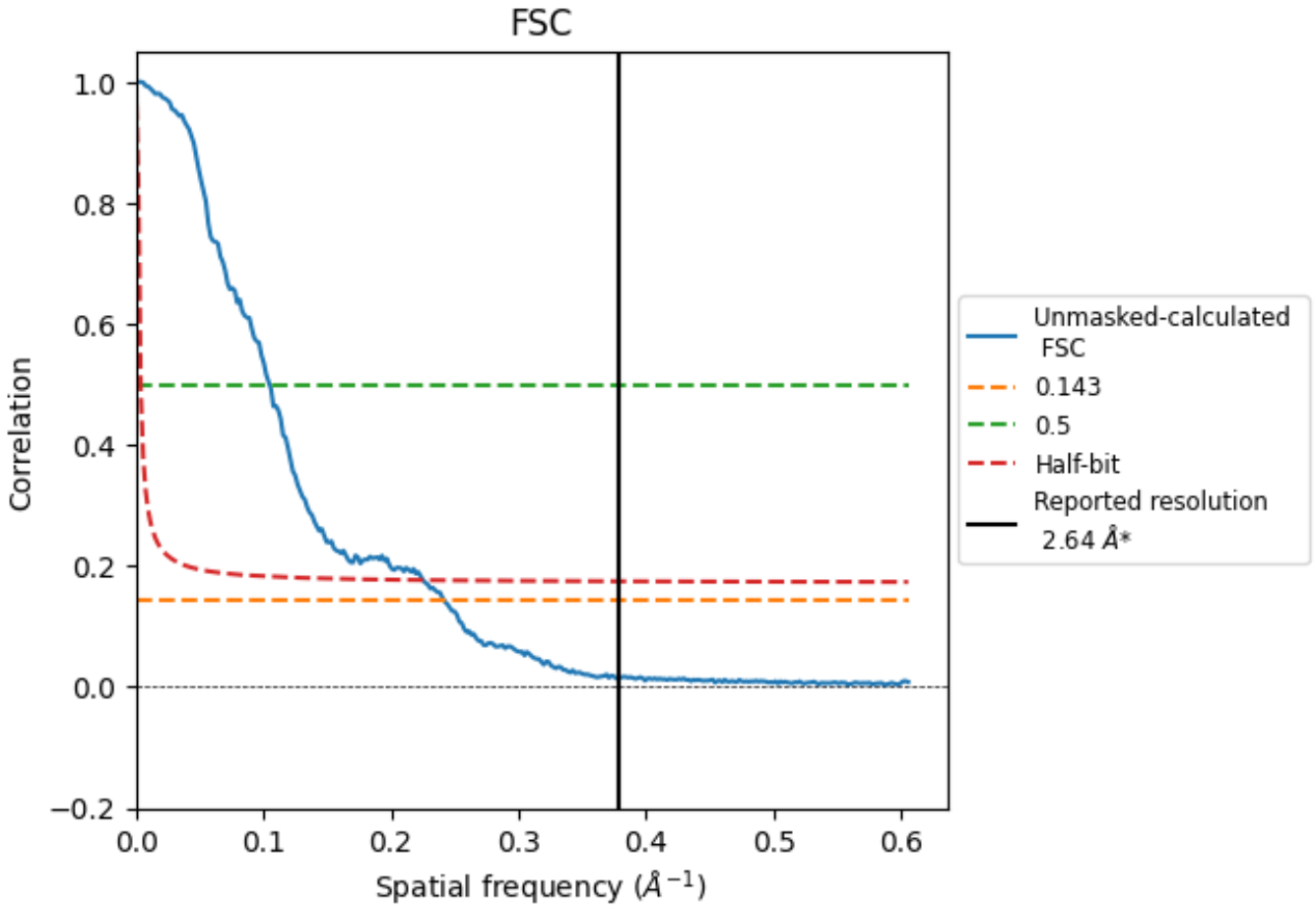


*Reported resolution corresponds to spatial frequency of 0.379 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.379 Å^{-1}

8.2 Resolution estimates (i)

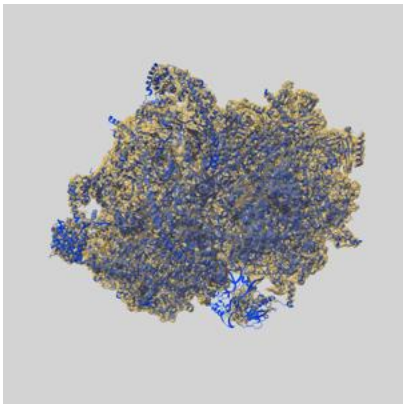
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	9.54	4.44

*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 4.14 differs from the reported value 2.64 by more than 10 %

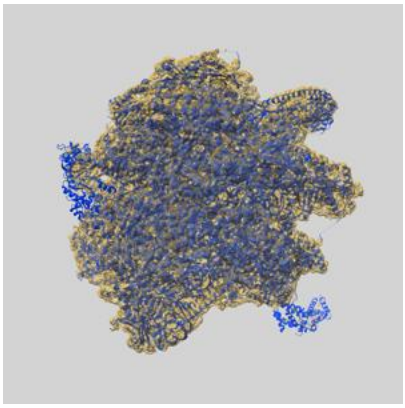
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54264 and PDB model 9RU6. Per-residue inclusion information can be found in section 3 on page 26.

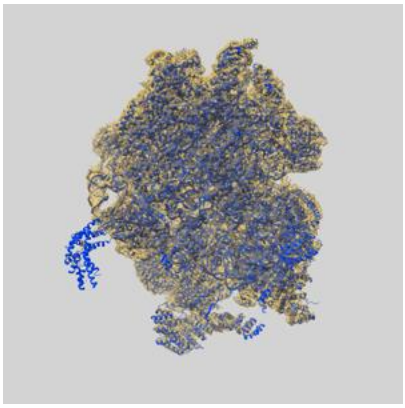
9.1 Map-model overlay



X



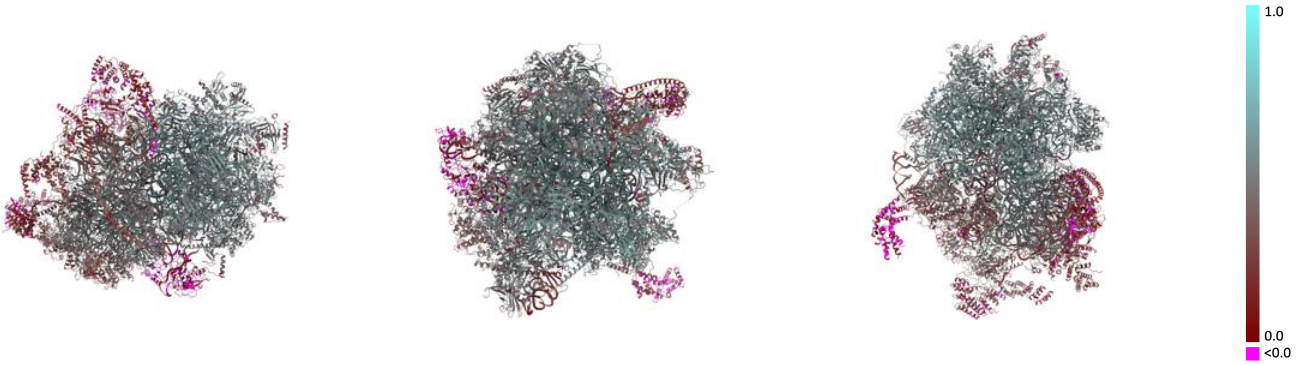
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24 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.

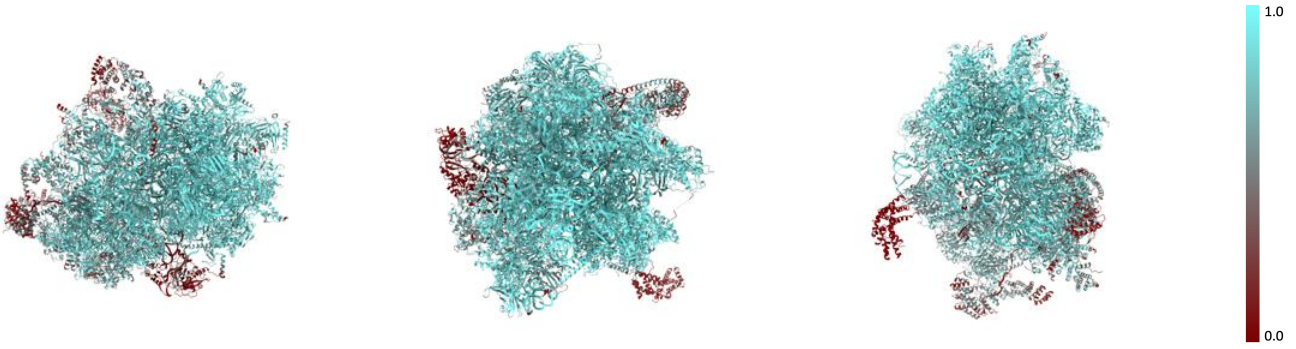
9.2 Q-score mapped to coordinate model (i)



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.

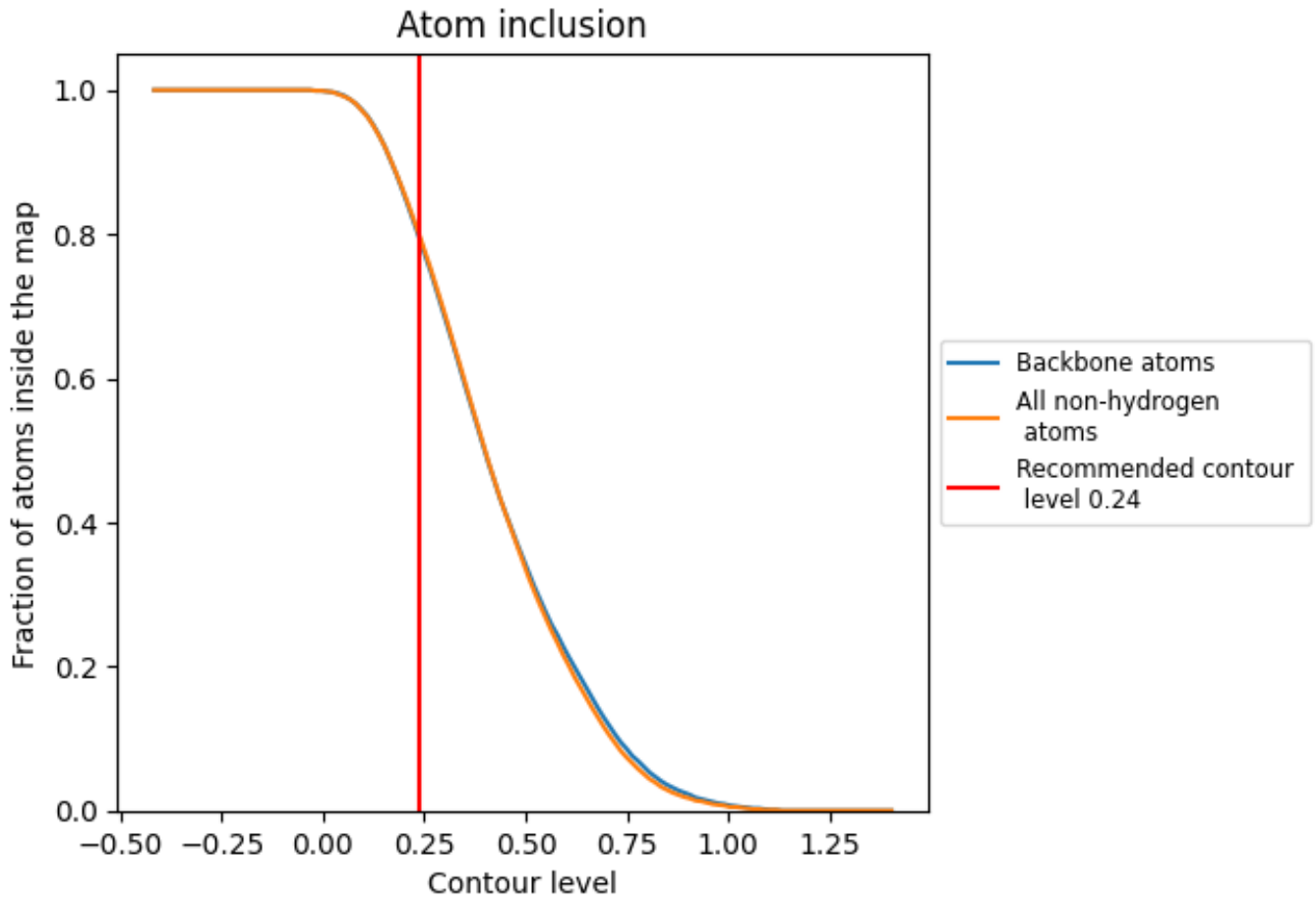
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.24).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 80% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.4390
0	0.8920	0.5290
1	0.8270	0.5130
2	0.9560	0.5850
3	0.9410	0.5860
4	0.9140	0.5600
5	0.8840	0.5100
6	0.8680	0.4750
7	0.8510	0.4760
8	0.6510	0.3450
9	0.8740	0.4930
A	0.9620	0.5480
A0	0.5100	0.2030
A1	0.6630	0.3270
A2	0.7120	0.4220
A3	0.7680	0.4820
A4	0.4060	0.2040
A5	0.6080	0.2940
AA	0.9570	0.4630
AB	0.7930	0.4460
AC	0.7410	0.4400
AD	0.7070	0.4200
AE	0.7780	0.4770
AF	0.7000	0.3910
AG	0.6910	0.3670
AH	0.6840	0.3830
AI	0.7970	0.4730
AJ	0.7560	0.4710
AK	0.8230	0.4300
AL	0.7260	0.4070
AM	0.6460	0.2760
AN	0.7840	0.4250
AO	0.6550	0.2780
AP	0.7980	0.4820
AQ	0.8130	0.4840



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Chain	Atom inclusion	Q-score
AR	0.6000	0.2440
AS	0.6850	0.3690
AT	0.7370	0.3810
AU	0.6700	0.2940
AV	0.4070	0.1380
AW	0.7630	0.4390
AX	0.7080	0.3320
AY	0.5360	0.2590
AZ	0.6900	0.3350
Aw	0.7480	0.2960
Ax	0.7810	0.3810
Ay	0.0680	0.1020
Az	0.3990	0.2390
B	0.9030	0.3540
D	0.9230	0.5570
E	0.8970	0.5450
F	0.9310	0.5570
H	0.4110	0.2560
I	0.5350	0.3220
J	0.7080	0.3230
K	0.9330	0.5580
L	0.8880	0.5400
M	0.9090	0.5510
N	0.8700	0.5380
O	0.9110	0.5460
P	0.8980	0.5230
Q	0.8320	0.5000
R	0.9280	0.5670
S	0.9040	0.5580
T	0.9060	0.5560
U	0.8380	0.4860
V	0.8280	0.4690
W	0.9020	0.5720
X	0.8470	0.5030
Y	0.8870	0.5210
Z	0.9180	0.5590
a	0.8270	0.4940
b	0.9210	0.5580
c	0.8660	0.5020
d	0.7840	0.4350
e	0.6450	0.2850
f	0.7080	0.4070

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Chain	Atom inclusion	Q-score
g	0.9060	0.5390
h	0.8760	0.4610
i	0.9450	0.5770
j	0.8590	0.4970
k	0.7110	0.4010
l	0.7270	0.3540
m	0.6680	0.3260
o	0.9370	0.5670
p	0.7680	0.4410
q	0.6450	0.3390
r	0.8830	0.5260
s	0.8900	0.5180
t	0.0990	0.2010
t1	0.4180	0.1790
u	0.0120	0.1550
v	0.0000	0.0660
w	0.0000	-0.0050
x	0.0000	0.0460
y	0.0080	0.0140
z	0.0660	0.0450