



Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 07:01 am BST

PDB ID : 7QI5
EMDB ID : EMD-13981
Title : Human mitochondrial ribosome in complex with mRNA, A/A-, P/P- and E/E-tRNAs at 2.63 Å resolution
Authors : Singh, V.; Itoh, Y.; Amunts, A.
Deposited on : 2021-12-14
Resolution : 2.63 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:

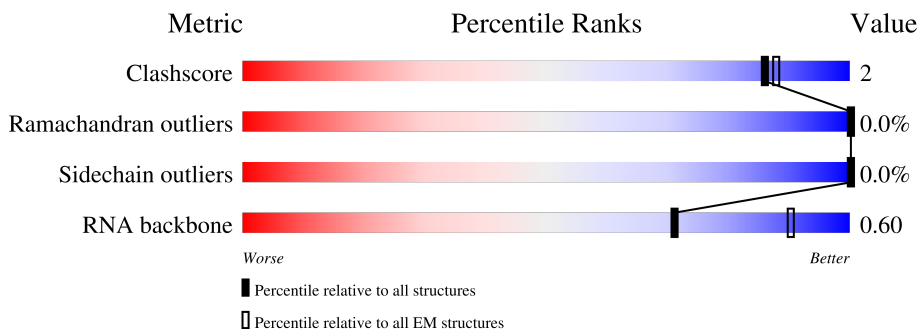
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.63 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.













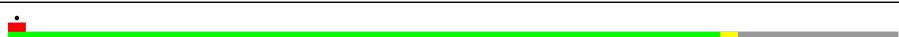


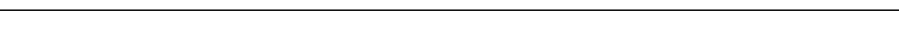
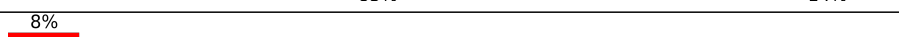
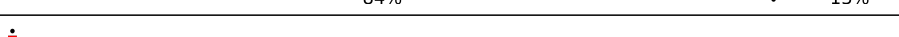
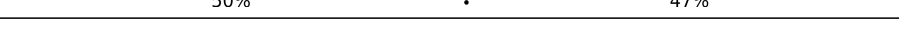


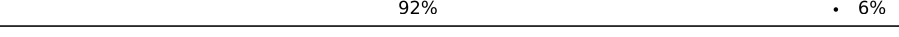
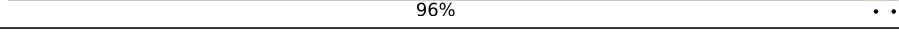




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	AA	954	76% 22%
2	AB	296	72% 24%
3	AC	167	73% 6% 21%
4	AD	430	76% 20%
5	AE	125	97%
6	AF	242	81% 5% 14%
7	AG	396	76% 7% 17%

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Mol	Chain	Length	Quality of chain
8	AH	201	 66% 30%
9	AI	194	 68% 29%
10	AJ	138	 72% 7% 22%
11	AK	128	 76% 21%
12	AL	257	 66% 32%
13	AM	137	 85% 13%
14	AN	130	 79% 5% 15%
15	AO	258	 73% 25%
16	AP	142	 68% 32%
17	AQ	87	 95%
18	AR	360	 80% 18%
19	AS	190	 68% 29%
20	AT	173	 94%
21	AU	205	 83% 14%
22	AV	414	 84% 13%
23	AW	187	 50% 47%
24	AX	398	 82% 7% 12%
25	AY	395	 36% 62%
26	AZ	106	 92% 6%
27	A0	217	 96%
28	A1	323	 80% 6% 14%
29	A2	118	 87% 12%
30	A3	199	 33% 65%
31	A4	689	 83% 15%
32	Aw	68	 72% 28%

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Mol	Chain	Length	Quality of chain
33	Ax	70	10% 80% 20%
34	Ay	70	79% 21%
35	Az	34	18% 62% 38%
36	A	1561	76% 21%
37	B	72	72% 25%
38	D	305	75% 22%
39	E	348	84% 12%
40	F	311	78% 19%
41	I	261	23% 77% 19%
42	J	192	25% 88% 9%
43	K	178	96%
44	L	145	74% 5% 21%
45	M	296	93%
46	N	251	86% 12%
47	O	175	85% 12%
48	P	180	78% 20%
49	Q	292	5% 78% 18%
50	R	149	91% 6%
51	S	205	77% 21%
52	T	206	80% 19%
53	U	153	10% 95% 5%
54	V	216	5% 88% 7% 5%
55	W	148	77% 22%
56	X	256	93% 5%
57	Y	250	71% 28%

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Mol	Chain	Length	Quality of chain
58	Z	161	73% 24%
59	0	188	55% 41%
60	1	65	78% 8% 14%
61	2	92	49% 50%
62	3	188	47% 49%
63	4	103	35% 63%
64	5	423	91% 7%
65	6	380	89% 7%
66	7	338	83% 13%
67	8	206	5% 74% 24%
68	9	137	88% 9%
69	a	142	7% 70% 30%
70	b	215	70% 30%
71	c	332	86% 14%
72	d	306	8% 79% 21%
73	e	279	5% 85% 15%
74	f	212	74% 26%
75	g	166	81% 19%
76	h	158	70% 30%
77	i	128	76% 24%
78	j	123	5% 76% 24%
79	k	112	5% 90% 10%
80	l	138	13% 59% 41%
81	m	128	9% 72% 28%
82	o	102	92% 8%

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Mol	Chain	Length	Quality of chain
83	p	206	 8% 71% 29%
84	q	222	 14% 74% 26%
85	r	196	 83% 17%
86	s	439	 88% 12%
87	t	198	 21% 23% 77%
87	u	198	 16% 16% 84%
87	v	198	 16% 16% 84%
87	w	198	 16% 16% 84%
87	x	198	 16% 16% 84%
87	y	198	 16% 16% 84%
88	H	267	 69% 7% 24%
89	z	325	 6% 77% 22%

2 Entry composition [i](#)

There are 101 unique types of molecules in this entry. The entry contains 343544 atoms, of which 153978 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 RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	AA	954	30564	9088	10304	3647	6571	954	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	AB	224	3627	1158	1809	328	322	10	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	AC	132	2172	699	1089	195	185	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	AD	343	5536	1713	2805	518	487	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	AF	208	3496	1104	1771	312	298	11	0	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	AG	327	5377	1710	2689	477	487	14	0	0

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	AH	140	2339	745	1187	194	210	3	0	0

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	AI	137	2081	642	1061	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	184	5F0	ASN	conflict	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	AJ	108	1728	521	889	169	143	6	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	AK	101	1748	537	886	179	141	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	AL	174	2994	925	1541	270	251	7	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	AM	119	1908	594	966	185	157	6	0	0

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	AN	110	1797	562	929	156	147	3	0	0

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	AO	193	3153	1014	1561	294	277	7	0	0

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	AP	97	1588	501	807	134	138	8	0	0

- Molecule 17 is a protein called MRPS21 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	AQ	86	1502	460	758	150	126	8	0	0

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	AR	295	4839	1533	2430	413	455	8	0	0

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	AS	135	2227	716	1116	198	196	1	0	0

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	AU	176	2989	916	1501	301	267	4	0	0

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	AV	362	5933	1904	2964	495	558	12	0	0

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	AW	100	1593	498	804	141	146	4	0	0

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	AX	352	5694	1822	2845	499	517	11	0	0

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	AY	149	2444	801	1198	207	234	4	0	0

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	AZ	100	1698	534	859	153	148	4	0	0

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	A0	215	3584	1130	1797	339	313	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	A1	279	4561	1435	2296	387	432	11	0	0

- Molecule 29 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	A2	117	1906	579	971	182	166	8	0	0

- Molecule 30 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	A3	70	1326	401	701	134	89	1	0	0

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	A4	588	9538	3053	4770	808	879	28	0	0

- Molecule 32 is a RNA chain called A/A-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
32	Aw	68	2159	646	725	248	472	68	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aw	26	U	G	conflict	GB 1896813690
Aw	34	A	U	conflict	GB 1896813690
Aw	35	A	C	conflict	GB 1896813690
Aw	36	C	G	conflict	GB 1896813690
Aw	73	U	A	conflict	GB 1896813690

- Molecule 33 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
33	Ax	70	2233	665	751	260	487	70	0	0

- Molecule 34 is a RNA chain called E/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
34	Ay	70	2235	665	752	261	487	70	0	0

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
35	Az	34	1079	324	360	123	238	34	0	0

- Molecule 36 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
36	A	1558	49871	14843	16801	5963	10706	1558	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	C	conflict	GB 208964619

- Molecule 37 is a RNA chain called mitochondrial tRNA^{Val}.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
37	B	72	2303	685	779	269	498	72	0	0

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 38 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
38	D	238	3780	1157	1921	376	317	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
39	E	305	4822	1545	2416	418	432	11	0	0

- Molecule 40 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
40	F	252	4097	1305	2066	370	350	6	0	0

- Molecule 41 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
41	I	212	3484	1088	1789	304	292	11	0	0

- Molecule 42 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
42	J	175	2739	847	1409	237	244	2	0	0

- Molecule 43 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
43	K	177	2907	936	1452	259	253	7	0	0

- Molecule 44 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	M	289	4699	1476	2385	427	405	6	0	0

- Molecule 46 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	N	222	3604	1143	1818	326	307	10	0	0

- Molecule 47 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	O	154	2554	792	1295	241	219	7	0	0

- Molecule 48 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	P	144	2339	733	1166	224	211	5	0	0

- Molecule 49 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	Q	239	4021	1277	2031	353	351	9	0	0

- Molecule 50 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	R	140	2369	732	1215	231	187	4	0	0

- Molecule 51 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	S	161	2659	835	1366	227	227	4	0	0

- Molecule 52 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
52	T	166	Total	C	H	N	O	S	0	0
			2781	875	1412	254	233	7		

- Molecule 53 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
53	U	152	Total	C	H	N	O	S	0	0
			2483	788	1232	234	226	3		

- Molecule 54 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
54	V	205	Total	C	H	N	O	S	0	0
			3365	1068	1689	298	302	8		

- Molecule 55 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
55	W	116	Total	C	H	N	O	S	0	0
			1840	577	936	171	153	3		

- Molecule 56 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
56	X	244	Total	C	H	N	O	S	0	0
			4105	1322	2061	352	365	5		

- Molecule 57 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
57	Y	181	Total	C	H	N	O	S	0	0
			3154	995	1598	298	259	4		

- Molecule 58 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
58	Z	122	Total	C	H	N	O	S	0	0
			2041	636	1045	186	171	3		

- Molecule 59 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
59	0	110	Total	C	H	N	O	S	0	0
			1815	554	917	176	162	6		

- Molecule 60 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
60	1	56	Total	C	H	N	O	S	0	0
			977	296	513	89	77	2		

- Molecule 61 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
61	2	46	Total	C	H	N	O	S	0	0
			784	233	407	83	60	1		

- Molecule 62 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
62	3	95	Total	C	H	N	O	S	0	0
			1716	539	884	162	128	3		

- Molecule 63 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
63	4	38	Total	C	H	N	O	S	0	0
			704	217	362	72	49	4		

- Molecule 64 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
64	5	394	Total	C	H	N	O	S	0	0
			6419	2073	3209	560	566	11		

- Molecule 65 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
65	6	354	Total	C	H	N	O	S	0	0
			5792	1881	2844	525	533	9		

- Molecule 66 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
66	7	294	4789	1529	2399	405	438	18	0	0

- Molecule 67 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
67	8	157	2696	844	1369	235	246	2	0	0

- Molecule 68 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
68	9	124	1985	644	988	170	181	2	0	0

- Molecule 69 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
69	a	100	1652	529	812	152	154	5	0	0

- Molecule 70 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
70	b	150	2392	744	1196	231	218	3	0	0

- Molecule 71 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
71	c	286	4621	1470	2322	397	423	9	0	0

- Molecule 72 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
72	d	241	3964	1273	1979	340	359	13	0	0

- Molecule 73 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
73	e	238	3848	1222	1917	339	364	6	0	0

- Molecule 74 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
74	f	157	2523	799	1271	207	242	4	0	0

- Molecule 75 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 76 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
76	h	110	1777	568	882	156	168	3	0	0

- Molecule 77 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
77	i	97	1687	532	859	165	127	4	0	0

- Molecule 78 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
78	j	94	1492	463	747	144	136	2	0	0

- Molecule 79 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
79	k	101	1559	479	785	148	142	5	0	0

- Molecule 80 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
80	l	82	1363	437	675	120	128	3	0	0

- Molecule 81 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
81	m	92	1551	488	760	159	142	2	0	0

- Molecule 82 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
82	o	94	1604	501	806	165	129	3	0	0

- Molecule 83 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
83	p	147	2429	748	1224	228	225	4	0	0

- Molecule 84 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
84	q	165	2765	865	1376	270	249	5	0	0

- Molecule 85 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
85	r	162	2671	839	1349	252	223	8	0	0

- Molecule 86 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
86	s	386	6298	2023	3143	559	559	14	0	0

- Molecule 87 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	t	46	Total	C	H	N	O	0	0
			732	228	378	56	70		
87	u	32	Total	C	H	N	O	0	0
			541	168	284	40	49		
87	v	32	Total	C	H	N	O	0	0
			541	168	284	40	49		
87	w	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
87	x	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
87	y	31	Total	C	H	N	O	0	0
			520	159	275	39	47		

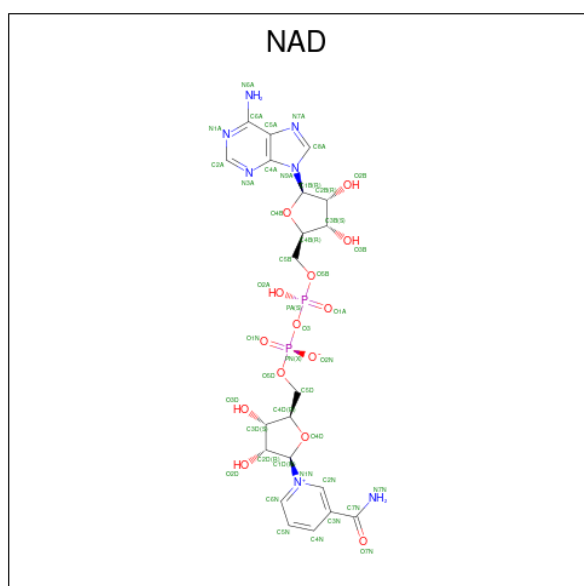
- Molecule 88 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
88	H	202	Total	C	H	N	O	S	0	0
			3397	1067	1736	304	286	4		

- Molecule 89 is a protein called 39S ribosomal protein L1, mitochondrial.

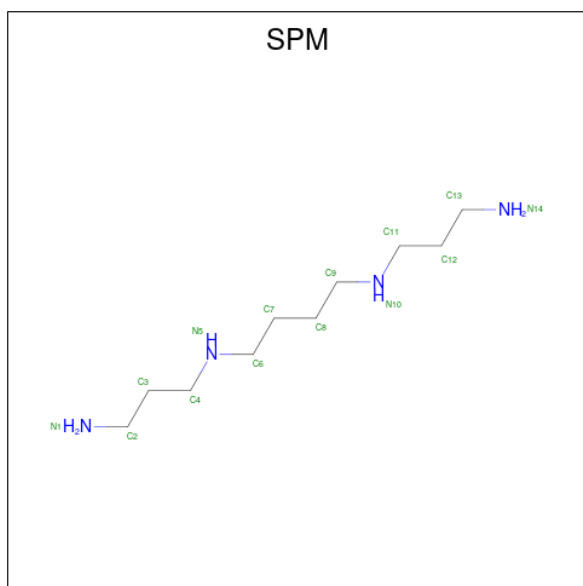
Mol	Chain	Residues	Atoms					AltConf	Trace	
89	z	252	Total	C	H	N	O	S	0	0
			4104	1304	2077	336	381	6		

- Molecule 90 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



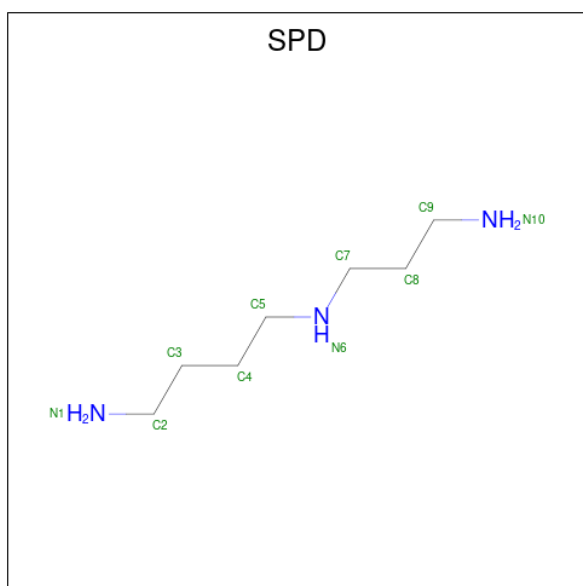
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
90	AA	1	70	21	26	7	14	2	0

- Molecule 91 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
91	AA	1	44	10	30	4	0

- Molecule 92 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms				AltConf
92	AA	1	Total	C	H	N	0
			32	7	22	3	
92	A	1	Total	C	H	N	0
			32	7	22	3	
92	A	1	Total	C	H	N	0
			32	7	22	3	
92	A	1	Total	C	H	N	0
			32	7	22	3	

- Molecule 93 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
93	AA	63	Total	Mg	0
			63	63	
93	AB	1	Total	Mg	0
			1	1	
93	AX	1	Total	Mg	0
			1	1	
93	A3	1	Total	Mg	0
			1	1	
93	A	138	Total	Mg	0
			138	138	
93	D	2	Total	Mg	0
			2	2	
93	E	1	Total	Mg	0
			1	1	
93	g	1	Total	Mg	0
			1	1	

- Molecule 94 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
94	AA	18	Total	K	0
			18	18	
94	A	29	Total	K	0
			29	29	
94	D	1	Total	K	0
			1	1	
94	M	1	Total	K	0
			1	1	
94	W	1	Total	K	0
			1	1	
94	3	1	Total	K	0
			1	1	

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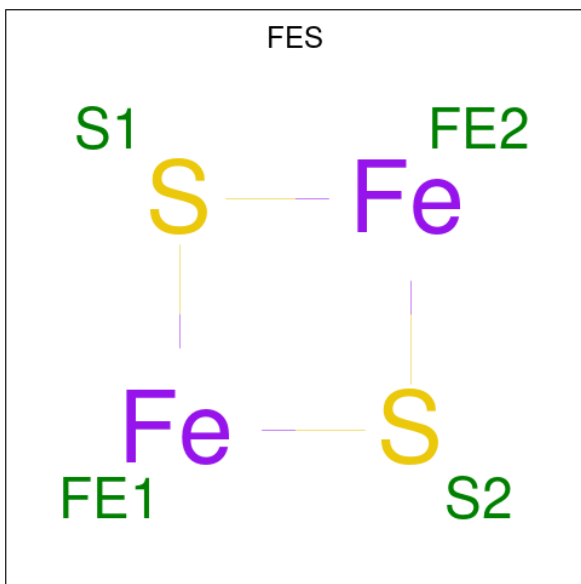
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Mol	Chain	Residues	Atoms	AltConf
94	6	1	Total K 1 1	0
94	i	1	Total K 1 1	0
94	o	1	Total K 1 1	0

- Molecule 95 is ZINC ION (three-letter code: ZN) (formula: Zn).

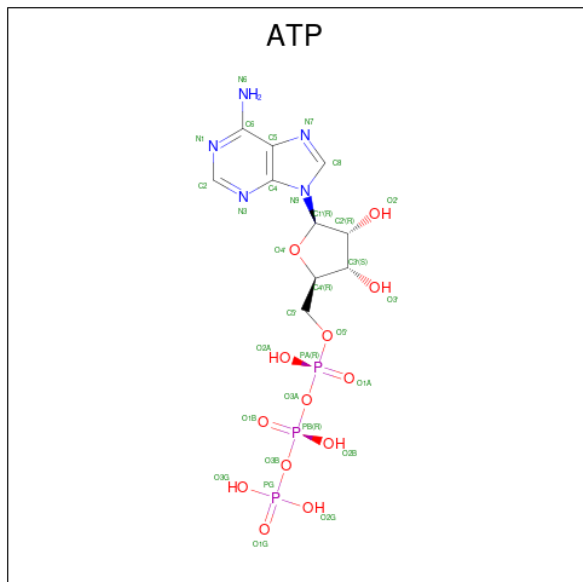
Mol	Chain	Residues	Atoms	AltConf
95	AO	1	Total Zn 1 1	0
95	0	1	Total Zn 1 1	0
95	4	1	Total Zn 1 1	0

- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



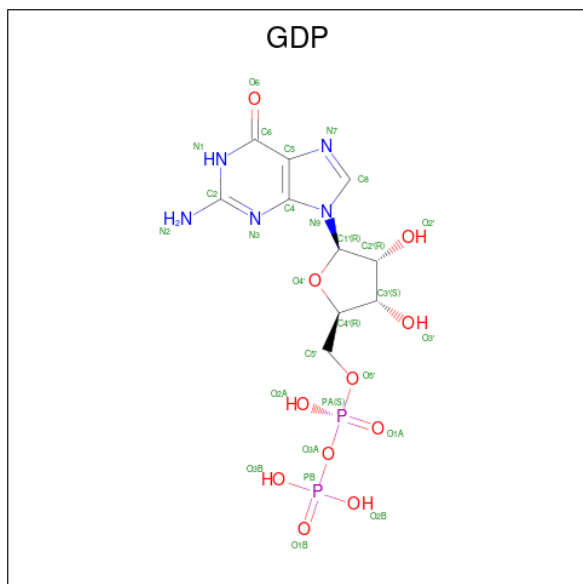
Mol	Chain	Residues	Atoms	AltConf
96	AP	1	Total Fe S 4 2 2	0
96	AT	1	Total Fe S 4 2 2	0
96	r	1	Total Fe S 4 2 2	0

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



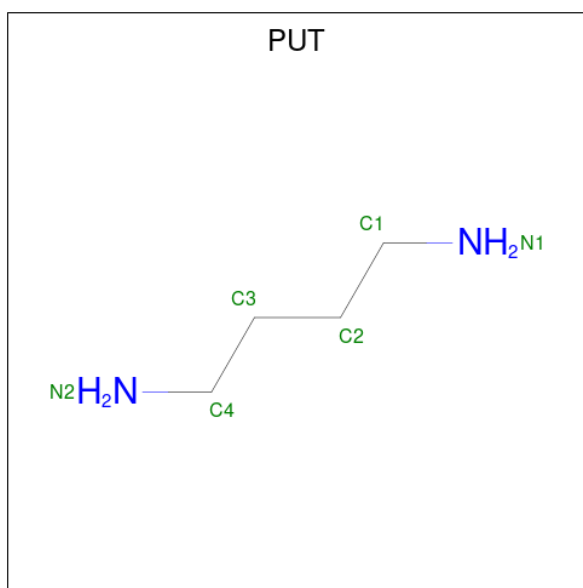
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
97	AX	1	43	10	12	5	13	3	0

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



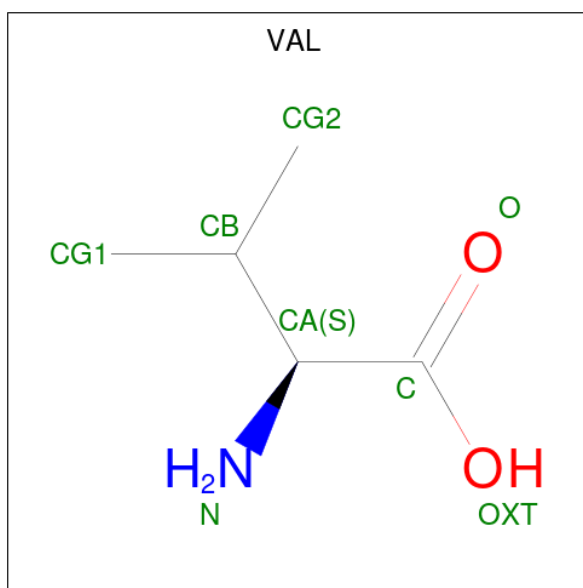
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
98	AX	1	40	10	12	5	11	2	0

- Molecule 99 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
99	A	1	20	4	14	2	0

- Molecule 100 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
100	B	1	18	5	11	1	1	0

- Molecule 101 is water.

Mol	Chain	Residues	Atoms		AltConf
101	AA	2039	Total 2039	O 2039	0
101	AB	78	Total 78	O 78	0
101	AC	55	Total 55	O 55	0
101	AD	82	Total 82	O 82	0
101	AE	27	Total 27	O 27	0
101	AF	39	Total 39	O 39	0
101	AG	64	Total 64	O 64	0
101	AH	57	Total 57	O 57	0
101	AI	39	Total 39	O 39	0
101	AJ	25	Total 25	O 25	0
101	AK	51	Total 51	O 51	0
101	AL	42	Total 42	O 42	0
101	AM	22	Total 22	O 22	0
101	AN	39	Total 39	O 39	0
101	AO	37	Total 37	O 37	0
101	AP	31	Total 31	O 31	0
101	AQ	77	Total 77	O 77	0
101	AR	11	Total 11	O 11	0
101	AS	25	Total 25	O 25	0
101	AT	44	Total 44	O 44	0
101	AU	8	Total 8	O 8	0
101	AW	16	Total 16	O 16	0

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Mol	Chain	Residues	Atoms		AltConf
101	AX	56	Total 56	O 56	0
101	AY	18	Total 18	O 18	0
101	AZ	30	Total 30	O 30	0
101	A0	1	Total 1	O 1	0
101	A1	35	Total 35	O 35	0
101	A2	32	Total 32	O 32	0
101	A3	50	Total 50	O 50	0
101	A4	9	Total 9	O 9	0
101	Aw	6	Total 6	O 6	0
101	Ax	7	Total 7	O 7	0
101	Ay	3	Total 3	O 3	0
101	Az	13	Total 13	O 13	0
101	A	2955	Total 2955	O 2955	0
101	B	66	Total 66	O 66	0
101	D	68	Total 68	O 68	0
101	E	66	Total 66	O 66	0
101	F	79	Total 79	O 79	0
101	I	27	Total 27	O 27	0
101	J	1	Total 1	O 1	0
101	K	57	Total 57	O 57	0
101	L	31	Total 31	O 31	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
101	M	51	51	51	0
101	N	58	58	58	0
101	O	33	33	33	0
101	P	81	81	81	0
101	Q	29	29	29	0
101	R	63	63	63	0
101	S	49	49	49	0
101	T	45	45	45	0
101	U	24	24	24	0
101	V	5	5	5	0
101	W	55	55	55	0
101	X	11	11	11	0
101	Y	25	25	25	0
101	Z	32	32	32	0
101	0	28	28	28	0
101	1	3	3	3	0
101	2	34	34	34	0
101	3	44	44	44	0
101	4	11	11	11	0
101	5	14	14	14	0
101	6	100	100	100	0

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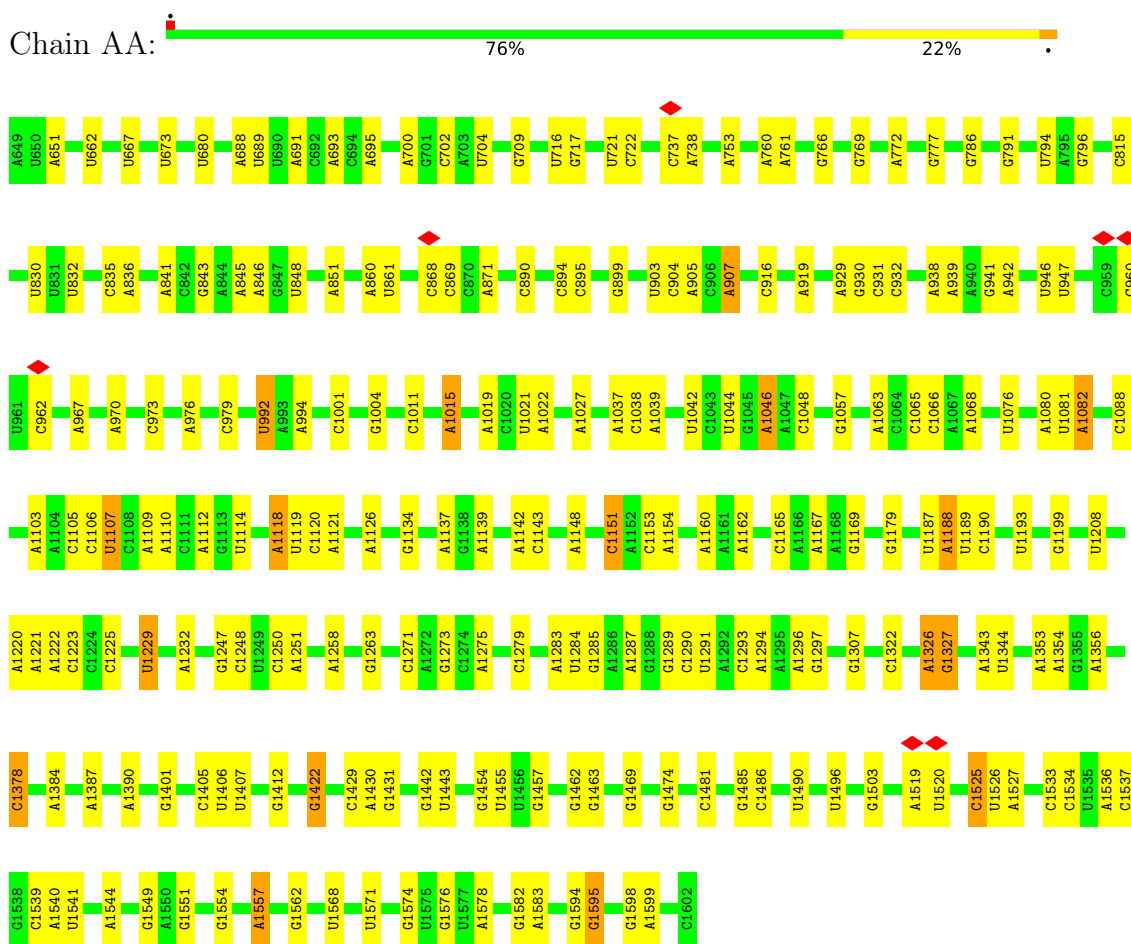
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Mol	Chain	Residues	Atoms		AltConf
101	7	15	Total 15	O 15	0
101	8	15	Total 15	O 15	0
101	9	17	Total 17	O 17	0
101	a	11	Total 11	O 11	0
101	b	35	Total 35	O 35	0
101	c	18	Total 18	O 18	0
101	d	9	Total 9	O 9	0
101	e	13	Total 13	O 13	0
101	f	19	Total 19	O 19	0
101	g	13	Total 13	O 13	0
101	i	46	Total 46	O 46	0
101	j	22	Total 22	O 22	0
101	k	5	Total 5	O 5	0
101	l	5	Total 5	O 5	0
101	m	8	Total 8	O 8	0
101	o	34	Total 34	O 34	0
101	p	8	Total 8	O 8	0
101	r	49	Total 49	O 49	0
101	s	51	Total 51	O 51	0
101	H	7	Total 7	O 7	0

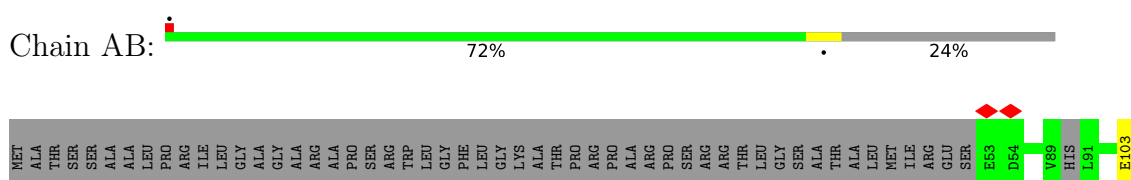
3 Residue-property plots [i](#)

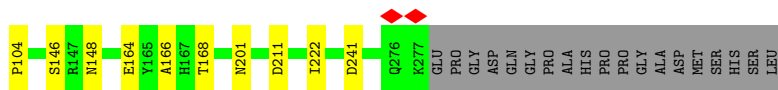
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 12S mitochondrial rRNA



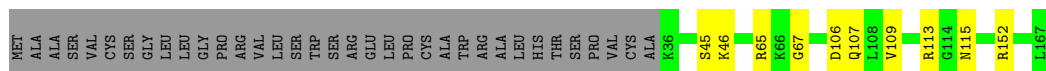
- Molecule 2: 28S ribosomal protein S2, mitochondrial





- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain AC:



- Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain AD:



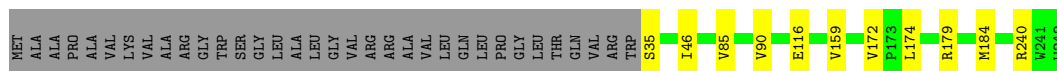
- Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain AE:



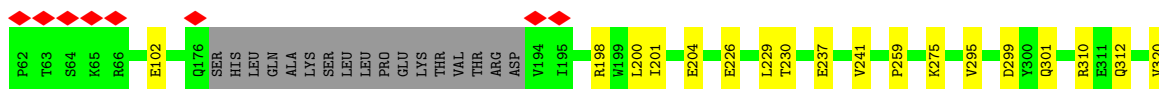
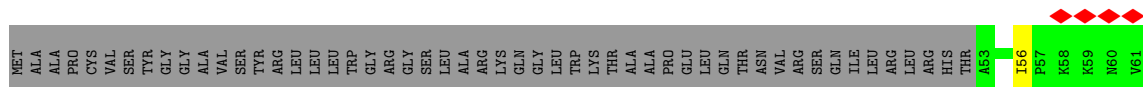
- Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain AF:



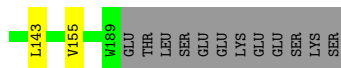
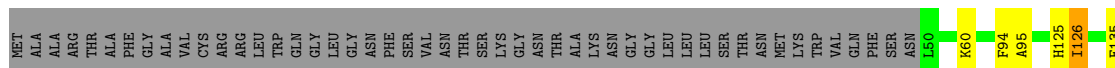
- Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain AG:

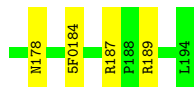
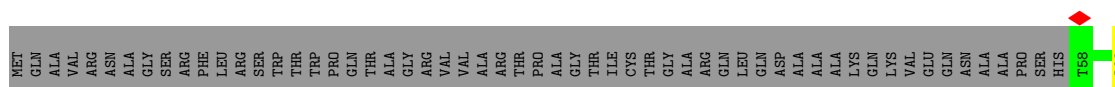




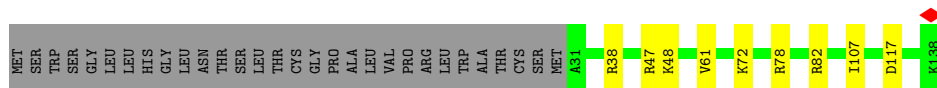
- Molecule 8: 28S ribosomal protein S10, mitochondrial



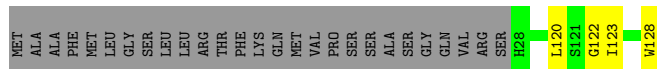
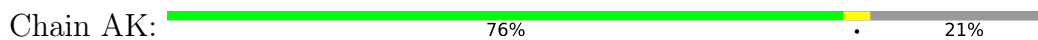
- Molecule 9: 28S ribosomal protein S11, mitochondrial



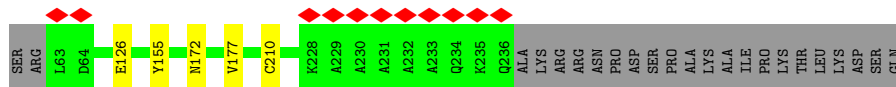
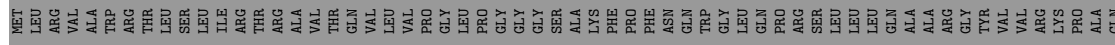
- Molecule 10: 28S ribosomal protein S12, mitochondrial




- Molecule 11: 28S ribosomal protein S14, mitochondrial

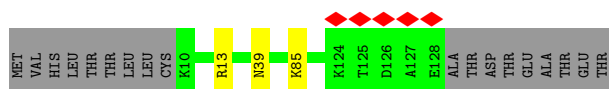


- Molecule 12: 28S ribosomal protein S15, mitochondrial




- Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain AM:  85% 13%




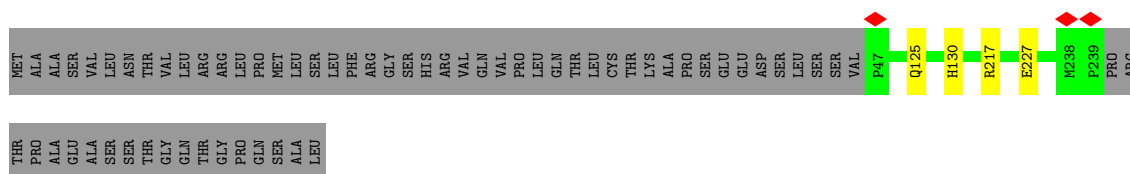
- Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain AN:  79% 5% 15%



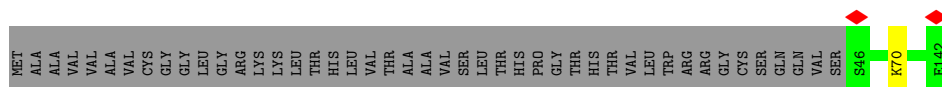
- Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain AO:  73% 25%



- Molecule 16: 28S ribosomal protein S18c, mitochondrial

Chain AP:  68% 32%




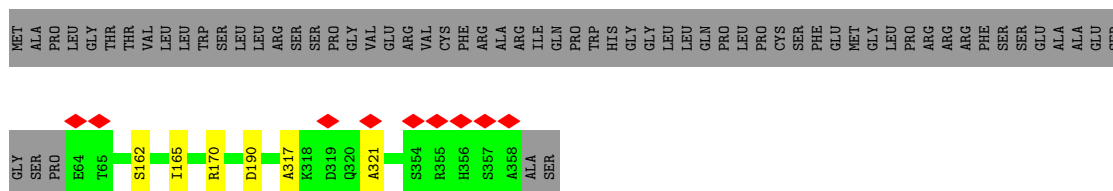
- Molecule 17: MRPS21 isoform 1

Chain AQ:  95%

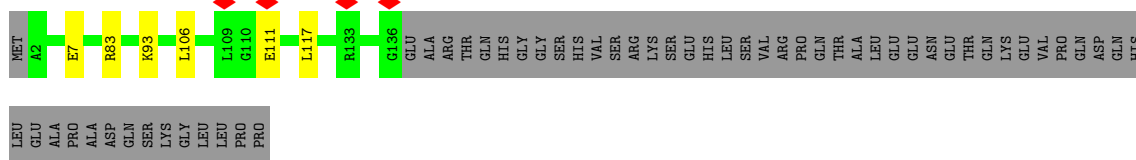


- Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain AR:  80% 18%



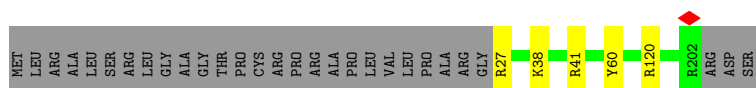
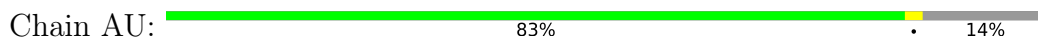
- Molecule 19: 28S ribosomal protein S23, mitochondrial



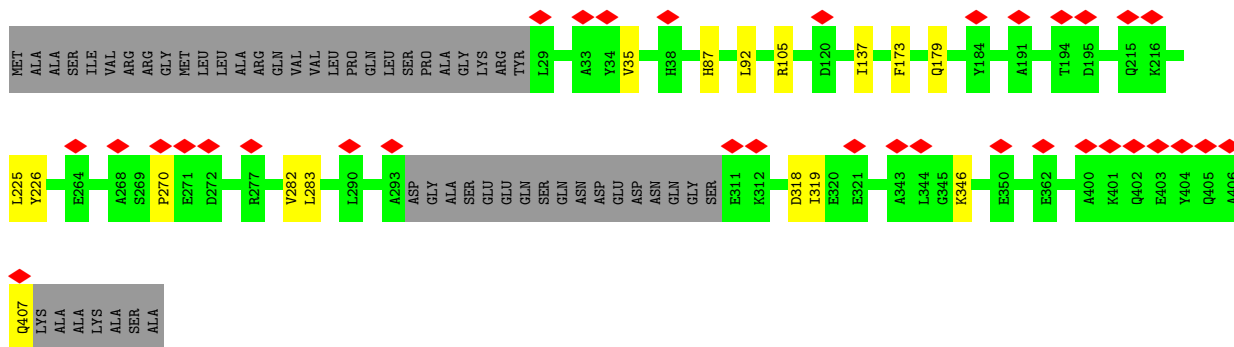
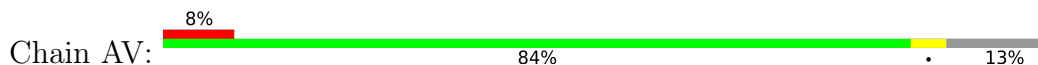
- Molecule 20: 28S ribosomal protein S25, mitochondrial



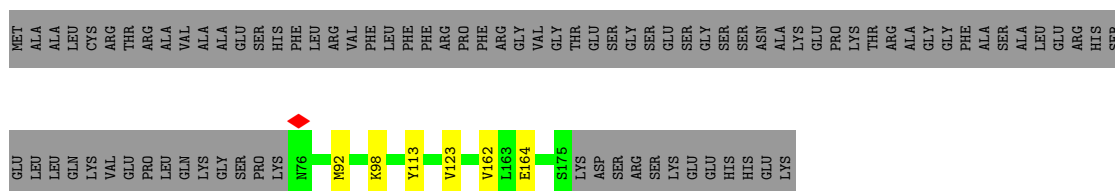
- Molecule 21: 28S ribosomal protein S26, mitochondrial



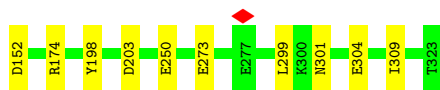
- Molecule 22: 28S ribosomal protein S27, mitochondrial



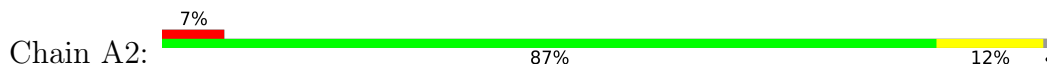
- Molecule 23: 28S ribosomal protein S28, mitochondrial



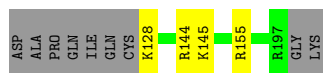
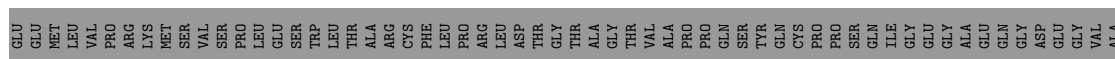
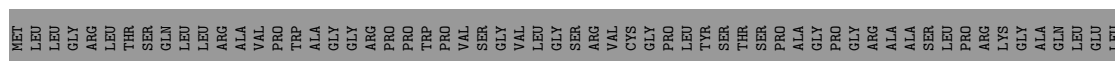
- Molecule 24: 28S ribosomal protein S29, mitochondrial



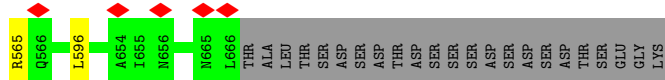
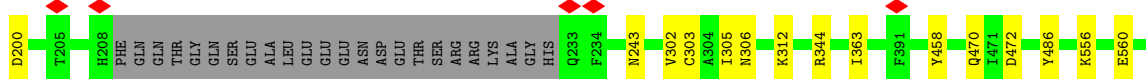
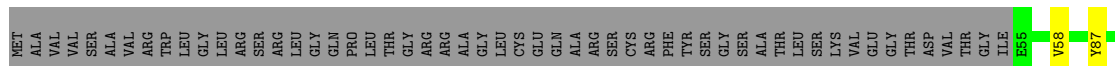
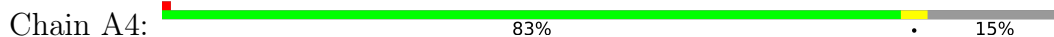
- Molecule 29: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1



- Molecule 30: Aurora kinase A-interacting protein



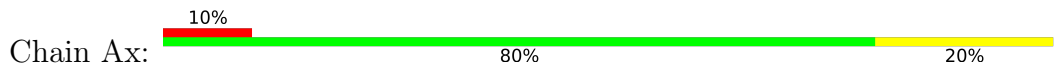
- Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

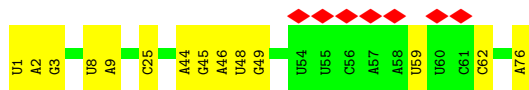


- Molecule 32: A/A-tRNA

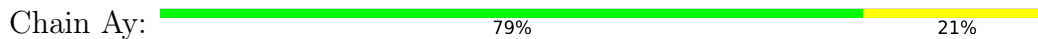


- Molecule 33: P/P-tRNA

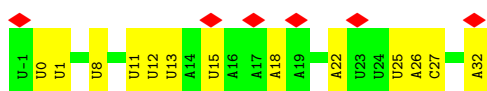




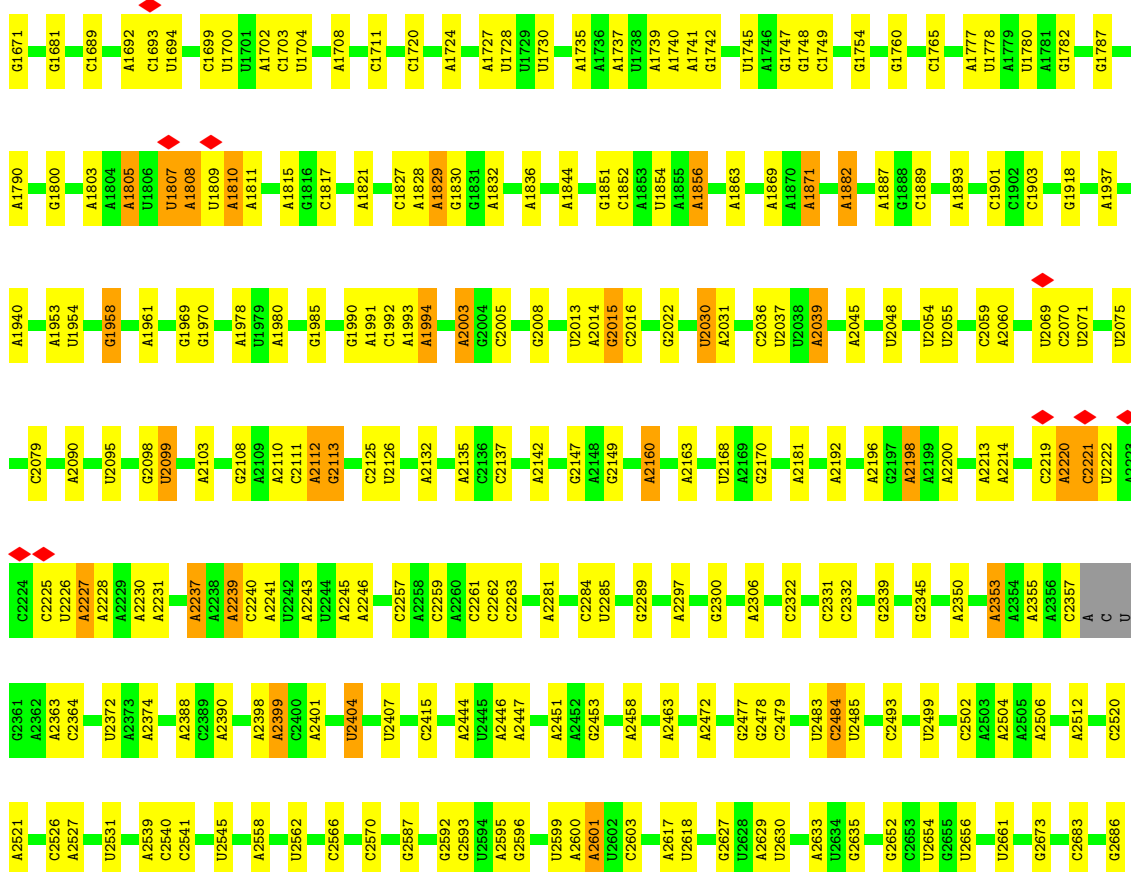
• Molecule 34: E/E-tRNA

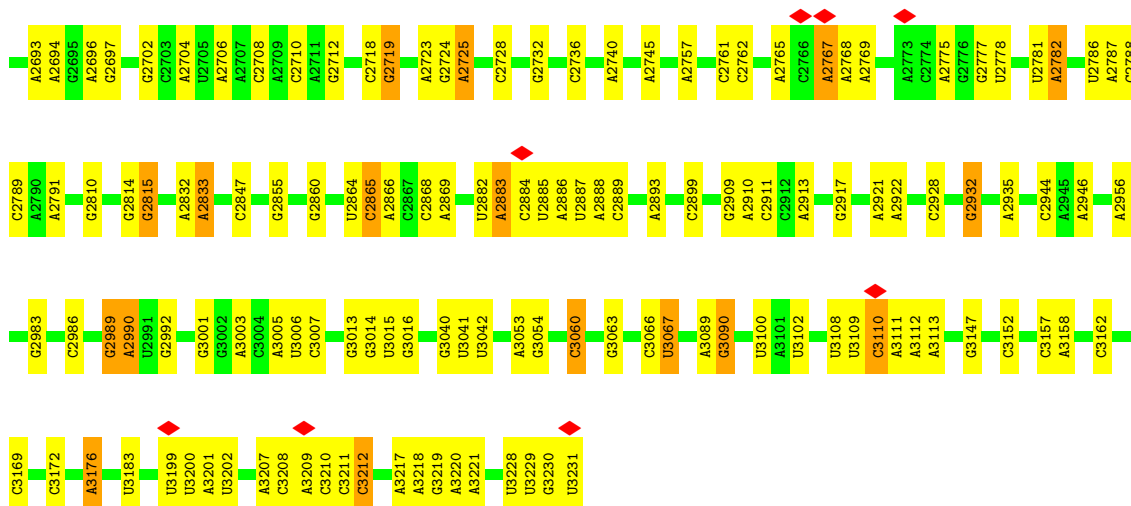


• Molecule 35: mRNA



• Molecule 36: 16S mitochondrial rRNA

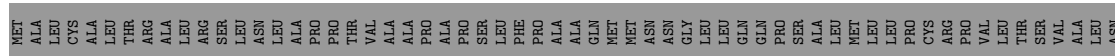
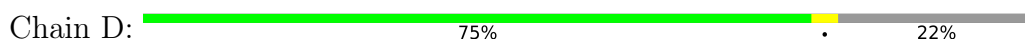




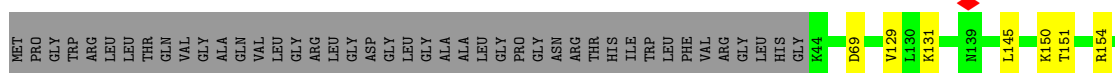
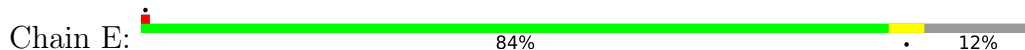
• Molecule 37: mitochondrial tRNA^{Val}



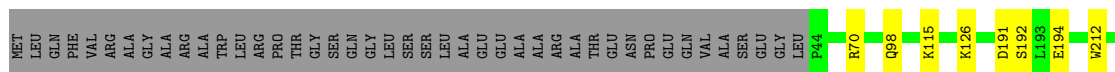
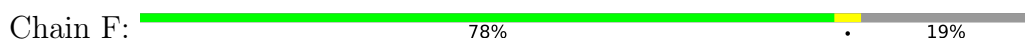
• Molecule 38: 39S ribosomal protein L2, mitochondrial

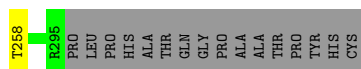


• Molecule 39: 39S ribosomal protein L3, mitochondrial

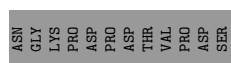
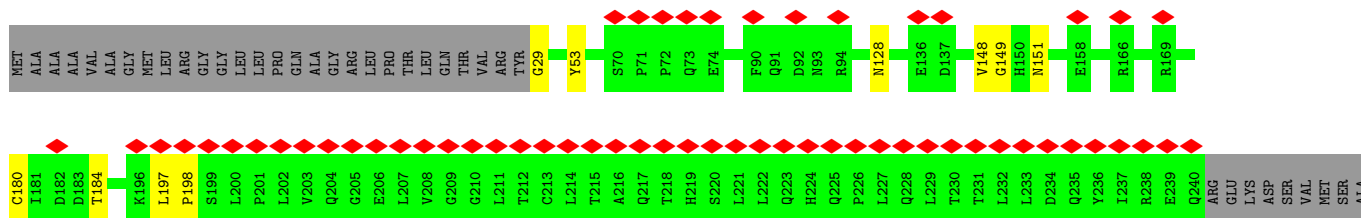
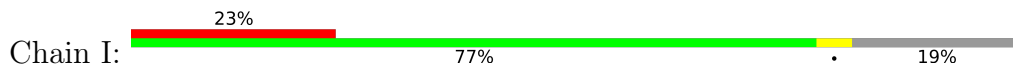


• Molecule 40: 39S ribosomal protein L4, mitochondrial

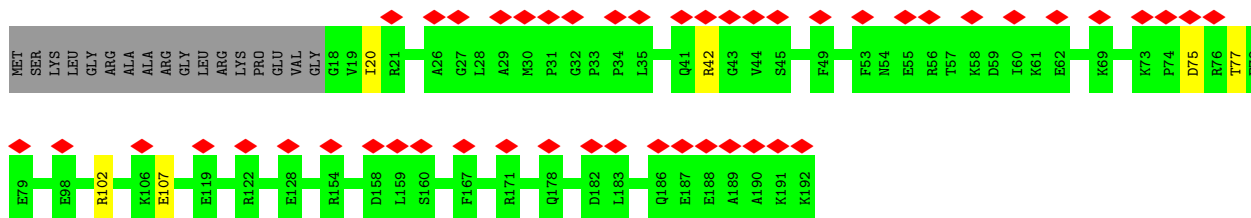
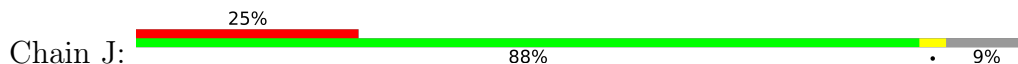




• Molecule 41: 39S ribosomal protein L10, mitochondrial



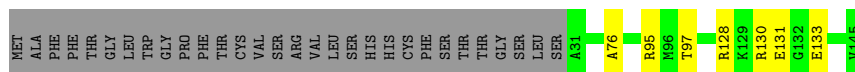
• Molecule 42: 39S ribosomal protein L11, mitochondrial



• Molecule 43: 39S ribosomal protein L13, mitochondrial



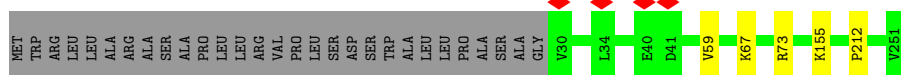
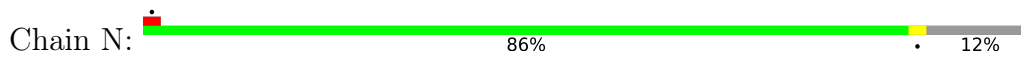
• Molecule 44: 39S ribosomal protein L14, mitochondrial



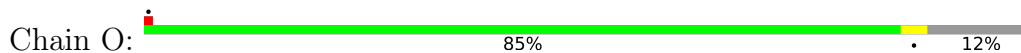
• Molecule 45: 39S ribosomal protein L15, mitochondrial



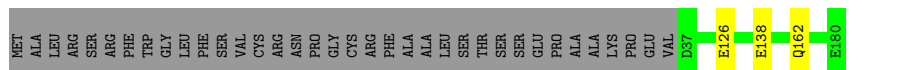
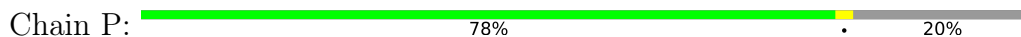
• Molecule 46: 39S ribosomal protein L16, mitochondrial



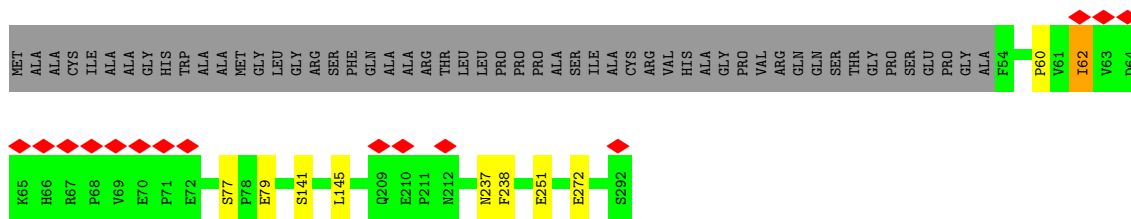
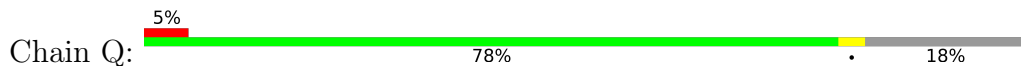
• Molecule 47: 39S ribosomal protein L17, mitochondrial



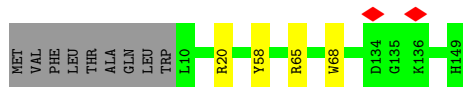
• Molecule 48: 39S ribosomal protein L18, mitochondrial



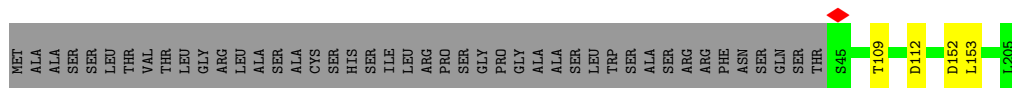
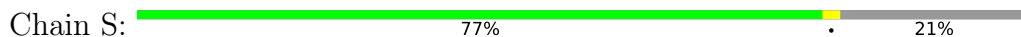
• Molecule 49: 39S ribosomal protein L19, mitochondrial



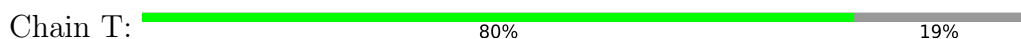
• Molecule 50: 39S ribosomal protein L20, mitochondrial

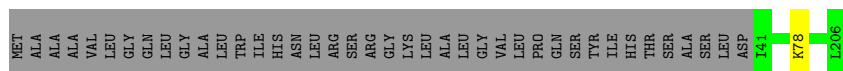


• Molecule 51: 39S ribosomal protein L21, mitochondrial

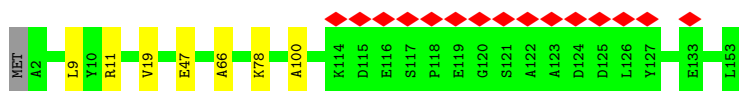


• Molecule 52: 39S ribosomal protein L22, mitochondrial

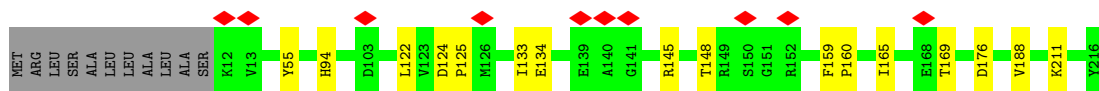
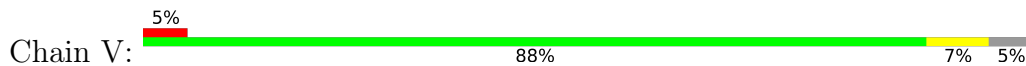




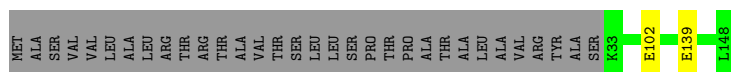
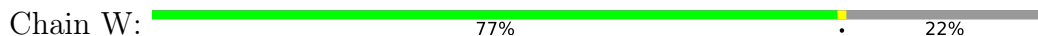
• Molecule 53: 39S ribosomal protein L23, mitochondrial



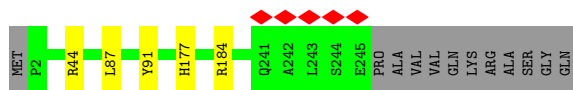
• Molecule 54: 39S ribosomal protein L24, mitochondrial



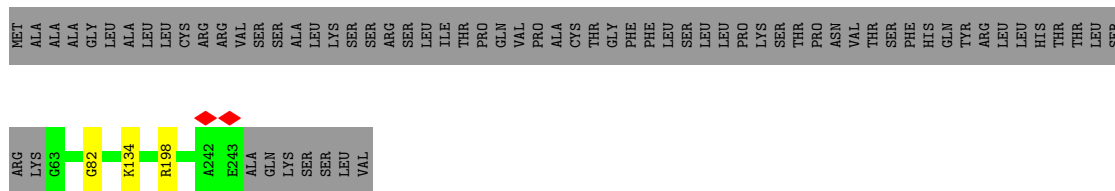
• Molecule 55: 39S ribosomal protein L27, mitochondrial



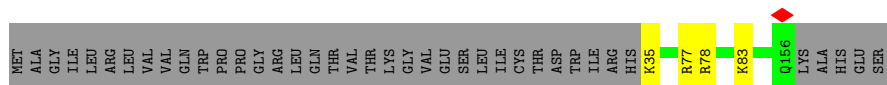
• Molecule 56: 39S ribosomal protein L28, mitochondrial



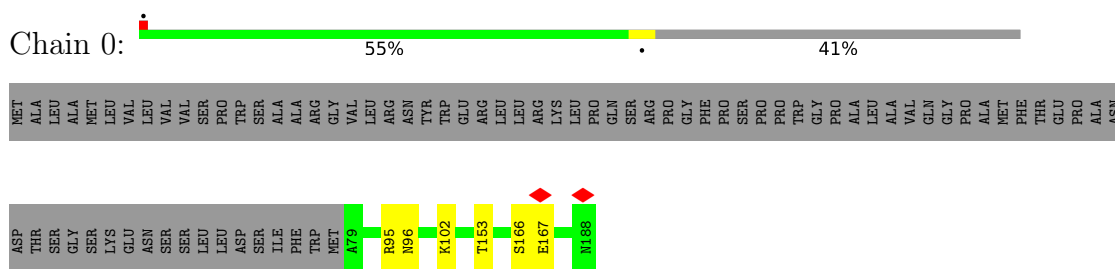
• Molecule 57: 39S ribosomal protein L47, mitochondrial



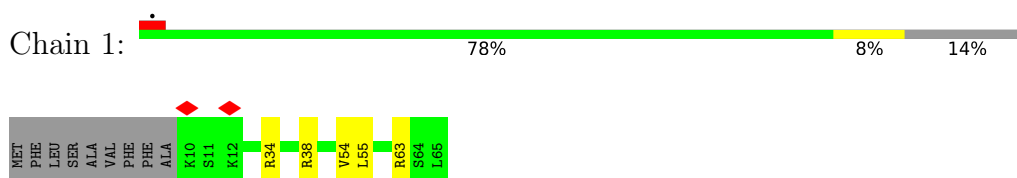
• Molecule 58: 39S ribosomal protein L30, mitochondrial



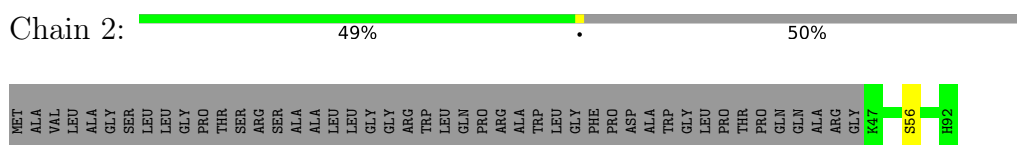
- Molecule 59: 39S ribosomal protein L32, mitochondrial



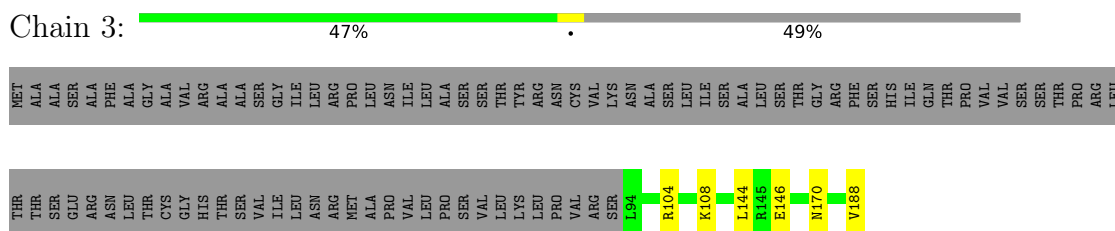
- Molecule 60: 39S ribosomal protein L33, mitochondrial



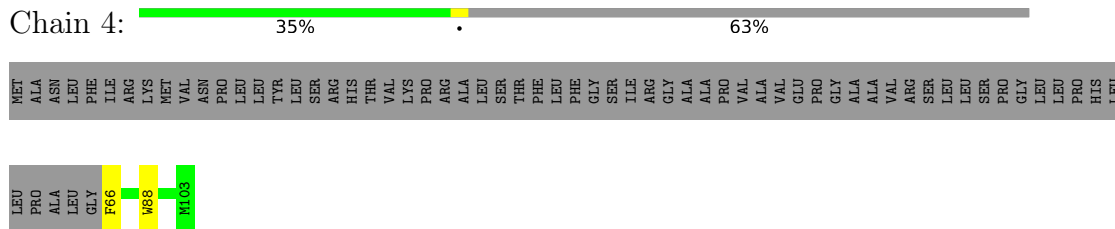
- Molecule 61: 39S ribosomal protein L34, mitochondrial



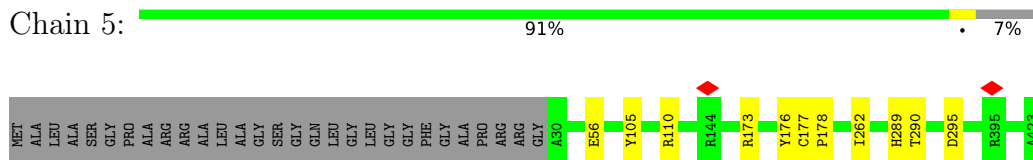
- Molecule 62: 39S ribosomal protein L35, mitochondrial




- Molecule 63: 39S ribosomal protein L36, mitochondrial

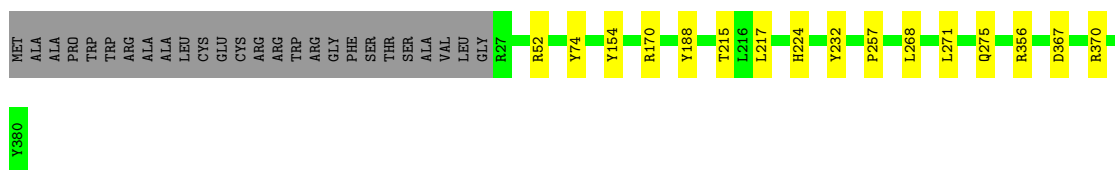


- Molecule 64: 39S ribosomal protein L37, mitochondrial




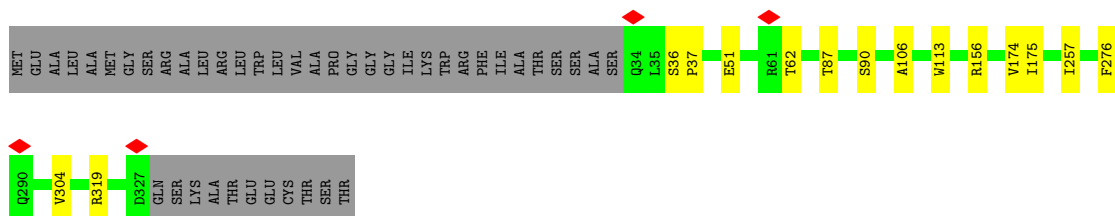
- Molecule 65: 39S ribosomal protein L38, mitochondrial

Chain 6:  89% 7%




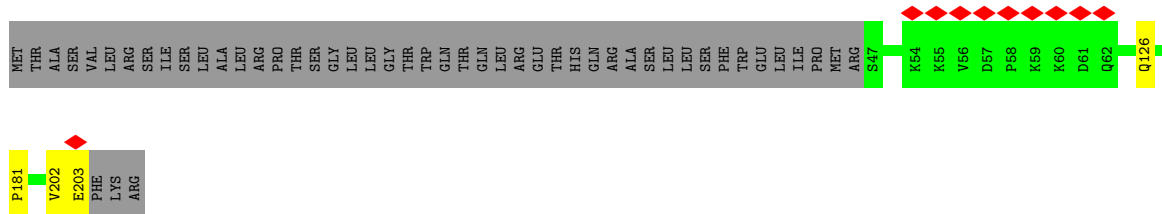
- Molecule 66: 39S ribosomal protein L39, mitochondrial

Chain 7:  83% 13%




- Molecule 67: 39S ribosomal protein L40, mitochondrial

Chain 8:  5% 74% 24%



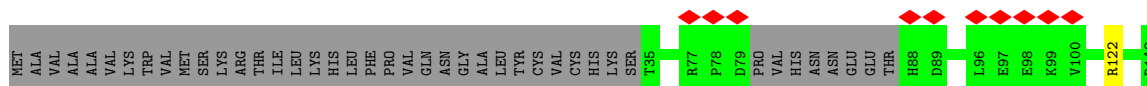
- Molecule 68: 39S ribosomal protein L41, mitochondrial

Chain 9:  88% 9%



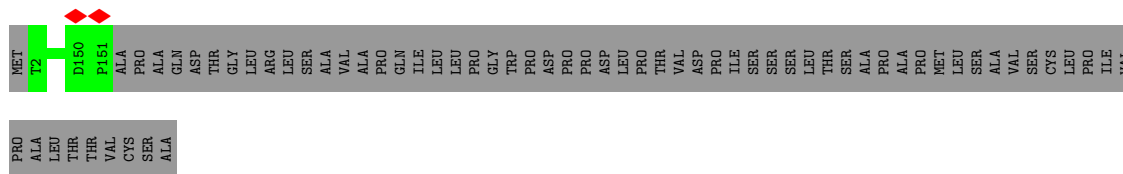
- Molecule 69: 39S ribosomal protein L42, mitochondrial

Chain a:  7% 70% 30%

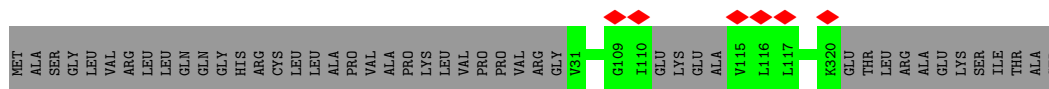
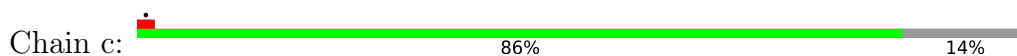


- Molecule 70: 39S ribosomal protein L43, mitochondrial

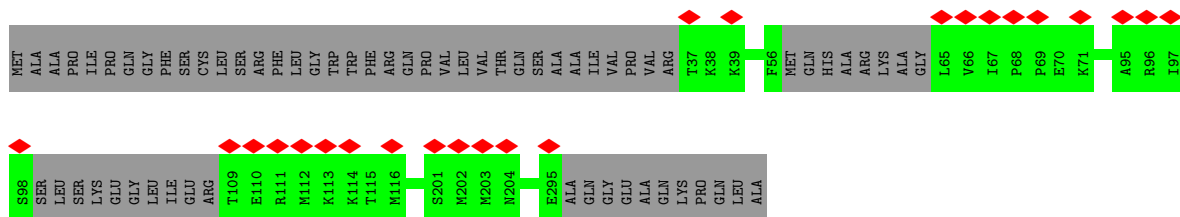
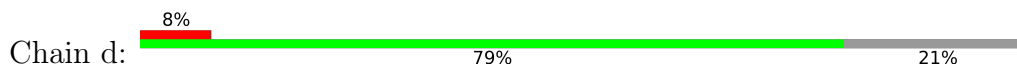
Chain b:  70% 30%



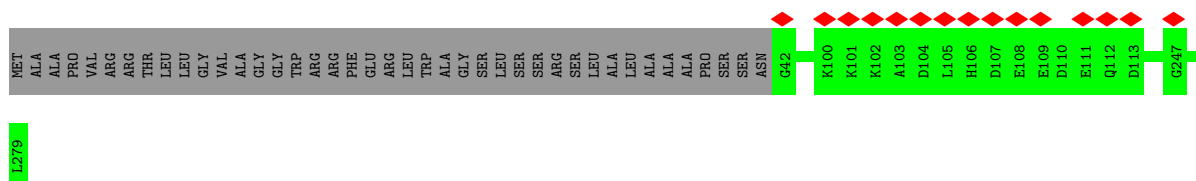
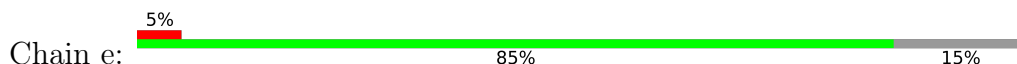
• Molecule 71: 39S ribosomal protein L44, mitochondrial



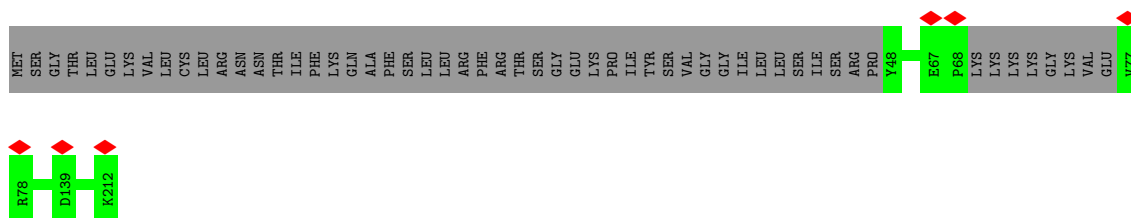
• Molecule 72: 39S ribosomal protein L45, mitochondrial



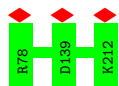
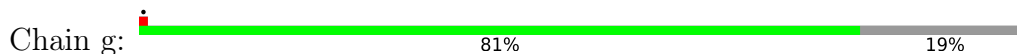
• Molecule 73: 39S ribosomal protein L46, mitochondrial

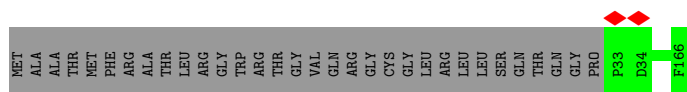


• Molecule 74: 39S ribosomal protein L48, mitochondrial

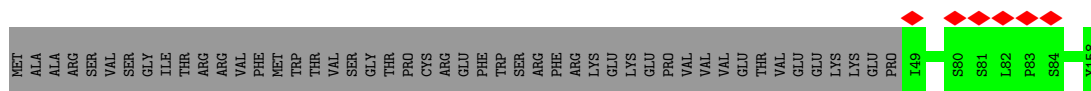


• Molecule 75: 39S ribosomal protein L49, mitochondrial

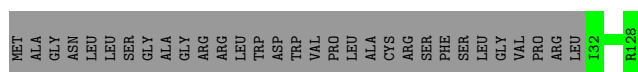




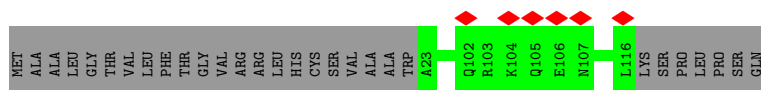
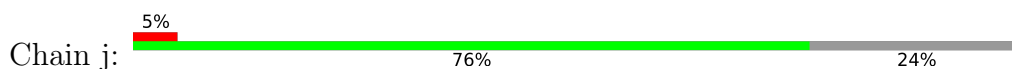
- Molecule 76: 39S ribosomal protein L50, mitochondrial



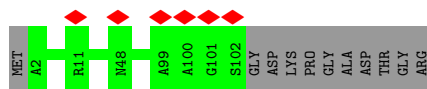
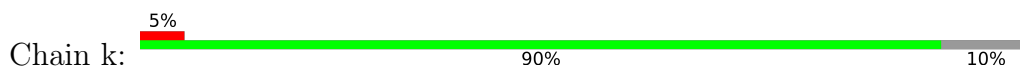
- Molecule 77: 39S ribosomal protein L51, mitochondrial



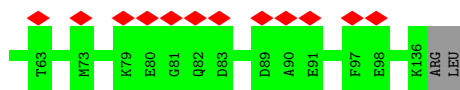
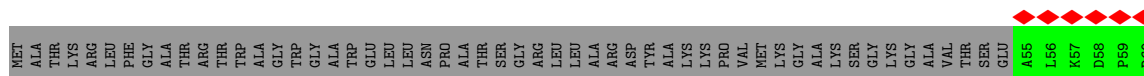
- Molecule 78: 39S ribosomal protein L52, mitochondrial



- Molecule 79: 39S ribosomal protein L53, mitochondrial

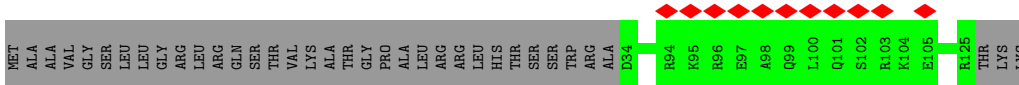


- Molecule 80: 39S ribosomal protein L54, mitochondrial

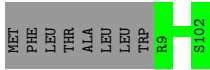


- Molecule 81: 39S ribosomal protein L55, mitochondrial

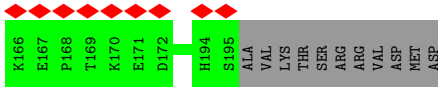
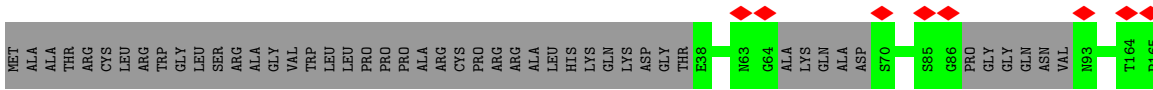




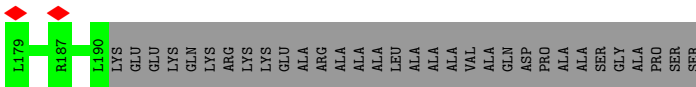
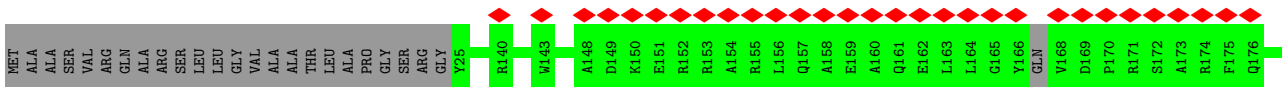
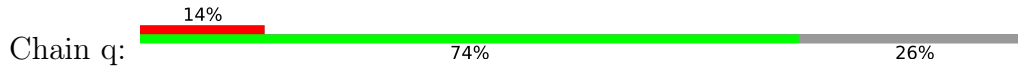
- Molecule 82: Ribosomal protein 63, mitochondrial



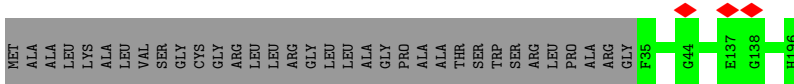
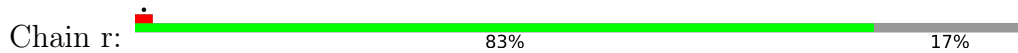
- Molecule 83: Peptidyl-tRNA hydrolase ICT1, mitochondrial



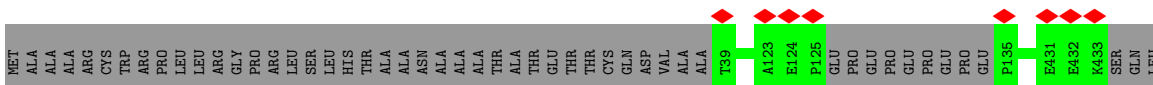
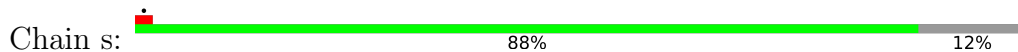
- Molecule 84: Growth arrest and DNA damage-inducible proteins-interacting protein 1



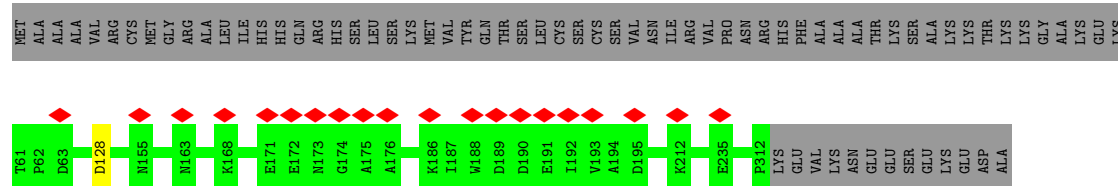
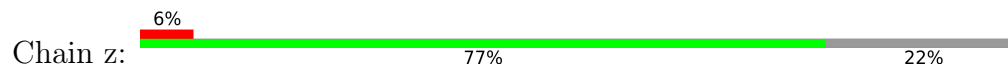
- Molecule 85: 39S ribosomal protein S18a, mitochondrial



- Molecule 86: 39S ribosomal protein S30, mitochondrial



• Molecule 89: 39S ribosomal protein L1, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82522	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	61.722	Depositor
Minimum map value	-28.634	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.267	Depositor
Recommended contour level	2.8	Depositor
Map size (\AA)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPM, MG, ZN, NAD, MA6, OMG, 2MG, THC, ATP, AYA, K, PSU, GDP, OMU, 5MU, PUT, 5MC, SAC, 5F0, B8T, SPD, FES, 1MA

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	AA	0.20	0/22537	0.67	0/35085
2	AB	0.24	0/1859	0.49	0/2513
3	AC	0.25	0/1113	0.48	0/1505
4	AD	0.24	0/2783	0.51	0/3724
5	AE	0.24	0/989	0.50	0/1335
6	AF	0.24	0/1767	0.47	0/2373
7	AG	0.24	0/2746	0.48	0/3681
8	AH	0.25	0/1178	0.47	0/1598
9	AI	0.25	0/1030	0.49	0/1386
10	AJ	0.25	0/855	0.55	0/1148
11	AK	0.22	0/880	0.57	0/1182
12	AL	0.24	0/1477	0.46	0/1974
13	AM	0.24	0/963	0.53	0/1295
14	AN	0.24	0/886	0.49	0/1199
15	AO	0.24	0/1648	0.48	0/2243
16	AP	0.24	0/798	0.44	0/1070
17	AQ	0.23	0/748	0.55	0/994
18	AR	0.23	0/2456	0.44	0/3317
19	AS	0.24	0/1138	0.50	0/1533
20	AT	0.24	0/1402	0.46	0/1883
21	AU	0.23	0/1510	0.53	0/2025
22	AV	0.23	0/3030	0.40	0/4093
23	AW	0.25	0/801	0.51	0/1079
24	AX	0.24	0/2921	0.44	0/3954
25	AY	0.24	0/1280	0.39	0/1725
26	AZ	0.25	0/857	0.49	0/1141
27	A0	0.23	0/1834	0.52	0/2484
28	A1	0.24	0/2313	0.45	0/3129
29	A2	0.24	0/941	0.54	0/1257
30	A3	0.23	0/636	0.58	0/839
31	A4	0.24	0/4877	0.43	0/6598

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Aw	0.30	1/1603 (0.1%)	0.65	0/2488
33	Ax	0.30	1/1655 (0.1%)	0.66	0/2569
34	Ay	0.29	1/1656 (0.1%)	0.66	0/2571
35	Az	0.16	0/803	0.68	0/1244
36	A	0.21	1/36876 (0.0%)	0.68	0/57402
37	B	0.34	1/1627 (0.1%)	0.67	0/2527
38	D	0.24	0/1896	0.56	0/2549
39	E	0.24	0/2475	0.46	0/3355
40	F	0.24	0/2090	0.51	0/2842
41	I	0.24	0/1731	0.48	0/2345
42	J	0.25	0/1348	0.48	0/1813
43	K	0.24	0/1490	0.47	0/2021
44	L	0.24	0/905	0.53	0/1218
45	M	0.25	0/2368	0.53	0/3195
46	N	0.24	0/1833	0.51	0/2468
47	O	0.23	0/1283	0.53	0/1727
48	P	0.24	0/1199	0.54	0/1623
49	Q	0.24	0/2039	0.50	0/2750
50	R	0.23	0/1175	0.54	0/1572
51	S	0.23	0/1320	0.52	0/1789
52	T	0.25	0/1403	0.51	0/1886
53	U	0.25	0/1274	0.54	0/1723
54	V	0.24	0/1721	0.52	0/2333
55	W	0.25	0/926	0.48	0/1244
56	X	0.25	0/2099	0.47	0/2837
57	Y	0.23	0/1593	0.50	0/2136
58	Z	0.23	0/1021	0.47	0/1378
59	0	0.23	0/913	0.52	0/1224
60	1	0.24	0/469	0.56	0/621
61	2	0.22	0/383	0.56	0/507
62	3	0.24	0/853	0.53	0/1136
63	4	0.24	0/350	0.55	0/461
64	5	0.24	0/3305	0.48	0/4502
65	6	0.26	0/3043	0.51	0/4140
66	7	0.24	0/2447	0.46	0/3310
67	8	0.24	0/1354	0.48	0/1819
68	9	0.26	0/1025	0.48	0/1379
69	a	0.24	0/866	0.50	0/1174
70	b	0.24	0/1211	0.54	0/1639
71	c	0.24	0/2347	0.47	0/3171
72	d	0.24	0/2039	0.47	0/2759
73	e	0.24	0/1970	0.47	0/2658
74	f	0.25	0/1273	0.44	0/1716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	g	0.24	0/1151	0.49	0/1569
76	h	0.23	0/918	0.45	0/1249
77	i	0.24	0/850	0.53	0/1135
78	j	0.24	0/760	0.51	0/1023
79	k	0.24	0/777	0.52	0/1048
80	l	0.23	0/707	0.49	0/960
81	m	0.23	0/805	0.58	0/1081
82	o	0.23	0/819	0.57	0/1097
83	p	0.23	0/1223	0.50	0/1641
84	q	0.24	0/1422	0.51	0/1916
85	r	0.24	0/1362	0.53	0/1846
86	s	0.24	0/3239	0.51	0/4400
87	t	0.23	0/358	0.35	0/486
87	u	0.22	0/259	0.34	0/350
87	v	0.22	0/259	0.34	0/350
87	w	0.22	0/246	0.35	0/331
87	x	0.22	0/246	0.34	0/331
87	y	0.22	0/246	0.34	0/331
88	H	0.24	0/1698	0.49	0/2292
89	z	0.25	0/2067	0.48	0/2793
All	All	0.23	5/190922 (0.0%)	0.57	0/271412

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	1671	G	OP3-P	-10.76	1.48	1.61
33	Ax	1	U	OP3-P	-10.61	1.48	1.61
32	Aw	1	U	OP3-P	-10.59	1.48	1.61
34	Ay	1	U	OP3-P	-10.59	1.48	1.61
37	B	1	C	OP3-P	-10.55	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	AA	20260	10304	10285	106	0
2	AB	1818	1809	1807	10	0
3	AC	1083	1089	1088	8	0
4	AD	2731	2805	2804	13	0
5	AE	972	1000	1000	1	0
6	AF	1725	1771	1769	11	0
7	AG	2688	2689	2687	18	0
8	AH	1152	1187	1183	7	0
9	AI	1020	1061	1053	4	0
10	AJ	839	889	887	10	0
11	AK	862	886	885	3	0
12	AL	1453	1541	1540	4	0
13	AM	942	966	965	3	0
14	AN	868	929	928	4	0
15	AO	1592	1561	1557	3	0
16	AP	781	807	806	1	0
17	AQ	744	758	758	4	0
18	AR	2409	2430	2428	4	0
19	AS	1111	1116	1115	4	0
20	AT	1371	1393	1393	4	0
21	AU	1488	1501	1499	5	0
22	AV	2969	2964	2961	11	0
23	AW	789	804	802	4	0
24	AX	2849	2845	2843	20	0
25	AY	1246	1198	1197	6	0
26	AZ	839	859	858	1	0
27	A0	1787	1797	1796	4	0
28	A1	2265	2296	2294	14	0
29	A2	935	971	971	10	0
30	A3	625	701	699	4	0
31	A4	4768	4770	4766	12	0
32	Aw	1434	725	725	0	0
33	Ax	1482	751	752	0	0
34	Ay	1483	752	753	0	0
35	Az	719	360	360	0	0
36	A	33070	16801	16795	161	0
37	B	1524	779	779	4	0
38	D	1859	1921	1920	7	0
39	E	2406	2416	2415	10	0
40	F	2031	2066	2065	6	0
41	I	1695	1789	1785	8	0
42	J	1330	1409	1407	3	0
43	K	1455	1452	1452	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	L	890	942	941	6	0
45	M	2314	2385	2384	10	0
46	N	1786	1818	1817	5	0
47	O	1259	1295	1294	4	0
48	P	1173	1166	1165	3	0
49	Q	1990	2031	2031	8	0
50	R	1154	1215	1214	3	0
51	S	1293	1366	1365	4	0
52	T	1369	1412	1410	1	0
53	U	1251	1232	1232	6	0
54	V	1676	1689	1687	12	0
55	W	904	936	935	2	0
56	X	2044	2061	2060	4	0
57	Y	1556	1598	1597	2	0
58	Z	996	1045	1044	3	0
59	0	898	917	916	5	0
60	1	464	513	511	3	0
61	2	377	407	406	1	0
62	3	832	884	883	6	0
63	4	342	362	361	2	0
64	5	3210	3209	3206	7	0
65	6	2948	2844	2841	12	0
66	7	2390	2399	2397	10	0
67	8	1327	1369	1368	3	0
68	9	997	988	987	3	0
69	a	840	812	810	0	0
70	b	1196	1196	1190	0	0
71	c	2299	2322	2320	0	0
72	d	1985	1979	1976	0	0
73	e	1931	1917	1916	0	0
74	f	1252	1271	1269	0	0
75	g	1113	1097	1097	0	0
76	h	895	882	881	0	0
77	i	828	859	857	0	0
78	j	745	747	746	0	0
79	k	774	785	784	0	0
80	l	688	675	674	0	0
81	m	791	760	796	0	0
82	o	798	806	804	0	0
83	p	1205	1224	1223	0	0
84	q	1389	1376	1374	0	0
85	r	1322	1349	1348	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	s	3155	3143	3139	0	0
87	t	354	378	377	0	0
87	u	257	284	283	0	0
87	v	257	284	283	0	0
87	w	245	275	275	0	0
87	x	245	275	275	0	0
87	y	245	275	275	0	0
88	H	1661	1736	1734	12	0
89	z	2027	2077	2076	0	0
90	AA	44	26	26	1	0
91	AA	14	30	26	0	0
92	A	30	66	57	0	0
92	AA	10	22	19	0	0
93	A	138	0	0	0	0
93	A3	1	0	0	0	0
93	AA	63	0	0	0	0
93	AB	1	0	0	0	0
93	AX	1	0	0	0	0
93	D	2	0	0	0	0
93	E	1	0	0	0	0
93	g	1	0	0	0	0
94	3	1	0	0	0	0
94	6	1	0	0	0	0
94	A	29	0	0	0	0
94	AA	18	0	0	0	0
94	D	1	0	0	0	0
94	M	1	0	0	0	0
94	W	1	0	0	0	0
94	i	1	0	0	0	0
94	o	1	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	12	12	0	0
99	A	6	14	12	0	0
100	B	7	11	8	1	0
101	0	28	0	0	2	0
101	1	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
101	2	34	0	0	0	0
101	3	44	0	0	2	0
101	4	11	0	0	0	0
101	5	14	0	0	1	0
101	6	100	0	0	4	0
101	7	15	0	0	0	0
101	8	15	0	0	2	0
101	9	17	0	0	0	0
101	A	2955	0	0	87	0
101	A0	1	0	0	0	0
101	A1	35	0	0	0	0
101	A2	32	0	0	0	0
101	A3	50	0	0	1	0
101	A4	9	0	0	0	0
101	AA	2039	0	0	60	0
101	AB	78	0	0	7	0
101	AC	55	0	0	3	0
101	AD	82	0	0	2	0
101	AE	27	0	0	0	0
101	AF	39	0	0	2	0
101	AG	64	0	0	3	0
101	AH	57	0	0	1	0
101	AI	39	0	0	2	0
101	AJ	25	0	0	2	0
101	AK	51	0	0	2	0
101	AL	42	0	0	2	0
101	AM	22	0	0	1	0
101	AN	39	0	0	0	0
101	AO	37	0	0	2	0
101	AP	31	0	0	1	0
101	AQ	77	0	0	1	0
101	AR	11	0	0	1	0
101	AS	25	0	0	0	0
101	AT	44	0	0	0	0
101	AU	8	0	0	2	0
101	AW	16	0	0	0	0
101	AX	56	0	0	4	0
101	AY	18	0	0	1	0
101	AZ	30	0	0	0	0
101	Aw	6	0	0	0	0
101	Ax	7	0	0	0	0
101	Ay	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
101	Az	13	0	0	0	0
101	B	66	0	0	0	0
101	D	68	0	0	0	0
101	E	66	0	0	2	0
101	F	79	0	0	3	0
101	H	7	0	0	1	0
101	I	27	0	0	3	0
101	J	1	0	0	0	0
101	K	57	0	0	2	0
101	L	31	0	0	4	0
101	M	51	0	0	2	0
101	N	58	0	0	1	0
101	O	33	0	0	0	0
101	P	81	0	0	3	0
101	Q	29	0	0	1	0
101	R	63	0	0	2	0
101	S	49	0	0	1	0
101	T	45	0	0	1	0
101	U	24	0	0	0	0
101	V	5	0	0	0	0
101	W	55	0	0	1	0
101	X	11	0	0	0	0
101	Y	25	0	0	0	0
101	Z	32	0	0	0	0
101	a	11	0	0	0	0
101	b	35	0	0	0	0
101	c	18	0	0	0	0
101	d	9	0	0	0	0
101	e	13	0	0	0	0
101	f	19	0	0	0	0
101	g	13	0	0	0	0
101	i	46	0	0	0	0
101	j	22	0	0	0	0
101	k	5	0	0	0	0
101	l	5	0	0	0	0
101	m	8	0	0	0	0
101	o	34	0	0	0	0
101	p	8	0	0	0	0
101	r	49	0	0	0	0
101	s	51	0	0	0	0
All	All	189566	153978	153838	573	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 (573) 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)
1:AA:1046:A:O2'	1:AA:1048:C:OP2	1.97	0.82
1:AA:1327:G:O6	101:AA:1801:HOH:O	1.99	0.80
36:A:3063:G:O2'	36:A:3066:C:OP2	1.98	0.80
36:A:3042:U:OP2	101:A:3501:HOH:O	1.99	0.78
13:AM:85:LYS:NZ	101:AM:201:HOH:O	2.18	0.77
36:A:2103:A:HO2'	58:Z:35:LYS:N	1.83	0.77
45:M:43:ARG:NH2	101:M:402:HOH:O	2.18	0.77
36:A:1777:A:N6	36:A:1780:U:OP2	2.18	0.76
36:A:3147:G:OP1	101:A:3502:HOH:O	2.03	0.76
36:A:3110:C:O2'	39:E:266:ARG:NH1	2.20	0.75
52:T:78:LYS:NZ	101:T:301:HOH:O	2.20	0.75
36:A:2708:C:O2'	59:O:96:ASN:OD1	2.04	0.74
50:R:20:ARG:NH2	101:R:202:HOH:O	2.19	0.74
11:AK:128:TRP:OXT	101:AK:201:HOH:O	2.05	0.74
49:Q:145:LEU:O	101:Q:301:HOH:O	2.05	0.74
6:AF:159:VAL:HG23	6:AF:172:VAL:HG21	1.70	0.74
36:A:2198:A:N1	101:A:3572:HOH:O	2.21	0.73
40:F:126:LYS:O	101:F:6501:HOH:O	2.05	0.73
1:AA:979:C:N3	101:AA:1850:HOH:O	2.21	0.73
62:3:170:ASN:O	101:3:301:HOH:O	2.06	0.73
36:A:2539:A:OP1	101:A:3507:HOH:O	2.07	0.73
1:AA:1151:C:N3	101:AA:1856:HOH:O	2.22	0.72
48:P:138:GLU:OE2	101:P:201:HOH:O	2.07	0.72
36:A:1703:C:OP2	101:A:3509:HOH:O	2.07	0.72
1:AA:1165:C:OP2	101:AA:1804:HOH:O	2.06	0.72
36:A:1970:G:O6	101:A:3503:HOH:O	2.06	0.72
36:A:2090:A:N7	101:A:3584:HOH:O	2.22	0.72
1:AA:1118:A:O2'	4:AD:351:ARG:NH2	2.22	0.72
36:A:2008:G:OP1	101:A:3506:HOH:O	2.07	0.72
1:AA:1139:A:OP2	101:AA:1802:HOH:O	2.05	0.72
36:A:2098:G:O2'	36:A:2099:U:OP2	2.06	0.72
36:A:2132:A:OP2	101:A:3508:HOH:O	2.07	0.72
39:E:337:VAL:O	101:E:501:HOH:O	2.07	0.72
36:A:2865:C:OP1	101:A:3504:HOH:O	2.06	0.72
1:AA:916:C:OP2	101:AA:1805:HOH:O	2.08	0.71
4:AD:127:ASN:OD1	101:AD:501:HOH:O	2.08	0.71
8:AH:94:PHE:CE1	28:A1:114:LEU:HD22	2.25	0.71
36:A:3090:G:N7	101:A:3582:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:2725:A:OP2	101:A:3510:HOH:O	2.08	0.71
7:AG:299:ASP:OD2	7:AG:301:GLN:NE2	2.23	0.71
1:AA:1057:G:OP2	101:AA:1803:HOH:O	2.06	0.71
3:AC:67:GLY:O	101:AC:201:HOH:O	2.07	0.71
24:AX:86:ARG:O	101:AX:601:HOH:O	2.08	0.71
36:A:2479:C:OP1	101:A:3505:HOH:O	2.06	0.71
1:AA:1169:G:N7	101:AA:1858:HOH:O	2.23	0.71
12:AL:210:CYS:O	101:AL:302:HOH:O	2.07	0.71
12:AL:172:ASN:O	101:AL:303:HOH:O	2.08	0.71
36:A:1856:A:OP2	36:A:2986:C:O2'	2.09	0.70
1:AA:976:A:N7	101:AA:1868:HOH:O	2.24	0.70
1:AA:1039:A:OP1	101:AA:1807:HOH:O	2.09	0.70
36:A:1863:A:OP2	101:A:3514:HOH:O	2.08	0.70
36:A:2453:G:OP2	101:A:3517:HOH:O	2.10	0.70
11:AK:122:GLY:O	101:AK:202:HOH:O	2.09	0.70
36:A:2240:C:OP2	101:A:3513:HOH:O	2.08	0.70
36:A:3015:U:OP1	101:A:3515:HOH:O	2.09	0.70
36:A:3176:A:OP2	101:A:3511:HOH:O	2.08	0.70
1:AA:1289:G:O2'	1:AA:1297:G:OP2	2.09	0.70
1:AA:1384:A:N7	101:AA:1873:HOH:O	2.25	0.70
48:P:126:GLU:OE2	101:P:203:HOH:O	2.10	0.70
36:A:2045:A:N7	101:A:3602:HOH:O	2.25	0.69
59:O:102:LYS:O	101:O:301:HOH:O	2.10	0.69
36:A:1782:G:OP2	101:A:3512:HOH:O	2.08	0.69
65:6:170:ARG:NH1	101:6:8105:HOH:O	2.22	0.69
1:AA:1015:A:N7	101:AA:1872:HOH:O	2.25	0.69
36:A:2003:A:N1	101:A:3598:HOH:O	2.24	0.69
56:X:44:ARG:NH2	88:H:84:GLU:OE1	2.26	0.69
18:AR:190:ASP:O	101:AR:401:HOH:O	2.10	0.69
1:AA:1027:A:N1	101:AA:1874:HOH:O	2.25	0.69
36:A:2404:U:OP1	101:A:3519:HOH:O	2.10	0.69
36:A:2740:A:N3	36:A:2921:A:O2'	2.24	0.69
1:AA:1401:G:OP2	101:AA:1814:HOH:O	2.11	0.69
36:A:1969:G:N7	101:A:3614:HOH:O	2.26	0.69
8:AH:135:GLU:OE1	101:AH:301:HOH:O	2.12	0.68
46:N:212:PRO:O	101:N:301:HOH:O	2.10	0.68
1:AA:970:A:N3	101:AA:1871:HOH:O	2.25	0.68
36:A:1730:U:OP2	101:A:3522:HOH:O	2.11	0.68
1:AA:1148:A:OP2	101:AA:1815:HOH:O	2.11	0.68
25:AY:318:GLU:OE1	101:AY:401:HOH:O	2.11	0.68
58:Z:78:ARG:O	58:Z:83:LYS:NZ	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:6:154:TYR:O	101:6:8103:HOH:O	2.11	0.68
1:AA:1287:A:OP2	4:AD:260:LYS:NZ	2.27	0.68
24:AX:167:ASP:OD1	101:AX:602:HOH:O	2.11	0.68
64:5:295:ASP:OD2	101:5:501:HOH:O	2.12	0.68
67:8:126:GLN:OE1	101:8:301:HOH:O	2.10	0.68
2:AB:164:GLU:OE2	101:AB:401:HOH:O	2.10	0.68
36:A:3014:G:OP1	101:A:3525:HOH:O	2.12	0.68
36:A:2111:C:OP2	101:A:3521:HOH:O	2.11	0.67
1:AA:1486:B8T:OP1	101:AA:1817:HOH:O	2.11	0.67
36:A:2526:C:OP1	101:A:3518:HOH:O	2.10	0.67
15:AO:125:GLN:O	101:AO:401:HOH:O	2.12	0.67
24:AX:393:ARG:O	101:AX:603:HOH:O	2.12	0.67
36:A:1830:G:OP2	101:A:3524:HOH:O	2.12	0.67
36:A:2562:U:O2'	38:D:284:ARG:O	2.07	0.67
36:A:2719:G:O6	101:A:3520:HOH:O	2.10	0.67
54:V:55:TYR:HB2	54:V:133:ILE:HD11	1.77	0.67
57:Y:134:LYS:NZ	68:9:76:TYR:OH	2.27	0.67
36:A:1739:A:OP2	101:A:3533:HOH:O	2.13	0.67
39:E:69:ASP:OD1	39:E:154:ARG:NH1	2.28	0.67
1:AA:1554:G:O6	101:AA:1821:HOH:O	2.13	0.67
36:A:1702:A:OP2	101:A:3526:HOH:O	2.12	0.67
36:A:1815:A:N1	101:A:3635:HOH:O	2.28	0.67
45:M:22:VAL:O	101:M:401:HOH:O	2.11	0.67
45:M:91:ARG:NH1	45:M:209:GLU:OE2	2.28	0.67
1:AA:941:G:OP2	101:AA:1822:HOH:O	2.13	0.66
1:AA:1063:A:OP2	101:AA:1818:HOH:O	2.12	0.66
1:AA:1485:G:OP2	101:AA:1820:HOH:O	2.13	0.66
36:A:2944:C:OP2	101:A:3534:HOH:O	2.13	0.66
36:A:2566:C:OP1	101:A:3528:HOH:O	2.12	0.66
65:6:275:GLN:O	101:6:8102:HOH:O	2.11	0.66
43:K:123:GLU:OE2	101:K:201:HOH:O	2.12	0.66
1:AA:992:U:O2'	1:AA:994:A:OP2	2.09	0.66
36:A:2196:A:O2'	36:A:2213:A:N1	2.28	0.66
55:W:139:GLU:OE1	101:W:301:HOH:O	2.12	0.66
1:AA:1112:A:N7	101:AA:1882:HOH:O	2.27	0.66
36:A:2704:A:N7	101:A:3622:HOH:O	2.27	0.66
88:H:178:ASN:OD1	88:H:179:ASN:N	2.28	0.66
1:AA:1068:A:OP2	101:AA:1819:HOH:O	2.13	0.66
2:AB:166:ALA:O	101:AB:403:HOH:O	2.14	0.66
10:AJ:117:ASP:OD1	101:AJ:201:HOH:O	2.13	0.66
24:AX:272:THR:OG1	24:AX:282:ILE:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1015:A:OP2	101:AA:1827:HOH:O	2.14	0.66
17:AQ:55:GLU:OE1	101:AQ:101:HOH:O	2.14	0.66
36:A:1778:U:OP2	101:A:3531:HOH:O	2.13	0.66
36:A:1852:C:OP1	101:A:3530:HOH:O	2.12	0.66
36:A:2388:A:OP2	101:A:3529:HOH:O	2.12	0.66
1:AA:1114:U:O4	101:AA:1810:HOH:O	2.10	0.65
36:A:1829:A:OP2	101:A:3535:HOH:O	2.14	0.65
67:8:181:PRO:O	101:8:302:HOH:O	2.13	0.65
36:A:2661:U:OP2	101:A:3539:HOH:O	2.15	0.65
44:L:76:ALA:O	101:L:202:HOH:O	2.15	0.65
36:A:2767:A:O2'	36:A:2769:A:N7	2.29	0.65
2:AB:148:ASN:OD1	101:AB:402:HOH:O	2.13	0.65
1:AA:1221:A:N3	101:AA:1895:HOH:O	2.29	0.65
41:I:151:ASN:O	101:I:301:HOH:O	2.14	0.65
62:3:144:LEU:O	101:3:302:HOH:O	2.14	0.65
1:AA:662:U:O4	101:AA:1811:HOH:O	2.10	0.65
31:A4:200:ASP:OD2	31:A4:243:ASN:N	2.30	0.65
36:A:2142:A:OP1	101:A:3537:HOH:O	2.14	0.65
22:AV:270:PRO:O	22:AV:346:LYS:NZ	2.30	0.64
28:A1:152:ASP:OD2	28:A1:174:ARG:NH1	2.29	0.64
1:AA:693:A:N7	101:AA:1898:HOH:O	2.30	0.64
36:A:1882:A:N7	101:A:3643:HOH:O	2.29	0.64
1:AA:667:U:OP1	101:AA:1826:HOH:O	2.14	0.64
4:AD:235:GLU:OE2	101:AD:502:HOH:O	2.14	0.64
36:A:2289:G:N7	101:A:3651:HOH:O	2.30	0.64
36:A:2030:U:H3	36:A:2095:U:HO2'	1.45	0.64
1:AA:1287:A:OP1	101:AA:1828:HOH:O	2.15	0.64
36:A:3013:G:HO2'	63:4:66:PHE:N	1.96	0.64
3:AC:113:ARG:NH1	101:AC:202:HOH:O	2.28	0.64
39:E:129:VAL:CG1	39:E:145:LEU:HD11	2.28	0.64
1:AA:1294:A:OP1	2:AB:201:ASN:ND2	2.30	0.63
36:A:1978:A:OP1	101:A:3541:HOH:O	2.15	0.63
44:L:130:ARG:NH1	44:L:133:GLU:OE2	2.31	0.63
36:A:1990:G:OP1	38:D:269:ARG:NH2	2.30	0.63
1:AA:905:A:O2'	1:AA:907:A:OP1	2.17	0.63
1:AA:895:C:O2	101:AA:1823:HOH:O	2.13	0.63
21:AU:38:LYS:NZ	101:AU:301:HOH:O	2.31	0.63
1:AA:1107:U:O4	30:A3:128:LYS:NZ	2.30	0.63
49:Q:77:SER:OG	49:Q:79:GLU:OE1	2.12	0.63
20:AT:132:ARG:NH1	20:AT:136:LEU:O	2.32	0.62
68:9:16:ASP:OD1	68:9:25:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:899:G:O2'	1:AA:907:A:N1	2.23	0.62
3:AC:152:ARG:NH1	31:A4:87:TYR:OH	2.33	0.62
7:AG:275:LYS:O	101:AG:402:HOH:O	2.16	0.62
29:A2:33:VAL:HG21	29:A2:104:LEU:HD23	1.82	0.61
36:A:2014:A:O2'	101:A:3546:HOH:O	2.16	0.61
36:A:2652:G:O6	101:A:3536:HOH:O	2.14	0.61
40:F:212:TRP:O	40:F:258:THR:OG1	2.14	0.61
66:7:175:ILE:O	66:7:319:ARG:NH2	2.33	0.61
1:AA:1154:A:OP2	30:A3:155:ARG:NH2	2.34	0.61
36:A:2447:A:OP2	101:A:3544:HOH:O	2.15	0.61
29:A2:64:ASP:OD1	29:A2:65:ALA:N	2.34	0.61
36:A:2702:G:OP2	101:A:3548:HOH:O	2.16	0.60
88:H:75:ARG:O	101:H:301:HOH:O	2.17	0.60
36:A:2005:C:N4	101:A:3666:HOH:O	2.32	0.60
36:A:3060:C:OP2	101:A:3549:HOH:O	2.17	0.60
39:E:129:VAL:HG11	39:E:145:LEU:HD11	1.84	0.60
36:A:2045:A:N3	101:A:3664:HOH:O	2.32	0.60
36:A:2545:U:O2'	101:A:3532:HOH:O	2.13	0.60
38:D:281:TRP:O	38:D:285:LYS:NZ	2.32	0.60
1:AA:1549:G:O6	101:AA:1831:HOH:O	2.16	0.60
36:A:2239:A:N7	101:A:3667:HOH:O	2.32	0.59
36:A:1787:G:N2	36:A:1790:A:OP2	2.34	0.59
36:A:2048:U:OP2	101:A:3550:HOH:O	2.17	0.59
36:A:2013:U:OP2	101:A:3543:HOH:O	2.15	0.59
1:AA:1574:G:OP1	101:AA:1830:HOH:O	2.16	0.59
65:6:367:ASP:OD1	65:6:370:ARG:NH1	2.35	0.59
7:AG:226:GLU:O	7:AG:230:THR:HG23	2.02	0.59
7:AG:295:VAL:HG22	7:AG:330:CYS:SG	2.42	0.58
7:AG:356:VAL:HG23	7:AG:361:VAL:HG23	1.85	0.58
53:U:11:ARG:NH2	54:V:211:LYS:O	2.36	0.58
1:AA:1222:A:N7	101:AA:1913:HOH:O	2.32	0.58
66:7:62:THR:HG23	66:7:62:THR:O	2.03	0.58
44:L:95:ARG:NH2	101:L:204:HOH:O	2.30	0.58
1:AA:1199:G:N1	1:AA:1422:G:OP2	2.37	0.58
59:0:153:THR:HG22	59:0:153:THR:O	2.04	0.57
50:R:58:TYR:OH	101:R:201:HOH:O	2.11	0.57
29:A2:48:GLU:OE1	29:A2:48:GLU:N	2.35	0.57
22:AV:226:TYR:HE1	22:AV:282:VAL:HG21	1.69	0.57
53:U:9:LEU:O	53:U:11:ARG:NH1	2.38	0.57
1:AA:700:A:N1	1:AA:709:G:O2'	2.33	0.57
36:A:1741:A:OP1	101:A:3551:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:2364:C:OP2	53:U:78:LYS:NZ	2.36	0.57
88:H:53:THR:N	88:H:86:THR:HG1	2.03	0.57
1:AA:1162:A:N7	101:AA:1915:HOH:O	2.32	0.57
22:AV:226:TYR:CE1	22:AV:282:VAL:HG21	2.40	0.56
36:A:1737:A:H61	36:A:1760:G:H1'	1.70	0.56
1:AA:970:A:O2'	101:AA:1808:HOH:O	2.09	0.56
36:A:2499:U:OP2	36:A:2504:A:N6	2.33	0.56
47:O:140:SER:O	47:O:146:ASN:ND2	2.39	0.56
1:AA:841:A:OP1	13:AM:39:ASN:ND2	2.38	0.56
1:AA:973:C:OP2	101:AA:1834:HOH:O	2.17	0.56
1:AA:1232:A:OP2	101:AA:1836:HOH:O	2.18	0.56
36:A:2196:A:N3	101:A:3675:HOH:O	2.32	0.56
36:A:2860:G:O6	101:A:3540:HOH:O	2.15	0.56
47:O:62:TYR:OH	49:Q:272:GLU:OE2	2.23	0.56
51:S:112:ASP:OD2	101:S:301:HOH:O	2.18	0.56
1:AA:1412:G:OP1	24:AX:279:LYS:NZ	2.38	0.56
31:A4:470:GLN:NE2	31:A4:472:ASP:OD2	2.38	0.56
36:A:2355:A:HO2'	36:A:2673:G:HO2'	1.51	0.56
36:A:2697:G:OP2	101:A:3553:HOH:O	2.18	0.56
40:F:70:ARG:NH2	40:F:194:GLU:OE1	2.39	0.56
31:A4:556:LYS:NZ	31:A4:560:GLU:OE2	2.39	0.56
36:A:1958:G:O2'	101:A:3538:HOH:O	2.14	0.56
36:A:2108:G:O6	46:N:67:LYS:NZ	2.38	0.55
36:A:3219:G:O2'	36:A:3221:A:OP2	2.20	0.55
22:AV:92:LEU:HD21	22:AV:137:ILE:HD11	1.89	0.54
36:A:1805:A:OP2	54:V:94:HIS:NE2	2.33	0.54
1:AA:689:U:OP1	101:AA:1838:HOH:O	2.18	0.54
1:AA:1021:U:OP2	29:A2:9:ARG:NH2	2.40	0.54
1:AA:1496:U:OP1	10:AJ:82:ARG:NH2	2.41	0.54
2:AB:211:ASP:OD2	101:AB:405:HOH:O	2.18	0.54
36:A:3152:C:OP1	49:Q:141:SER:OG	2.15	0.54
1:AA:930:G:O6	10:AJ:47:ARG:NH2	2.40	0.54
1:AA:1263:G:N2	101:AA:1958:HOH:O	2.38	0.54
36:A:1953:A:O2'	36:A:2463:A:OP1	2.25	0.54
36:A:1800:G:N1	36:A:1803:A:OP2	2.40	0.54
1:AA:1037:A:OP2	101:AA:1839:HOH:O	2.18	0.54
36:A:2059:C:N4	101:A:3783:HOH:O	2.41	0.54
36:A:3006:U:OP2	101:A:3557:HOH:O	2.19	0.54
1:AA:843:G:N2	1:AA:846:A:OP2	2.36	0.54
1:AA:1595:G:OP2	101:AA:1833:HOH:O	2.17	0.54
20:AT:91:GLU:OE1	21:AU:120:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:1720:C:OP2	101:A:3555:HOH:O	2.18	0.54
36:A:2512:A:O2'	36:A:2541:C:OP1	2.20	0.54
29:A2:99:LEU:HD11	29:A2:103:LYS:HB2	1.89	0.54
14:AN:8:VAL:O	14:AN:11:ARG:NH1	2.40	0.54
19:AS:83:ARG:NH1	19:AS:93:LYS:O	2.41	0.53
1:AA:760:A:OP1	101:AA:1841:HOH:O	2.19	0.53
1:AA:1134:G:OP2	10:AJ:38:ARG:NH2	2.40	0.53
1:AA:1142:A:OP1	101:AA:1842:HOH:O	2.19	0.53
36:A:1742:G:O2'	36:A:1754:G:O6	2.21	0.53
36:A:2458:A:O2'	39:E:215:PHE:O	2.23	0.53
65:6:215:THR:OG1	65:6:275:GLN:OE1	2.23	0.53
7:AG:337:ARG:NH2	101:AG:408:HOH:O	2.42	0.53
1:AA:1525:C:O5'	22:AV:105:ARG:NH2	2.42	0.53
6:AF:116:GLU:OE1	101:AF:301:HOH:O	2.19	0.53
19:AS:7:GLU:N	19:AS:7:GLU:OE1	2.40	0.53
1:AA:1576:G:OP2	101:AA:1840:HOH:O	2.18	0.52
36:A:2531:U:O4	38:D:246:ARG:NH2	2.42	0.52
1:AA:1294:A:N1	101:AA:1930:HOH:O	2.34	0.52
4:AD:245:VAL:HG22	4:AD:271:ALA:HB1	1.90	0.52
9:AI:178:ASN:ND2	101:AI:205:HOH:O	2.41	0.52
15:AO:217:ARG:NH1	15:AO:227:GLU:OE2	2.42	0.52
24:AX:151:LEU:CD2	24:AX:247:LEU:HD22	2.39	0.52
36:A:1747:G:OP2	36:A:1749:C:N4	2.41	0.52
2:AB:241:ASP:CG	101:AB:404:HOH:O	2.47	0.52
48:P:162:GLN:NE2	101:P:210:HOH:O	2.36	0.52
36:A:1749:C:OP2	36:A:2899:C:O2'	2.27	0.52
47:O:144:LEU:HD12	66:7:174:VAL:HG11	1.92	0.52
2:AB:241:ASP:OD1	101:AB:404:HOH:O	2.18	0.51
36:A:1745:U:O4	62:3:108:LYS:NZ	2.41	0.51
38:D:257:ILE:O	38:D:262:ARG:NH1	2.40	0.51
1:AA:894:C:N4	10:AJ:117:ASP:OD2	2.43	0.51
36:A:2989:G:O2'	101:A:3523:HOH:O	2.11	0.51
65:6:188:TYR:OH	101:6:8101:HOH:O	2.07	0.51
1:AA:1022:A:OP1	101:AA:1845:HOH:O	2.19	0.51
8:AH:125:HIS:CE1	8:AH:126:ILE:HG23	2.45	0.51
28:A1:46:ARG:HB2	28:A1:47:PRO:HD3	1.92	0.51
1:AA:702:C:OP1	1:AA:848:U:O2'	2.27	0.51
1:AA:1326:A:OP1	101:AA:1837:HOH:O	2.18	0.51
36:A:2237:A:OP2	101:A:3561:HOH:O	2.19	0.51
40:F:98:GLN:NE2	101:F:6509:HOH:O	2.44	0.51
24:AX:81:HIS:CD2	24:AX:190:ASN:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A1:250:GLU:OE2	28:A1:301:ASN:ND2	2.44	0.51
10:AJ:78:ARG:NH2	10:AJ:117:ASP:OD2	2.43	0.50
14:AN:67:ARG:NH1	14:AN:80:GLU:OE2	2.44	0.50
24:AX:183:GLU:N	24:AX:183:GLU:OE1	2.41	0.50
36:A:2221:C:OP2	101:A:3556:HOH:O	2.18	0.50
1:AA:1485:G:O6	101:AA:1843:HOH:O	2.19	0.50
41:I:128:ASN:OD1	101:I:302:HOH:O	2.19	0.50
56:X:177:HIS:O	56:X:184:ARG:NH1	2.44	0.50
1:AA:1004:G:O2'	9:AI:98:GLN:NE2	2.44	0.50
36:A:2866:A:OP2	101:A:3558:HOH:O	2.19	0.50
46:N:73:ARG:O	46:N:155:LYS:NZ	2.45	0.50
51:S:109:THR:HG22	51:S:112:ASP:OD2	2.11	0.50
54:V:188:VAL:O	54:V:188:VAL:HG23	2.11	0.50
1:AA:1229:U:O2'	1:AA:1442:G:O4'	2.30	0.50
3:AC:109:VAL:HG23	28:A1:103:LEU:HD11	1.93	0.50
36:A:2170:G:OP1	101:A:3564:HOH:O	2.19	0.50
36:A:3089:A:H3'	36:A:3090:G:H5''	1.94	0.50
1:AA:1443:U:OP2	101:AA:1844:HOH:O	2.19	0.50
7:AG:200:LEU:HD11	7:AG:204:GLU:HB3	1.94	0.50
36:A:3001:G:N7	101:A:3693:HOH:O	2.35	0.50
4:AD:340:ILE:HG22	4:AD:340:ILE:O	2.12	0.50
36:A:2110:A:H5'	46:N:67:LYS:HZ3	1.77	0.50
36:A:2149:G:OP1	101:A:3568:HOH:O	2.20	0.50
62:3:188:VAL:O	65:6:356:ARG:NH2	2.44	0.50
36:A:1740:A:OP1	101:A:3560:HOH:O	2.19	0.49
24:AX:297:MET:HE3	24:AX:306:ILE:HG21	1.93	0.49
36:A:2075:U:O2'	36:A:2833:A:N7	2.34	0.49
36:A:2477:G:OP1	101:A:3565:HOH:O	2.19	0.49
66:7:156:ARG:HG3	66:7:156:ARG:HH11	1.77	0.49
36:A:1817:C:OP2	101:A:3567:HOH:O	2.20	0.49
44:L:97:THR:OG1	101:L:201:HOH:O	2.14	0.49
36:A:1760:G:OP1	45:M:196:ARG:NE	2.39	0.49
49:Q:237:ASN:OD1	49:Q:238:PHE:N	2.46	0.49
36:A:1851:G:H2'	36:A:2693:A:N7	2.28	0.49
28:A1:198:TYR:OH	28:A1:203:ASP:OD1	2.22	0.49
56:X:91:TYR:CE2	88:H:79:VAL:HG11	2.47	0.49
1:AA:845:A:H4'	21:AU:60:TYR:CE2	2.47	0.49
3:AC:106:ASP:OD1	3:AC:107:GLN:N	2.42	0.49
36:A:1735:A:H2'	36:A:1735:A:N3	2.28	0.49
36:A:2712:G:OP1	101:A:3563:HOH:O	2.19	0.49
1:AA:1486:B8T:O2'	101:AA:1848:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:I:53:TYR:O	101:I:303:HOH:O	2.20	0.49
7:AG:259:PRO:O	101:AG:403:HOH:O	2.20	0.48
36:A:2472:A:OP2	101:A:3566:HOH:O	2.20	0.48
4:AD:312:TYR:N	4:AD:331:ASP:OD2	2.45	0.48
51:S:109:THR:N	51:S:112:ASP:OD2	2.45	0.48
1:AA:769:G:OP2	14:AN:73:ARG:NH2	2.45	0.48
6:AF:172:VAL:HG12	6:AF:240:ARG:HD3	1.94	0.48
37:B:76:A:O2'	100:B:101:VAL:O	2.30	0.48
6:AF:159:VAL:CG2	6:AF:172:VAL:HG21	2.42	0.48
36:A:2777:G:N3	88:H:179:ASN:ND2	2.61	0.48
66:7:257:ILE:O	66:7:257:ILE:HG13	2.14	0.48
29:A2:33:VAL:HG22	29:A2:105:ASN:OD1	2.13	0.48
29:A2:15:ASN:OD1	29:A2:17:ARG:NH1	2.46	0.48
36:A:2016:C:OP2	45:M:59:ARG:NH1	2.47	0.48
36:A:2160:A:OP2	63:4:88:TRP:NE1	2.40	0.48
59:0:95:ARG:O	101:0:302:HOH:O	2.20	0.48
1:AA:1455:U:OP1	101:AA:1847:HOH:O	2.20	0.48
36:A:2339:G:OP2	101:A:3569:HOH:O	2.20	0.48
36:A:3089:A:H3'	36:A:3090:G:C5'	2.44	0.48
15:AO:130:HIS:ND1	101:AO:403:HOH:O	2.26	0.48
18:AR:162:SER:O	18:AR:170:ARG:NH1	2.47	0.48
65:6:257:PRO:HB3	65:6:268:LEU:HD21	1.95	0.48
7:AG:102:GLU:OE1	7:AG:102:GLU:N	2.43	0.47
51:S:152:ASP:OD1	51:S:153:LEU:N	2.48	0.47
60:1:34:ARG:NH1	60:1:38:ARG:O	2.47	0.47
66:7:276:PHE:HB2	66:7:304:VAL:HG22	1.96	0.47
41:I:148:VAL:HG23	41:I:148:VAL:O	2.14	0.47
1:AA:702:C:OP1	21:AU:41:ARG:NH2	2.45	0.47
1:AA:1080:A:O2'	1:AA:1082:A:N7	2.43	0.47
28:A1:299:LEU:HD21	28:A1:309:ILE:HD13	1.96	0.47
42:J:75:ASP:OD1	42:J:77:THR:HG22	2.15	0.47
47:O:64:LYS:NZ	47:O:100:GLN:O	2.48	0.47
64:5:173:ARG:HA	64:5:176:TYR:CE1	2.50	0.47
1:AA:1378:C:O2	24:AX:389:SER:OG	2.30	0.47
36:A:3201:A:H2'	36:A:3202:U:O4'	2.15	0.47
36:A:2725:A:N7	36:A:2990:A:N6	2.64	0.46
22:AV:173:PHE:O	22:AV:179:GLN:NE2	2.48	0.46
1:AA:1557:A:OP1	10:AJ:72:LYS:N	2.47	0.46
4:AD:268:PHE:HB3	7:AG:56:ILE:HD11	1.98	0.46
19:AS:106:LEU:HB2	19:AS:117:LEU:HD11	1.98	0.46
24:AX:108:LEU:HD23	24:AX:141:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1520:U:OP2	22:AV:407:GLN:NE2	2.46	0.46
27:A0:13:GLU:OE2	27:A0:16:ARG:NH1	2.49	0.46
36:A:1954:U:O4	101:A:3562:HOH:O	2.19	0.46
46:N:59:VAL:O	46:N:59:VAL:HG13	2.15	0.46
1:AA:1188:A:OP2	1:AA:1429:C:O2'	2.21	0.46
5:AE:17:GLU:OE1	5:AE:17:GLU:N	2.48	0.46
24:AX:153:LEU:HD21	24:AX:244:LEU:CD2	2.45	0.46
1:AA:1454:G:OP2	7:AG:377:ARG:NH1	2.44	0.46
6:AF:159:VAL:HG23	6:AF:172:VAL:CG2	2.44	0.46
7:AG:198:ARG:NH1	7:AG:201:ILE:HG23	2.31	0.46
45:M:250:ASP:OD1	45:M:251:GLU:N	2.49	0.46
1:AA:1598:G:OP2	101:AA:1851:HOH:O	2.21	0.46
36:A:2220:A:HO2'	36:A:2221:C:P	2.36	0.46
41:I:128:ASN:ND2	41:I:149:GLY:O	2.49	0.46
56:X:87:LEU:O	88:H:78:ARG:NH1	2.47	0.46
1:AA:1038:C:O2'	12:AL:155:TYR:OH	2.31	0.46
6:AF:85:VAL:HG22	24:AX:379:GLU:OE1	2.16	0.46
53:U:47:GLU:OE1	53:U:47:GLU:N	2.45	0.46
54:V:124:ASP:OD1	54:V:125:PRO:HD2	2.16	0.46
14:AN:93:ASP:O	14:AN:97:GLY:N	2.44	0.45
24:AX:153:LEU:HD12	24:AX:187:TRP:HZ2	1.81	0.45
88:H:146:LEU:O	88:H:150:GLY:N	2.45	0.45
1:AA:1044:U:OP1	1:AA:1110:A:O2'	2.30	0.45
25:AY:377:ARG:O	25:AY:381:ASN:ND2	2.49	0.45
37:B:38:C:OP1	65:6:52:ARG:NH1	2.50	0.45
1:AA:1583:MA6:OP1	30:A3:145:LYS:NZ	2.48	0.45
20:AT:92:THR:O	20:AT:92:THR:HG22	2.16	0.45
36:A:2883:A:N3	36:A:2883:A:H2'	2.31	0.45
42:J:20:ILE:HD11	42:J:42:ARG:HD3	1.98	0.45
90:AA:1701:NAD:O2D	101:AA:1849:HOH:O	2.20	0.45
36:A:2946:A:OP2	101:A:3571:HOH:O	2.21	0.45
88:H:223:VAL:N	88:H:231:VAL:O	2.45	0.45
40:F:115:LYS:NZ	101:F:6510:HOH:O	2.44	0.45
22:AV:35:VAL:O	22:AV:35:VAL:HG12	2.17	0.45
62:3:146:GLU:HA	62:3:146:GLU:OE1	2.17	0.45
31:A4:305:ILE:HG22	31:A4:306:ASN:N	2.32	0.45
36:A:1889:C:OP1	45:M:133:LYS:NZ	2.43	0.45
36:A:2353:A:O2'	36:A:2355:A:OP2	2.17	0.45
42:J:102:ARG:N	42:J:107:GLU:OE2	2.49	0.45
54:V:169:THR:HG22	54:V:169:THR:O	2.16	0.45
1:AA:709:G:OP1	13:AM:13:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A4:303:CYS:SG	31:A4:344:ARG:NH2	2.89	0.44
1:AA:769:G:N2	1:AA:772:A:OP2	2.44	0.44
1:AA:1431:G:O2'	1:AA:1457:G:O6	2.32	0.44
36:A:2259:C:O2'	36:A:2261:C:OP2	2.24	0.44
36:A:2281:A:O2'	101:A:3559:HOH:O	2.19	0.44
36:A:1871:A:N3	62:3:104:ARG:NH2	2.65	0.44
45:M:177:ALA:HA	45:M:222:TYR:CD1	2.53	0.44
18:AR:317:ALA:O	18:AR:321:ALA:N	2.50	0.44
24:AX:119:TYR:OH	28:A1:273:GLU:OE2	2.22	0.44
29:A2:99:LEU:HD11	29:A2:103:LYS:CB	2.47	0.44
31:A4:58:VAL:O	31:A4:58:VAL:HG23	2.17	0.44
49:Q:251:GLU:OE1	49:Q:251:GLU:HA	2.16	0.44
54:V:176:ASP:OD1	57:Y:82:GLY:N	2.51	0.44
36:A:2137:C:OP2	58:Z:77:ARG:NH1	2.49	0.44
37:B:44:A:H2'	37:B:45:G:O4'	2.17	0.44
36:A:2135:A:N3	36:A:2135:A:H2'	2.33	0.44
38:D:207:ILE:HG22	38:D:207:ILE:O	2.18	0.44
53:U:66:ALA:HB2	53:U:100:ALA:HA	1.99	0.44
54:V:122:LEU:HD22	54:V:133:ILE:HD13	2.00	0.44
26:AZ:46:LYS:HA	26:AZ:49:TYR:CE1	2.53	0.44
31:A4:458:TYR:HB3	31:A4:486:TYR:CD1	2.53	0.44
1:AA:1490:U:O2'	101:AA:1812:HOH:O	2.10	0.44
36:A:2231:A:N3	36:A:3003:A:O2'	2.39	0.44
36:A:3211:C:HO2'	36:A:3212:C:H5	1.59	0.44
54:V:134:GLU:HG3	54:V:148:THR:HG22	1.99	0.44
66:7:51:GLU:OE1	66:7:51:GLU:HA	2.18	0.44
64:5:289:HIS:CE1	64:5:290:THR:HG1	2.33	0.43
1:AA:1208:U:OP1	101:AA:1852:HOH:O	2.21	0.43
41:I:180:CYS:SG	41:I:184:THR:N	2.92	0.43
43:K:67:PHE:HB3	43:K:71:LYS:HB2	2.00	0.43
49:Q:62:ILE:HG23	49:Q:62:ILE:O	2.17	0.43
54:V:159:PHE:CD1	54:V:160:PRO:HD2	2.53	0.43
1:AA:1293:C:N4	17:AQ:80:ARG:O	2.51	0.43
4:AD:415:GLN:NE2	4:AD:417:MET:SD	2.92	0.43
7:AG:312:GLN:OE1	7:AG:345:ARG:NH1	2.51	0.43
10:AJ:48:LYS:NZ	101:AJ:207:HOH:O	2.47	0.43
28:A1:113:HIS:CD2	28:A1:114:LEU:HG	2.53	0.43
31:A4:596:LEU:H	31:A4:596:LEU:HD12	1.84	0.43
36:A:1807:U:O2'	36:A:1808:A:OP2	2.28	0.43
36:A:2506:A:H1'	36:A:2601:A:N6	2.33	0.43
3:AC:115:ASN:ND2	25:AY:309:LYS:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A3:144:ARG:NH2	101:A3:304:HOH:O	2.51	0.43
36:A:1991:A:H5'	36:A:1992:C:OP1	2.19	0.43
39:E:151:THR:HG23	39:E:171:PRO:HB2	2.00	0.43
1:AA:1088:C:O2'	101:AA:1824:HOH:O	2.14	0.43
8:AH:155:VAL:HG21	28:A1:129:PHE:HB2	2.01	0.43
36:A:2710:C:O2'	36:A:3220:A:N1	2.38	0.43
39:E:131:LYS:O	39:E:145:LEU:HD12	2.18	0.43
88:H:65:ALA:HB2	88:H:71:PRO:HA	2.00	0.43
3:AC:65:ARG:NH1	101:AC:205:HOH:O	2.38	0.43
8:AH:155:VAL:HG21	28:A1:129:PHE:CB	2.49	0.43
41:I:197:LEU:HD23	41:I:198:PRO:O	2.18	0.43
1:AA:691:A:N7	1:AA:716:U:O2'	2.50	0.42
7:AG:229:LEU:HD13	7:AG:241:VAL:HG11	2.01	0.42
24:AX:153:LEU:HD21	24:AX:244:LEU:HD22	2.01	0.42
36:A:2015:G:O4'	45:M:56:GLU:HG3	2.19	0.42
36:A:2075:U:OP1	101:A:3577:HOH:O	2.21	0.42
36:A:2855:G:O6	101:A:3552:HOH:O	2.18	0.42
7:AG:237:GLU:OE1	7:AG:237:GLU:N	2.51	0.42
9:AI:189:ARG:NH2	101:AI:208:HOH:O	2.53	0.42
28:A1:86:ARG:NH1	28:A1:96:PRO:O	2.50	0.42
36:A:2112:A:H4'	36:A:2113:G:OP1	2.19	0.42
43:K:16:ARG:O	101:K:202:HOH:O	2.21	0.42
44:L:95:ARG:NH2	101:L:207:HOH:O	2.51	0.42
66:7:87:THR:O	66:7:90:SER:OG	2.30	0.42
1:AA:1279:C:O2'	1:AA:1296:A:N1	2.48	0.42
18:AR:162:SER:HB2	18:AR:165:ILE:HD12	2.01	0.42
36:A:2039:A:N1	36:A:2932:G:O2'	2.45	0.42
1:AA:894:C:OP1	101:AA:1846:HOH:O	2.20	0.42
8:AH:60:LYS:NZ	28:A1:128:ASP:OD2	2.38	0.42
3:AC:45:SER:OG	3:AC:46:LYS:N	2.51	0.42
21:AU:27:ARG:N	101:AU:303:HOH:O	2.51	0.42
55:W:102:GLU:OE2	65:6:74:TYR:N	2.53	0.42
88:H:238:VAL:HG12	88:H:239:ASN:N	2.35	0.42
1:AA:1322:C:N3	4:AD:234:LYS:NZ	2.66	0.42
25:AY:255:ARG:NH1	25:AY:256:LEU:O	2.53	0.42
27:A0:37:ASP:O	27:A0:41:LEU:N	2.52	0.42
28:A1:304:GLU:OE2	28:A1:309:ILE:HD11	2.20	0.42
36:A:2483:U:H2'	36:A:2484:C:O4'	2.19	0.42
36:A:2868:C:H2'	36:A:2869:A:O4'	2.20	0.42
65:6:217:LEU:HD11	65:6:271:LEU:HD12	2.01	0.42
1:AA:1066:C:O2'	9:AI:187:ARG:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:95:ALA:HB3	8:AH:143:LEU:HD21	2.01	0.42
17:AQ:80:ARG:NH2	23:AW:164:GLU:OE1	2.45	0.42
6:AF:90:VAL:HG13	6:AF:184:MET:CE	2.50	0.42
7:AG:320:VAL:HG21	7:AG:352:LEU:HD21	2.00	0.42
36:A:2814:G:O2'	36:A:2983:G:OP1	2.38	0.42
50:R:65:ARG:HA	50:R:68:TRP:CE3	2.55	0.42
53:U:19:VAL:O	53:U:19:VAL:HG13	2.20	0.42
54:V:165:ILE:HG21	68:9:76:TYR:CD2	2.55	0.42
2:AB:103:GLU:N	2:AB:104:PRO:CD	2.82	0.41
27:A0:63:ARG:NH2	27:A0:110:ASP:OD2	2.53	0.41
36:A:1980:A:OP1	61:2:56:SER:OG	2.32	0.41
37:B:12:U:O2'	37:B:14:A:OP1	2.38	0.41
2:AB:222:ILE:O	101:AB:406:HOH:O	2.22	0.41
6:AF:46:ILE:O	6:AF:46:ILE:HG22	2.20	0.41
27:A0:158:GLU:O	27:A0:158:GLU:HG2	2.21	0.41
101:A:3796:HOH:O	41:I:29:GLY:N	2.53	0.41
67:8:202:VAL:O	67:8:203:GLU:HB3	2.20	0.41
25:AY:259:PHE:HB2	31:A4:363:ILE:HD11	2.02	0.41
36:A:2099:U:OP1	101:A:3574:HOH:O	2.21	0.41
64:5:56:GLU:O	64:5:56:GLU:HG3	2.19	0.41
4:AD:112:LYS:NZ	4:AD:235:GLU:O	2.53	0.41
6:AF:35:SER:N	101:AF:304:HOH:O	2.53	0.41
45:M:149:THR:O	45:M:149:THR:HG22	2.19	0.41
1:AA:1057:G:H4'	1:AA:1578:A:H4'	2.02	0.41
16:AP:70:LYS:NZ	101:AP:303:HOH:O	2.53	0.41
23:AW:92:MET:O	23:AW:98:LYS:NZ	2.54	0.41
23:AW:162:VAL:O	23:AW:162:VAL:HG12	2.20	0.41
65:6:224:HIS:HA	65:6:232:TYR:CE2	2.56	0.41
4:AD:198:TRP:HA	4:AD:201:ILE:HD12	2.03	0.41
22:AV:318:ASP:OD1	22:AV:319:ILE:N	2.54	0.41
36:A:2306:A:OP1	101:A:3573:HOH:O	2.21	0.41
64:5:105:TYR:CE1	64:5:262:ILE:HD12	2.56	0.41
1:AA:1065:C:H2'	1:AA:1066:C:O4'	2.21	0.41
1:AA:1143:C:N4	101:AA:1853:HOH:O	2.22	0.41
22:AV:87:HIS:ND1	49:Q:60:PRO:HB2	2.36	0.41
24:AX:103:LYS:N	24:AX:104:PRO:CD	2.83	0.41
36:A:1958:G:OP1	101:A:3576:HOH:O	2.21	0.41
36:A:2398:A:H2'	36:A:2399:A:O4'	2.21	0.41
64:5:110:ARG:O	64:5:110:ARG:HG3	2.20	0.41
31:A4:302:VAL:O	31:A4:312:LYS:NZ	2.51	0.41
36:A:2227:A:N3	36:A:2227:A:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:2728:C:H4'	36:A:2815:OMG:HM22	2.02	0.41
36:A:2778:U:OP1	36:A:2782:A:N6	2.48	0.41
36:A:2909:G:OP1	60:1:63:ARG:NH1	2.47	0.41
43:K:7:ALA:HB3	43:K:8:PRO:HD3	2.02	0.41
88:H:208:LEU:HB3	88:H:209:PRO:HD2	2.03	0.41
1:AA:894:C:H41	10:AJ:78:ARG:NH2	2.19	0.41
7:AG:310:ARG:NE	24:AX:383:LEU:O	2.54	0.41
7:AG:337:ARG:HG3	7:AG:338:SER:N	2.36	0.41
17:AQ:63:ILE:HD13	29:A2:6:LEU:HD21	2.03	0.41
24:AX:129:GLU:OE1	101:AX:605:HOH:O	2.22	0.41
29:A2:59:ASN:ND2	29:A2:66:CYS:SG	2.87	0.41
36:A:2595:A:H2'	36:A:2596:G:O4'	2.21	0.41
44:L:128:ARG:O	44:L:131:GLU:HG3	2.20	0.41
54:V:133:ILE:HD12	54:V:145:ARG:HB3	2.02	0.41
59:0:166:SER:OG	59:0:167:GLU:N	2.54	0.41
4:AD:363:ALA:O	4:AD:367:GLY:N	2.53	0.41
6:AF:174:LEU:O	6:AF:179:ARG:NH1	2.53	0.41
20:AT:6:ARG:HG2	20:AT:7:PHE:CD2	2.56	0.41
24:AX:384:SER:O	24:AX:385:ASN:HB3	2.20	0.41
25:AY:290:ASN:OD1	25:AY:290:ASN:O	2.38	0.41
31:A4:560:GLU:O	31:A4:565:ARG:NH1	2.51	0.41
36:A:1961:A:N1	101:A:3730:HOH:O	2.37	0.41
36:A:1994:A:H61	36:A:2736:C:H4'	1.86	0.41
38:D:230:SER:O	38:D:231:LYS:HB2	2.20	0.41
64:5:177:CYS:HB3	64:5:178:PRO:HD3	2.02	0.41
66:7:36:SER:HB2	66:7:37:PRO:HD2	2.02	0.41
19:AS:111:GLU:HB2	19:AS:117:LEU:HD13	2.03	0.40
36:A:3067:PSU:OP1	39:E:234:THR:OG1	2.24	0.40
22:AV:225:LEU:HD11	22:AV:283:LEU:HD22	2.02	0.40
23:AW:113:TYR:CD1	23:AW:123:VAL:HG22	2.56	0.40
36:A:2757:A:N1	36:A:2789:C:O2'	2.50	0.40
40:F:191:ASP:OD1	40:F:192:SER:N	2.51	0.40
60:1:54:VAL:HG12	60:1:55:LEU:N	2.37	0.40
66:7:106:ALA:O	66:7:113:TRP:N	2.46	0.40
10:AJ:61:VAL:HG22	10:AJ:107:ILE:CD1	2.52	0.40
11:AK:120:LEU:HB3	11:AK:123:ILE:HD12	2.03	0.40
12:AL:126:GLU:HG2	12:AL:177:VAL:HG11	2.03	0.40
36:A:1810:A:H2'	36:A:1811:A:O4'	2.21	0.40
2:AB:146:SER:O	2:AB:168:THR:HA	2.22	0.40
6:AF:90:VAL:HG13	6:AF:184:MET:HE2	2.03	0.40
36:A:2257:C:OP2	101:A:3580:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:717:G:O2'	101:AA:1854:HOH:O	2.22	0.40
39:E:281:ASN:ND2	101:E:513:HOH:O	2.54	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	
2	AB	220/296 (74%)	218 (99%)	2 (1%)	0	100	100
3	AC	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
4	AD	341/430 (79%)	331 (97%)	10 (3%)	0	100	100
5	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
6	AF	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
7	AG	323/396 (82%)	315 (98%)	8 (2%)	0	100	100
8	AH	138/201 (69%)	137 (99%)	0	1 (1%)	22	32
9	AI	134/194 (69%)	133 (99%)	1 (1%)	0	100	100
10	AJ	106/138 (77%)	105 (99%)	1 (1%)	0	100	100
11	AK	99/128 (77%)	99 (100%)	0	0	100	100
12	AL	172/257 (67%)	170 (99%)	2 (1%)	0	100	100
13	AM	117/137 (85%)	117 (100%)	0	0	100	100
14	AN	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
15	AO	191/258 (74%)	188 (98%)	3 (2%)	0	100	100
16	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
17	AQ	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
18	AR	293/360 (81%)	284 (97%)	9 (3%)	0	100	100
19	AS	133/190 (70%)	133 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	AU	174/205 (85%)	174 (100%)	0	0	100	100
22	AV	358/414 (86%)	351 (98%)	7 (2%)	0	100	100
23	AW	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
24	AX	350/398 (88%)	342 (98%)	7 (2%)	1 (0%)	41	56
25	AY	147/395 (37%)	147 (100%)	0	0	100	100
26	AZ	98/106 (92%)	97 (99%)	1 (1%)	0	100	100
27	A0	213/217 (98%)	209 (98%)	4 (2%)	0	100	100
28	A1	277/323 (86%)	273 (99%)	4 (1%)	0	100	100
29	A2	115/118 (98%)	115 (100%)	0	0	100	100
30	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
31	A4	584/689 (85%)	577 (99%)	7 (1%)	0	100	100
38	D	236/305 (77%)	231 (98%)	5 (2%)	0	100	100
39	E	303/348 (87%)	298 (98%)	4 (1%)	1 (0%)	41	56
40	F	250/311 (80%)	245 (98%)	5 (2%)	0	100	100
41	I	210/261 (80%)	200 (95%)	10 (5%)	0	100	100
42	J	173/192 (90%)	173 (100%)	0	0	100	100
43	K	175/178 (98%)	173 (99%)	2 (1%)	0	100	100
44	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
45	M	287/296 (97%)	284 (99%)	3 (1%)	0	100	100
46	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
47	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
48	P	142/180 (79%)	142 (100%)	0	0	100	100
49	Q	237/292 (81%)	235 (99%)	1 (0%)	1 (0%)	34	48
50	R	138/149 (93%)	138 (100%)	0	0	100	100
51	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
52	T	164/206 (80%)	164 (100%)	0	0	100	100
53	U	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
54	V	203/216 (94%)	199 (98%)	4 (2%)	0	100	100
55	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
56	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
58	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
59	0	108/188 (57%)	108 (100%)	0	0	100	100
60	1	54/65 (83%)	54 (100%)	0	0	100	100
61	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
62	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
63	4	36/103 (35%)	36 (100%)	0	0	100	100
64	5	392/423 (93%)	384 (98%)	8 (2%)	0	100	100
65	6	352/380 (93%)	344 (98%)	8 (2%)	0	100	100
66	7	292/338 (86%)	284 (97%)	8 (3%)	0	100	100
67	8	155/206 (75%)	153 (99%)	2 (1%)	0	100	100
68	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
69	a	96/142 (68%)	95 (99%)	1 (1%)	0	100	100
70	b	148/215 (69%)	146 (99%)	2 (1%)	0	100	100
71	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
72	d	235/306 (77%)	231 (98%)	4 (2%)	0	100	100
73	e	236/279 (85%)	230 (98%)	6 (2%)	0	100	100
74	f	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
75	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
76	h	108/158 (68%)	108 (100%)	0	0	100	100
77	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
78	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
79	k	99/112 (88%)	99 (100%)	0	0	100	100
80	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
81	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
82	o	92/102 (90%)	91 (99%)	1 (1%)	0	100	100
83	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
84	q	161/222 (72%)	160 (99%)	1 (1%)	0	100	100
85	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
86	s	382/439 (87%)	375 (98%)	7 (2%)	0	100	100
87	t	44/198 (22%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	u	30/198 (15%)	30 (100%)	0	0	100	100
87	v	30/198 (15%)	30 (100%)	0	0	100	100
87	w	29/198 (15%)	29 (100%)	0	0	100	100
87	x	29/198 (15%)	29 (100%)	0	0	100	100
87	y	29/198 (15%)	29 (100%)	0	0	100	100
88	H	200/267 (75%)	194 (97%)	6 (3%)	0	100	100
89	z	250/325 (77%)	237 (95%)	12 (5%)	1 (0%)	34	48
All	All	14696/19484 (75%)	14471 (98%)	220 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AH	126	ILE
89	z	128	ASP
24	AX	81	HIS
39	E	150	LYS
49	Q	62	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	197/249 (79%)	197 (100%)	0	100	100
3	AC	115/143 (80%)	115 (100%)	0	100	100
4	AD	286/357 (80%)	286 (100%)	0	100	100
5	AE	104/107 (97%)	104 (100%)	0	100	100
6	AF	185/209 (88%)	185 (100%)	0	100	100
7	AG	285/342 (83%)	285 (100%)	0	100	100
8	AH	130/180 (72%)	130 (100%)	0	100	100
9	AI	104/146 (71%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	93/118 (79%)	93 (100%)	0	100	100
11	AK	91/113 (80%)	91 (100%)	0	100	100
12	AL	158/226 (70%)	158 (100%)	0	100	100
13	AM	97/113 (86%)	97 (100%)	0	100	100
14	AN	96/115 (84%)	96 (100%)	0	100	100
15	AO	174/230 (76%)	174 (100%)	0	100	100
16	AP	88/123 (72%)	88 (100%)	0	100	100
17	AQ	78/79 (99%)	78 (100%)	0	100	100
18	AR	264/318 (83%)	264 (100%)	0	100	100
19	AS	116/164 (71%)	116 (100%)	0	100	100
20	AT	153/157 (98%)	153 (100%)	0	100	100
21	AU	152/174 (87%)	152 (100%)	0	100	100
22	AV	325/364 (89%)	325 (100%)	0	100	100
23	AW	87/158 (55%)	87 (100%)	0	100	100
24	AX	311/351 (89%)	311 (100%)	0	100	100
25	AY	137/357 (38%)	137 (100%)	0	100	100
26	AZ	90/95 (95%)	90 (100%)	0	100	100
27	A0	188/189 (100%)	188 (100%)	0	100	100
28	A1	257/291 (88%)	257 (100%)	0	100	100
29	A2	100/101 (99%)	100 (100%)	0	100	100
30	A3	65/166 (39%)	65 (100%)	0	100	100
31	A4	526/609 (86%)	526 (100%)	0	100	100
38	D	192/245 (78%)	192 (100%)	0	100	100
39	E	260/290 (90%)	260 (100%)	0	100	100
40	F	219/262 (84%)	219 (100%)	0	100	100
41	I	194/232 (84%)	194 (100%)	0	100	100
42	J	138/150 (92%)	138 (100%)	0	100	100
43	K	154/155 (99%)	154 (100%)	0	100	100
44	L	98/124 (79%)	98 (100%)	0	100	100
45	M	245/249 (98%)	245 (100%)	0	100	100
46	N	189/211 (90%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	O	134/150 (89%)	134 (100%)	0	100	100
48	P	126/155 (81%)	126 (100%)	0	100	100
49	Q	221/256 (86%)	221 (100%)	0	100	100
50	R	118/126 (94%)	118 (100%)	0	100	100
51	S	146/180 (81%)	146 (100%)	0	100	100
52	T	146/176 (83%)	146 (100%)	0	100	100
53	U	134/135 (99%)	134 (100%)	0	100	100
54	V	183/191 (96%)	183 (100%)	0	100	100
55	W	94/119 (79%)	94 (100%)	0	100	100
56	X	220/229 (96%)	220 (100%)	0	100	100
57	Y	163/223 (73%)	162 (99%)	1 (1%)	86	93
58	Z	113/147 (77%)	113 (100%)	0	100	100
59	0	99/164 (60%)	99 (100%)	0	100	100
60	1	53/60 (88%)	53 (100%)	0	100	100
61	2	40/72 (56%)	40 (100%)	0	100	100
62	3	88/166 (53%)	88 (100%)	0	100	100
63	4	37/89 (42%)	37 (100%)	0	100	100
64	5	353/368 (96%)	353 (100%)	0	100	100
65	6	313/332 (94%)	313 (100%)	0	100	100
66	7	270/303 (89%)	270 (100%)	0	100	100
67	8	146/190 (77%)	146 (100%)	0	100	100
68	9	104/112 (93%)	104 (100%)	0	100	100
69	a	96/133 (72%)	95 (99%)	1 (1%)	76	86
70	b	131/185 (71%)	131 (100%)	0	100	100
71	c	251/288 (87%)	251 (100%)	0	100	100
72	d	223/274 (81%)	223 (100%)	0	100	100
73	e	207/236 (88%)	207 (100%)	0	100	100
74	f	139/188 (74%)	139 (100%)	0	100	100
75	g	124/148 (84%)	124 (100%)	0	100	100
76	h	104/148 (70%)	104 (100%)	0	100	100
77	i	86/110 (78%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	j	74/97 (76%)	74 (100%)	0	100	100
79	k	83/90 (92%)	83 (100%)	0	100	100
80	l	76/116 (66%)	76 (100%)	0	100	100
81	m	85/113 (75%)	85 (100%)	0	100	100
82	o	80/87 (92%)	80 (100%)	0	100	100
83	p	135/181 (75%)	135 (100%)	0	100	100
84	q	142/178 (80%)	142 (100%)	0	100	100
85	r	147/169 (87%)	147 (100%)	0	100	100
86	s	340/381 (89%)	340 (100%)	0	100	100
87	t	40/158 (25%)	40 (100%)	0	100	100
87	u	31/158 (20%)	31 (100%)	0	100	100
87	v	31/158 (20%)	31 (100%)	0	100	100
87	w	30/158 (19%)	30 (100%)	0	100	100
87	x	30/158 (19%)	30 (100%)	0	100	100
87	y	30/158 (19%)	30 (100%)	0	100	100
88	H	182/228 (80%)	182 (100%)	0	100	100
89	z	226/287 (79%)	226 (100%)	0	100	100
All	All	13165/16790 (78%)	13163 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	Y	198	ARG
69	a	122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
4	AD	302	HIS
4	AD	356	GLN
5	AE	56	GLN
6	AF	113	GLN
6	AF	146	HIS
8	AH	125	HIS
9	AI	87	HIS

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Mol	Chain	Res	Type
9	AI	96	GLN
9	AI	178	ASN
10	AJ	105	HIS
18	AR	288	GLN
20	AT	101	HIS
21	AU	188	ASN
22	AV	380	GLN
24	AX	69	ASN
24	AX	159	HIS
24	AX	250	GLN
28	A1	185	HIS
31	A4	306	ASN
38	D	221	ASN
39	E	125	GLN
39	E	281	ASN
40	F	98	GLN
40	F	188	HIS
46	N	181	HIS
47	O	100	GLN
49	Q	139	GLN
51	S	118	ASN
53	U	84	ASN
53	U	98	GLN
58	Z	150	HIS
59	0	120	HIS
64	5	331	ASN
64	5	367	ASN
65	6	320	GLN
65	6	354	GLN
69	a	126	HIS
70	b	58	ASN
70	b	131	HIS
73	e	252	HIS
77	i	124	HIS
82	o	21	HIS
82	o	94	HIS
86	s	239	ASN
89	z	241	HIS
89	z	266	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	950/954 (99%)	135 (14%)	1 (0%)
32	Aw	67/68 (98%)	18 (26%)	0
33	Ax	68/70 (97%)	13 (19%)	0
34	Ay	68/70 (97%)	14 (20%)	0
35	Az	32/34 (94%)	13 (40%)	0
36	A	1556/1561 (99%)	224 (14%)	3 (0%)
37	B	71/72 (98%)	12 (16%)	0
All	All	2812/2829 (99%)	429 (15%)	4 (0%)

All (429) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	651	A
1	AA	673	U
1	AA	680	U
1	AA	688	A
1	AA	695	A
1	AA	704	U
1	AA	721	U
1	AA	722	C
1	AA	737	C
1	AA	738	A
1	AA	753	A
1	AA	761	A
1	AA	766	G
1	AA	777	G
1	AA	786	G
1	AA	791	G
1	AA	794	U
1	AA	796	G
1	AA	815	C
1	AA	830	U
1	AA	832	U
1	AA	835	C
1	AA	836	A
1	AA	851	A
1	AA	860	A
1	AA	861	U
1	AA	868	C
1	AA	869	C
1	AA	871	A
1	AA	890	C
1	AA	903	U

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Mol	Chain	Res	Type
1	AA	904	C
1	AA	907	A
1	AA	919	A
1	AA	929	A
1	AA	931	C
1	AA	932	C
1	AA	938	A
1	AA	939	A
1	AA	942	A
1	AA	946	U
1	AA	947	U
1	AA	960	C
1	AA	962	C
1	AA	967	A
1	AA	992	U
1	AA	1001	C
1	AA	1011	C
1	AA	1015	A
1	AA	1019	A
1	AA	1042	U
1	AA	1046	A
1	AA	1081	U
1	AA	1082	A
1	AA	1103	A
1	AA	1105	C
1	AA	1106	C
1	AA	1107	U
1	AA	1109	A
1	AA	1118	A
1	AA	1119	U
1	AA	1120	C
1	AA	1121	A
1	AA	1126	A
1	AA	1137	A
1	AA	1151	C
1	AA	1153	C
1	AA	1160	A
1	AA	1167	A
1	AA	1179	G
1	AA	1187	U
1	AA	1188	A
1	AA	1189	U

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Mol	Chain	Res	Type
1	AA	1190	C
1	AA	1193	U
1	AA	1220	A
1	AA	1223	C
1	AA	1225	C
1	AA	1229	U
1	AA	1247	G
1	AA	1248	C
1	AA	1250	C
1	AA	1251	A
1	AA	1258	A
1	AA	1271	C
1	AA	1273	G
1	AA	1275	A
1	AA	1283	A
1	AA	1284	U
1	AA	1285	G
1	AA	1290	C
1	AA	1291	U
1	AA	1307	G
1	AA	1326	A
1	AA	1327	G
1	AA	1343	A
1	AA	1344	U
1	AA	1353	A
1	AA	1354	A
1	AA	1356	A
1	AA	1378	C
1	AA	1387	A
1	AA	1390	A
1	AA	1405	C
1	AA	1406	U
1	AA	1407	U
1	AA	1422	G
1	AA	1430	A
1	AA	1462	G
1	AA	1463	G
1	AA	1469	G
1	AA	1474	G
1	AA	1481	C
1	AA	1503	G
1	AA	1519	A

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Mol	Chain	Res	Type
1	AA	1525	C
1	AA	1526	U
1	AA	1527	A
1	AA	1533	C
1	AA	1534	C
1	AA	1536	A
1	AA	1537	C
1	AA	1539	C
1	AA	1540	A
1	AA	1541	U
1	AA	1544	A
1	AA	1551	G
1	AA	1557	A
1	AA	1562	G
1	AA	1568	U
1	AA	1571	U
1	AA	1582	G
1	AA	1594	G
1	AA	1595	G
1	AA	1599	A
32	Aw	3	G
32	Aw	7	A
32	Aw	9	A
32	Aw	16	A
32	Aw	21	A
32	Aw	22	A
32	Aw	30	G
32	Aw	46	A
32	Aw	49	U
32	Aw	50	A
32	Aw	55	A
32	Aw	56	A
32	Aw	61	U
32	Aw	65	A
32	Aw	68	U
32	Aw	71	C
32	Aw	73	U
32	Aw	74	C
33	Ax	2	A
33	Ax	3	G
33	Ax	8	U
33	Ax	9	A

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Mol	Chain	Res	Type
33	Ax	25	C
33	Ax	44	A
33	Ax	45	G
33	Ax	46	A
33	Ax	48	U
33	Ax	49	G
33	Ax	59	U
33	Ax	62	C
33	Ax	76	A
34	Ay	3	G
34	Ay	4	G
34	Ay	23	A
34	Ay	28	C
34	Ay	29	U
34	Ay	30	G
34	Ay	37	A
34	Ay	44	A
34	Ay	45	G
34	Ay	48	U
34	Ay	49	G
34	Ay	59	U
34	Ay	75	C
34	Ay	76	A
35	Az	0	U
35	Az	1	U
35	Az	8	U
35	Az	11	U
35	Az	12	U
35	Az	13	U
35	Az	15	U
35	Az	18	A
35	Az	22	A
35	Az	25	U
35	Az	26	A
35	Az	27	C
35	Az	32	A
36	A	1681	G
36	A	1689	C
36	A	1692	A
36	A	1693	C
36	A	1694	U
36	A	1699	C

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Mol	Chain	Res	Type
36	A	1700	U
36	A	1704	U
36	A	1708	A
36	A	1711	C
36	A	1724	A
36	A	1727	A
36	A	1728	U
36	A	1748	G
36	A	1765	C
36	A	1805	A
36	A	1807	U
36	A	1808	A
36	A	1809	U
36	A	1810	A
36	A	1821	A
36	A	1827	C
36	A	1828	A
36	A	1829	A
36	A	1832	A
36	A	1836	A
36	A	1844	A
36	A	1854	U
36	A	1856	A
36	A	1869	A
36	A	1871	A
36	A	1882	A
36	A	1887	A
36	A	1893	A
36	A	1901	C
36	A	1903	C
36	A	1918	G
36	A	1937	A
36	A	1940	A
36	A	1958	G
36	A	1985	G
36	A	1993	A
36	A	1994	A
36	A	2003	A
36	A	2015	G
36	A	2022	G
36	A	2030	U
36	A	2031	A

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Mol	Chain	Res	Type
36	A	2036	C
36	A	2037	U
36	A	2039	A
36	A	2054	U
36	A	2055	U
36	A	2060	A
36	A	2069	U
36	A	2070	C
36	A	2071	U
36	A	2079	C
36	A	2099	U
36	A	2113	G
36	A	2125	C
36	A	2126	U
36	A	2147	G
36	A	2160	A
36	A	2163	A
36	A	2168	U
36	A	2181	A
36	A	2192	A
36	A	2198	A
36	A	2200	A
36	A	2214	A
36	A	2219	C
36	A	2220	A
36	A	2221	C
36	A	2222	U
36	A	2225	C
36	A	2226	U
36	A	2227	A
36	A	2228	A
36	A	2230	A
36	A	2237	A
36	A	2239	A
36	A	2241	A
36	A	2243	A
36	A	2245	A
36	A	2246	A
36	A	2262	C
36	A	2263	C
36	A	2284	C
36	A	2285	U

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Mol	Chain	Res	Type
36	A	2297	A
36	A	2300	G
36	A	2322	C
36	A	2331	C
36	A	2332	C
36	A	2345	G
36	A	2350	A
36	A	2353	A
36	A	2357	C
36	A	2363	A
36	A	2372	U
36	A	2374	A
36	A	2390	A
36	A	2399	A
36	A	2401	A
36	A	2404	U
36	A	2407	U
36	A	2415	C
36	A	2444	A
36	A	2446	A
36	A	2451	A
36	A	2478	G
36	A	2484	C
36	A	2485	U
36	A	2493	C
36	A	2502	C
36	A	2520	C
36	A	2521	A
36	A	2527	A
36	A	2540	C
36	A	2558	A
36	A	2570	C
36	A	2587	G
36	A	2592	G
36	A	2593	G
36	A	2599	U
36	A	2600	A
36	A	2601	A
36	A	2603	C
36	A	2618	U
36	A	2627	G
36	A	2629	A

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Mol	Chain	Res	Type
36	A	2630	U
36	A	2633	A
36	A	2635	G
36	A	2654	U
36	A	2656	U
36	A	2683	C
36	A	2686	G
36	A	2694	A
36	A	2696	A
36	A	2706	A
36	A	2718	C
36	A	2719	G
36	A	2723	A
36	A	2724	G
36	A	2725	A
36	A	2732	G
36	A	2745	A
36	A	2761	C
36	A	2762	C
36	A	2765	A
36	A	2767	A
36	A	2768	A
36	A	2775	A
36	A	2781	U
36	A	2782	A
36	A	2786	U
36	A	2787	A
36	A	2788	C
36	A	2791	A
36	A	2810	G
36	A	2832	A
36	A	2833	A
36	A	2847	C
36	A	2864	U
36	A	2865	C
36	A	2882	U
36	A	2883	A
36	A	2884	C
36	A	2885	U
36	A	2886	A
36	A	2887	U
36	A	2888	A

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Mol	Chain	Res	Type
36	A	2889	C
36	A	2893	A
36	A	2910	A
36	A	2911	C
36	A	2913	A
36	A	2917	G
36	A	2922	A
36	A	2928	C
36	A	2932	G
36	A	2935	A
36	A	2956	A
36	A	2989	G
36	A	2990	A
36	A	2992	G
36	A	3005	A
36	A	3007	C
36	A	3016	G
36	A	3041	U
36	A	3053	A
36	A	3054	G
36	A	3060	C
36	A	3090	G
36	A	3100	U
36	A	3102	U
36	A	3108	U
36	A	3109	U
36	A	3110	C
36	A	3111	A
36	A	3112	A
36	A	3113	A
36	A	3157	C
36	A	3158	A
36	A	3162	C
36	A	3169	C
36	A	3172	C
36	A	3176	A
36	A	3183	U
36	A	3199	U
36	A	3200	U
36	A	3207	A
36	A	3208	C
36	A	3209	A

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Mol	Chain	Res	Type
36	A	3210	C
36	A	3212	C
36	A	3217	A
36	A	3218	A
36	A	3228	U
36	A	3229	U
36	A	3230	G
36	A	3231	U
37	B	8	U
37	B	16	C
37	B	21	A
37	B	45	G
37	B	48	U
37	B	54	C
37	B	55	U
37	B	56	U
37	B	58	A
37	B	64	A
37	B	69	U
37	B	76	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1539	C
36	A	2030	U
36	A	2112	A
36	A	2245	A

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

20 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
79	AYA	k	2	79	6,7,8	0.83	0	5,8,10	0.52	0
1	5MU	AA	1076	1	19,22,23	0.62	0	28,32,35	1.20	3 (10%)
36	OMU	A	3039	94,36	19,22,23	0.27	0	26,31,34	0.42	0
37	2MG	B	10	37	18,26,27	1.16	2 (11%)	16,38,41	0.88	1 (6%)
17	AYA	AQ	2	17	6,7,8	0.79	0	5,8,10	0.51	0
37	PSU	B	39	37	18,21,22	0.78	0	22,30,33	2.54	4 (18%)
53	AYA	U	2	53	6,7,8	0.80	0	5,8,10	0.58	0
29	AYA	A2	2	29	6,7,8	0.80	0	5,8,10	0.56	0
36	OMG	A	3040	32,36	18,26,27	0.92	1 (5%)	19,38,41	0.61	0
37	1MA	B	9	37	16,25,26	1.16	2 (12%)	18,37,40	0.88	1 (5%)
36	OMG	A	2815	94,36,33	18,26,27	0.94	2 (11%)	19,38,41	0.62	0
43	SAC	K	2	43	7,8,9	0.24	0	8,9,11	0.56	0
36	PSU	A	3067	36	18,21,22	0.79	0	22,30,33	2.56	5 (22%)
70	THC	b	2	70	8,9,10	0.29	0	9,11,13	0.54	0
1	MA6	AA	1584	1	18,26,27	0.75	0	19,38,41	0.54	0
9	5F0	AI	184	9	8,8,9	0.58	0	7,9,11	1.17	1 (14%)
36	1MA	A	2617	36	16,25,26	1.15	3 (18%)	18,37,40	0.91	1 (5%)
1	B8T	AA	1486	93,1	19,22,23	0.31	0	26,31,34	0.32	0
1	MA6	AA	1583	1	18,26,27	0.74	0	19,38,41	0.55	0
1	5MC	AA	1488	1	18,22,23	0.31	0	26,32,35	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	AYA	k	2	79	-	1/4/6/8	-
1	5MU	AA	1076	1	-	0/7/25/26	0/2/2/2
36	OMU	A	3039	94,36	-	0/9/27/28	0/2/2/2
37	2MG	B	10	37	-	0/5/27/28	0/3/3/3
17	AYA	AQ	2	17	-	1/4/6/8	-
37	PSU	B	39	37	-	0/7/25/26	0/2/2/2
53	AYA	U	2	53	-	0/4/6/8	-
29	AYA	A2	2	29	-	0/4/6/8	-
36	OMG	A	3040	32,36	-	0/5/27/28	0/3/3/3
37	1MA	B	9	37	-	0/3/25/26	0/3/3/3
36	OMG	A	2815	94,36,33	-	0/5/27/28	0/3/3/3
43	SAC	K	2	43	-	0/7/8/10	-
36	PSU	A	3067	36	-	0/7/25/26	0/2/2/2
70	THC	b	2	70	-	0/8/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	AA	1584	1	-	2/7/29/30	0/3/3/3
9	5F0	AI	184	9	-	0/9/9/10	-
36	1MA	A	2617	36	-	0/3/25/26	0/3/3/3
1	B8T	AA	1486	93,1	-	0/7/27/28	0/2/2/2
1	MA6	AA	1583	1	-	0/7/29/30	0/3/3/3
1	5MC	AA	1488	1	-	0/7/25/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	9	1MA	C6-N6	3.10	1.35	1.27
36	A	2617	1MA	C6-N6	3.09	1.35	1.27
37	B	10	2MG	C8-N7	-3.04	1.29	1.35
37	B	10	2MG	C5-C6	-2.39	1.42	1.47
36	A	2815	OMG	C5-C6	-2.25	1.42	1.47
36	A	3040	OMG	C5-C6	-2.21	1.42	1.47
37	B	9	1MA	C5-C4	-2.14	1.37	1.43
36	A	2617	1MA	C5-C4	-2.10	1.37	1.43
36	A	2815	OMG	C8-N7	-2.08	1.31	1.35
36	A	2617	1MA	C8-N7	-2.01	1.31	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	39	PSU	N1-C2-N3	8.06	124.26	115.13
36	A	3067	PSU	N1-C2-N3	8.05	124.25	115.13
37	B	39	PSU	C4-N3-C2	-6.54	116.92	126.34
36	A	3067	PSU	C4-N3-C2	-6.53	116.92	126.34
1	AA	1076	5MU	C4-N3-C2	-4.78	121.17	127.35
36	A	3067	PSU	O2-C2-N1	-3.66	118.76	122.79
37	B	39	PSU	O2-C2-N1	-3.62	118.81	122.79
9	AI	184	5F0	O-C-CB	-2.74	117.45	125.43
1	AA	1076	5MU	C5-C4-N3	2.63	117.56	115.31
37	B	39	PSU	O2-C2-N3	-2.59	116.93	121.82
36	A	3067	PSU	O2-C2-N3	-2.56	116.98	121.82
1	AA	1076	5MU	N3-C2-N1	2.23	117.85	114.89
36	A	3067	PSU	O4'-C1'-C2'	2.18	108.22	105.14
37	B	10	2MG	O6-C6-C5	2.17	128.61	124.37
37	B	9	1MA	N1-C6-N6	2.09	125.08	119.77
36	A	2617	1MA	N1-C6-N6	2.07	125.03	119.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1584	MA6	C5-C6-N6-C9
79	k	2	AYA	C-CA-N-CT
1	AA	1584	MA6	C4'-C5'-O5'-P
17	AQ	2	AYA	CB-CA-N-CT

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	2815	OMG	1	0
36	A	3067	PSU	1	0
1	AA	1486	B8T	2	0
1	AA	1583	MA6	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 278 ligands modelled in this entry, 265 are monoatomic - leaving 13 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	$\# Z > 2$
92	SPD	A	3302	-	9,9,9	0.33	0	8,8,8	1.17	0
92	SPD	A	3303	-	9,9,9	0.34	0	8,8,8	1.12	0
98	GDP	AX	503	-	24,30,30	0.88	1 (4%)	30,47,47	0.61	0
92	SPD	AA	1703	-	9,9,9	0.29	0	8,8,8	1.31	2 (25%)
96	FES	AP	201	16,5	0,4,4	-	-	-	-	-
96	FES	AT	201	20,13	0,4,4	-	-	-	-	-
97	ATP	AX	501	93	26,33,33	0.75	0	31,52,52	0.65	0
99	PUT	A	3304	-	5,5,5	0.24	0	4,4,4	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
96	FES	r	201	41,85	0,4,4	-	-	-		
90	NAD	AA	1701	93	42,48,48	0.57	0	50,73,73	0.65	1 (2%)
91	SPM	AA	1702	-	13,13,13	0.28	0	12,12,12	0.97	0
92	SPD	A	3301	-	9,9,9	0.27	0	8,8,8	1.18	0
100	VAL	B	101	37	4,6,7	0.52	0	6,7,9	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	SPD	A	3302	-	-	0/7/7/7	-
92	SPD	A	3303	-	-	2/7/7/7	-
98	GDP	AX	503	-	-	0/12/32/32	0/3/3/3
92	SPD	AA	1703	-	-	0/7/7/7	-
99	PUT	A	3304	-	-	0/3/3/3	-
97	ATP	AX	501	93	-	0/18/38/38	0/3/3/3
96	FES	AP	201	16,5	-	-	0/1/1/1
96	FES	AT	201	20,13	-	-	0/1/1/1
96	FES	r	201	41,85	-	-	0/1/1/1
90	NAD	AA	1701	93	-	0/26/62/62	0/5/5/5
91	SPM	AA	1702	-	-	0/11/11/11	-
92	SPD	A	3301	-	-	1/7/7/7	-
100	VAL	B	101	37	-	0/5/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
98	AX	503	GDP	C5-C6	-2.20	1.42	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	AA	1701	NAD	C5A-C6A-N6A	2.31	123.87	120.35
92	AA	1703	SPD	C4-C5-N6	-2.24	106.09	112.14
92	AA	1703	SPD	C8-C7-N6	-2.09	106.49	112.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

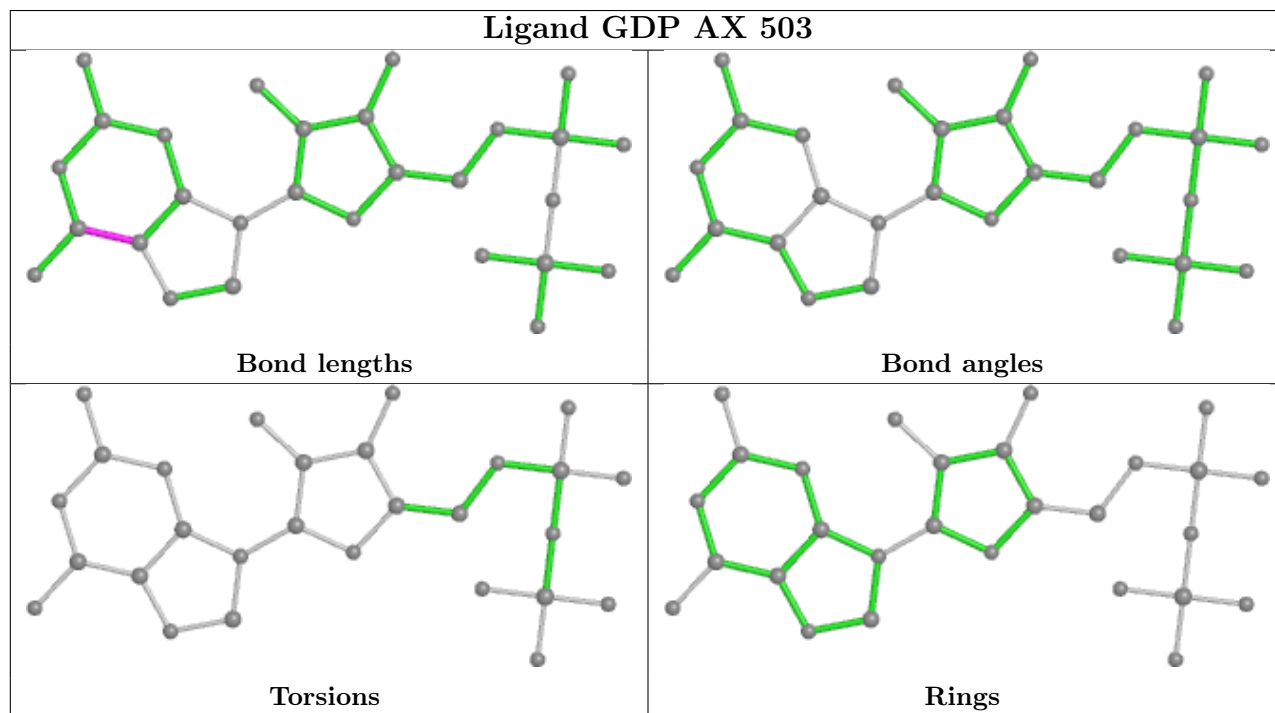
Mol	Chain	Res	Type	Atoms
92	A	3303	SPD	C4-C5-N6-C7
92	A	3301	SPD	N6-C7-C8-C9
92	A	3303	SPD	C8-C7-N6-C5

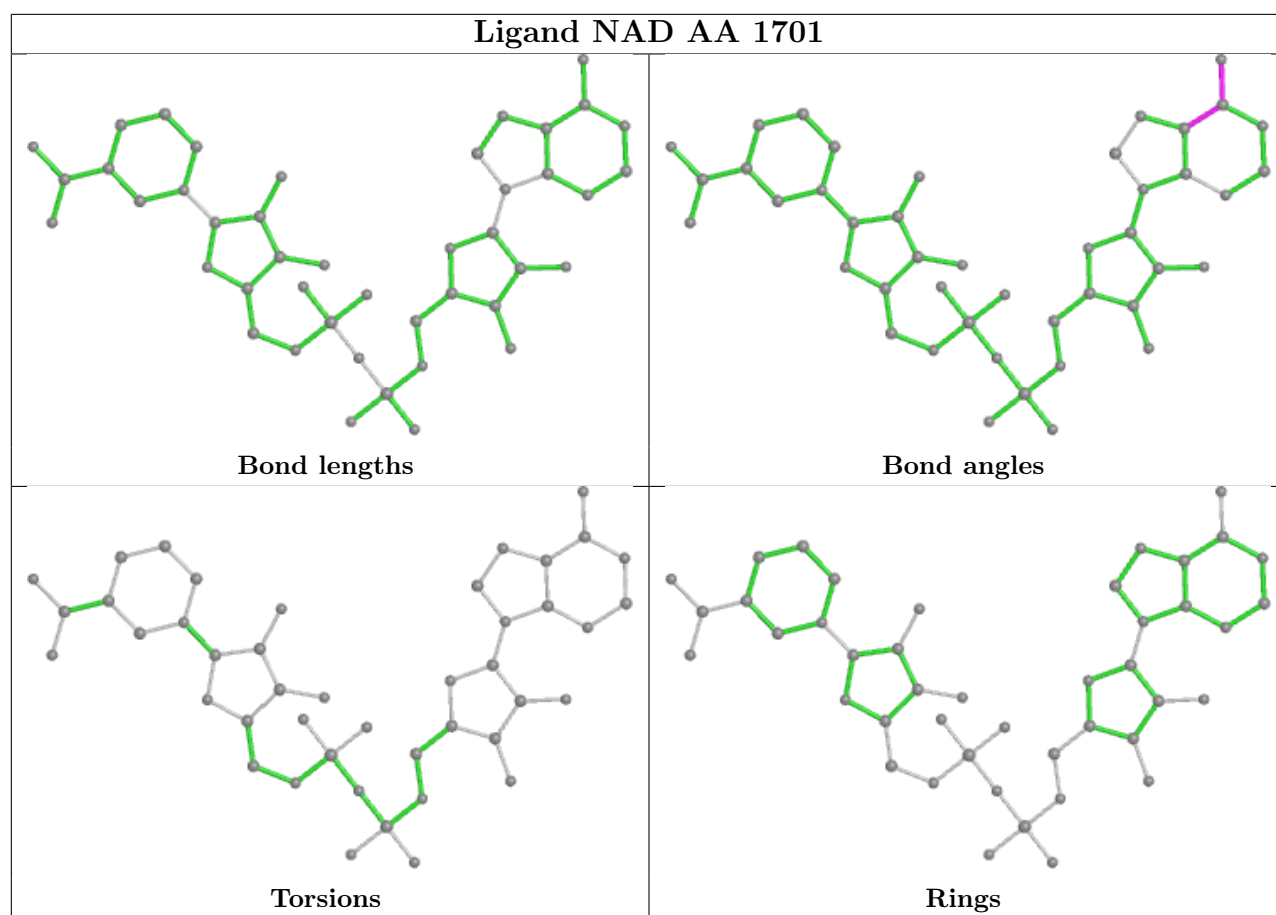
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	AA	1701	NAD	1	0
100	B	101	VAL	1	0

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





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	Ay	1
33	Ax	1
35	Az	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	9.67
1	Ax	15:A	O3'	21:A	P	8.73
1	Az	3:A	O3'	4:A	P	3.00

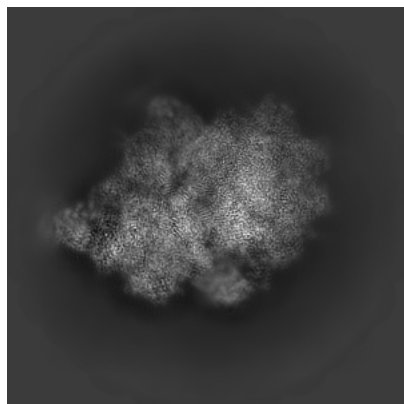
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13981. These allow visual inspection of the internal detail of the map and identification of artifacts.

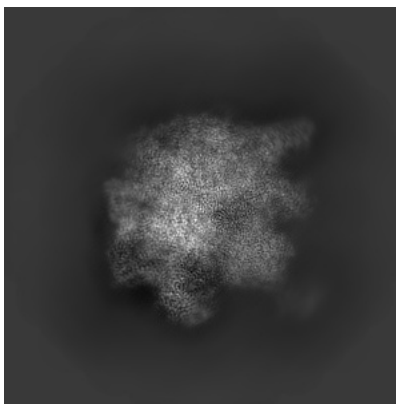
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

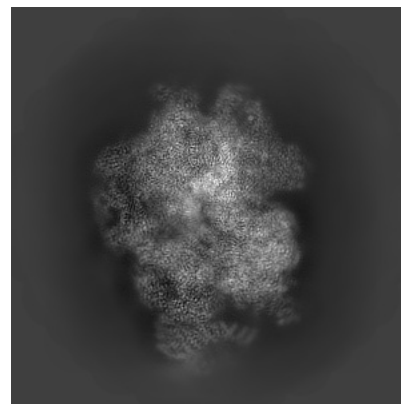
6.1.1 Primary map



X

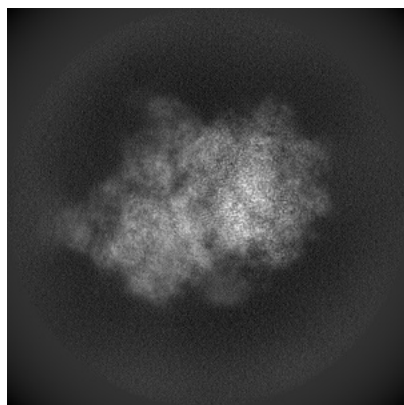


Y

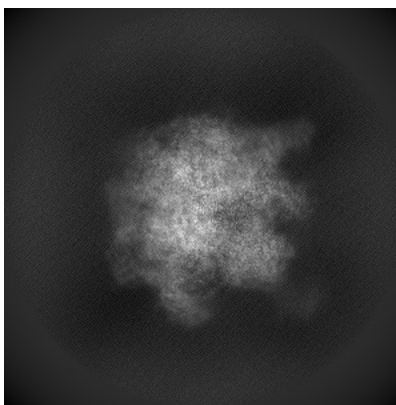


Z

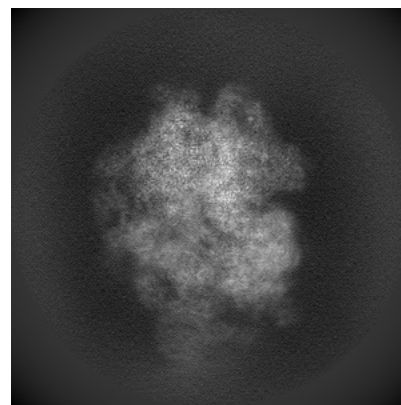
6.1.2 Raw map



X



Y

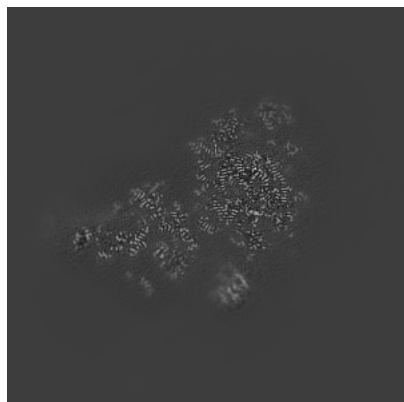


Z

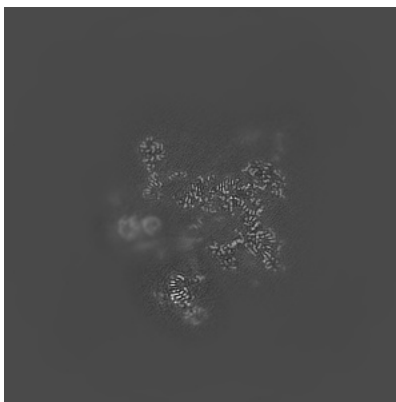
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

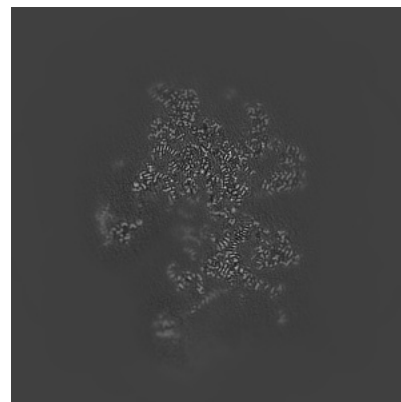
6.2.1 Primary map



X Index: 270

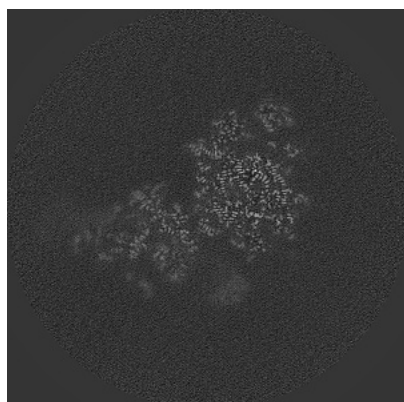


Y Index: 270

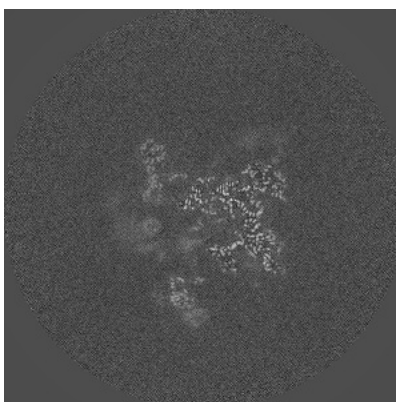


Z Index: 270

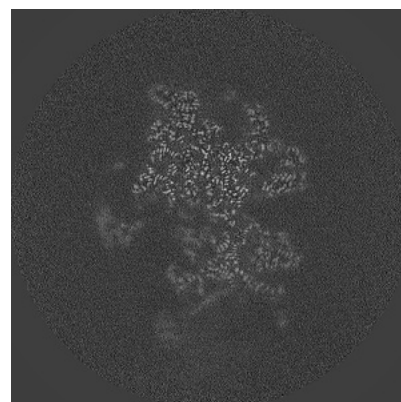
6.2.2 Raw map



X Index: 270



Y Index: 270

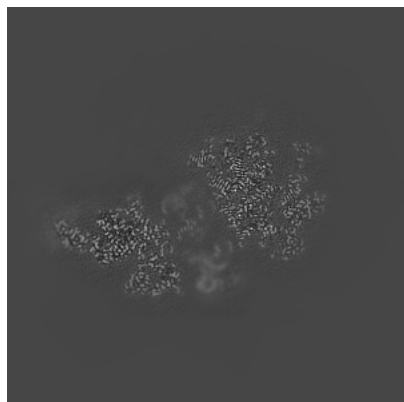


Z Index: 270

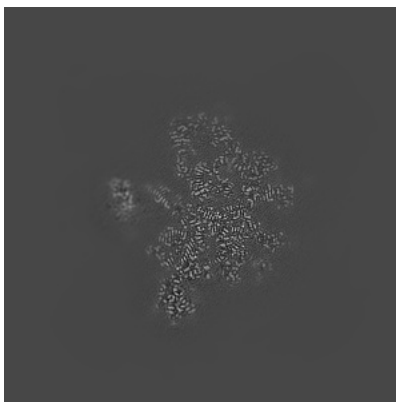
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

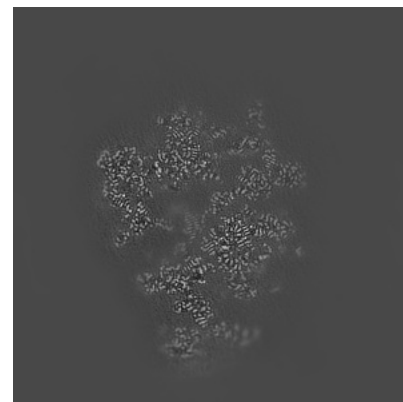
6.3.1 Primary map



X Index: 237

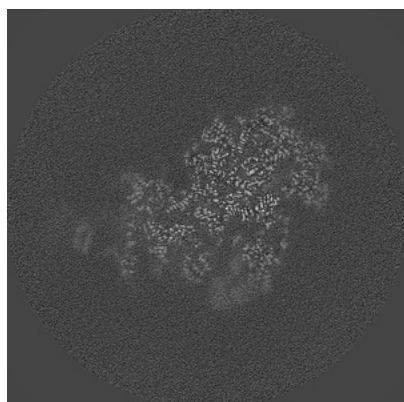


Y Index: 318

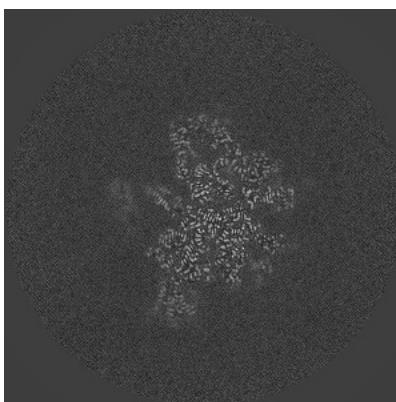


Z Index: 240

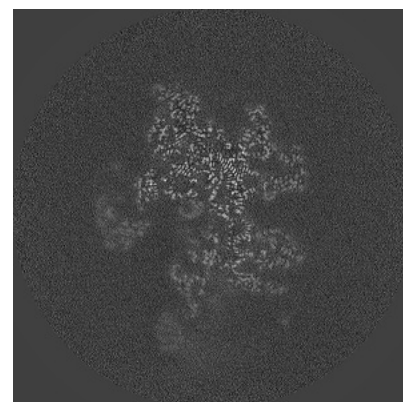
6.3.2 Raw map



X Index: 289



Y Index: 318

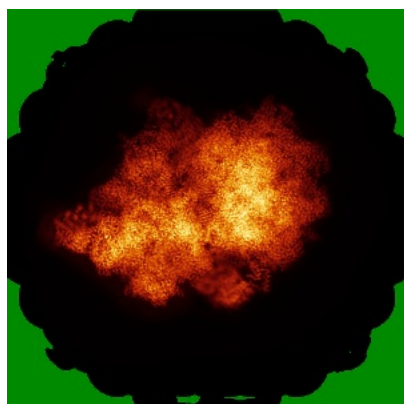


Z Index: 265

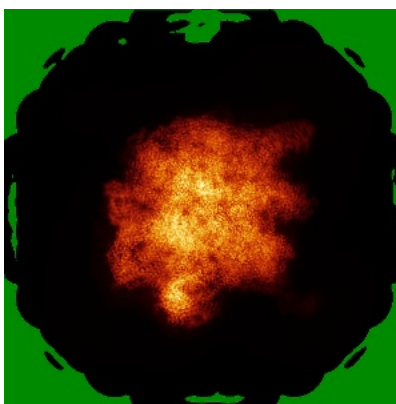
The images above show the largest variance slices of the map in three orthogonal directions.

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

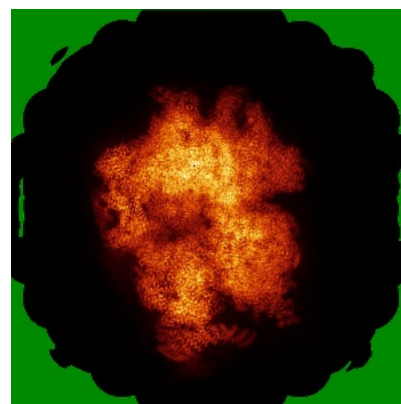
6.4.1 Primary map



X

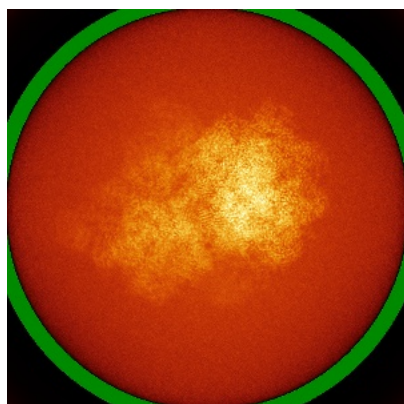


Y

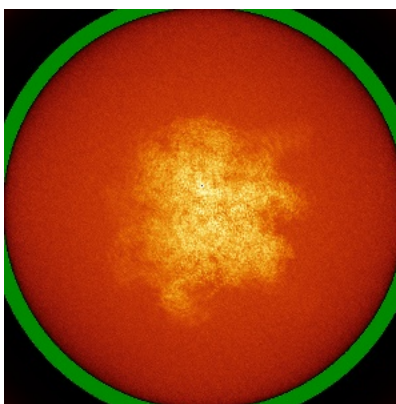


Z

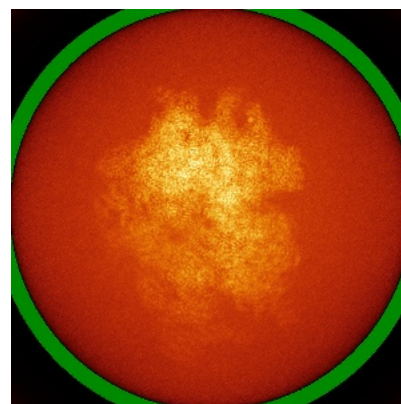
6.4.2 Raw map



X



Y

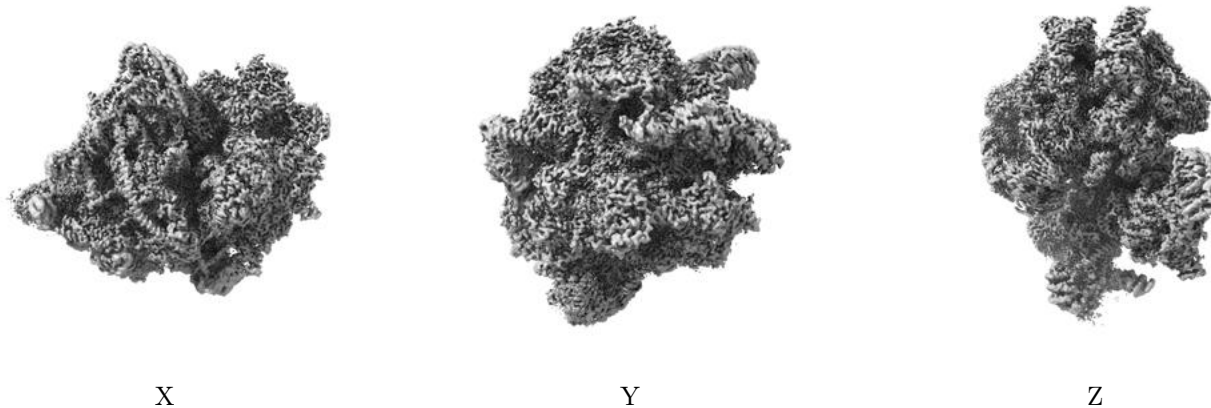


Z

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

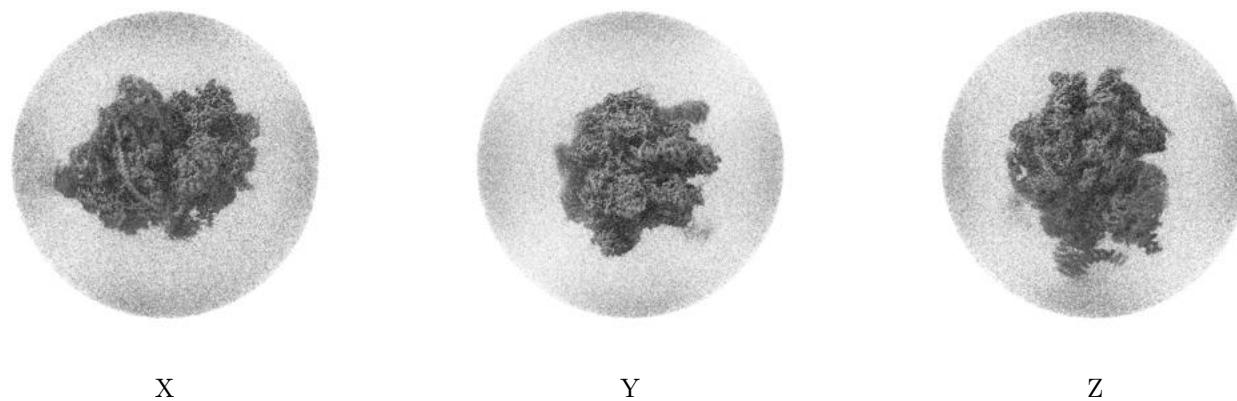
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

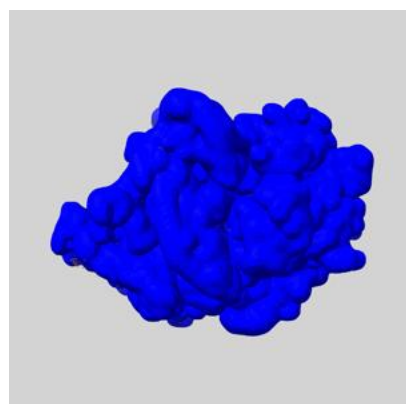
6.6 Mask visualisation [i](#)

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

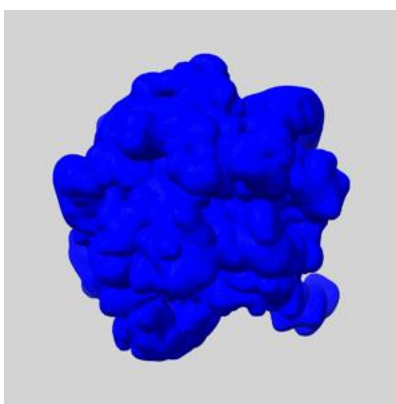
A mask typically either:

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

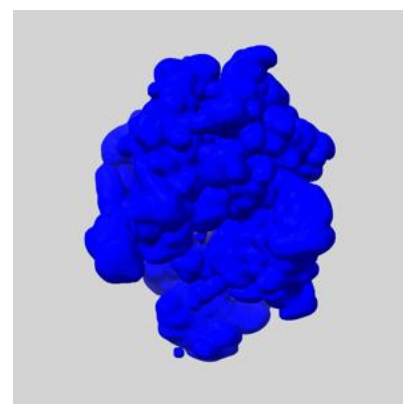
6.6.1 emd_13981_msk_1.map [i](#)



X

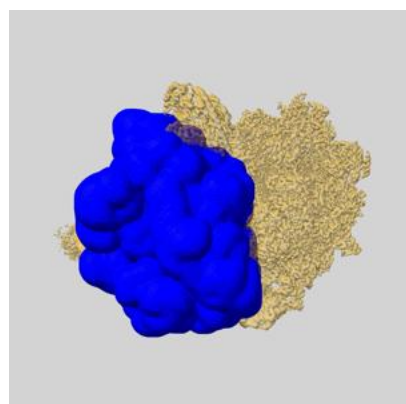


Y

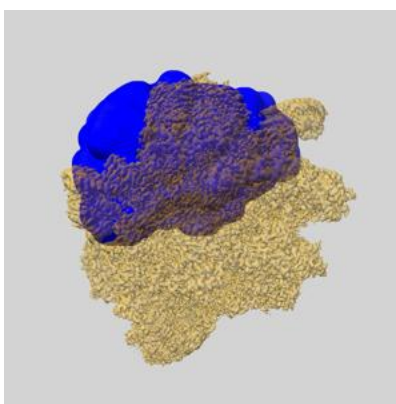


Z

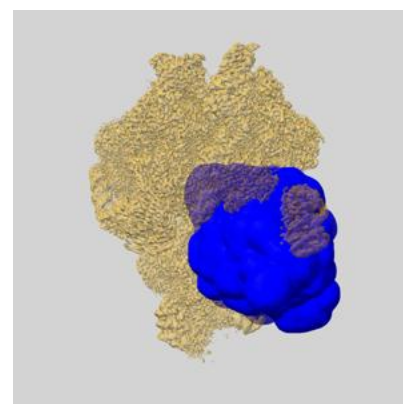
6.6.2 emd_13981_msk_2.map [i](#)



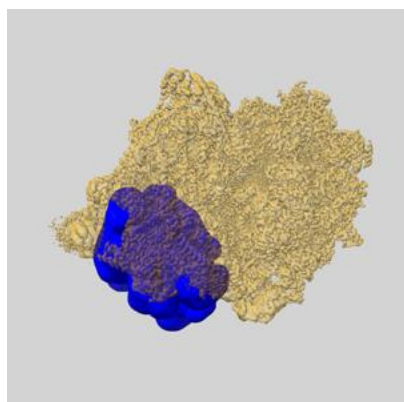
X



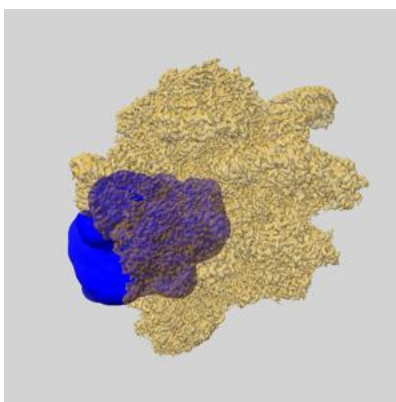
Y



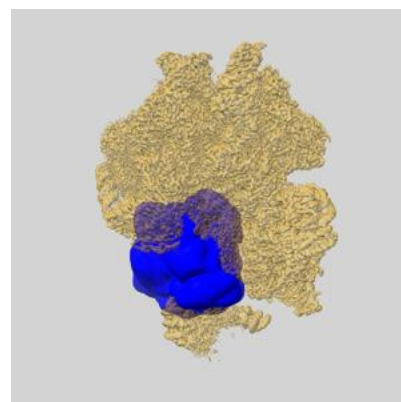
Z

6.6.3 `emd_13981_msk_3.map` ⓘ

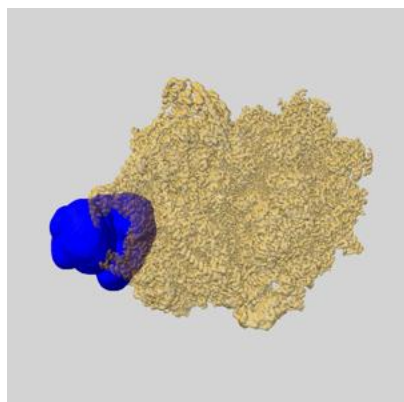
X



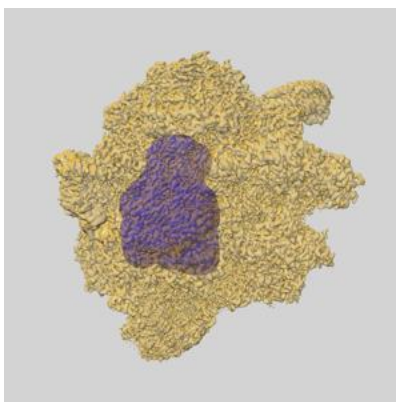
Y



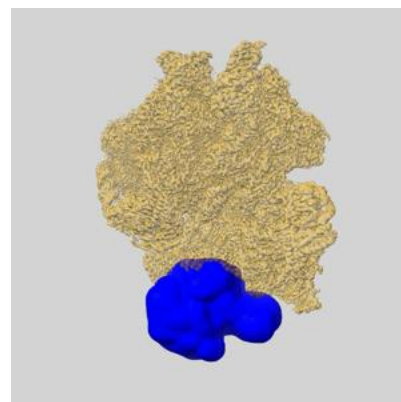
Z

6.6.4 `emd_13981_msk_4.map` ⓘ

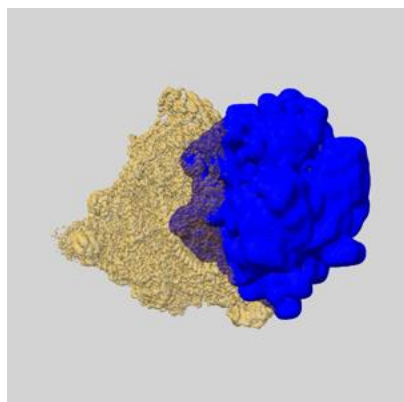
X



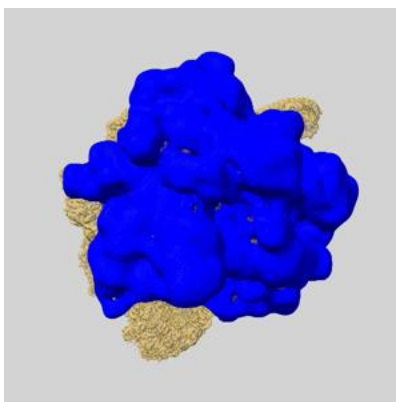
Y



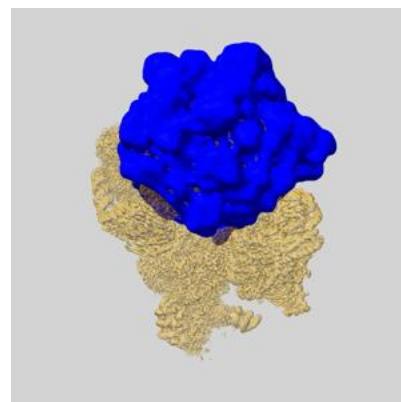
Z

6.6.5 `emd_13981_msk_5.map` ⓘ

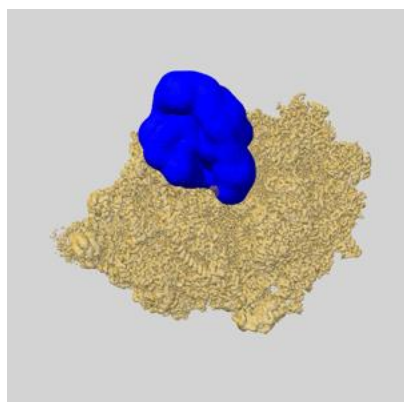
X



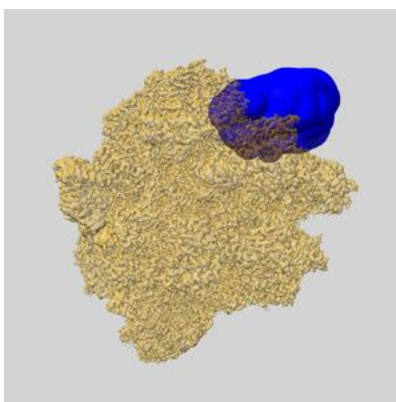
Y



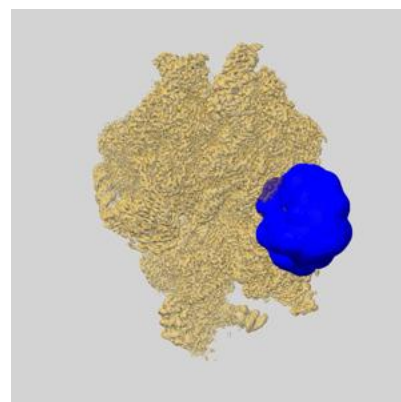
Z

6.6.6 emd_13981_msk_6.map [i](#)

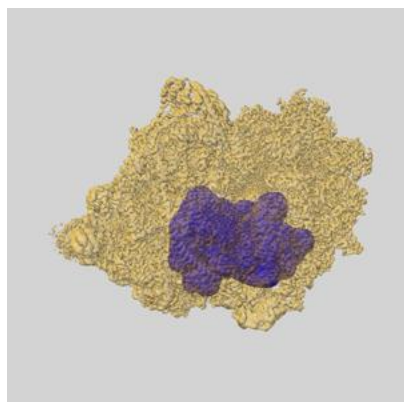
X



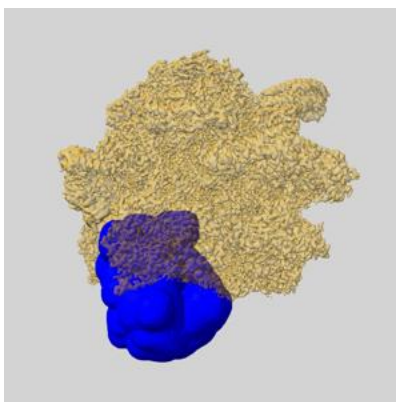
Y



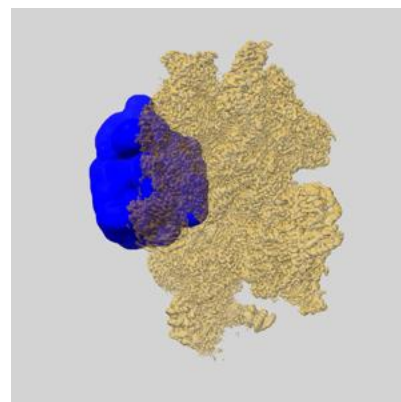
Z

6.6.7 emd_13981_msk_7.map [i](#)

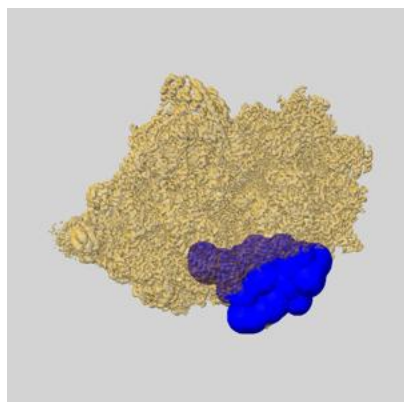
X



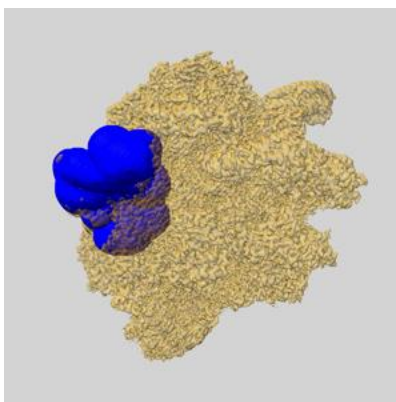
Y



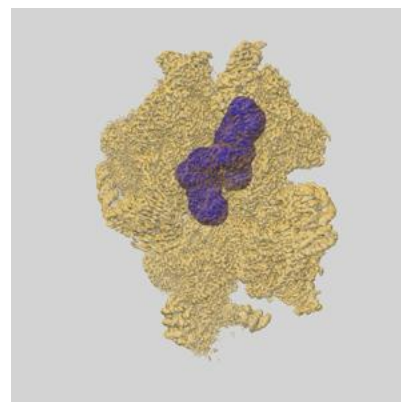
Z

6.6.8 emd_13981_msk_8.map [i](#)

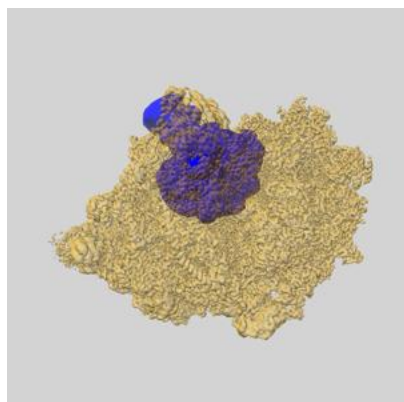
X



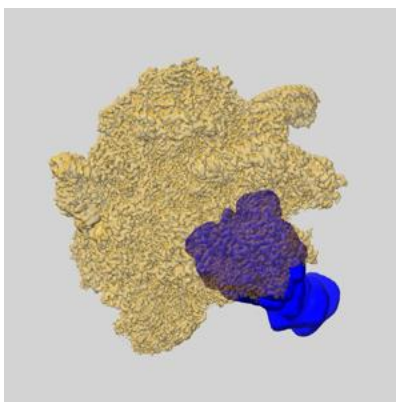
Y



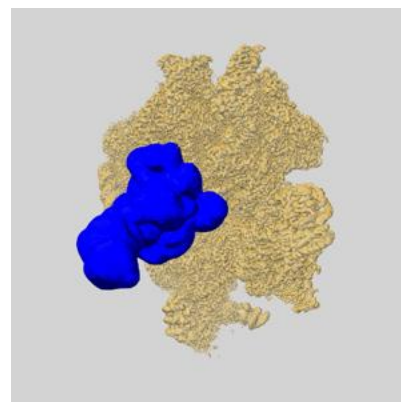
Z

6.6.9 emd_13981_msk_9.map [i](#)

X



Y

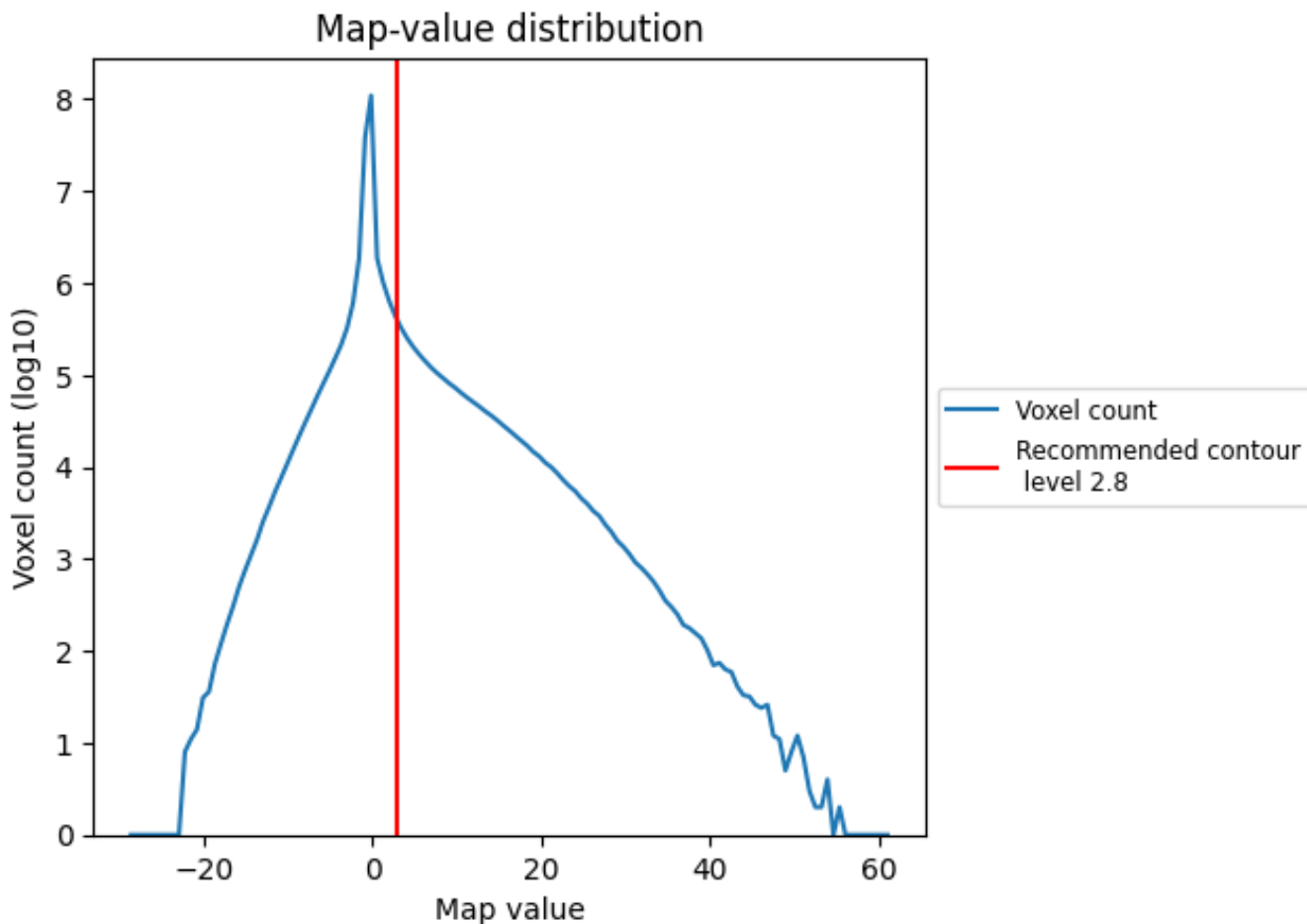


Z

7 Map analysis [i](#)

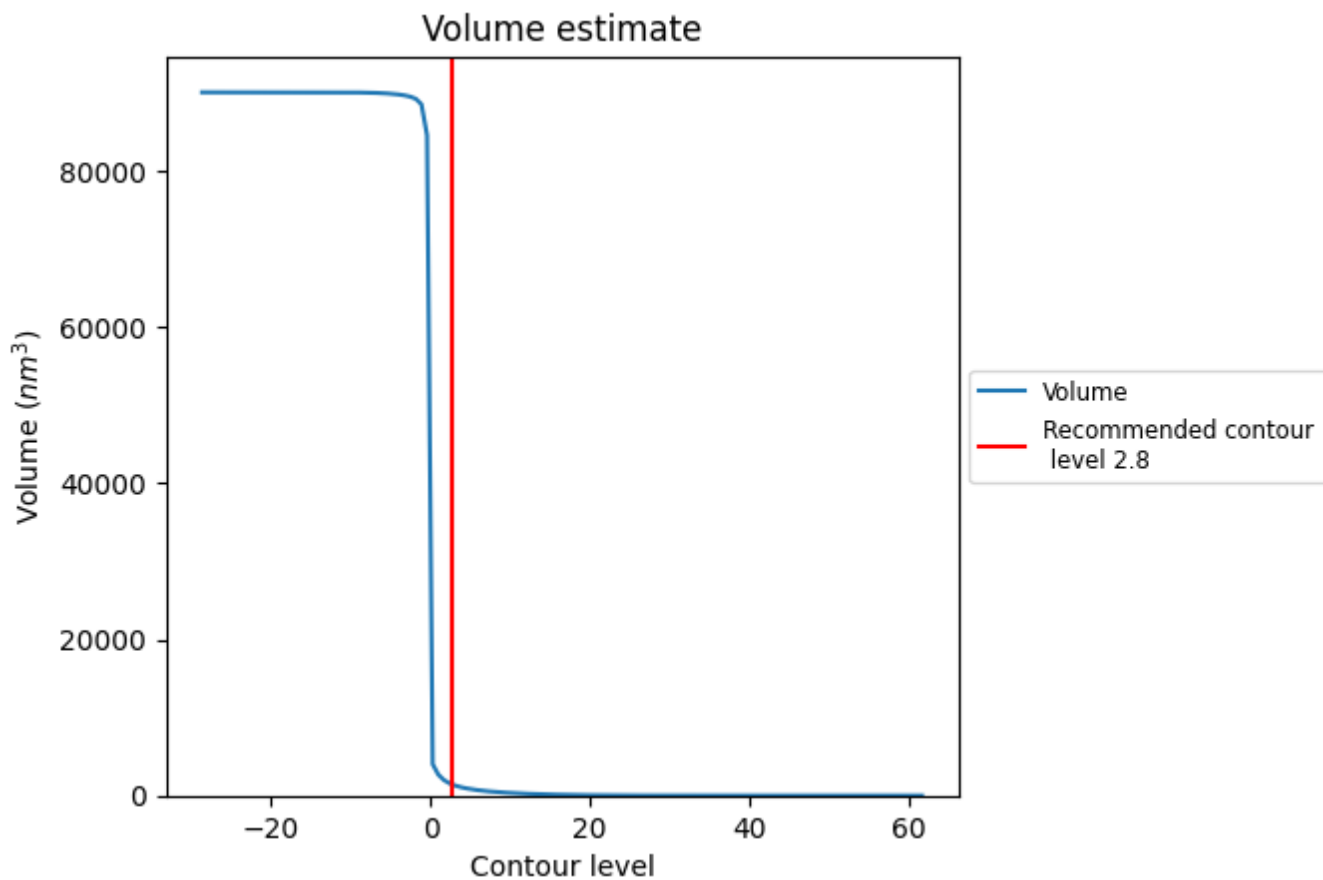
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

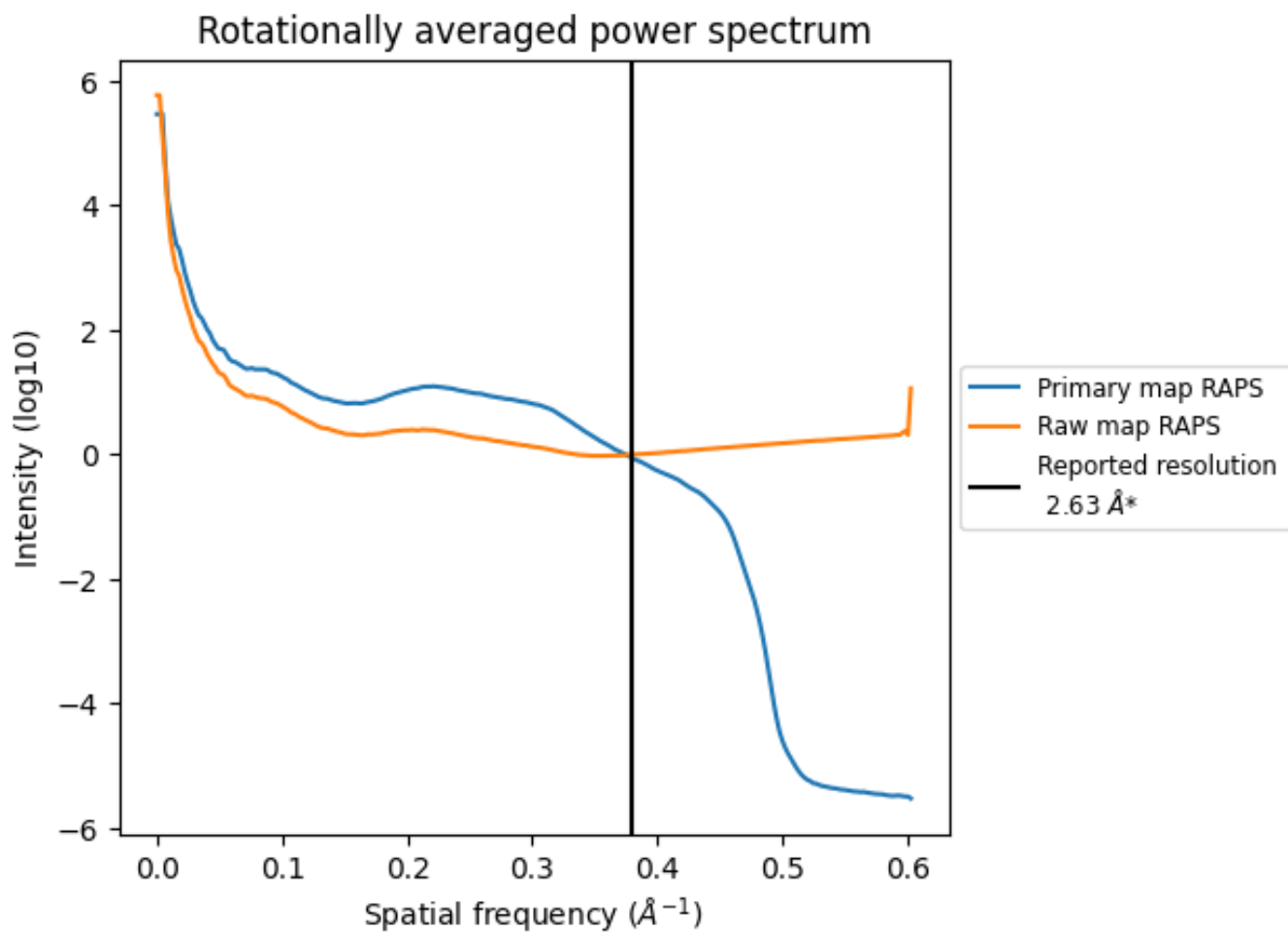
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1416 nm^3 ; this corresponds to an approximate mass of 1279 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](#)

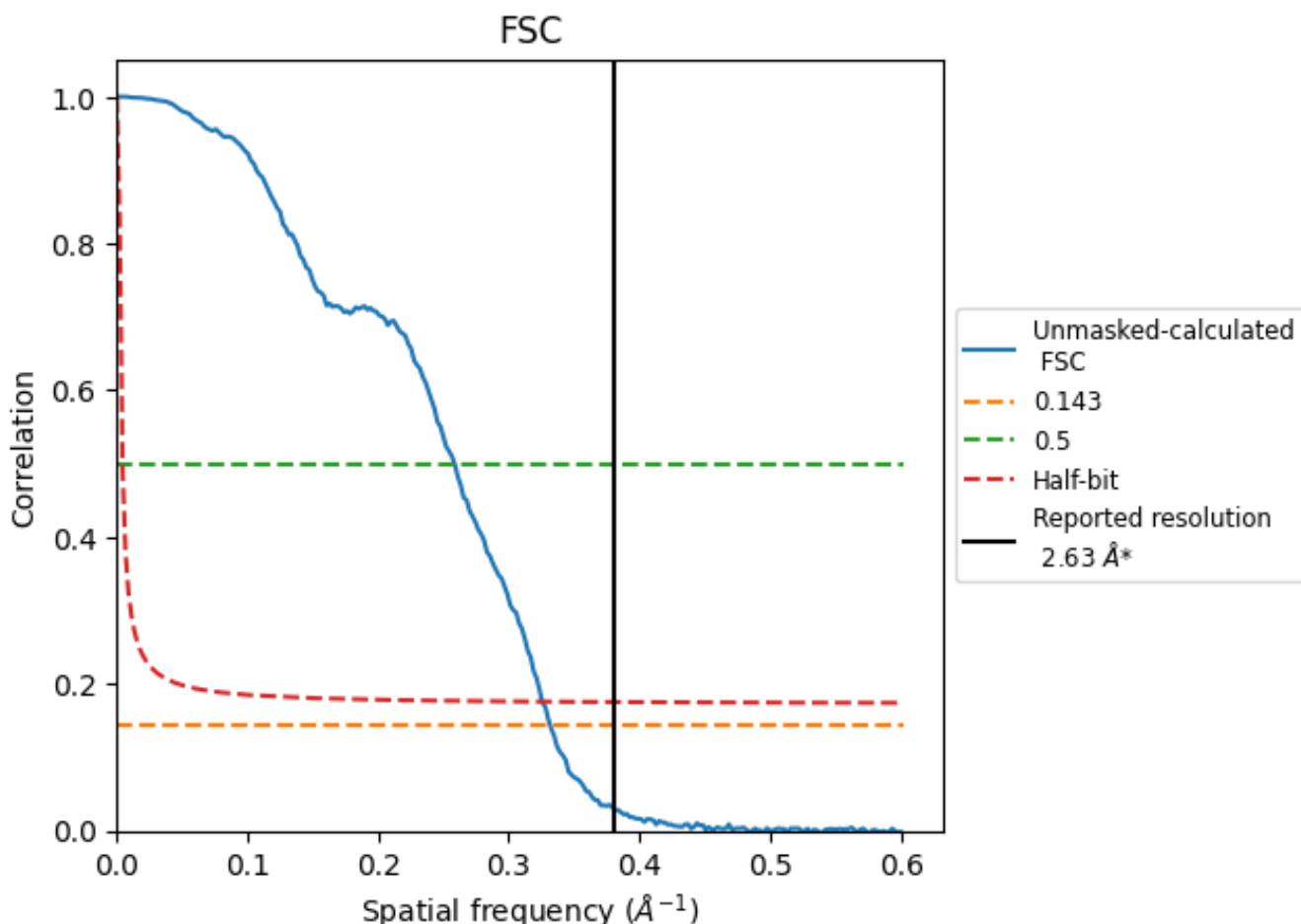


*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

8.2 Resolution estimates [i](#)

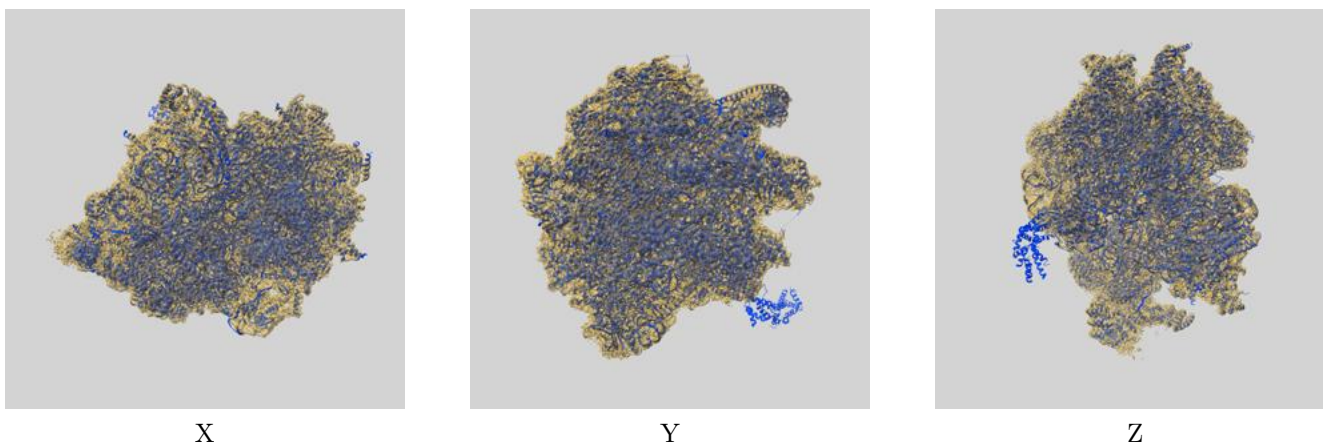
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.01	3.87	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.01 differs from the reported value 2.63 by more than 10 %

9 Map-model fit [i](#)

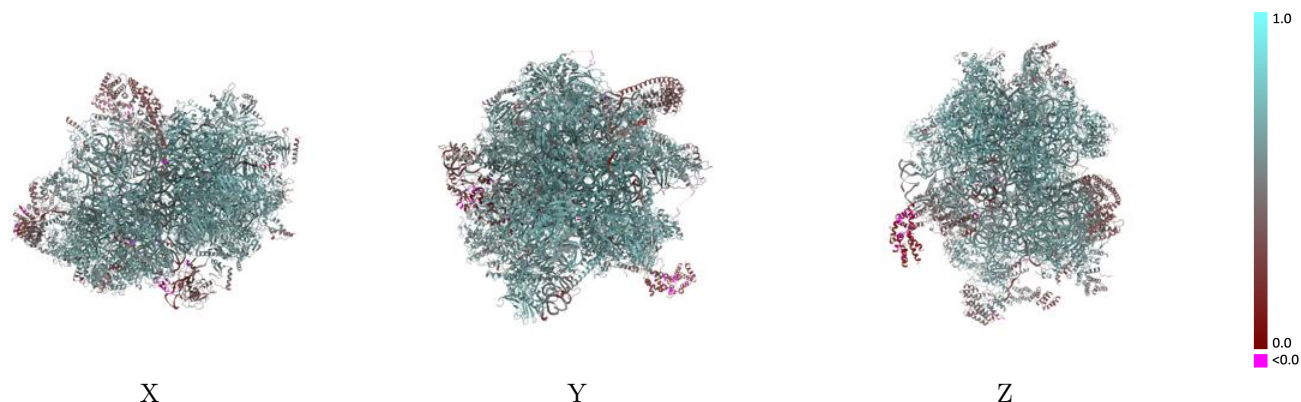
This section contains information regarding the fit between EMDB map EMD-13981 and PDB model 7QI5. Per-residue inclusion information can be found in section 3 on page 30.

9.1 Map-model overlay [i](#)



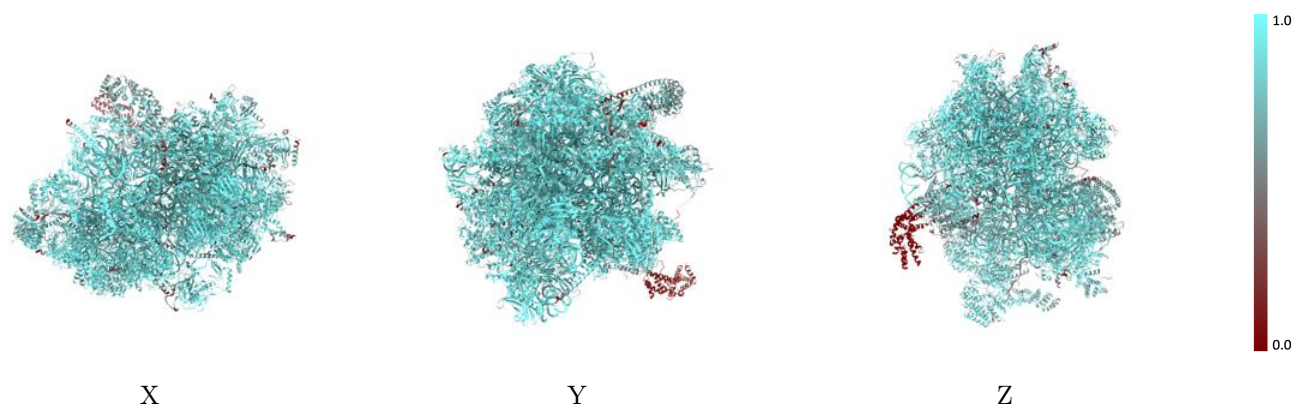
The images above show the 3D surface view of the map at the recommended contour level 2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



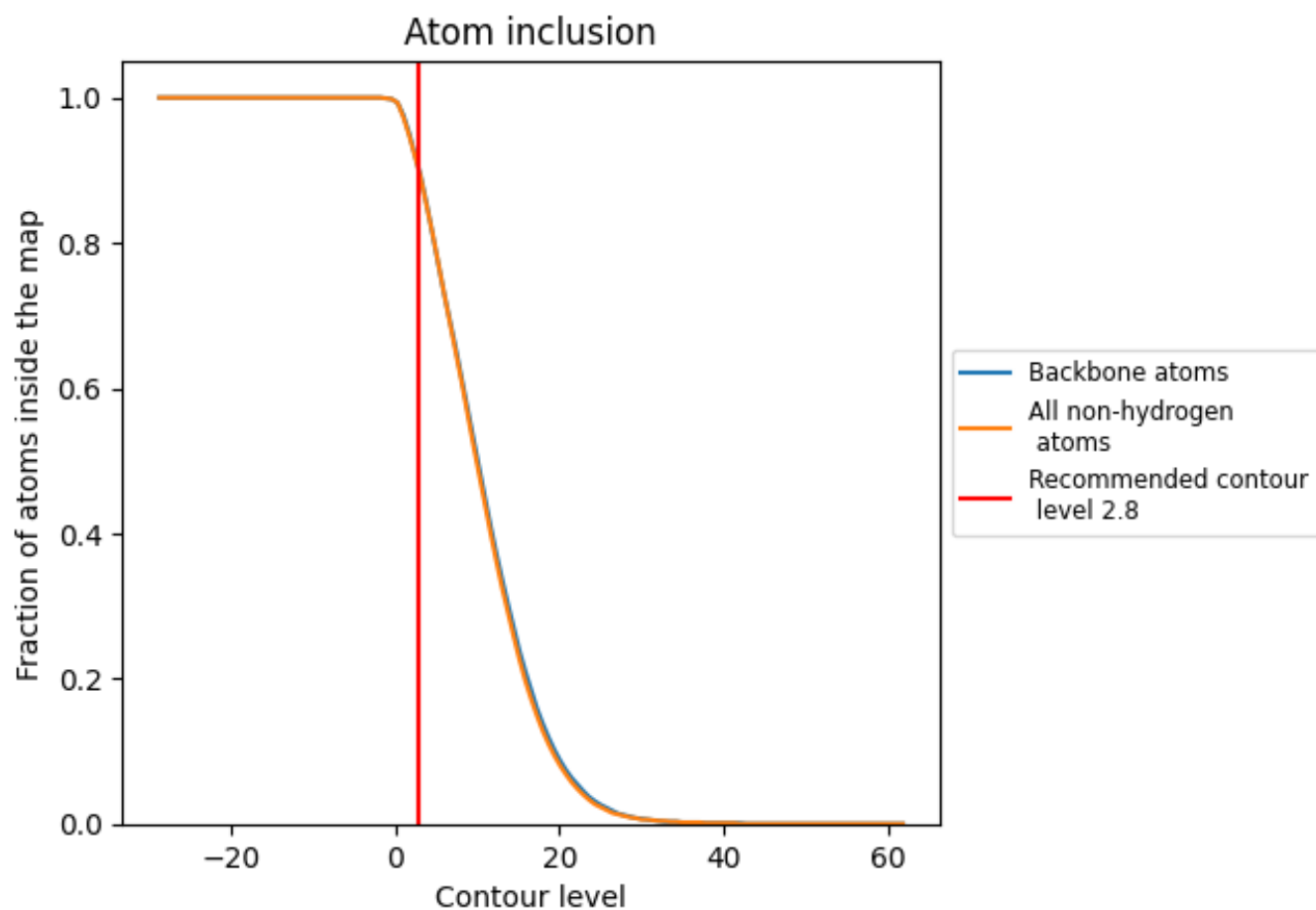
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.8).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.5940
0	 0.9130	 0.6410
1	 0.8960	 0.6060
2	 0.9950	 0.7280
3	 0.9860	 0.7160
4	 0.9660	 0.6610
5	 0.9290	 0.6170
6	 0.9530	 0.6300
7	 0.8520	 0.5690
8	 0.8120	 0.5150
9	 0.8730	 0.5940
A	 0.9740	 0.6620
A0	 0.8550	 0.5140
A1	 0.9160	 0.5830
A2	 0.8650	 0.5540
A3	 0.9400	 0.6400
A4	 0.8730	 0.4560
AA	 0.9850	 0.6450
AB	 0.9400	 0.6180
AC	 0.9830	 0.6680
AD	 0.9130	 0.5920
AE	 0.9320	 0.6050
AF	 0.9390	 0.6000
AG	 0.8930	 0.5650
AH	 0.9540	 0.6210
AI	 0.9480	 0.6230
AJ	 0.9340	 0.6190
AK	 0.9820	 0.6700
AL	 0.8780	 0.5730
AM	 0.9220	 0.5940
AN	 0.9450	 0.6240
AO	 0.9220	 0.5860
AP	 0.9380	 0.6290
AQ	 0.9690	 0.6520
AR	 0.8710	 0.5340







































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Chain	Atom inclusion	Q-score
AS	0.8610	0.5460
AT	0.9190	0.5990
AU	0.8660	0.5350
AV	0.6510	0.3600
AW	0.9170	0.5840
AX	0.9500	0.6050
AY	0.8340	0.5200
AZ	0.9290	0.6050
Aw	0.7910	0.4180
Ax	0.8270	0.4800
Ay	0.9240	0.3230
Az	0.7050	0.3920
B	0.9690	0.5600
D	0.9640	0.6670
E	0.9470	0.6590
F	0.9670	0.6800
H	0.9110	0.4640
I	0.5630	0.4350
J	0.5080	0.3640
K	0.9680	0.6860
L	0.9550	0.6610
M	0.9590	0.6740
N	0.9310	0.6530
O	0.9460	0.6600
P	0.9790	0.6660
Q	0.8730	0.6150
R	0.9680	0.6990
S	0.9500	0.6680
T	0.9680	0.6820
U	0.8550	0.6020
V	0.8480	0.5720
W	0.9770	0.6850
X	0.9070	0.6100
Y	0.9380	0.6460
Z	0.9430	0.6700
a	0.8450	0.5740
b	0.9620	0.6690
c	0.9000	0.6090
d	0.7810	0.5240
e	0.8530	0.5230
f	0.8710	0.5550
g	0.9290	0.6400

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Chain	Atom inclusion	Q-score
h	 0.8450	 0.5610
i	 0.9770	 0.7080
j	 0.8710	 0.5990
k	 0.7530	 0.5080
l	 0.5990	 0.4290
m	 0.7940	 0.4870
o	 0.9700	 0.6960
p	 0.8070	 0.5350
q	 0.6890	 0.4570
r	 0.9260	 0.6280
s	 0.9350	 0.6330
t	 0.0680	 0.2330
u	 0.0000	 0.2200
v	 0.0000	 0.1390
w	 0.0000	 0.0470
x	 0.0000	 0.0870
y	 0.0000	 0.0550
z	 0.8680	 0.2230