



Full wwPDB EM Validation Report ⓘ

Sep 8, 2026 – 04:54 am BST

PDB ID : 8ANY / pdb_00008any
EMDB ID : EMD-15544
Title : Human mitochondrial ribosome in complex with LRPPRC, SLIRP, A-site, P-site, E-site tRNAs and mRNA
Authors : Singh, V.; Itoh, Y.; Amunts, A.
Deposited on : 2022-08-06
Resolution : 2.85 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

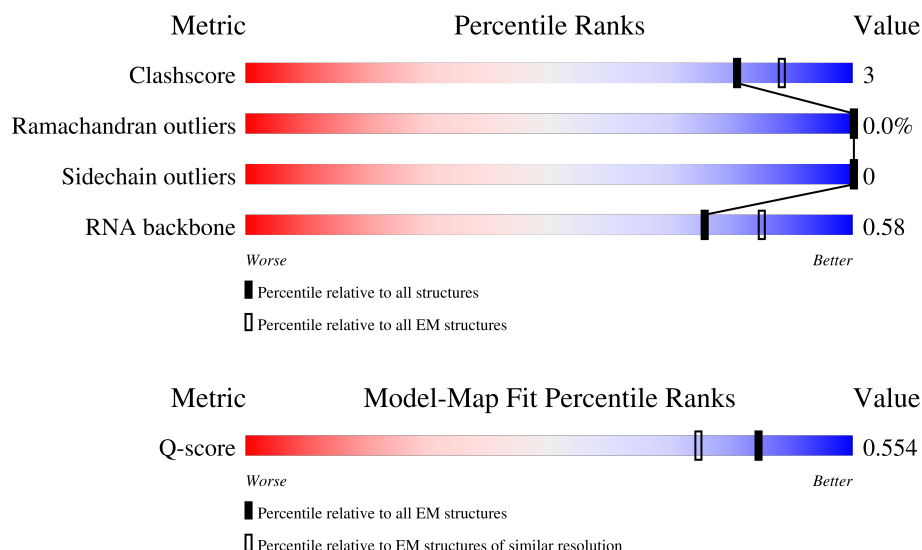
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 Å.

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



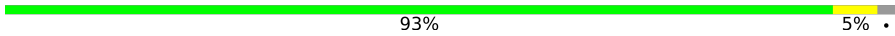
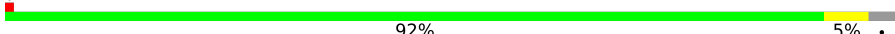
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	
2	AB	296	
3	AC	167	

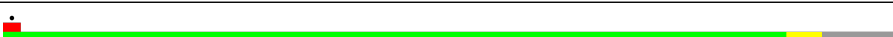
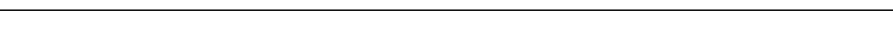
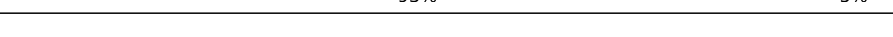
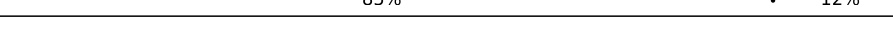
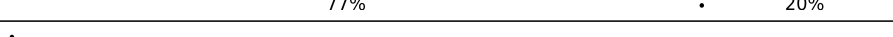
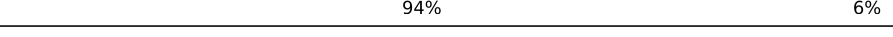
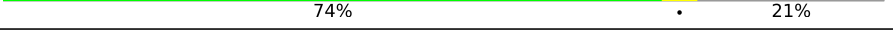
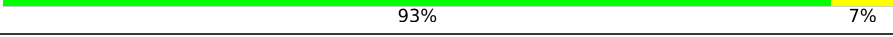
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Mol	Chain	Length	Quality of chain
4	AD	430	
5	AE	125	
6	AF	242	
7	AG	396	
8	AH	201	
9	AI	194	
10	AJ	138	
11	AK	128	
12	AL	257	
13	AM	137	
14	AN	130	
15	AO	258	
16	AP	142	
17	AQ	87	
18	AR	360	
19	AS	190	
20	AT	173	
21	AU	205	
22	AV	414	
23	AW	187	
24	AX	398	
25	AZ	106	
26	A0	217	
27	A1	323	
28	A2	118	

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Mol	Chain	Length	Quality of chain
29	A3	199	
30	Aw	68	
31	Ax	70	
32	Ay	70	
33	A	1561	
34	B	72	
35	D	305	
36	E	348	
37	F	311	
38	I	261	
39	J	192	
40	K	178	
41	L	145	
42	M	296	
43	N	251	
44	O	175	
45	P	180	
46	Q	292	
47	R	149	
48	S	205	
49	T	206	
50	U	153	
51	V	216	
52	W	148	
53	X	256	

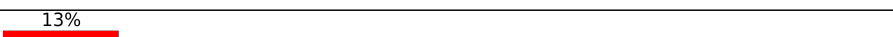
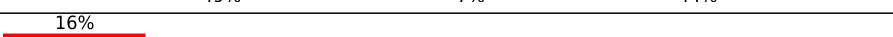
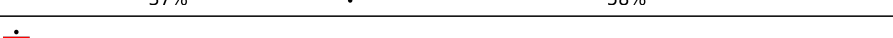
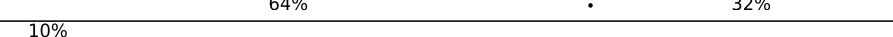
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Mol	Chain	Length	Quality of chain
54	Y	250	
55	Z	161	
56	0	188	
57	1	65	
58	2	92	
59	3	188	
60	4	103	
61	5	423	
62	6	380	
63	7	338	
64	8	206	
65	9	137	
66	a	142	
67	b	215	
68	c	332	
69	d	306	
70	e	279	
71	f	212	
72	g	166	
73	h	158	
74	i	128	
75	j	123	
76	k	112	
77	l	138	
78	m	128	

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Mol	Chain	Length	Quality of chain
79	o	102	
80	p	206	
81	q	222	
82	r	196	
83	s	439	
84	t	198	
84	u	198	
84	v	198	
84	w	198	
84	x	198	
84	y	198	
85	H	267	
86	z	325	
87	AY	395	
88	A5	1394	
89	A4	689	
90	A6	109	
91	Az	42	

2 Entry composition

There are 103 unique types of molecules in this entry. The entry contains 355123 atoms, of which 160326 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
1	AA	954	Total	C	H	N	O	P	0	0
			30565	9088	10305	3647	6571	954		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	225	Total	C	H	N	O	S	0	0
			3654	1164	1826	331	323	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	AC	132	Total	C	H	N	O	S	0	0
			2179	699	1096	195	185	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AD	343	Total	C	H	N	O	S	0	0
			5545	1713	2814	518	487	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	AE	122	Total	C	H	N	O	S	0	0
			1976	614	1004	177	177	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	AF	208	Total	C	H	N	O	S	0	0
			3503	1104	1778	312	298	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	AG	327	Total	C	H	N	O	S	0	0
			5385	1710	2697	477	487	14		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	AH	140	Total	C	H	N	O	S	0	0
			2343	745	1191	194	210	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AI	137	Total	C	H	N	O	S	0	0
			2086	642	1066	192	182	4		

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
10	AJ	108	Total	C	H	N	O	S	0	0
			1731	521	892	169	143	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AK	101	Total	C	H	N	O	S	0	0
			1751	537	889	179	141	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AL	174	Total	C	H	N	O	S	0	0
			2998	925	1545	270	251	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AM	119	Total	C	H	N	O	S	0	0
			1914	594	972	185	157	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AN	110	Total	C	H	N	O	S	0	0
			1801	562	933	156	147	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AO	193	Total	C	H	N	O	S	0	0
			3162	1014	1570	294	277	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AP	97	Total	C	H	N	O	S	0	0
			1590	501	809	134	138	8		

- Molecule 17 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AQ	86	Total	C	H	N	O	S	0	0
			1504	460	760	150	126	8		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AR	295	Total	C	H	N	O	S	0	0
			4845	1533	2436	413	455	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AS	135	Total	C	H	N	O	S	0	0
			2228	716	1117	198	196	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AT	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AU	176	Total	C	H	N	O	S	0	0
			2993	916	1505	301	267	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AV	362	Total	C	H	N	O	S	0	0
			5941	1904	2972	495	558	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	100	Total	C	H	N	O	S	0	0
			1595	498	806	141	146	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	352	Total	C	H	N	O	S	0	0
			5708	1822	2859	499	517	11		

- Molecule 25 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AZ	100	Total	C	H	N	O	S	0	0
			1701	534	862	153	148	4		

- Molecule 26 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	A0	215	Total	C	H	N	O	S	0	0
			3589	1130	1802	339	313	5		

- Molecule 27 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	A1	277	Total	C	H	N	O	S	0	0
			4526	1424	2281	382	428	11		

- Molecule 28 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

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

- Molecule 29 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	A3	70	Total	C	H	N	O	S	0	0
			1327	401	702	134	89	1		

- Molecule 30 is a RNA chain called A/A-tRNA.

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

- Molecule 31 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Ax	70	Total	C	H	N	O	P	0	0
			2232	665	750	260	487	70		

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

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

- Molecule 33 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	A	1558	Total	C	H	N	O	P	0	0
			49872	14843	16802	5963	10706	1558		

- Molecule 34 is a RNA chain called mitochondrial tRNA^{Val}.

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

- Molecule 35 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	D	238	Total	C	H	N	O	S	0	0
			3787	1157	1928	376	317	9		

- Molecule 36 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	E	305	Total	C	H	N	O	S	0	0
			4830	1545	2424	418	432	11		

- Molecule 37 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	F	252	Total	C	H	N	O	S	0	0
			4106	1305	2075	370	350	6		

- Molecule 38 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	I	212	Total	C	H	N	O	S	0	0
			3489	1088	1794	304	292	11		

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

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

- Molecule 40 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	K	177	Total	C	H	N	O	S	0	0
			2915	936	1460	259	253	7		

- Molecule 41 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	L	115	Total	C	H	N	O	S	0	0
			1835	559	945	171	155	5		

- Molecule 42 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	M	289	Total	C	H	N	O	S	0	0
			4701	1476	2387	427	405	6		

- Molecule 43 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	N	222	Total	C	H	N	O	S	0	0
			3610	1143	1824	326	307	10		

- Molecule 44 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	O	154	Total	C	H	N	O	S	0	0
			2557	792	1298	241	219	7		

- Molecule 45 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	P	144	Total	C	H	N	O	S	0	0
			2344	733	1171	224	211	5		

- Molecule 46 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	Q	238	Total	C	H	N	O	S	0	0
			4004	1268	2025	352	350	9		

- Molecule 47 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	R	140	Total	C	H	N	O	S	0	0
			2374	732	1220	231	187	4		

- Molecule 48 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	S	161	Total	C	H	N	O	S	0	0
			2662	835	1369	227	227	4		

- Molecule 49 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	T	166	Total	C	H	N	O	S	0	0
			2786	875	1417	254	233	7		

- Molecule 50 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	U	152	Total	C	H	N	O	S	0	0
			2486	788	1235	234	226	3		

- Molecule 51 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	V	205	Total	C	H	N	O	S	0	0
			3367	1068	1691	298	302	8		

- Molecule 52 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	W	116	Total	C	H	N	O	S	0	0
			1847	577	943	171	153	3		

- Molecule 53 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	X	244	Total	C	H	N	O	S	0	0
			4109	1322	2065	352	365	5		

- Molecule 54 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Y	181	Total	C	H	N	O	S	0	0
			3159	995	1603	298	259	4		

- Molecule 55 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Z	122	Total	C	H	N	O	S	0	0
			2048	636	1052	186	171	3		

- Molecule 56 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	0	110	Total	C	H	N	O	S	0	0
			1817	554	919	176	162	6		

- Molecule 57 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	1	56	Total	C	H	N	O	S	0	0
			977	296	513	89	77	2		

- Molecule 58 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	2	46	Total	C	H	N	O	S	0	0
			786	233	409	83	60	1		

- Molecule 59 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	3	95	Total	C	H	N	O	S	0	0
			1718	539	886	162	128	3		

- Molecule 60 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	4	38	Total	C	H	N	O	S	0	0
			705	217	363	72	49	4		

- Molecule 61 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	5	394	Total	C	H	N	O	S	0	0
			6432	2073	3222	560	566	11		

- Molecule 62 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	6	354	Total	C	H	N	O	S	0	0
			5802	1881	2854	525	533	9		

- Molecule 63 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	7	294	Total	C	H	N	O	S	0	0
			4796	1529	2406	405	438	18		

- Molecule 64 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	8	157	Total	C	H	N	O	S	0	0
			2698	844	1371	235	246	2		

- Molecule 65 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	9	124	Total	C	H	N	O	S	0	0
			1985	644	988	170	181	2		

- Molecule 66 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	a	100	Total	C	H	N	O	S	0	0
			1659	529	819	152	154	5		

- Molecule 67 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	b	151	Total	C	H	N	O	S	0	0
			2395	744	1199	231	218	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	2	ACE	-	acetylation	UNP Q8N983

- Molecule 68 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	c	286	Total	C	H	N	O	S	0	0
			4624	1470	2325	397	423	9		

- Molecule 69 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	d	241	Total	C	H	N	O	S	0	0
			3971	1273	1986	340	359	13		

- Molecule 70 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	e	238	Total	C	H	N	O	S	0	0
			3853	1222	1922	339	364	6		

- Molecule 71 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	f	157	Total	C	H	N	O	S	0	0
			2529	799	1277	207	242	4		

- Molecule 72 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	g	134	Total	C	H	N	O	S	0	0
			2214	719	1101	193	199	2		

- Molecule 73 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	h	110	Total	C	H	N	O	S	0	0
			1780	568	885	156	168	3		

- Molecule 74 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	i	97	Total	C	H	N	O	S	0	0
			1690	532	862	165	127	4		

- Molecule 75 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 76 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	k	101	Total	C	H	N	O	S	0	0
			1562	479	788	148	142	5		

- Molecule 77 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	l	82	Total	C	H	N	O	S	0	0
			1364	437	676	120	128	3		

- Molecule 78 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	m	92	Total	C	H	N	O	S	0	0
			1554	488	763	159	142	2		

- Molecule 79 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	o	94	Total	C	H	N	O	S	0	0
			1608	501	810	165	129	3		

- Molecule 80 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	p	147	Total	C	H	N	O	S	0	0
			2433	748	1228	228	225	4		

- Molecule 81 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	q	165	Total	C	H	N	O	S	0	0
			2766	865	1377	270	249	5		

- Molecule 82 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	r	162	Total	C	H	N	O	S	0	0
			2677	839	1355	252	223	8		

- Molecule 83 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	s	386	Total	C	H	N	O	S	0	0
			6306	2023	3151	559	559	14		

- Molecule 84 is a protein called 39S ribosomal protein L12, mitochondrial.

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

- Molecule 85 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	H	202	Total	C	H	N	O	S	0	0
			3398	1067	1737	304	286	4		

- Molecule 86 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	z	252	Total	C	H	N	O	S	0	0
			4107	1304	2080	336	381	6		

- Molecule 87 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	AY	221	Total	C	H	N	O	S	0	0
			3622	1159	1787	319	352	5		

- Molecule 88 is a protein called Leucine-rich PPR motif-containing protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	A5	581	Total	C	H	N	O	S	0	0
			9336	2959	4690	790	871	26		

- Molecule 89 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	A4	595	Total	C	H	N	O	S	0	0
			9643	3080	4828	815	892	28		

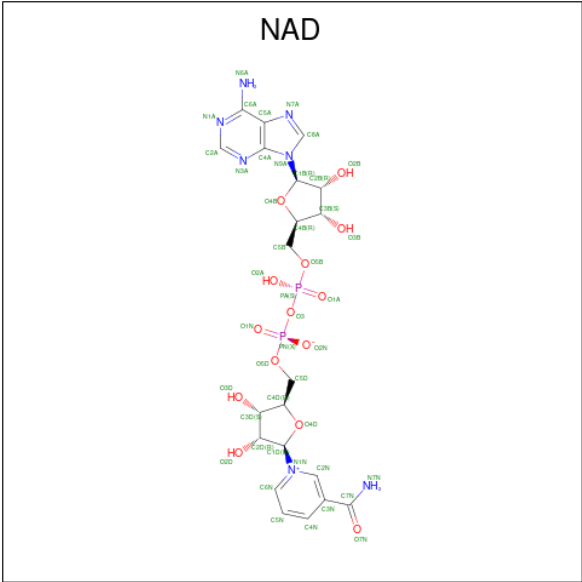
- Molecule 90 is a protein called SRA stem-loop-interacting RNA-binding protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
90	A6	74	Total	C	H	N	O	S	0	0
			1197	384	594	115	103	1		

- Molecule 91 is a RNA chain called mRNA.

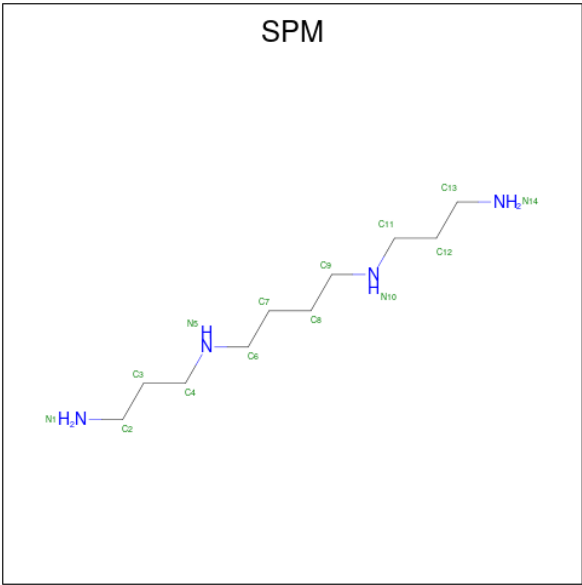
Mol	Chain	Residues	Atoms						AltConf	Trace
91	Az	42	Total	C	H	N	O	P	0	0
			1325	396	445	144	298	42		

- Molecule 92 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



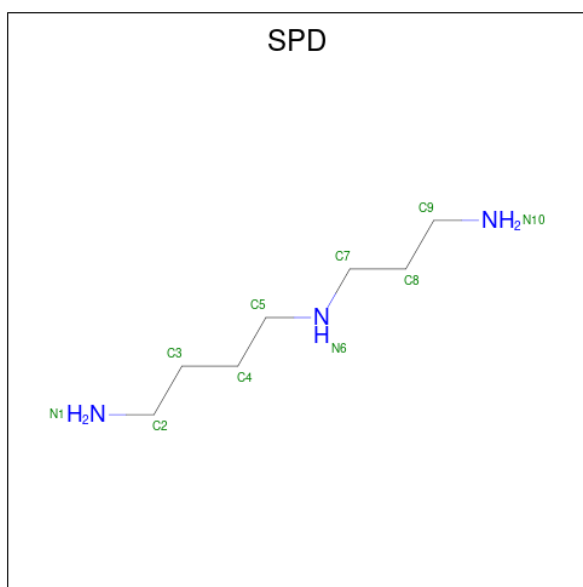
Mol	Chain	Residues	Atoms						AltConf
92	AA	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 93 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



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

- Molecule 94 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



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

- Molecule 95 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
95	AA	62	Total	Mg	0
			62	62	
95	AB	1	Total	Mg	0
			1	1	
95	AX	1	Total	Mg	0
			1	1	
95	A3	1	Total	Mg	0
			1	1	
95	Aw	1	Total	Mg	0
			1	1	
95	A	136	Total	Mg	0
			136	136	
95	D	2	Total	Mg	0
			2	2	
95	E	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
95	g	1	Total 1	Mg 1	0

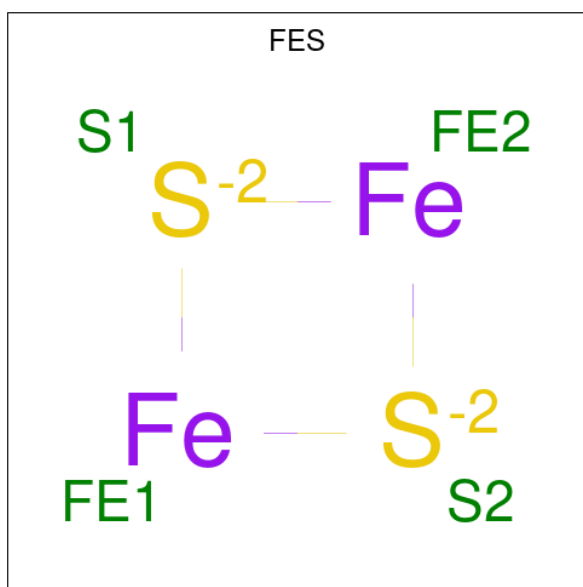
- Molecule 96 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
96	AA	16	Total 16	K 16	0
96	A	28	Total 28	K 28	0
96	D	1	Total 1	K 1	0
96	M	1	Total 1	K 1	0
96	P	1	Total 1	K 1	0
96	i	1	Total 1	K 1	0
96	o	1	Total 1	K 1	0

- Molecule 97 is ZINC ION (CCD ID: ZN) (formula: Zn).

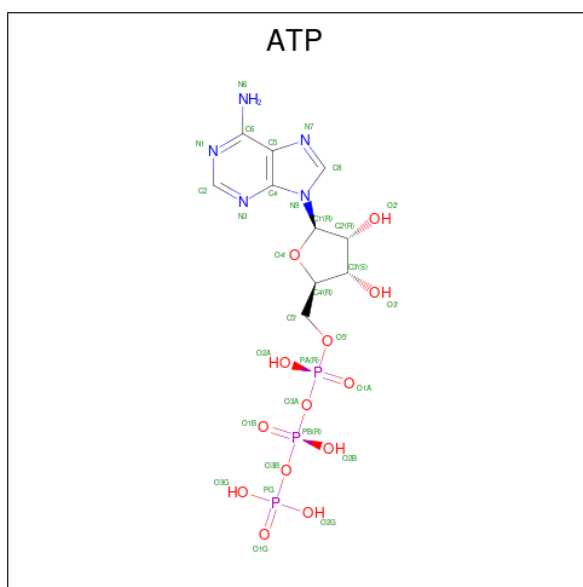
Mol	Chain	Residues	Atoms		AltConf
97	AO	1	Total 1	Zn 1	0
97	0	1	Total 1	Zn 1	0
97	4	1	Total 1	Zn 1	0

- Molecule 98 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 99 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



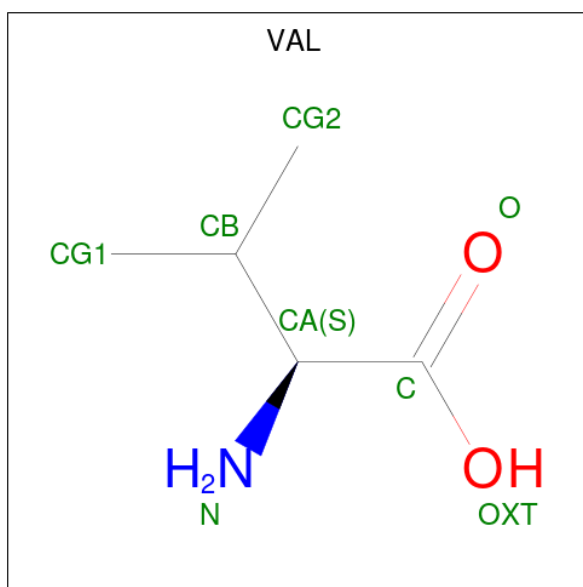
Mol	Chain	Residues	Atoms						AltConf
99	AX	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

-
- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including the amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected in a diphosphate chain, with the first phosphate linked to the 5' carbon of the ribose and the second phosphate linked to the first. The structure is labeled with various atoms and bonds, including the nitrogenous base, the sugar, and the phosphate groups.

PUT

The diagram shows the chemical structure of Putrescine (PUT), a linear diamine. It consists of a four-carbon chain. The first carbon (C1) is bonded to an amino group (NH₂, N1). The second carbon (C2) is bonded to a hydrogen atom (H2). The third carbon (C3) is bonded to a hydrogen atom (H3). The fourth carbon (C4) is bonded to an amino group (NH₂, N2). The atoms are labeled with green text: C1, C2, C3, C4, N1, N2, H1, H2, H3, H4. The bonds are shown as a zigzag line.





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

- Molecule 103 is water.

Mol	Chain	Residues	Atoms		AltConf
103	AA	1747	Total	O	0
			1747	1747	
103	AB	60	Total	O	0
			60	60	
103	AC	48	Total	O	0
			48	48	
103	AD	66	Total	O	0
			66	66	
103	AE	20	Total	O	0
			20	20	
103	AF	29	Total	O	0
			29	29	
103	AG	53	Total	O	0
			53	53	
103	AH	46	Total	O	0
			46	46	
103	AI	30	Total	O	0
			30	30	
103	AJ	14	Total	O	0
			14	14	
103	AK	49	Total	O	0
			49	49	

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Mol	Chain	Residues	Atoms		AltConf
103	AL	42	Total 42	O 42	0
103	AM	13	Total 13	O 13	0
103	AN	29	Total 29	O 29	0
103	AO	33	Total 33	O 33	0
103	AP	23	Total 23	O 23	0
103	AQ	52	Total 52	O 52	0
103	AR	9	Total 9	O 9	0
103	AS	18	Total 18	O 18	0
103	AT	26	Total 26	O 26	0
103	AU	4	Total 4	O 4	0
103	AW	9	Total 9	O 9	0
103	AX	44	Total 44	O 44	0
103	AZ	24	Total 24	O 24	0
103	A0	2	Total 2	O 2	0
103	A1	36	Total 36	O 36	0
103	A2	26	Total 26	O 26	0
103	A3	43	Total 43	O 43	0
103	Aw	4	Total 4	O 4	0
103	Ax	8	Total 8	O 8	0
103	Ay	1	Total 1	O 1	0
103	A	2847	Total 2847	O 2847	0

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Mol	Chain	Residues	Atoms		AltConf
103	B	55	Total 55	O 55	0
103	D	68	Total 68	O 68	0
103	E	57	Total 57	O 57	0
103	F	74	Total 74	O 74	0
103	I	21	Total 21	O 21	0
103	K	68	Total 68	O 68	0
103	L	27	Total 27	O 27	0
103	M	46	Total 46	O 46	0
103	N	50	Total 50	O 50	0
103	O	34	Total 34	O 34	0
103	P	69	Total 69	O 69	0
103	Q	26	Total 26	O 26	0
103	R	59	Total 59	O 59	0
103	S	43	Total 43	O 43	0
103	T	47	Total 47	O 47	0
103	U	25	Total 25	O 25	0
103	V	6	Total 6	O 6	0
103	W	49	Total 49	O 49	0
103	X	11	Total 11	O 11	0
103	Y	23	Total 23	O 23	0
103	Z	35	Total 35	O 35	0

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Mol	Chain	Residues	Atoms		AltConf
103	0	27	Total 27	O 27	0
103	1	2	Total 2	O 2	0
103	2	33	Total 33	O 33	0
103	3	43	Total 43	O 43	0
103	4	11	Total 11	O 11	0
103	5	15	Total 15	O 15	0
103	6	69	Total 69	O 69	0
103	7	11	Total 11	O 11	0
103	8	14	Total 14	O 14	0
103	9	16	Total 16	O 16	0
103	a	9	Total 9	O 9	0
103	b	32	Total 32	O 32	0
103	c	16	Total 16	O 16	0
103	d	6	Total 6	O 6	0
103	e	8	Total 8	O 8	0
103	f	18	Total 18	O 18	0
103	g	10	Total 10	O 10	0
103	i	50	Total 50	O 50	0
103	j	21	Total 21	O 21	0
103	l	1	Total 1	O 1	0
103	m	8	Total 8	O 8	0

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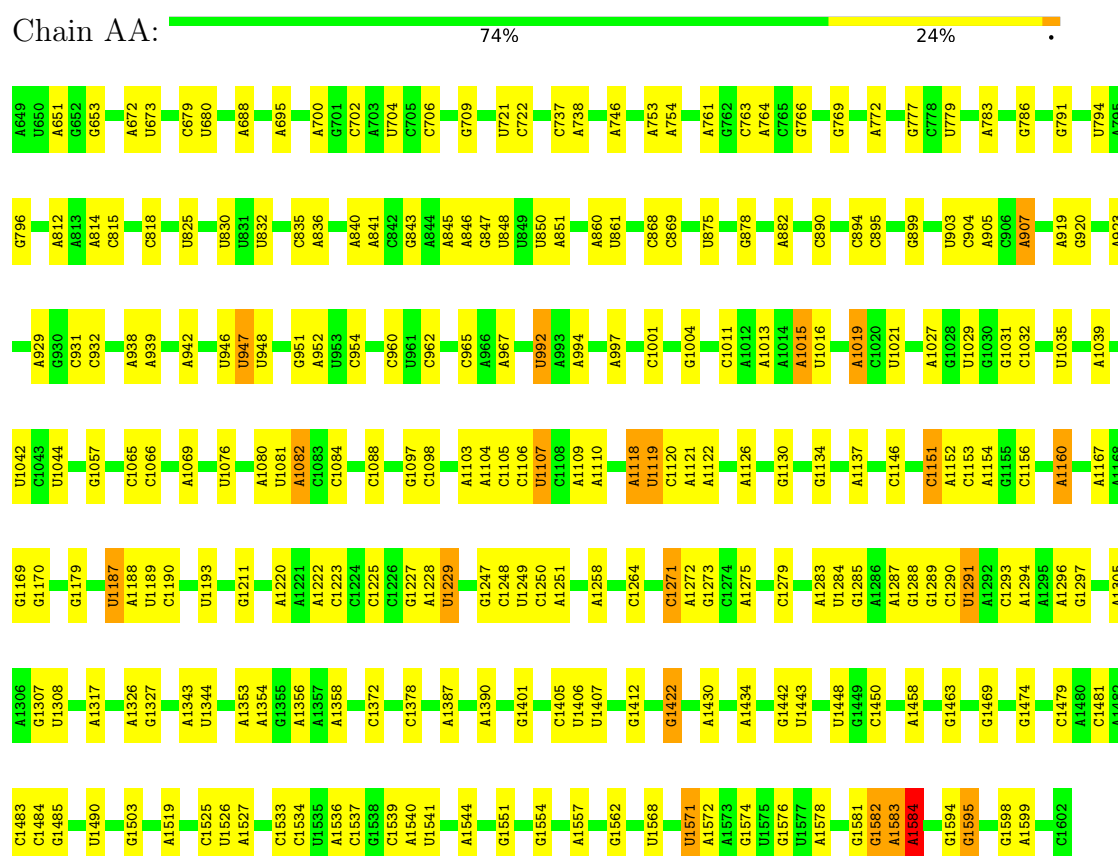
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Mol	Chain	Residues	Atoms		AltConf
103	o	33	Total 33	O 33	0
103	p	4	Total 4	O 4	0
103	r	35	Total 35	O 35	0
103	s	40	Total 40	O 40	0
103	H	7	Total 7	O 7	0
103	AY	20	Total 20	O 20	0
103	A4	7	Total 7	O 7	0
103	Az	12	Total 12	O 12	0

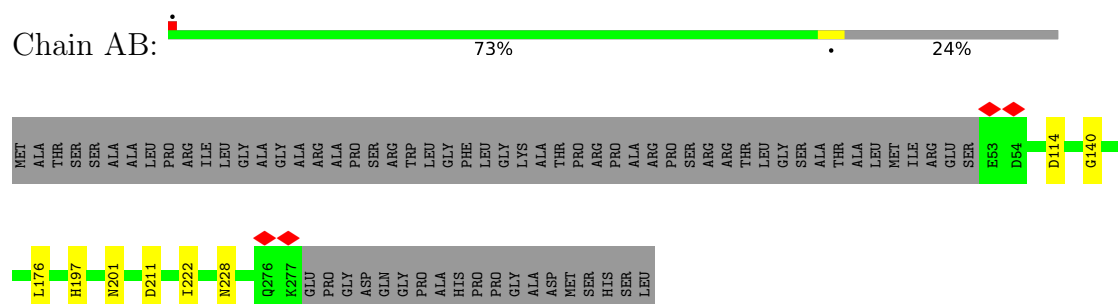
3 Residue-property plots

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

• Molecule 1: 12S mitochondrial rRNA

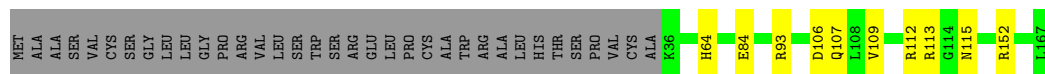


• Molecule 2: 28S ribosomal protein S2, mitochondrial



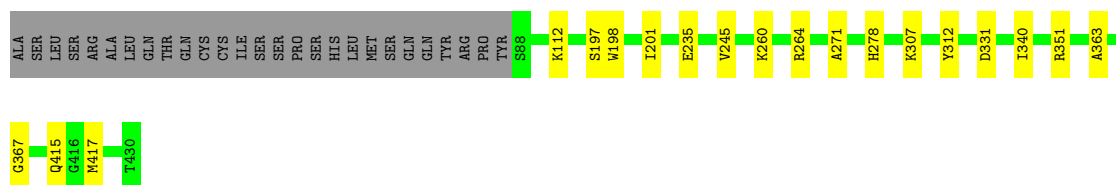
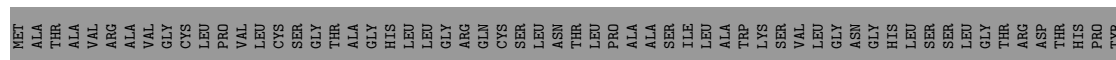
- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain AC:  73% 6% 21%

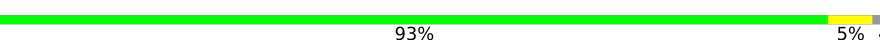


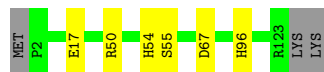
- Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain AD:  75% 20%



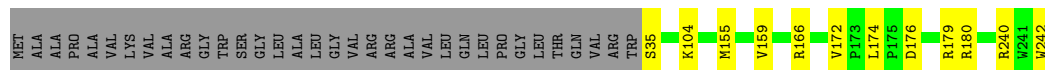
- Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain AE:  93% 5% 2%



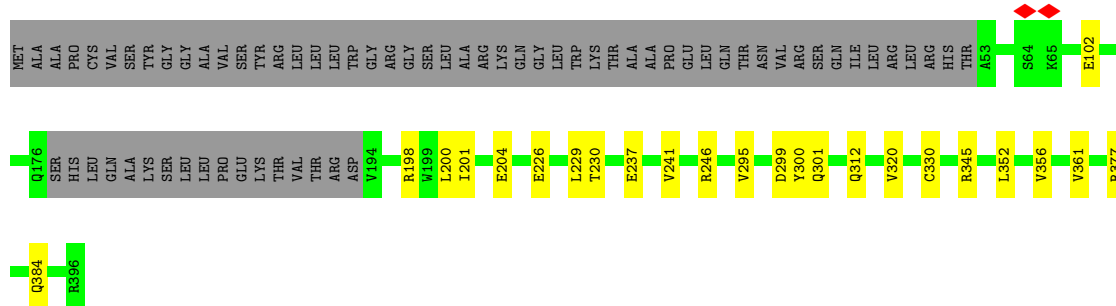
- Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain AF:  81% 5% 14%



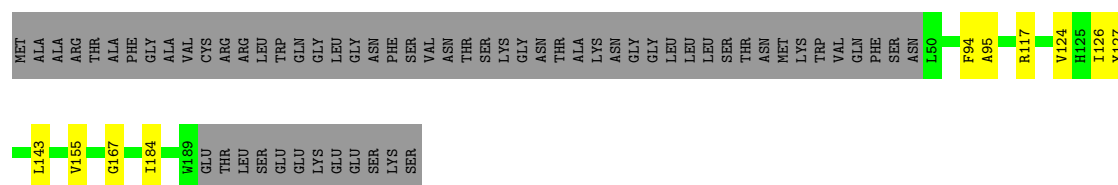
- Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain AG:  76% 6% 17%



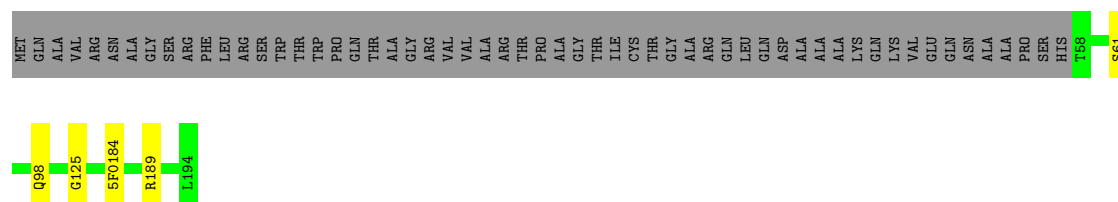
- Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain AH:  65% 5% 30%



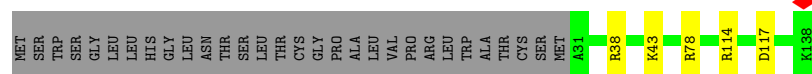
- Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain AI:  68% 0% 32%



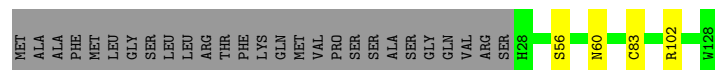
- Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain AJ:  75% 0% 25%



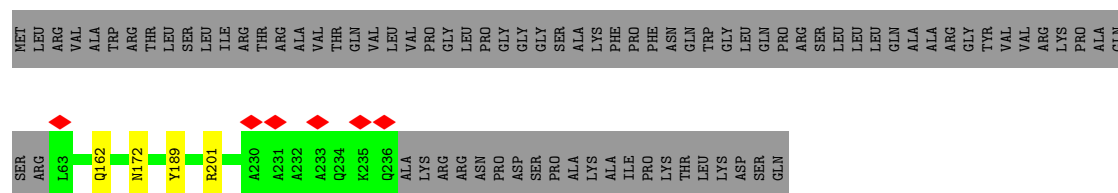
- Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain AK:  76% 0% 24%



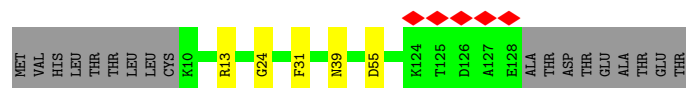
- Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain AL:  66% 0% 34%



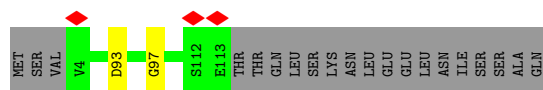
- Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain AM:  83% 0% 17%



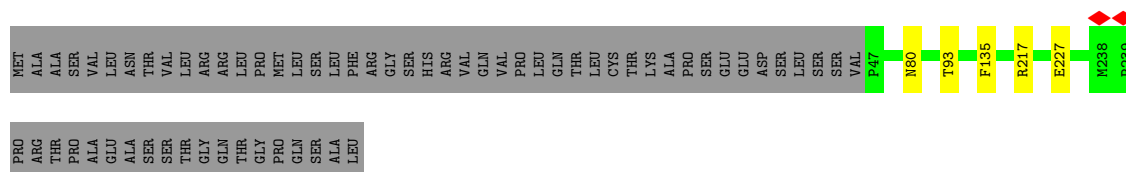
- Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain AN:  83% 15%



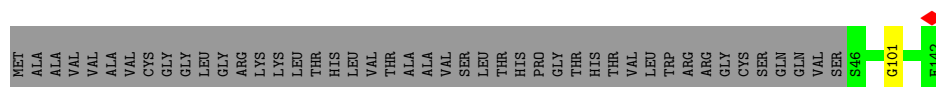
- Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain AO:  73% 25%

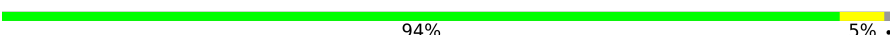


- Molecule 16: 28S ribosomal protein S18c, mitochondrial

Chain AP:  68% 32%



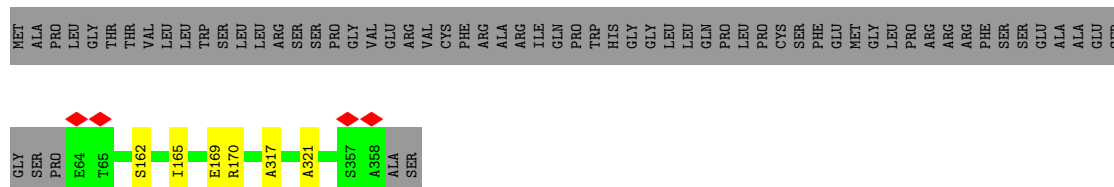
- Molecule 17: 28S ribosomal protein S21, mitochondrial

Chain AQ:  94% 5%



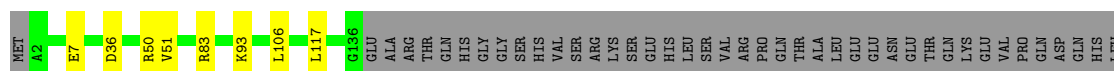
- Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain AR:  80% 18%



- Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain AS:  67% 29%



GLU
ALA
PRO
ALA
ASP
GLN
SER
LYS
LEU
LEU
PRO
PRO

- Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain AT:  92% 5%

MET P2 F47 I52 E91 T92 K108 K121 R132 L136 Q146 K168 A169 ASP ALA GLN ASP

- Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain AU:  84% 14%

MET LEU ARG ALA SER LEU SER ARG LEU GLY GLY ALA THR PRO CYS ARG PRO ARG ALA PRO LEU VAL LEU PRO ALA ARG GLY R27 D49 Y60 R120 R202 ARG ASP SER

- Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain AV:  84% 13%

MET ALA ALA SER ILE VAL ARG ARG GLY GLY MET LEU LEU ALA ARG GLN VAL LEU PRO GLN LEU LEU PRO SER SER ALA ALA LYS TYR L29 V35 K39 D52 L92 I137 L225 Y226 P270 V282 L283 L293 ASP GLY ALA SER GLU GLU SER GLN ASN ASP

GLU ASP ASN GLN GLY SER E311 D318 I319 K346 E376 Q407 LYS ALA ALA LYS ALA SER ALA

- Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain AW:  52% 47%

MET ALA ALA LEU LEU CYS ARG THR ARG ALA VAL LEU ALA ALA ARG GLU SER HIS PHE LEU ARG VAL PHE LEU PHE PHE ARG PRO PHE ARG GLY VAL GLY THR GLU SER GLY SER SER ASN VAL LYS GLU PRO LYS THR ARG ALA GLY PHE ALA SER LEU LEU ARG HIS SER

GLU LEU LEU GLN LYS VAL GLU PRO LEU LEU GLN LYS ARG GLY SER PRO LYS N76 M92 K98 V162 S175 LYS ASP SER GLN ARG SER GLN LYS LEU HIS HIS GLU LYS

- Molecule 24: 28S ribosomal protein S29, mitochondrial

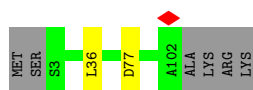
Chain AX:  82% 6% 12%

MET MET LEU LYS ILE THR ARG LEU LEU ILE ILE SER ARG HIS HIS LYS LEU ASP PRO ARG GLY ARG PHE LEU HIS MET GLY THR GLN ALA ARG GLN LEU ILE LEU ASP ASN GLN VAL PRO VAL VAL GLU SER PRO PRO ARG A47 E81 L108 Y119 R123 V141 L151 I152

L153 H159 D167 S171 E183 N190 Y208 L244 K245 E246 L247 T265 N266 T272 K279 T282 M297 L337 N385 E392 L398

- Molecule 25: 28S ribosomal protein S33, mitochondrial

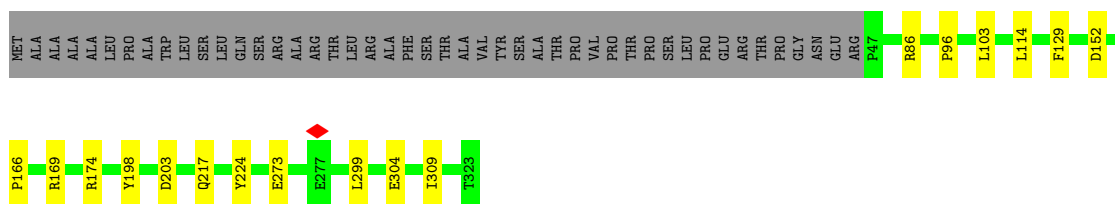
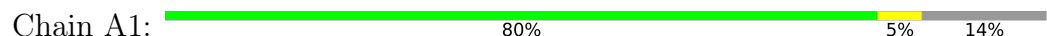
Chain AZ:  92% 6%



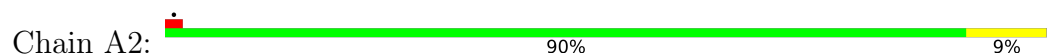
- Molecule 26: 28S ribosomal protein S34, mitochondrial



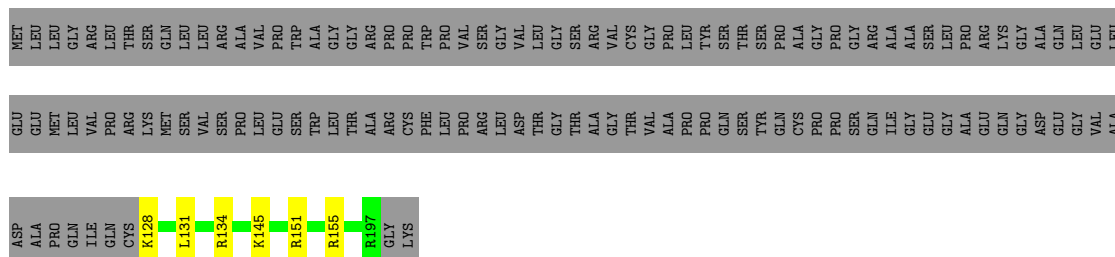
- Molecule 27: 28S ribosomal protein S35, mitochondrial



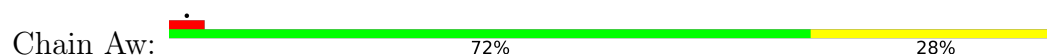
- Molecule 28: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1



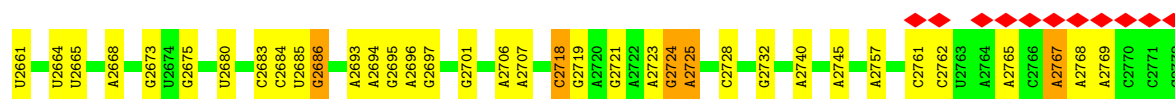
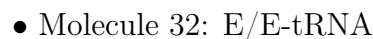
- Molecule 29: Aurora kinase A-interacting protein

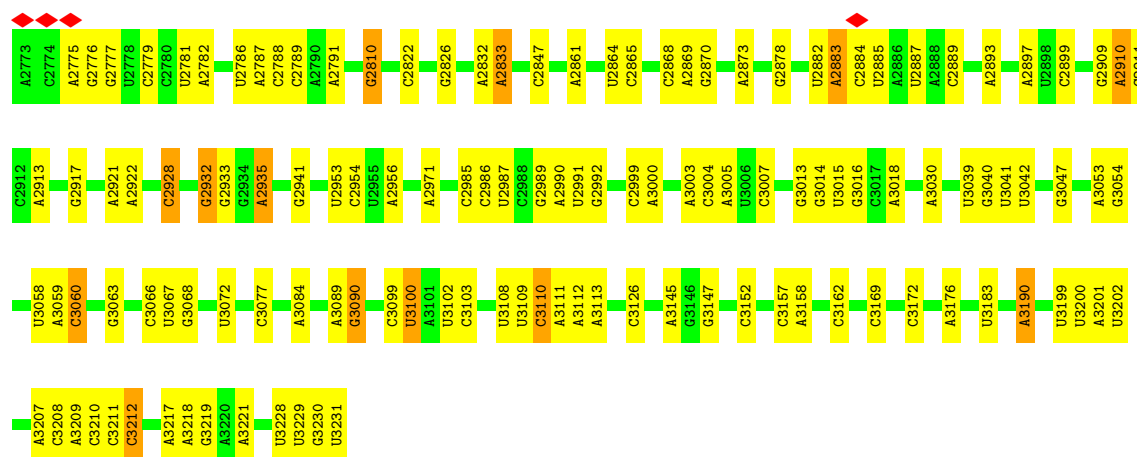


- Molecule 30: A/A-tRNA

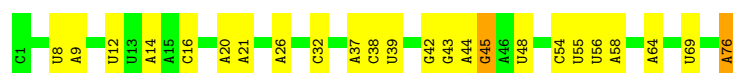


- Molecule 31: P/P-tRNA

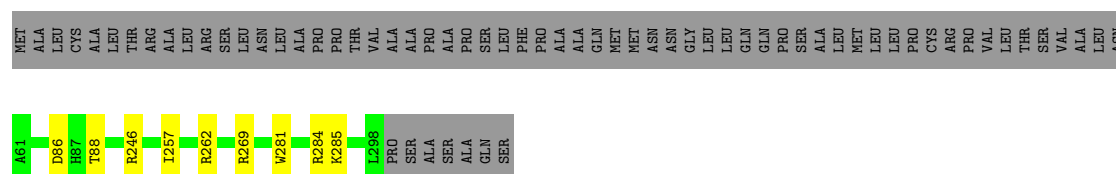




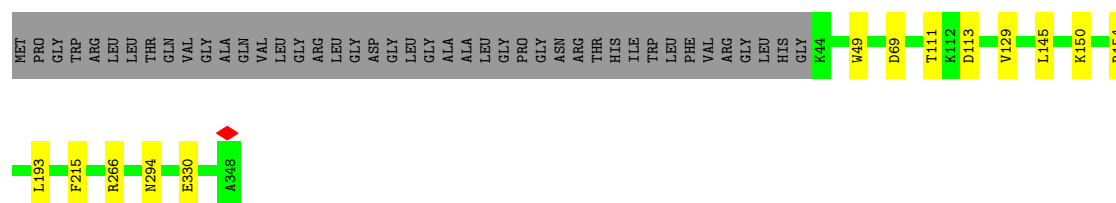
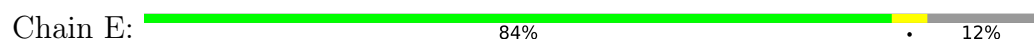
- Molecule 34: mitochondrial tRNAVal



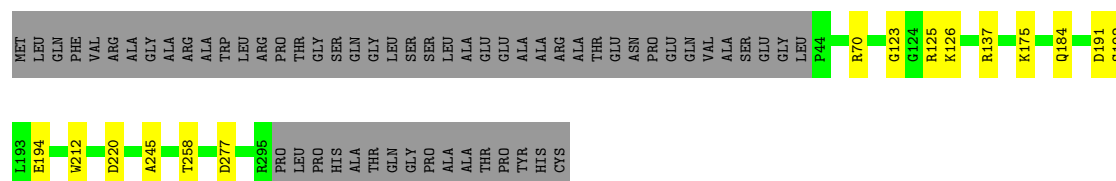
- Molecule 35: 39S ribosomal protein L2, mitochondrial



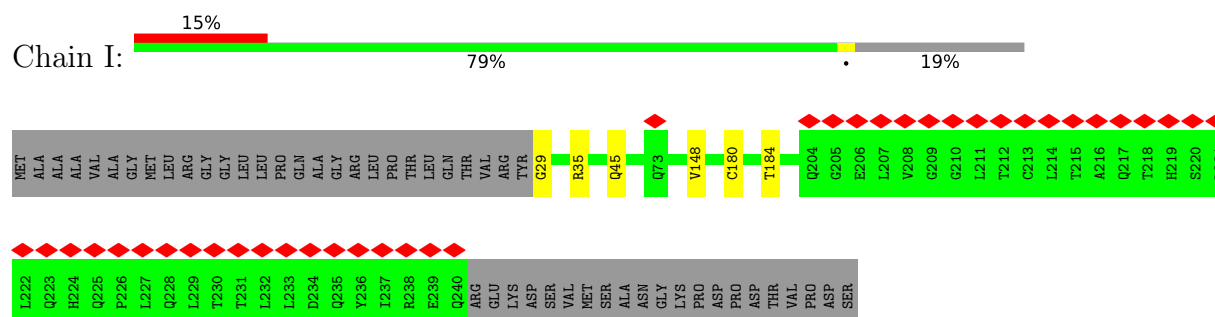
- Molecule 36: 39S ribosomal protein L3, mitochondrial



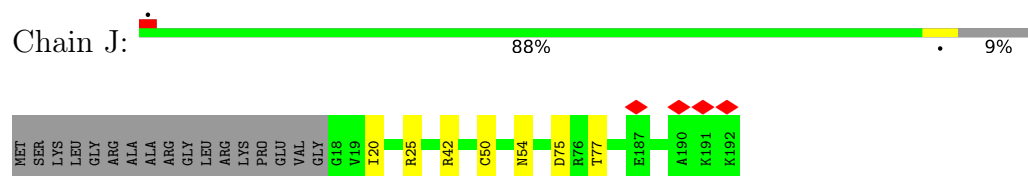
- Molecule 37: 39S ribosomal protein L4, mitochondrial



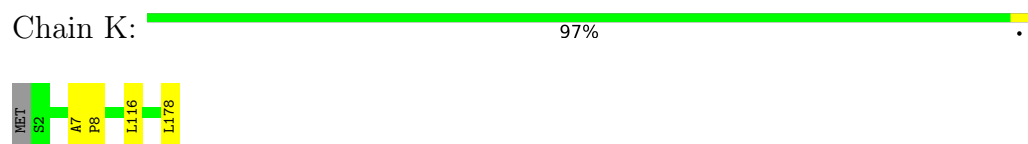
- Molecule 38: 39S ribosomal protein L10, mitochondrial



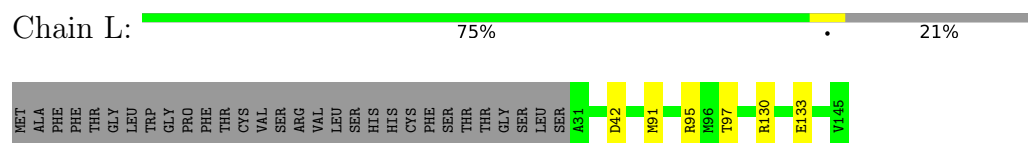
- Molecule 39: 39S ribosomal protein L11, mitochondrial



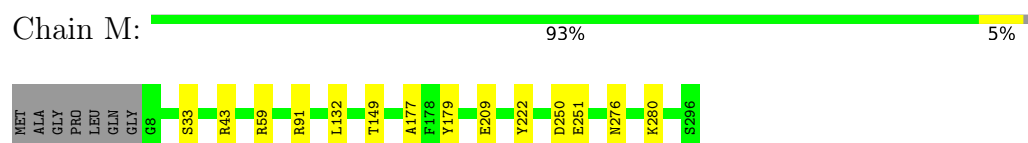
- Molecule 40: 39S ribosomal protein L13, mitochondrial



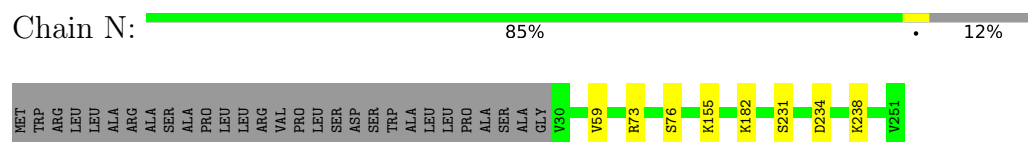
- Molecule 41: 39S ribosomal protein L14, mitochondrial



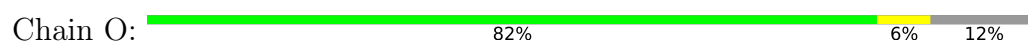
- Molecule 42: 39S ribosomal protein L15, mitochondrial

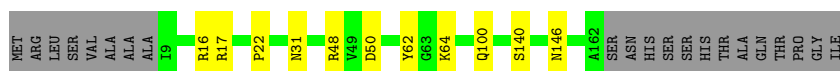


- Molecule 43: 39S ribosomal protein L16, mitochondrial

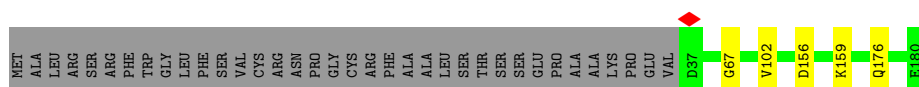
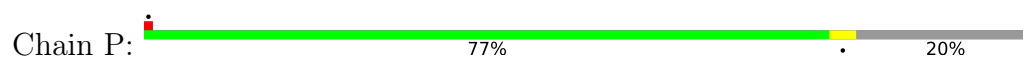


- Molecule 44: 39S ribosomal protein L17, mitochondrial

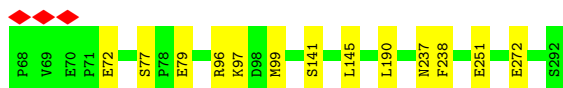
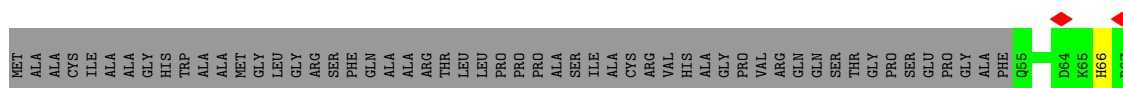
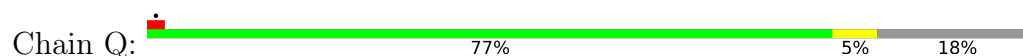




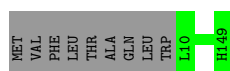
- Molecule 45: 39S ribosomal protein L18, mitochondrial



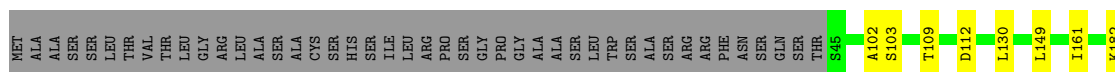
- Molecule 46: 39S ribosomal protein L19, mitochondrial



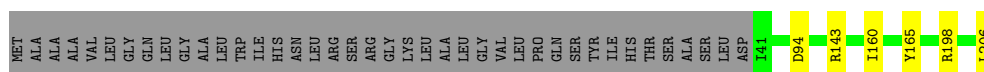
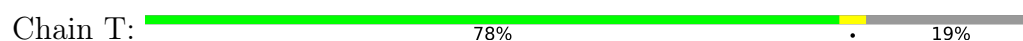
- Molecule 47: 39S ribosomal protein L20, mitochondrial



- Molecule 48: 39S ribosomal protein L21, mitochondrial



- Molecule 49: 39S ribosomal protein L22, mitochondrial



- Molecule 50: 39S ribosomal protein L23, mitochondrial





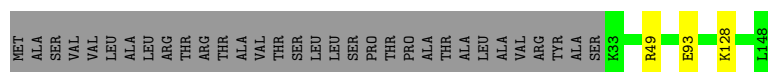
- Molecule 51: 39S ribosomal protein L24, mitochondrial

Chain V: 88% 6% 5%



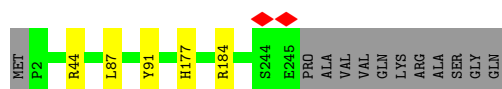
- Molecule 52: 39S ribosomal protein L27, mitochondrial

Chain W: 76% 22%



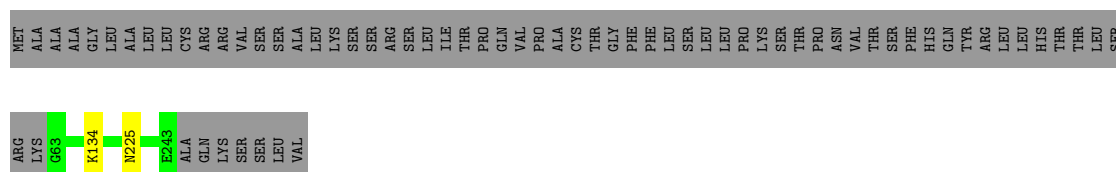
- Molecule 53: 39S ribosomal protein L28, mitochondrial

Chain X: 93% 5%



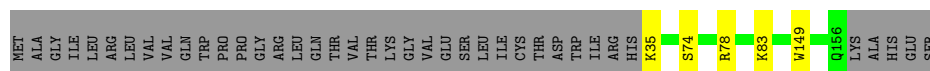
- Molecule 54: 39S ribosomal protein L47, mitochondrial

Chain Y: 72% 28%



- Molecule 55: 39S ribosomal protein L30, mitochondrial

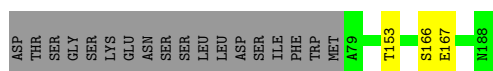
Chain Z: 73% 24%



- Molecule 56: 39S ribosomal protein L32, mitochondrial

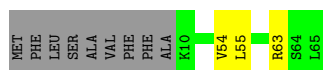
Chain 0: 57% 41%





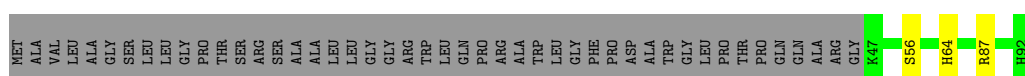
- Molecule 57: 39S ribosomal protein L33, mitochondrial

Chain 1: 82% 5% 14%



- Molecule 58: 39S ribosomal protein L34, mitochondrial

Chain 2: 47% 0% 50%



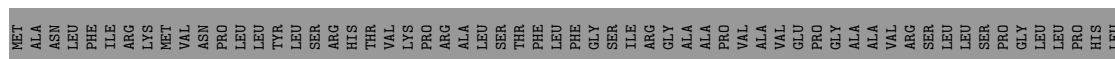
- Molecule 59: 39S ribosomal protein L35, mitochondrial

Chain 3: 46% 5% 49%



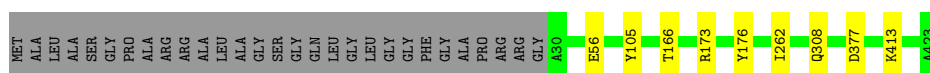
- Molecule 60: 39S ribosomal protein L36, mitochondrial

Chain 4: 33% 0% 63%



- Molecule 61: 39S ribosomal protein L37, mitochondrial

Chain 5: 91% 0% 7%



- Molecule 62: 39S ribosomal protein L38, mitochondrial

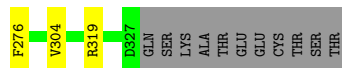
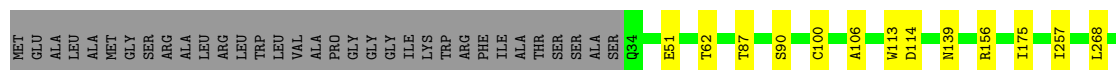
Chain 6: 88% 5% 7%





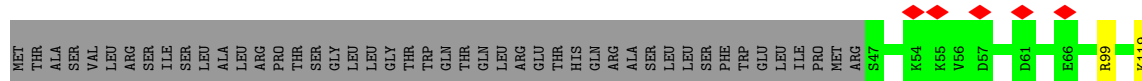
- Molecule 63: 39S ribosomal protein L39, mitochondrial

Chain 7: 82% 5% 13%



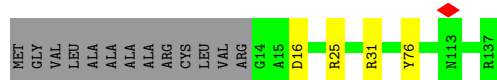
- Molecule 64: 39S ribosomal protein L40, mitochondrial

Chain 8: 74% 24%



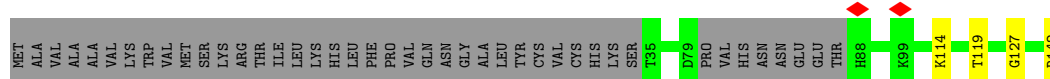
- Molecule 65: 39S ribosomal protein L41, mitochondrial

Chain 9: 88% 9%



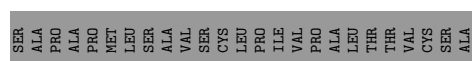
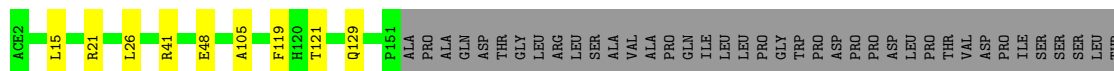
- Molecule 66: 39S ribosomal protein L42, mitochondrial

Chain a: 68% 30%



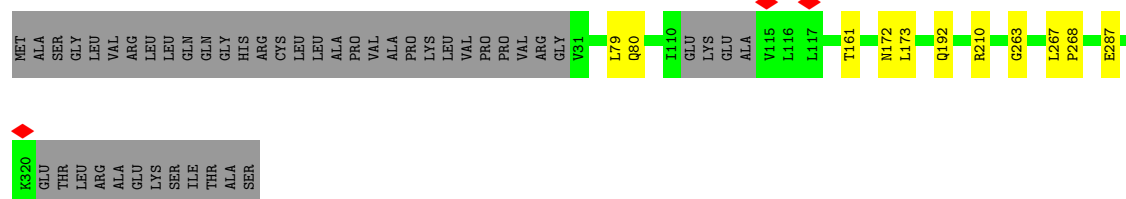
- Molecule 67: Large ribosomal subunit protein mL43

Chain b: 66% 30%



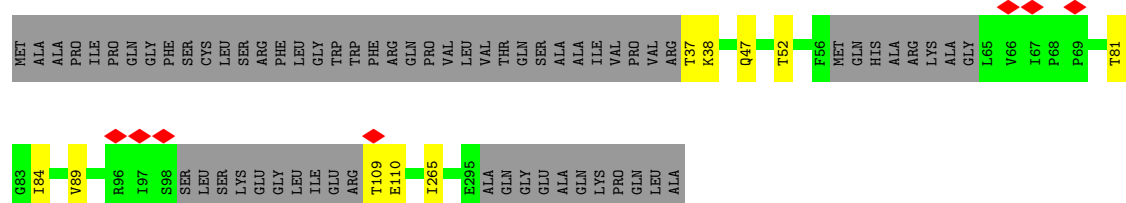
- Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c:  83% 14%



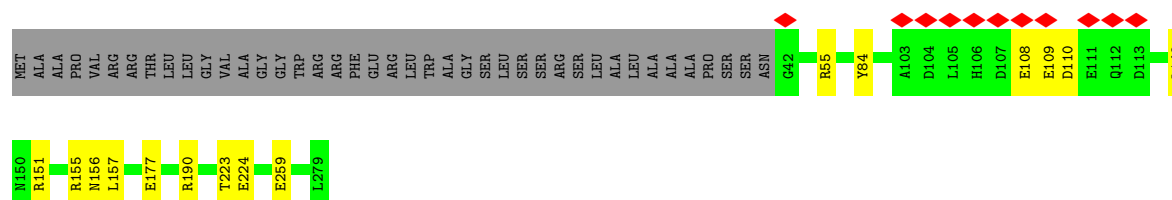
- Molecule 69: 39S ribosomal protein L45, mitochondrial

Chain d:  75% 21%



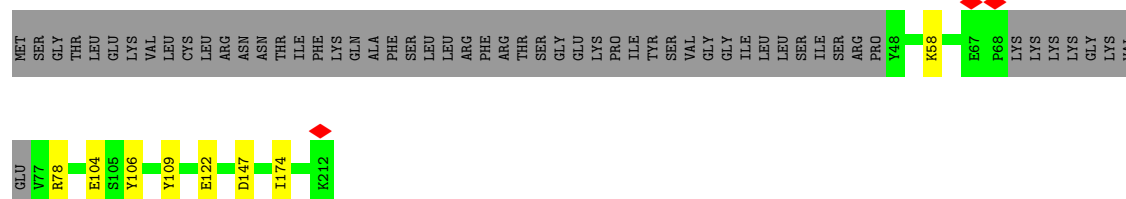
- Molecule 70: 39S ribosomal protein L46, mitochondrial

Chain e:  80% 5% 15%



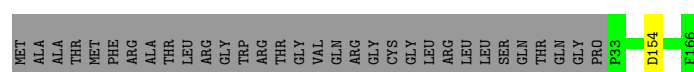
- Molecule 71: 39S ribosomal protein L48, mitochondrial

Chain f:  70% 26%

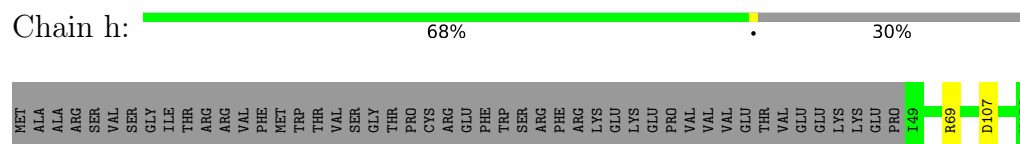


- Molecule 72: 39S ribosomal protein L49, mitochondrial

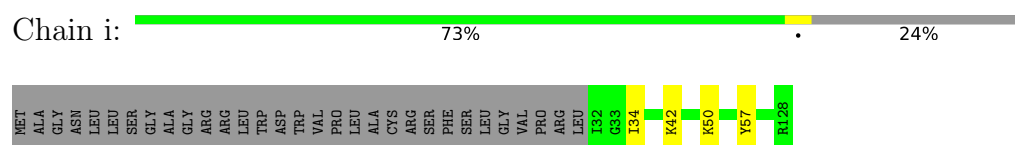
Chain g:  80% 19%



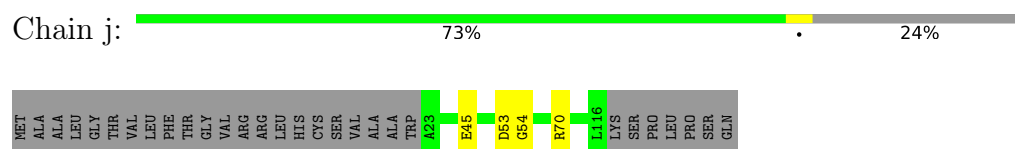
- Molecule 73: 39S ribosomal protein L50, mitochondrial



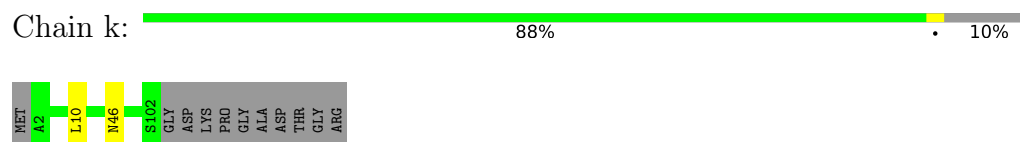
- Molecule 74: 39S ribosomal protein L51, mitochondrial



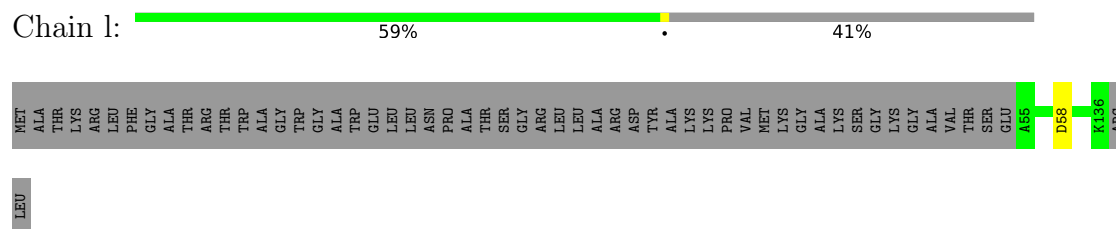
- Molecule 75: 39S ribosomal protein L52, mitochondrial



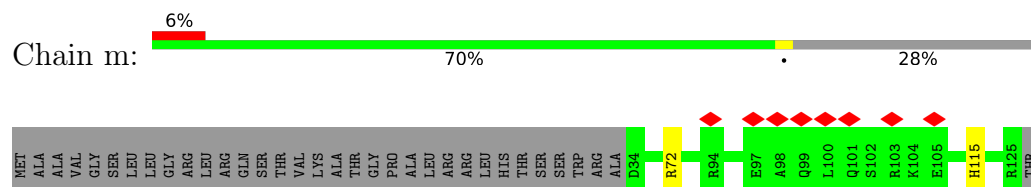
- Molecule 76: 39S ribosomal protein L53, mitochondrial



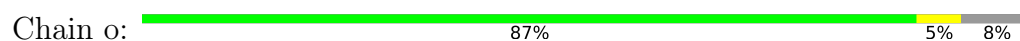
- Molecule 77: 39S ribosomal protein L54, mitochondrial



- Molecule 78: 39S ribosomal protein L55, mitochondrial

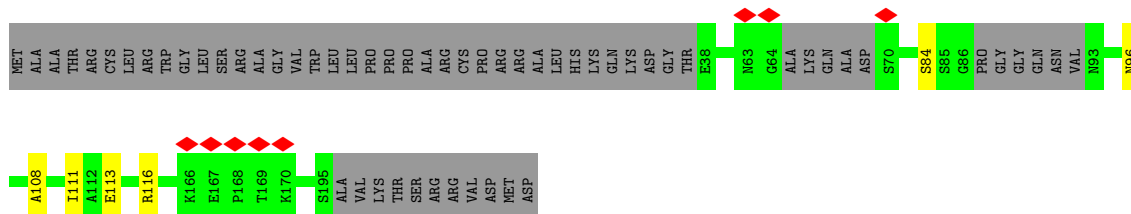


- Molecule 79: Ribosomal protein 63, mitochondrial

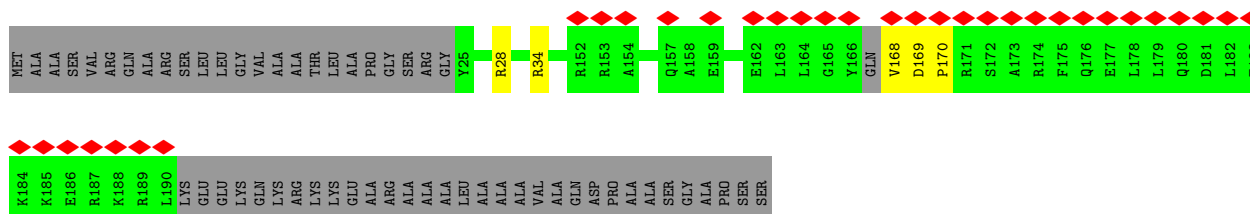




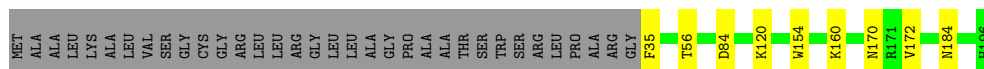
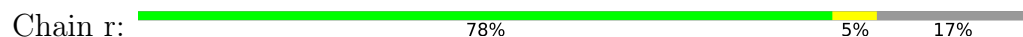
- Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial



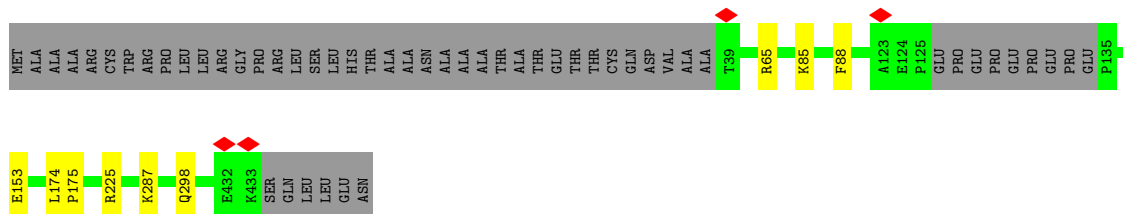
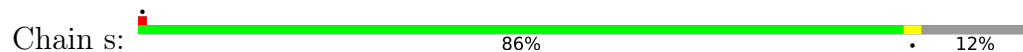
- Molecule 81: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 82: 39S ribosomal protein S18a, mitochondrial

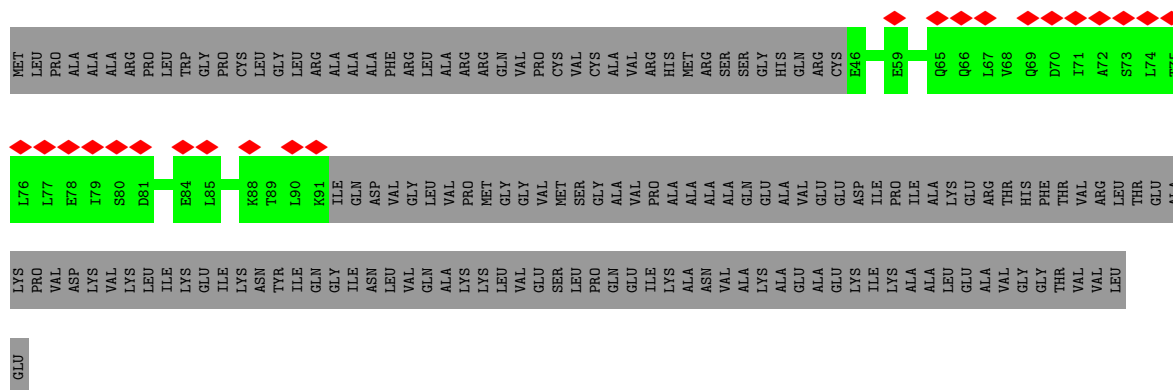


- Molecule 83: 39S ribosomal protein S30, mitochondrial

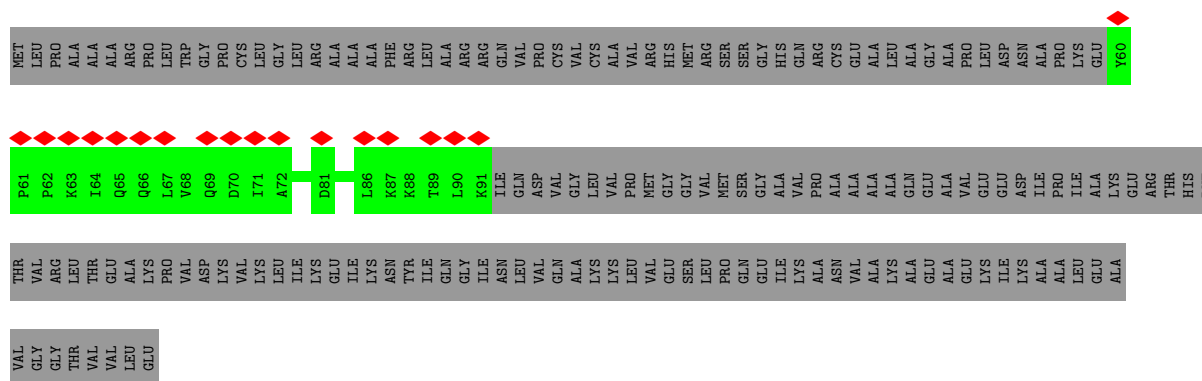


- Molecule 84: 39S ribosomal protein L12, mitochondrial

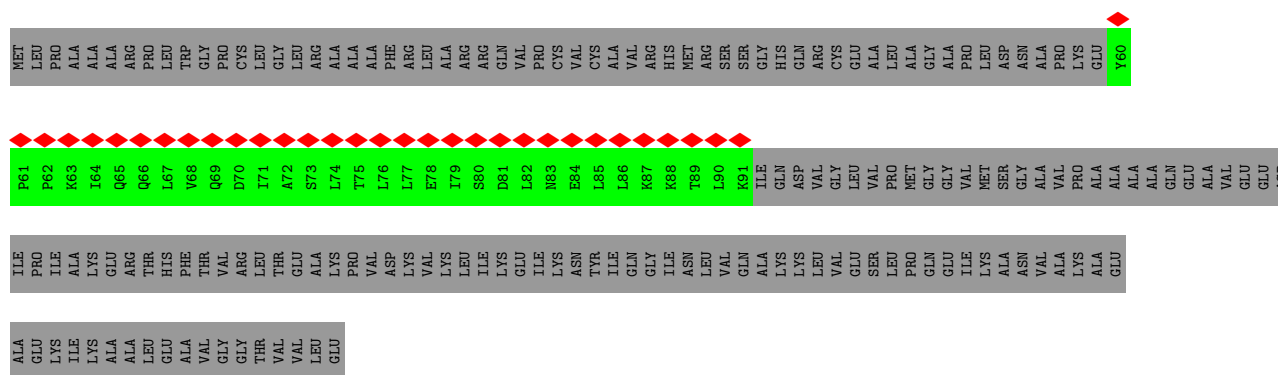




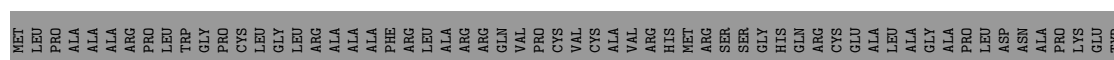
- Molecule 84: 39S ribosomal protein L12, mitochondrial

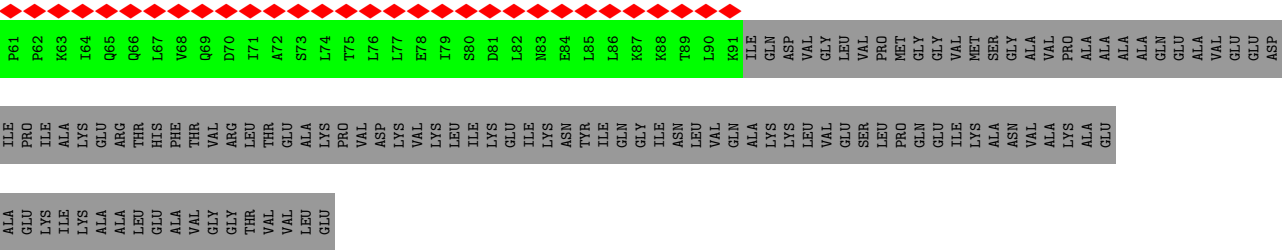


- Molecule 84: 39S ribosomal protein L12, mitochondrial

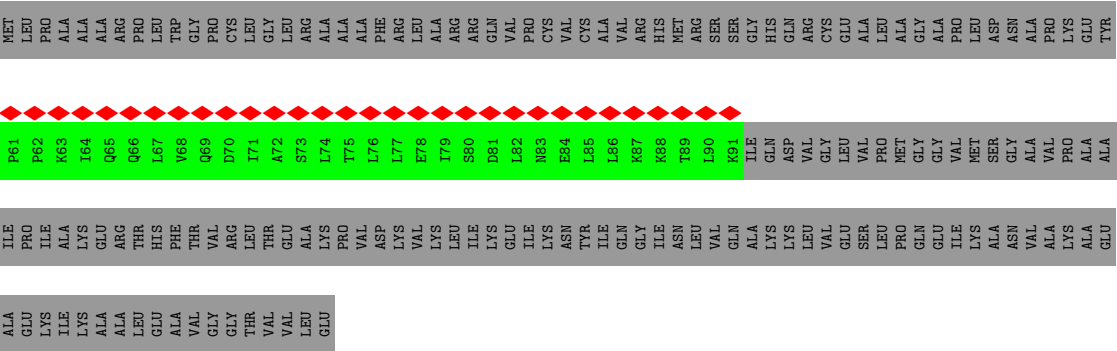


- Molecule 84: 39S ribosomal protein L12, mitochondrial

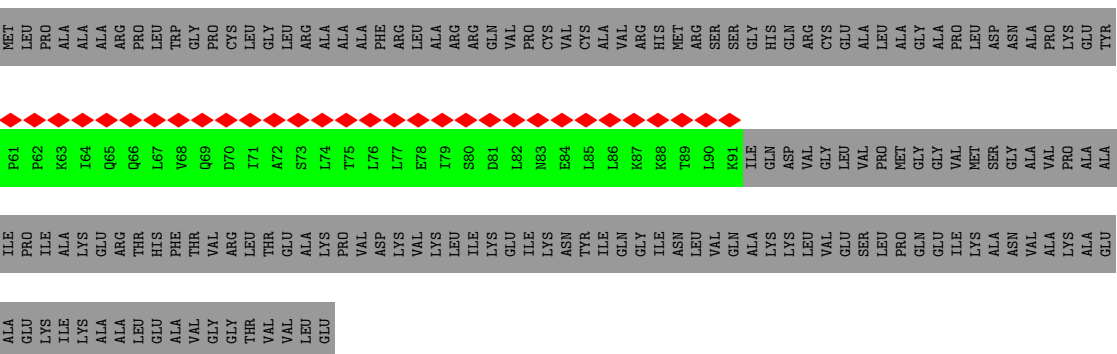




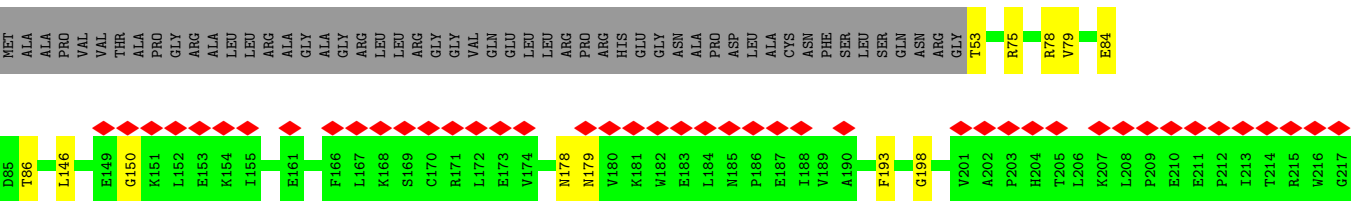
• Molecule 84: 39S ribosomal protein L12, mitochondrial

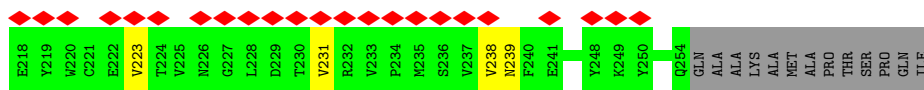


• Molecule 84: 39S ribosomal protein L12, mitochondrial



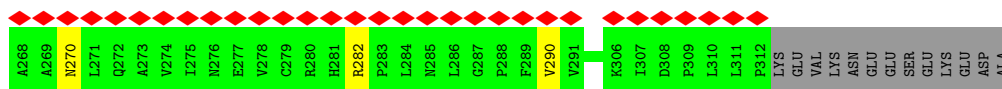
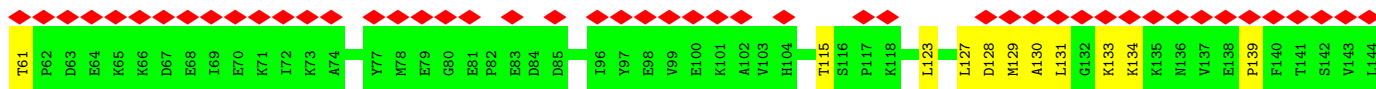
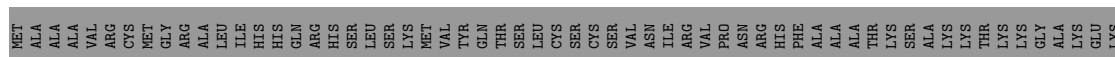
• Molecule 85: 39S ribosomal protein L9, mitochondrial





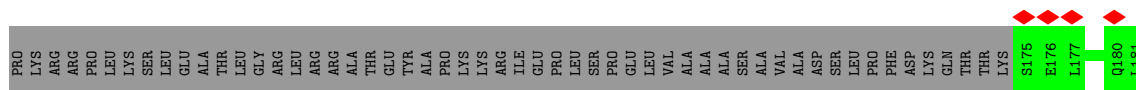
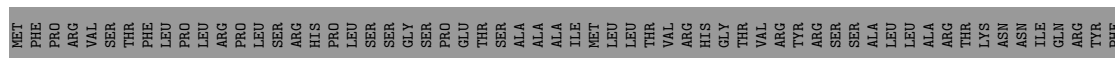
- Molecule 86: 39S ribosomal protein L1, mitochondrial

Chain z: 60% 70% 8% 22%



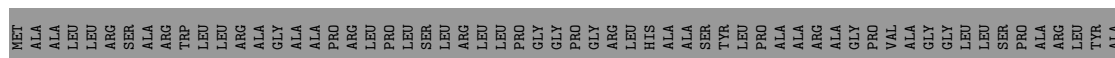
- Molecule 87: 28S ribosomal protein S31, mitochondrial

Chain AY: 13% 49% 7% 44%



- Molecule 88: Leucine-rich PPR motif-containing protein, mitochondrial

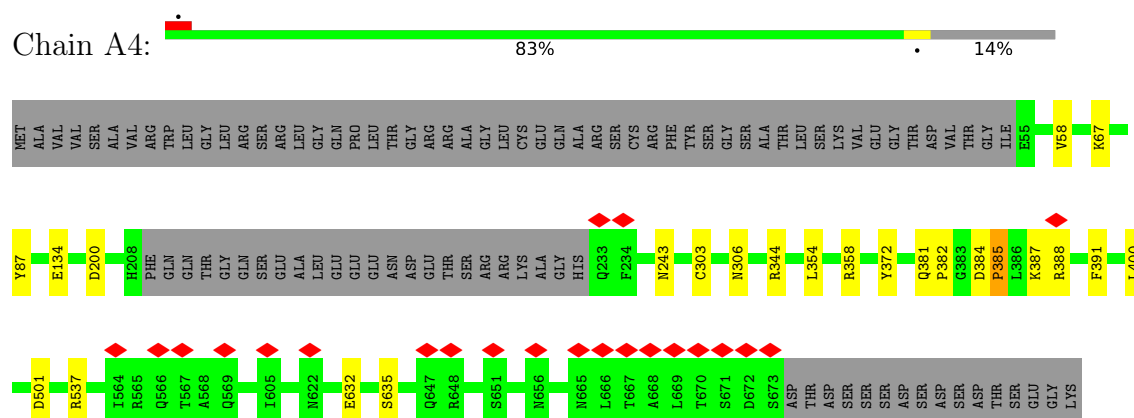
Chain A5: 16% 37% 58%





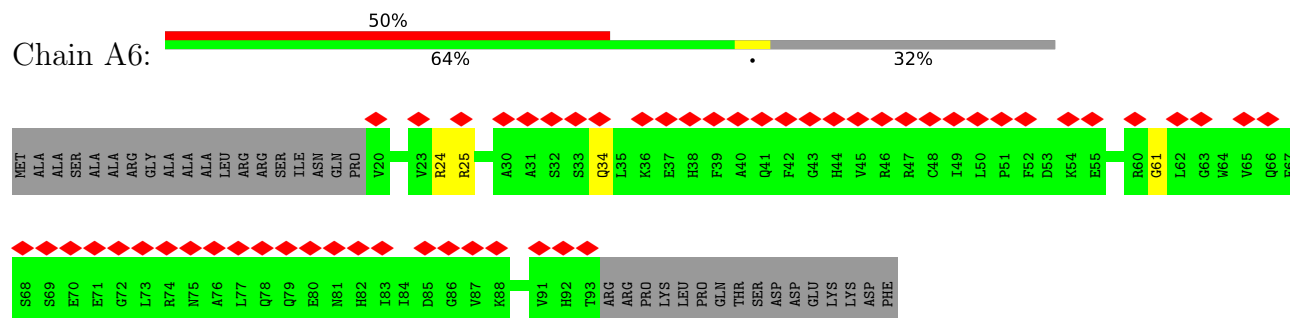
- Molecule 89: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4:



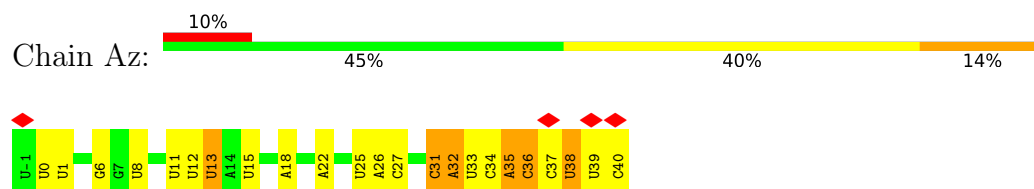
- Molecule 90: SRA stem-loop-interacting RNA-binding protein, mitochondrial

Chain A6:



- Molecule 91: mRNA

Chain Az:



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	0.335	Depositor
Minimum map value	-0.152	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	531.2, 531.2, 531.2	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.12	0/22537	0.19	0/35085
2	AB	0.09	0/1871	0.24	0/2531
3	AC	0.10	0/1113	0.24	0/1505
4	AD	0.09	0/2783	0.21	0/3724
5	AE	0.08	0/989	0.21	0/1335
6	AF	0.08	0/1767	0.21	0/2373
7	AG	0.09	0/2746	0.21	0/3681
8	AH	0.11	0/1178	0.25	0/1598
9	AI	0.08	0/1030	0.21	0/1386
10	AJ	0.10	0/855	0.25	0/1148
11	AK	0.09	0/880	0.21	0/1182
12	AL	0.08	0/1477	0.20	0/1974
13	AM	0.09	0/963	0.24	0/1295
14	AN	0.09	0/886	0.23	0/1199
15	AO	0.09	0/1648	0.22	0/2243
16	AP	0.10	0/798	0.24	0/1070
17	AQ	0.10	0/748	0.22	0/994
18	AR	0.08	0/2456	0.19	0/3317
19	AS	0.08	0/1138	0.19	0/1533
20	AT	0.09	0/1402	0.24	0/1883
21	AU	0.07	0/1510	0.17	0/2025
22	AV	0.09	0/3030	0.20	0/4093
23	AW	0.09	0/801	0.22	0/1079
24	AX	0.09	0/2921	0.23	0/3954
25	AZ	0.09	0/857	0.22	0/1141
26	A0	0.10	0/1834	0.24	0/2484
27	A1	0.09	0/2293	0.22	0/3102
28	A2	0.08	0/941	0.23	0/1257
29	A3	0.10	0/636	0.25	0/839
30	Aw	0.05	0/1603	0.13	0/2488
31	Ax	0.08	0/1655	0.16	0/2569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ay	0.06	0/1656	0.15	0/2571
33	A	0.12	0/36876	0.21	0/57402
34	B	0.10	0/1627	0.17	0/2527
35	D	0.09	0/1896	0.25	0/2549
36	E	0.10	0/2475	0.25	0/3355
37	F	0.11	0/2090	0.27	0/2842
38	I	0.10	0/1731	0.25	0/2345
39	J	0.08	0/1348	0.21	0/1813
40	K	0.10	0/1490	0.24	0/2021
41	L	0.09	0/905	0.25	0/1218
42	M	0.10	0/2368	0.27	0/3195
43	N	0.10	0/1833	0.24	0/2468
44	O	0.09	0/1283	0.23	0/1727
45	P	0.12	0/1199	0.24	0/1623
46	Q	0.09	0/2027	0.23	0/2734
47	R	0.10	0/1175	0.22	0/1572
48	S	0.11	0/1320	0.28	0/1789
49	T	0.11	0/1403	0.27	0/1886
50	U	0.10	0/1274	0.24	0/1723
51	V	0.09	0/1721	0.24	0/2333
52	W	0.11	0/926	0.24	0/1244
53	X	0.10	0/2099	0.22	0/2837
54	Y	0.09	0/1593	0.22	0/2136
55	Z	0.10	0/1021	0.27	0/1378
56	0	0.10	0/913	0.23	0/1224
57	1	0.09	0/469	0.24	0/621
58	2	0.11	0/383	0.27	0/507
59	3	0.11	0/853	0.26	0/1136
60	4	0.10	0/350	0.22	0/461
61	5	0.10	0/3305	0.24	0/4502
62	6	0.12	0/3043	0.24	0/4140
63	7	0.09	0/2447	0.25	0/3310
64	8	0.09	0/1354	0.23	0/1819
65	9	0.10	0/1025	0.24	0/1379
66	a	0.11	0/866	0.27	0/1174
67	b	0.12	0/1219	0.25	0/1651
68	c	0.09	0/2347	0.22	0/3171
69	d	0.09	0/2039	0.22	0/2759
70	e	0.08	0/1970	0.22	0/2658
71	f	0.10	0/1273	0.21	0/1716
72	g	0.11	0/1151	0.24	0/1569
73	h	0.08	0/918	0.19	0/1249
74	i	0.11	0/850	0.24	0/1135

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	j	0.11	0/760	0.25	0/1023
76	k	0.08	0/777	0.19	0/1048
77	l	0.08	0/707	0.24	0/960
78	m	0.08	0/805	0.20	0/1081
79	o	0.11	0/819	0.26	0/1097
80	p	0.08	0/1223	0.21	0/1641
81	q	0.08	0/1422	0.19	0/1916
82	r	0.10	0/1362	0.26	0/1846
83	s	0.10	0/3239	0.24	0/4400
84	t	0.06	0/358	0.18	0/486
84	u	0.07	0/259	0.18	0/350
84	v	0.06	0/259	0.15	0/350
84	w	0.08	0/246	0.17	0/331
84	x	0.07	0/246	0.16	0/331
84	y	0.07	0/246	0.16	0/331
85	H	0.09	0/1698	0.22	0/2292
86	z	0.10	0/2067	0.27	0/2793
87	AY	0.11	0/1877	0.26	0/2524
88	A5	0.10	0/4737	0.27	0/6398
89	A4	0.09	0/4924	0.23	0/6663
90	A6	0.08	0/619	0.22	0/835
91	Az	0.10	0/981	0.24	0/1522
All	All	0.10	0/197088	0.22	0/279774

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	10305	10285	129	0
2	AB	1828	1826	1815	9	0
3	AC	1083	1096	1088	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AD	2731	2814	2804	13	0
5	AE	972	1004	1000	4	0
6	AF	1725	1778	1769	9	0
7	AG	2688	2697	2687	17	0
8	AH	1152	1191	1183	10	0
9	AI	1020	1066	1053	5	0
10	AJ	839	892	887	6	0
11	AK	862	889	885	4	0
12	AL	1453	1545	1540	4	0
13	AM	942	972	965	4	0
14	AN	868	933	928	1	0
15	AO	1592	1570	1557	4	0
16	AP	781	809	806	1	0
17	AQ	744	760	758	5	0
18	AR	2409	2436	2428	4	0
19	AS	1111	1117	1115	6	0
20	AT	1371	1396	1393	6	0
21	AU	1488	1505	1499	3	0
22	AV	2969	2972	2961	9	0
23	AW	789	806	802	2	0
24	AX	2849	2859	2843	18	0
25	AZ	839	862	858	2	0
26	A0	1787	1802	1796	7	0
27	A1	2245	2281	2276	14	0
28	A2	935	971	971	10	0
29	A3	625	702	699	6	0
30	Aw	1434	725	725	2	0
31	Ax	1482	750	752	8	0
32	Ay	1483	752	753	4	0
33	A	33070	16802	16798	244	0
34	B	1524	779	779	13	0
35	D	1859	1928	1920	6	0
36	E	2406	2424	2415	10	0
37	F	2031	2075	2065	10	0
38	I	1695	1794	1785	5	0
39	J	1330	1409	1407	4	0
40	K	1455	1460	1452	3	0
41	L	890	945	941	5	0
42	M	2314	2387	2384	10	0
43	N	1786	1824	1817	7	0
44	O	1259	1298	1294	8	0
45	P	1173	1171	1165	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Q	1979	2025	2022	11	0
47	R	1154	1220	1214	0	0
48	S	1293	1369	1365	9	0
49	T	1369	1417	1410	6	0
50	U	1251	1235	1232	8	0
51	V	1676	1691	1687	11	0
52	W	904	943	935	4	0
53	X	2044	2065	2060	4	0
54	Y	1556	1603	1597	2	0
55	Z	996	1052	1044	4	0
56	0	898	919	916	2	0
57	1	464	513	511	2	0
58	2	377	409	406	3	0
59	3	832	886	883	8	0
60	4	342	363	361	4	0
61	5	3210	3222	3206	6	0
62	6	2948	2854	2841	15	0
63	7	2390	2406	2397	11	0
64	8	1327	1371	1368	5	0
65	9	997	988	987	4	0
66	a	840	819	810	4	0
67	b	1196	1199	1195	9	0
68	c	2299	2325	2320	8	0
69	d	1985	1986	1976	9	0
70	e	1931	1922	1916	9	0
71	f	1252	1277	1269	6	0
72	g	1113	1101	1097	1	0
73	h	895	885	881	1	0
74	i	828	862	857	4	0
75	j	745	747	746	3	0
76	k	774	788	784	1	0
77	l	688	676	674	1	0
78	m	791	763	796	2	0
79	o	798	810	804	6	0
80	p	1205	1228	1223	4	0
81	q	1389	1377	1374	4	0
82	r	1322	1355	1348	10	0
83	s	3155	3151	3139	8	0
84	t	354	378	377	0	0
84	u	257	284	283	0	0
84	v	257	284	283	0	0
84	w	245	275	275	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	x	245	275	275	0	0
84	y	245	275	275	0	0
85	H	1661	1737	1734	12	0
86	z	2027	2080	2076	20	0
87	AY	1835	1787	1780	23	0
88	A5	4646	4690	4674	44	0
89	A4	4815	4828	4810	17	0
90	A6	603	594	588	3	0
91	Az	880	445	445	7	0
92	AA	44	26	26	0	0
93	AA	14	30	26	0	0
94	A	30	66	57	0	0
94	AA	10	22	19	0	0
95	A	136	0	0	0	0
95	A3	1	0	0	0	0
95	AA	62	0	0	0	0
95	AB	1	0	0	0	0
95	AX	1	0	0	0	0
95	Aw	1	0	0	0	0
95	D	2	0	0	0	0
95	E	1	0	0	0	0
95	g	1	0	0	0	0
96	A	28	0	0	0	0
96	AA	16	0	0	1	0
96	D	1	0	0	0	0
96	M	1	0	0	0	0
96	P	1	0	0	1	0
96	i	1	0	0	0	0
96	o	1	0	0	0	0
97	0	1	0	0	0	0
97	4	1	0	0	0	0
97	AO	1	0	0	0	0
98	AP	4	0	0	0	0
98	AT	4	0	0	0	0
98	r	4	0	0	0	0
99	AX	31	12	12	0	0
100	AX	28	12	12	0	0
101	A	6	14	12	0	0
102	B	7	11	8	1	0
103	0	27	0	0	0	0
103	1	2	0	0	0	0
103	2	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
103	3	43	0	0	2	0
103	4	11	0	0	1	0
103	5	15	0	0	1	0
103	6	69	0	0	6	0
103	7	11	0	0	2	0
103	8	14	0	0	3	0
103	9	16	0	0	0	0
103	A	2847	0	0	153	0
103	A0	2	0	0	0	0
103	A1	36	0	0	0	0
103	A2	26	0	0	3	0
103	A3	43	0	0	2	0
103	A4	7	0	0	2	0
103	AA	1747	0	0	87	0
103	AB	60	0	0	8	0
103	AC	48	0	0	4	0
103	AD	66	0	0	3	0
103	AE	20	0	0	1	0
103	AF	29	0	0	1	0
103	AG	53	0	0	2	0
103	AH	46	0	0	4	0
103	AI	30	0	0	4	0
103	AJ	14	0	0	3	0
103	AK	49	0	0	3	0
103	AL	42	0	0	2	0
103	AM	13	0	0	0	0
103	AN	29	0	0	0	0
103	AO	33	0	0	3	0
103	AP	23	0	0	1	0
103	AQ	52	0	0	4	0
103	AR	9	0	0	0	0
103	AS	18	0	0	2	0
103	AT	26	0	0	1	0
103	AU	4	0	0	0	0
103	AW	9	0	0	0	0
103	AX	44	0	0	3	0
103	AY	20	0	0	0	0
103	AZ	24	0	0	2	0
103	Aw	4	0	0	1	0
103	Ax	8	0	0	1	0
103	Ay	1	0	0	1	0
103	Az	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
103	B	55	0	0	8	0
103	D	68	0	0	0	0
103	E	57	0	0	3	0
103	F	74	0	0	5	0
103	H	7	0	0	1	0
103	I	21	0	0	2	0
103	K	68	0	0	1	0
103	L	27	0	0	3	0
103	M	46	0	0	4	0
103	N	50	0	0	3	0
103	O	34	0	0	2	0
103	P	69	0	0	5	0
103	Q	26	0	0	2	0
103	R	59	0	0	0	0
103	S	43	0	0	4	0
103	T	47	0	0	3	0
103	U	25	0	0	2	0
103	V	6	0	0	0	0
103	W	49	0	0	3	0
103	X	11	0	0	0	0
103	Y	23	0	0	1	0
103	Z	35	0	0	1	0
103	a	9	0	0	2	0
103	b	32	0	0	4	0
103	c	16	0	0	2	0
103	d	6	0	0	2	0
103	e	8	0	0	0	0
103	f	18	0	0	2	0
103	g	10	0	0	0	0
103	i	50	0	0	1	0
103	j	21	0	0	0	0
103	l	1	0	0	0	0
103	m	8	0	0	0	0
103	o	33	0	0	4	0
103	p	4	0	0	0	0
103	r	35	0	0	6	0
103	s	40	0	0	4	0
All	All	194797	160326	159801	879	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 3.

All (879) 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)
33:A:2317:G:OP2	103:A:3501:HOH:O	1.82	0.96
1:AA:1485:G:OP2	103:AA:1801:HOH:O	1.90	0.90
96:P:201:K:K	103:P:327:HOH:O	1.83	0.88
33:A:3047:G:N7	103:A:3564:HOH:O	2.08	0.86
30:Aw:76:A:O3'	33:A:3072:U:O4	1.93	0.86
71:f:106:TYR:OH	71:f:174:ILE:O	1.93	0.86
17:AQ:46:GLU:O	103:AQ:101:HOH:O	1.95	0.84
33:A:1914:A:OP2	103:A:3502:HOH:O	1.96	0.81
33:A:2685:U:OP1	103:A:3503:HOH:O	1.98	0.81
33:A:2035:U:OP2	103:A:3505:HOH:O	1.98	0.81
33:A:2724:G:O6	103:A:3504:HOH:O	1.98	0.81
1:AA:1574:G:OP1	103:AA:1803:HOH:O	1.99	0.81
33:A:3063:G:O2'	33:A:3066:C:OP2	1.98	0.81
49:T:165:TYR:O	103:T:301:HOH:O	1.98	0.81
33:A:2878:G:OP2	103:A:3509:HOH:O	1.99	0.81
82:r:35:PHE:N	82:r:56:THR:HG1	1.78	0.81
33:A:2515:U:O4	103:A:3508:HOH:O	1.99	0.80
31:Ax:75:C:O2	103:Ax:101:HOH:O	1.97	0.80
33:A:2668:A:OP2	103:A:3510:HOH:O	1.99	0.80
1:AA:1571:U:OP1	103:AA:1805:HOH:O	1.99	0.79
33:A:1908:A:OP2	103:A:3507:HOH:O	1.99	0.79
33:A:2740:A:N3	33:A:2921:A:O2'	2.15	0.79
49:T:160:ILE:O	103:T:302:HOH:O	1.99	0.79
1:AA:1288:G:N7	103:AA:1854:HOH:O	2.15	0.79
33:A:2104:A:N7	103:A:3616:HOH:O	2.16	0.79
33:A:1794:A:OP1	103:A:3515:HOH:O	2.01	0.79
33:A:1777:A:N6	33:A:1780:U:OP2	2.15	0.79
33:A:3042:U:OP2	103:A:3516:HOH:O	2.01	0.79
59:3:159:ASP:OD2	103:3:201:HOH:O	2.00	0.79
33:A:1975:U:O2	103:A:3512:HOH:O	2.00	0.78
33:A:2296:U:OP1	103:A:3511:HOH:O	2.00	0.78
8:AH:124:VAL:O	103:AH:301:HOH:O	2.00	0.78
33:A:1739:A:OP2	103:A:3506:HOH:O	1.99	0.78
16:AP:101:GLY:O	103:AP:301:HOH:O	2.01	0.78
1:AA:895:C:O2	103:AA:1806:HOH:O	2.00	0.78
2:AB:222:ILE:O	103:AB:401:HOH:O	2.00	0.78
33:A:3013:G:HO2'	60:4:66:PHE:N	1.81	0.78
1:AA:1130:G:N7	103:AA:1857:HOH:O	2.15	0.78
3:AC:84:GLU:OE2	103:AC:201:HOH:O	2.01	0.78
33:A:2985:C:OP1	103:A:3521:HOH:O	2.02	0.78
1:AA:1110:A:N7	103:AA:1860:HOH:O	2.16	0.77
1:AA:653:G:N3	103:AA:1863:HOH:O	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1358:A:O2'	31:Ax:30:G:OP1	2.02	0.77
33:A:1995:A:OP2	103:A:3519:HOH:O	2.02	0.77
1:AA:1097:G:N7	103:AA:1868:HOH:O	2.17	0.77
33:A:2470:G:O6	103:A:3522:HOH:O	2.03	0.77
34:B:42:G:OP2	103:B:201:HOH:O	2.01	0.77
36:E:49:TRP:O	103:E:502:HOH:O	2.03	0.77
36:E:193:LEU:O	103:E:501:HOH:O	2.03	0.77
1:AA:1576:G:OP2	103:AA:1809:HOH:O	2.03	0.77
33:A:2267:U:OP2	103:A:3517:HOH:O	2.01	0.77
33:A:3014:G:OP1	103:A:3520:HOH:O	2.02	0.77
1:AA:841:A:N3	103:AA:1871:HOH:O	2.18	0.77
103:AA:1803:HOH:O	29:A3:134:ARG:NH1	2.16	0.77
9:AI:189:ARG:NH1	103:AI:203:HOH:O	2.18	0.77
33:A:1825:A:OP2	103:A:3518:HOH:O	2.01	0.77
33:A:2076:C:OP2	103:A:3524:HOH:O	2.03	0.77
1:AA:895:C:N3	103:AA:1862:HOH:O	2.16	0.76
1:AA:1107:U:O4	29:A3:128:LYS:NZ	2.19	0.76
33:A:1835:A:OP1	103:A:3530:HOH:O	2.04	0.76
25:AZ:77:ASP:OD2	103:AZ:201:HOH:O	2.03	0.76
8:AH:127:TYR:O	103:AH:302:HOH:O	2.03	0.76
33:A:3152:C:OP1	46:Q:141:SER:OG	2.04	0.76
33:A:2718:C:O2	103:A:3532:HOH:O	2.04	0.76
62:6:367:ASP:OD1	62:6:370:ARG:NH1	2.19	0.76
33:A:2111:C:OP2	103:A:3529:HOH:O	2.03	0.76
33:A:3099:C:OP1	103:A:3535:HOH:O	2.04	0.76
1:AA:1443:U:OP2	103:AA:1814:HOH:O	2.04	0.76
9:AI:189:ARG:NH2	103:AI:204:HOH:O	2.19	0.76
33:A:2460:A:N7	103:A:3639:HOH:O	2.18	0.76
33:A:1867:A:OP1	103:A:3526:HOH:O	2.03	0.76
33:A:2149:G:OP1	103:A:3536:HOH:O	2.04	0.76
88:A5:309:ILE:HG23	88:A5:321:VAL:HG13	1.68	0.76
1:AA:1015:A:OP2	103:AA:1815:HOH:O	2.04	0.76
1:AA:1027:A:N1	103:AA:1874:HOH:O	2.19	0.75
1:AA:1084:C:OP1	103:AA:1811:HOH:O	2.03	0.75
45:P:176:GLN:O	103:P:301:HOH:O	2.05	0.75
34:B:32:C:O2	103:B:203:HOH:O	2.03	0.75
33:A:1849:C:OP2	103:A:3534:HOH:O	2.04	0.75
33:A:2017:U:OP1	103:A:3525:HOH:O	2.03	0.75
1:AA:1289:G:O2'	1:AA:1297:G:OP2	2.03	0.75
3:AC:93:ARG:O	103:AC:202:HOH:O	2.04	0.75
33:A:1923:C:OP2	103:A:3539:HOH:O	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:A:2728:C:OP2	103:A:3540:HOH:O	2.05	0.75
1:AA:1151:C:N3	103:AA:1876:HOH:O	2.20	0.75
34:B:43:G:N7	103:B:205:HOH:O	2.18	0.75
33:A:2477:G:OP1	103:A:3533:HOH:O	2.04	0.74
79:o:24:PRO:O	103:o:301:HOH:O	2.04	0.74
1:AA:764:A:N1	103:AA:1875:HOH:O	2.19	0.74
1:AA:1015:A:N7	103:AA:1872:HOH:O	2.18	0.74
33:A:2132:A:OP2	103:A:3528:HOH:O	2.03	0.74
62:6:52:ARG:O	103:6:401:HOH:O	2.04	0.74
1:AA:1152:A:OP2	103:AA:1810:HOH:O	2.03	0.74
33:A:2098:G:O2'	33:A:2099:U:OP2	2.04	0.74
1:AA:965:C:O2	103:AA:1818:HOH:O	2.06	0.74
54:Y:225:ASN:OD1	103:Y:301:HOH:O	2.05	0.74
33:A:1941:G:N7	103:A:3643:HOH:O	2.20	0.74
1:AA:779:U:O4	103:AA:1820:HOH:O	2.06	0.74
33:A:2910:A:N7	103:A:3650:HOH:O	2.21	0.74
42:M:132:LEU:O	103:M:401:HOH:O	2.03	0.74
52:W:49:ARG:O	103:W:201:HOH:O	2.04	0.74
33:A:1796:A:OP2	103:A:3527:HOH:O	2.03	0.74
33:A:2654:U:OP1	103:A:3542:HOH:O	2.06	0.74
2:AB:228:ASN:O	103:AB:402:HOH:O	2.04	0.74
33:A:1850:U:OP1	103:A:3546:HOH:O	2.06	0.74
33:A:1673:U:O4	103:A:3547:HOH:O	2.06	0.73
33:A:2621:G:N7	103:A:3646:HOH:O	2.20	0.73
33:A:2317:G:N7	103:A:3652:HOH:O	2.21	0.73
34:B:38:C:N3	103:B:203:HOH:O	2.20	0.73
82:r:160:LYS:O	103:r:301:HOH:O	2.06	0.73
62:6:225:LEU:O	103:6:402:HOH:O	2.05	0.73
79:o:48:TRP:O	103:o:302:HOH:O	2.06	0.73
33:A:2535:A:OP1	103:A:3549:HOH:O	2.06	0.73
33:A:3100:U:OP2	103:A:3537:HOH:O	2.04	0.73
1:AA:754:A:N3	103:AA:1882:HOH:O	2.22	0.73
1:AA:1434:A:OP1	103:AA:1823:HOH:O	2.06	0.73
1:AA:679:C:O2	103:AA:1821:HOH:O	2.06	0.72
4:AD:307:LYS:O	103:AD:501:HOH:O	2.08	0.72
33:A:2013:U:OP2	103:A:3545:HOH:O	2.06	0.72
33:A:2701:G:OP2	103:A:3557:HOH:O	2.07	0.72
33:A:2833:A:OP2	103:A:3552:HOH:O	2.07	0.72
64:8:126:GLN:OE1	103:8:301:HOH:O	2.08	0.72
45:P:102:VAL:O	103:P:302:HOH:O	2.06	0.72
51:V:55:TYR:HB2	51:V:133:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:211:ASP:OD2	103:AB:403:HOH:O	2.08	0.72
11:AK:102:ARG:NH2	103:AK:202:HOH:O	2.22	0.72
1:AA:1029:U:OP1	103:AA:1822:HOH:O	2.06	0.72
1:AA:1122:A:OP1	103:AA:1819:HOH:O	2.06	0.72
33:A:1943:A:N1	103:A:3668:HOH:O	2.23	0.72
33:A:2008:G:N7	103:A:3649:HOH:O	2.21	0.72
89:A4:67:LYS:O	103:A4:701:HOH:O	2.08	0.72
33:A:1674:A:OP2	103:A:3551:HOH:O	2.07	0.72
33:A:2654:U:OP2	103:A:3555:HOH:O	2.07	0.72
6:AF:176:ASP:OD2	6:AF:180:ARG:NH1	2.23	0.72
22:AV:226:TYR:HE1	22:AV:282:VAL:HG21	1.55	0.72
33:A:1990:G:OP1	35:D:269:ARG:NH2	2.22	0.72
33:A:1909:A:N7	103:A:3666:HOH:O	2.23	0.72
33:A:2196:A:O2'	33:A:2213:A:N1	2.22	0.72
33:A:2277:U:O4	103:A:3559:HOH:O	2.08	0.72
59:3:178:GLN:OE1	103:3:202:HOH:O	2.08	0.72
33:A:3147:G:OP1	103:A:3550:HOH:O	2.07	0.71
60:4:102:GLN:NE2	103:4:301:HOH:O	2.22	0.71
20:AT:132:ARG:NH1	20:AT:136:LEU:O	2.22	0.71
24:AX:392:GLU:OE2	103:AX:601:HOH:O	2.08	0.71
1:AA:847:G:OP2	103:AA:1827:HOH:O	2.07	0.71
33:A:1856:A:OP2	33:A:2986:C:O2'	2.08	0.71
33:A:1962:A:OP1	103:A:3556:HOH:O	2.07	0.71
33:A:2003:A:N1	103:A:3671:HOH:O	2.23	0.71
33:A:2045:A:N7	103:A:3659:HOH:O	2.22	0.71
33:A:3103:C:OP1	103:A:3565:HOH:O	2.08	0.71
53:X:44:ARG:NH2	85:H:84:GLU:OE1	2.23	0.71
33:A:2528:G:OP2	103:A:3558:HOH:O	2.08	0.71
43:N:238:LYS:O	103:N:301:HOH:O	2.08	0.71
67:b:129:GLN:O	103:b:302:HOH:O	2.09	0.71
1:AA:1066:C:OP2	103:AA:1829:HOH:O	2.08	0.71
33:A:1817:C:OP2	103:A:3570:HOH:O	2.09	0.70
67:b:26:LEU:O	103:b:301:HOH:O	2.09	0.70
1:AA:1598:G:N2	103:AA:1884:HOH:O	2.23	0.70
33:A:1844:A:OP2	103:A:3553:HOH:O	2.07	0.70
1:AA:1211:G:O6	103:AA:1832:HOH:O	2.08	0.70
3:AC:113:ARG:NH1	103:AC:204:HOH:O	2.24	0.70
34:B:38:C:OP1	62:6:52:ARG:NH1	2.24	0.70
2:AB:197:HIS:O	103:AB:404:HOH:O	2.08	0.70
50:U:52:ASP:OD2	103:U:201:HOH:O	2.07	0.70
33:A:2933:G:OP2	103:A:3568:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:51:VAL:O	103:AS:201:HOH:O	2.08	0.70
19:AS:36:ASP:O	103:AS:202:HOH:O	2.09	0.70
33:A:2664:U:OP2	103:A:3560:HOH:O	2.08	0.70
69:d:47:GLN:O	103:d:401:HOH:O	2.09	0.70
43:N:76:SER:O	103:N:302:HOH:O	2.09	0.70
66:a:114:LYS:O	103:a:201:HOH:O	2.08	0.70
82:r:84:ASP:O	103:r:302:HOH:O	2.09	0.70
83:s:65:ARG:O	103:s:501:HOH:O	2.09	0.70
2:AB:176:LEU:O	103:AB:405:HOH:O	2.09	0.70
34:B:26:A:OP2	103:B:204:HOH:O	2.10	0.69
1:AA:1069:A:OP2	103:AA:1833:HOH:O	2.09	0.69
43:N:234:ASP:OD1	103:N:303:HOH:O	2.10	0.69
88:A5:232:GLU:OE2	88:A5:236:SER:OG	2.10	0.69
1:AA:1118:A:O2'	4:AD:351:ARG:NH2	2.25	0.69
62:6:153:GLU:OE1	103:6:404:HOH:O	2.09	0.69
33:A:2305:U:O2	103:A:3563:HOH:O	2.08	0.69
1:AA:1317:A:N7	103:AA:1890:HOH:O	2.25	0.69
33:A:2497:U:OP2	103:A:3576:HOH:O	2.11	0.69
33:A:2953:U:O4	103:A:3579:HOH:O	2.11	0.69
33:A:3030:A:OP2	103:A:3577:HOH:O	2.11	0.69
42:M:43:ARG:NH2	103:M:407:HOH:O	2.26	0.69
1:AA:1227:G:N7	103:AA:1895:HOH:O	2.26	0.69
1:AA:1287:A:OP2	4:AD:260:LYS:NZ	2.25	0.69
33:A:2673:G:O6	103:A:3573:HOH:O	2.10	0.69
20:AT:108:LYS:O	103:AT:301:HOH:O	2.10	0.69
29:A3:131:LEU:O	103:A3:301:HOH:O	2.11	0.69
37:F:184:GLN:OE1	103:F:401:HOH:O	2.11	0.69
52:W:128:LYS:NZ	103:W:204:HOH:O	2.24	0.69
28:A2:5:SER:O	103:A2:201:HOH:O	2.10	0.68
2:AB:114:ASP:OD2	103:AB:406:HOH:O	2.10	0.68
1:AA:1554:G:OP2	103:AA:1835:HOH:O	2.11	0.68
82:r:172:VAL:O	103:r:303:HOH:O	2.10	0.68
1:AA:947:U:OP1	103:AA:1838:HOH:O	2.12	0.68
37:F:125:ARG:O	103:F:402:HOH:O	2.11	0.68
83:s:88:PHE:O	103:s:502:HOH:O	2.10	0.68
37:F:126:LYS:O	103:F:403:HOH:O	2.12	0.68
1:AA:1187:U:O4	103:AA:1825:HOH:O	2.07	0.68
33:A:2446:A:OP1	103:A:3575:HOH:O	2.10	0.68
33:A:2680:U:O4	103:A:3562:HOH:O	2.08	0.68
33:A:2868:C:OP2	103:A:3578:HOH:O	2.11	0.68
1:AA:1595:G:N7	103:AA:1902:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:117:PHE:O	103:AG:402:HOH:O	2.11	0.68
1:AA:840:A:N7	103:AA:1899:HOH:O	2.27	0.68
33:A:2873:A:N1	103:A:3690:HOH:O	2.27	0.68
33:A:2779:C:OP1	86:z:115:THR:OG1	2.11	0.68
36:E:69:ASP:OD1	36:E:154:ARG:NH1	2.27	0.68
1:AA:1222:A:N7	103:AA:1903:HOH:O	2.27	0.67
1:AA:1305:A:N7	103:AA:1901:HOH:O	2.27	0.67
46:Q:190:LEU:O	103:Q:301:HOH:O	2.10	0.67
33:A:2686:G:OP2	103:A:3587:HOH:O	2.12	0.67
41:L:91:MET:O	103:L:201:HOH:O	2.12	0.67
15:AO:135:PHE:O	103:AO:401:HOH:O	2.12	0.67
33:A:1778:U:O4	103:A:3566:HOH:O	2.08	0.67
1:AA:1479:C:OP1	103:AA:1839:HOH:O	2.12	0.67
33:A:3060:C:OP2	103:A:3585:HOH:O	2.12	0.67
1:AA:1448:U:O4'	103:AA:1836:HOH:O	2.11	0.67
1:AA:1572:A:OP2	103:AA:1842:HOH:O	2.13	0.67
33:A:1747:G:OP2	33:A:1749:C:N4	2.27	0.67
33:A:2531:U:O4	35:D:246:ARG:NH2	2.27	0.67
37:F:123:GLY:O	103:F:404:HOH:O	2.13	0.67
3:AC:152:ARG:NH1	89:A4:87:TYR:OH	2.28	0.67
33:A:2501:C:OP2	103:A:3588:HOH:O	2.13	0.67
33:A:2680:U:OP2	103:A:3590:HOH:O	2.13	0.67
33:A:3110:C:O2'	36:E:266:ARG:NH1	2.28	0.67
88:A5:630:LEU:HD22	88:A5:638:LEU:HB3	1.75	0.67
89:A4:134:GLU:OE2	103:A4:702:HOH:O	2.12	0.67
8:AH:94:PHE:CE1	27:A1:114:LEU:HD22	2.29	0.67
12:AL:172:ASN:OD1	103:AL:302:HOH:O	2.11	0.67
71:f:58:LYS:O	103:f:301:HOH:O	2.11	0.67
33:A:1906:G:O6	103:A:3586:HOH:O	2.12	0.67
63:7:175:ILE:O	63:7:319:ARG:NH2	2.27	0.67
4:AD:197:SER:OG	103:AD:502:HOH:O	2.11	0.67
71:f:104:GLU:OE1	103:f:302:HOH:O	2.12	0.67
46:Q:145:LEU:O	103:Q:302:HOH:O	2.12	0.66
75:j:45:GLU:OE2	75:j:70:ARG:NH2	2.28	0.66
1:AA:672:A:N7	103:AA:1898:HOH:O	2.27	0.66
1:AA:905:A:O2'	1:AA:907:A:OP1	2.14	0.66
48:S:161:ILE:O	103:S:302:HOH:O	2.14	0.66
63:7:139:ASN:OD1	103:7:401:HOH:O	2.12	0.66
1:AA:920:G:OP2	103:AA:1844:HOH:O	2.13	0.66
31:Ax:9:A:O2'	31:Ax:10:G:N7	2.27	0.66
33:A:2016:C:OP2	42:M:59:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:A:2656:U:OP1	103:A:3591:HOH:O	2.13	0.66
33:A:3077:C:OP1	103:A:3601:HOH:O	2.14	0.66
87:AY:225:ARG:NH2	88:A5:304:ASP:OD1	2.29	0.66
33:A:3015:U:OP1	103:A:3589:HOH:O	2.13	0.66
2:AB:173:GLY:O	103:AB:407:HOH:O	2.13	0.66
33:A:2533:A:OP2	103:A:3592:HOH:O	2.13	0.66
36:E:294:ASN:OD1	103:E:503:HOH:O	2.13	0.66
55:Z:74:SER:O	103:Z:201:HOH:O	2.14	0.66
1:AA:899:G:O2'	1:AA:907:A:N1	2.26	0.66
33:A:2002:G:OP1	69:d:38:LYS:NZ	2.21	0.66
33:A:2013:U:OP1	103:A:3598:HOH:O	2.13	0.66
82:r:170:ASN:O	103:r:304:HOH:O	2.14	0.66
33:A:1830:G:OP2	103:A:3605:HOH:O	2.14	0.65
33:A:2074:A:O3'	103:A:3600:HOH:O	2.14	0.65
33:A:3058:U:OP2	103:A:3606:HOH:O	2.14	0.65
34:B:37:A:N7	103:B:207:HOH:O	2.29	0.65
48:S:149:LEU:O	103:S:301:HOH:O	2.12	0.65
33:A:1932:G:N7	103:A:3711:HOH:O	2.29	0.65
40:K:116:LEU:O	103:K:201:HOH:O	2.14	0.65
28:A2:17:ARG:O	103:A2:202:HOH:O	2.13	0.65
1:AA:1422:G:N7	103:AA:1906:HOH:O	2.28	0.65
33:A:2614:U:OP2	103:A:3612:HOH:O	2.15	0.65
32:Ay:76:A:N1	103:Ay:101:HOH:O	2.28	0.65
42:M:33:SER:O	103:M:402:HOH:O	2.13	0.65
88:A5:192:ASN:O	88:A5:192:ASN:ND2	2.30	0.65
33:A:2103:A:HO2'	55:Z:35:LYS:N	1.94	0.65
33:A:2935:A:N1	103:A:3725:HOH:O	2.30	0.65
67:b:105:ALA:O	103:b:303:HOH:O	2.14	0.65
33:A:2388:A:OP2	103:A:3615:HOH:O	2.15	0.65
33:A:2767:A:O2'	33:A:2769:A:N7	2.29	0.65
33:A:1787:G:N2	33:A:1790:A:OP2	2.28	0.65
1:AA:1450:C:OP2	103:AA:1848:HOH:O	2.14	0.65
1:AA:1483:C:OP1	103:AA:1847:HOH:O	2.14	0.65
33:A:3145:A:N7	103:A:3719:HOH:O	2.29	0.65
52:W:93:GLU:OE2	103:W:202:HOH:O	2.15	0.65
1:AA:1154:A:OP2	29:A3:155:ARG:NH2	2.29	0.64
33:A:1869:A:OP1	103:A:3610:HOH:O	2.14	0.64
33:A:2297:A:H5'	103:A:5158:HOH:O	1.97	0.64
33:A:2941:G:O6	103:A:3599:HOH:O	2.14	0.64
49:T:94:ASP:OD1	103:T:303:HOH:O	2.14	0.64
33:A:1772:A:OP2	103:A:3608:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Z:78:ARG:O	55:Z:83:LYS:NZ	2.31	0.64
61:5:308:GLN:O	103:5:502:HOH:O	2.14	0.64
1:AA:700:A:N1	1:AA:709:G:O2'	2.30	0.64
22:AV:226:TYR:CE1	22:AV:282:VAL:HG21	2.33	0.64
48:S:102:ALA:O	48:S:103:SER:OG	2.14	0.64
1:AA:1160:A:N1	103:AA:1920:HOH:O	2.30	0.64
10:AJ:114:ARG:NH2	103:AJ:202:HOH:O	2.28	0.64
33:A:2142:A:N3	103:A:3721:HOH:O	2.29	0.64
15:AO:93:THR:O	103:AO:403:HOH:O	2.15	0.64
44:O:22:PRO:O	103:O:201:HOH:O	2.15	0.64
46:Q:77:SER:OG	46:Q:79:GLU:OE1	2.16	0.64
48:S:182:LYS:NZ	103:S:303:HOH:O	2.15	0.64
33:A:1775:A:OP2	103:A:3613:HOH:O	2.15	0.64
33:A:2511:C:OP2	103:A:3609:HOH:O	2.14	0.64
53:X:177:HIS:O	53:X:184:ARG:NH1	2.31	0.64
74:i:34:ILE:O	103:i:301:HOH:O	2.14	0.64
24:AX:119:TYR:OH	27:A1:273:GLU:OE2	2.11	0.63
33:A:2037:U:O4	103:A:3580:HOH:O	2.11	0.63
22:AV:270:PRO:O	22:AV:346:LYS:NZ	2.31	0.63
44:O:31:ASN:O	103:O:202:HOH:O	2.15	0.63
33:A:1848:U:OP2	103:A:3611:HOH:O	2.15	0.63
33:A:1848:U:O4	103:A:3583:HOH:O	2.11	0.63
33:A:2721:G:N7	103:A:3730:HOH:O	2.31	0.63
1:AA:1032:C:OP2	103:AA:1852:HOH:O	2.15	0.63
33:A:1749:C:OP2	33:A:2899:C:O2'	2.15	0.63
1:AA:1013:A:O2'	103:AA:1802:HOH:O	1.99	0.63
63:7:100:CYS:O	103:7:402:HOH:O	2.15	0.63
33:A:1998:U:O2	103:A:3595:HOH:O	2.13	0.63
64:8:132:GLU:OE2	71:f:109:TYR:OH	2.16	0.62
27:A1:152:ASP:OD2	27:A1:174:ARG:NH1	2.31	0.62
50:U:9:LEU:O	50:U:11:ARG:NH1	2.33	0.62
24:AX:167:ASP:OD1	103:AX:603:HOH:O	2.16	0.62
41:L:130:ARG:NH1	41:L:133:GLU:OE2	2.32	0.62
25:AZ:36:LEU:O	103:AZ:202:HOH:O	2.16	0.62
33:A:1970:G:O6	103:A:3584:HOH:O	2.11	0.62
1:AA:1170:G:O6	103:AA:1845:HOH:O	2.13	0.62
80:p:108:ALA:O	80:p:116:ARG:NH1	2.33	0.62
33:A:2822:C:OP1	103:A:3621:HOH:O	2.16	0.61
2:AB:140:GLY:O	103:AB:408:HOH:O	2.16	0.61
33:A:1906:G:OP1	103:A:3619:HOH:O	2.16	0.61
33:A:3040:OMG:OP1	103:A:3617:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1082:A:OP1	103:AA:1865:HOH:O	2.16	0.61
33:A:2562:U:O2'	35:D:284:ARG:O	2.14	0.61
68:c:80:GLN:O	68:c:210:ARG:NH2	2.33	0.61
74:i:57:TYR:OH	81:q:28:ARG:O	2.15	0.61
1:AA:1156:C:OP1	103:AA:1864:HOH:O	2.16	0.61
33:A:2030:U:H3	33:A:2095:U:HO2'	1.46	0.61
17:AQ:51:ARG:NH1	103:AQ:103:HOH:O	2.33	0.61
33:A:1849:C:N4	103:A:3583:HOH:O	2.32	0.61
33:A:2030:U:N3	33:A:2095:U:O2'	2.33	0.61
33:A:2281:A:O2'	103:A:3544:HOH:O	2.06	0.61
33:A:2697:G:O6	103:A:3614:HOH:O	2.15	0.61
86:z:139:PRO:CB	86:z:245:VAL:HG21	2.31	0.61
1:AA:1098:C:OP2	103:AA:1858:HOH:O	2.16	0.61
38:I:29:GLY:N	103:I:302:HOH:O	2.32	0.61
85:H:178:ASN:OD1	85:H:179:ASN:N	2.34	0.61
88:A5:252:GLU:OE2	88:A5:277:TYR:OH	2.19	0.61
33:A:1805:A:OP2	51:V:94:HIS:NE2	2.31	0.60
17:AQ:57:TYR:OH	103:AQ:102:HOH:O	2.09	0.60
33:A:1737:A:H61	33:A:1760:G:H1'	1.65	0.60
24:AX:171:SER:OG	103:AX:602:HOH:O	2.08	0.60
1:AA:1104:A:OP2	103:AA:1859:HOH:O	2.16	0.60
45:P:159:LYS:O	103:P:304:HOH:O	2.15	0.60
1:AA:1019:A:N3	103:AA:1921:HOH:O	2.30	0.60
1:AA:1169:G:O6	103:AA:1861:HOH:O	2.16	0.60
33:A:2372:U:OP2	103:A:3624:HOH:O	2.16	0.60
42:M:179:TYR:O	103:M:403:HOH:O	2.16	0.60
32:Ay:75:C:O2'	32:Ay:76:A:OP1	2.19	0.59
33:A:1979:U:OP2	103:A:3623:HOH:O	2.16	0.59
1:AA:1134:G:OP2	10:AJ:38:ARG:NH2	2.34	0.59
36:E:330:GLU:OE2	46:Q:97:LYS:NZ	2.36	0.59
1:AA:992:U:O2'	1:AA:994:A:OP2	2.11	0.59
69:d:84:ILE:CD1	69:d:265:ILE:HD11	2.32	0.59
89:A4:200:ASP:OD2	89:A4:243:ASN:N	2.34	0.59
89:A4:306:ASN:ND2	91:Az:33:U:O5'	2.36	0.59
1:AA:709:G:OP1	13:AM:13:ARG:NH2	2.35	0.59
15:AO:80:ASN:ND2	103:AO:404:HOH:O	2.34	0.59
3:AC:109:VAL:HG23	27:A1:103:LEU:HD11	1.84	0.59
66:a:119:THR:OG1	103:a:202:HOH:O	2.17	0.59
33:A:2146:A:OP2	103:A:3626:HOH:O	2.17	0.59
34:B:76:A:O3'	102:B:101:VAL:HG12	2.02	0.59
45:P:67:GLY:O	103:P:305:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:A:2566:C:OP2	103:A:3620:HOH:O	2.16	0.59
42:M:91:ARG:NH1	42:M:209:GLU:OE2	2.36	0.58
1:AA:1401:G:OP2	103:AA:1867:HOH:O	2.17	0.58
33:A:1745:U:O4	59:3:108:LYS:NZ	2.36	0.58
64:8:133:ARG:NH1	103:8:304:HOH:O	2.35	0.58
80:p:111:ILE:O	80:p:116:ARG:NH1	2.36	0.58
7:AG:226:GLU:O	7:AG:230:THR:HG23	2.03	0.58
88:A5:321:VAL:HG11	88:A5:353:VAL:HG13	1.84	0.58
1:AA:1272:A:N6	103:AA:1923:HOH:O	2.31	0.58
70:e:108:GLU:O	70:e:110:ASP:N	2.36	0.58
20:AT:91:GLU:OE1	21:AU:120:ARG:NH2	2.35	0.58
33:A:2266:U:OP2	103:A:3627:HOH:O	2.17	0.58
1:AA:1412:G:OP1	24:AX:279:LYS:NZ	2.35	0.58
1:AA:1294:A:OP1	2:AB:201:ASN:ND2	2.38	0.57
33:A:2878:G:N7	103:A:3743:HOH:O	2.32	0.57
61:5:377:ASP:OD2	61:5:413:LYS:NZ	2.30	0.57
7:AG:356:VAL:HG23	7:AG:361:VAL:HG23	1.86	0.57
33:A:2429:A:OP1	103:A:3629:HOH:O	2.18	0.57
54:Y:134:LYS:NZ	65:9:76:TYR:OH	2.33	0.57
24:AX:272:THR:OG1	24:AX:282:ILE:O	2.22	0.57
62:6:170:ARG:NH1	103:6:406:HOH:O	2.33	0.57
87:AY:250:ILE:O	89:A4:358:ARG:NE	2.37	0.57
87:AY:335:GLU:OE1	87:AY:348:ARG:NH2	2.37	0.57
75:j:53:ASP:OD1	75:j:54:GLY:N	2.37	0.57
1:AA:1249:U:O4	103:AA:1851:HOH:O	2.15	0.57
56:0:153:THR:HG22	56:0:153:THR:O	2.05	0.57
33:A:1768:G:OP1	74:i:50:LYS:NZ	2.38	0.56
1:AA:1088:C:O2'	103:AA:1824:HOH:O	2.07	0.56
9:AI:61:SER:O	103:AI:202:HOH:O	2.17	0.56
33:A:2276:C:OP2	103:A:3631:HOH:O	2.18	0.56
49:T:198:ARG:NH2	68:c:287:GLU:OE1	2.38	0.56
59:3:188:VAL:O	62:6:356:ARG:NH2	2.38	0.56
7:AG:312:GLN:OE1	7:AG:345:ARG:NH1	2.39	0.56
1:AA:1146:C:O2'	103:AA:1837:HOH:O	2.12	0.56
4:AD:312:TYR:N	4:AD:331:ASP:OD2	2.37	0.56
33:A:2897:A:OP2	103:A:3625:HOH:O	2.17	0.56
33:A:3059:A:N6	103:A:3692:HOH:O	2.27	0.56
33:A:2259:C:O2'	33:A:2261:C:OP2	2.23	0.56
33:A:2274:A:N6	103:A:3819:HOH:O	2.39	0.56
96:AA:1772:K:K	103:AA:2450:HOH:O	0.49	0.55
7:AG:295:VAL:HG22	7:AG:330:CYS:SG	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:A:2104:A:OP1	43:N:231:SER:OG	2.20	0.55
44:O:62:TYR:OH	46:Q:272:GLU:OE2	2.22	0.55
53:X:87:LEU:O	85:H:78:ARG:NH1	2.38	0.55
88:A5:484:CYS:SG	88:A5:485:PHE:N	2.79	0.55
33:A:1973:G:OP1	103:A:3628:HOH:O	2.17	0.55
71:f:78:ARG:NH2	71:f:122:GLU:OE1	2.39	0.55
1:AA:1044:U:OP1	1:AA:1110:A:O2'	2.22	0.55
51:V:188:VAL:O	51:V:188:VAL:HG23	2.07	0.55
86:z:61:THR:HG22	86:z:131:LEU:CD2	2.36	0.55
87:AY:182:GLN:HB3	88:A5:182:THR:HG22	1.89	0.55
45:P:156:ASP:OD2	62:6:126:ARG:NH1	2.40	0.55
1:AA:850:U:O2'	103:AA:1812:HOH:O	2.03	0.55
19:AS:83:ARG:NH1	19:AS:93:LYS:O	2.39	0.55
28:A2:64:ASP:OD1	28:A2:65:ALA:N	2.39	0.55
33:A:3084:A:N1	103:A:3756:HOH:O	2.33	0.55
63:7:62:THR:HG23	63:7:62:THR:O	2.07	0.55
87:AY:208:MET:O	88:A5:224:LYS:NZ	2.39	0.55
3:AC:112:ARG:NH1	103:AC:207:HOH:O	2.39	0.55
33:A:2276:C:OP1	74:i:42:LYS:NZ	2.39	0.55
85:H:53:THR:N	85:H:86:THR:HG1	2.05	0.55
33:A:2342:U:O4	103:A:3622:HOH:O	2.16	0.54
33:A:2826:G:OP1	52:W:49:ARG:NH1	2.39	0.54
1:AA:948:U:O2'	103:AA:1866:HOH:O	2.17	0.54
33:A:1953:A:O2'	33:A:2463:A:OP1	2.25	0.54
103:AA:1919:HOH:O	7:AG:384:GLN:NE2	2.40	0.54
19:AS:7:GLU:N	19:AS:7:GLU:OE1	2.40	0.54
88:A5:400:VAL:HG12	88:A5:400:VAL:O	2.08	0.54
22:AV:92:LEU:HD21	22:AV:137:ILE:HD11	1.90	0.54
33:A:2661:U:OP2	103:A:3638:HOH:O	2.18	0.54
33:A:2725:A:OP2	103:A:3637:HOH:O	2.18	0.54
86:z:230:ILE:N	86:z:231:PRO:HD2	2.23	0.54
37:F:70:ARG:NH2	37:F:194:GLU:OE1	2.41	0.54
86:z:127:LEU:O	86:z:129:MET:N	2.41	0.54
33:A:1800:G:N1	33:A:1803:A:OP2	2.41	0.53
86:z:139:PRO:HB2	86:z:245:VAL:HG21	1.90	0.53
87:AY:182:GLN:NE2	88:A5:185:LEU:HD13	2.24	0.53
33:A:2065:A:O2'	33:A:2066:C:OP2	2.20	0.53
63:7:106:ALA:O	63:7:113:TRP:N	2.40	0.53
64:8:119:LYS:O	103:8:302:HOH:O	2.19	0.53
17:AQ:51:ARG:NE	103:AQ:105:HOH:O	2.41	0.53
86:z:130:ALA:O	86:z:282:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:AY:244:LEU:HD13	89:A4:391:PHE:CD2	2.43	0.53
15:AO:217:ARG:NH1	15:AO:227:GLU:OE2	2.41	0.53
36:E:129:VAL:HG11	36:E:145:LEU:HD11	1.89	0.53
37:F:137:ARG:NH1	103:F:408:HOH:O	2.38	0.53
1:AA:769:G:N2	1:AA:772:A:OP2	2.40	0.53
11:AK:83:CYS:O	103:AK:201:HOH:O	2.19	0.53
33:A:2458:A:O2'	36:E:215:PHE:O	2.22	0.53
35:D:281:TRP:O	35:D:285:LYS:NZ	2.41	0.53
87:AY:225:ARG:NH1	87:AY:229:ASP:OD2	2.41	0.53
50:U:11:ARG:NH2	51:V:211:LYS:O	2.41	0.53
67:b:21:ARG:NH1	68:c:79:LEU:O	2.41	0.53
1:AA:1021:U:OP2	28:A2:9:ARG:NH2	2.42	0.53
44:O:64:LYS:NZ	44:O:100:GLN:O	2.42	0.53
64:8:99:ARG:NH1	70:e:84:TYR:O	2.42	0.53
7:AG:320:VAL:HG21	7:AG:352:LEU:HD21	1.90	0.53
33:A:2236:C:OP2	103:A:3641:HOH:O	2.19	0.52
65:9:16:ASP:OD1	65:9:25:ARG:NH2	2.42	0.52
85:H:146:LEU:O	85:H:150:GLY:N	2.41	0.52
87:AY:214:ALA:O	87:AY:217:ARG:N	2.39	0.52
33:A:1793:G:OP2	103:A:3640:HOH:O	2.19	0.52
33:A:2364:C:OP2	50:U:78:LYS:NZ	2.42	0.52
48:S:109:THR:HG22	48:S:112:ASP:OD2	2.09	0.52
31:Ax:34:U:H3	91:Az:6:G:H1	1.56	0.52
33:A:2160:A:OP2	60:4:88:TRP:NE1	2.37	0.52
33:A:3068:G:OP2	33:A:3068:G:N2	2.42	0.52
4:AD:245:VAL:HG22	4:AD:271:ALA:HB1	1.91	0.52
6:AF:240:ARG:NH2	6:AF:242:TRP:OXT	2.42	0.52
24:AX:183:GLU:N	24:AX:183:GLU:OE1	2.40	0.52
33:A:2777:G:N3	85:H:179:ASN:ND2	2.58	0.52
87:AY:232:TYR:O	87:AY:234:ASN:N	2.42	0.52
29:A3:151:ARG:NE	103:A3:303:HOH:O	2.27	0.52
85:H:193:PHE:O	85:H:198:GLY:N	2.43	0.52
1:AA:763:C:N4	103:AA:1986:HOH:O	2.42	0.52
87:AY:192:ARG:O	87:AY:194:ALA:N	2.43	0.52
88:A5:309:ILE:HG21	88:A5:357:ILE:HD11	1.92	0.52
33:A:2861:A:OP2	103:A:3633:HOH:O	2.18	0.52
33:A:2932:G:OP2	103:A:3636:HOH:O	2.18	0.52
62:6:215:THR:OG1	62:6:275:GLN:OE1	2.27	0.52
86:z:139:PRO:HB3	86:z:245:VAL:HG21	1.92	0.52
31:Ax:46:A:O2'	31:Ax:48:U:O4'	2.28	0.52
38:I:35:ARG:O	103:I:301:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:z:239:ASN:OD1	86:z:240:GLY:N	2.42	0.52
1:AA:1228:A:N7	103:AA:1944:HOH:O	2.34	0.51
1:AA:1293:C:N4	17:AQ:80:ARG:O	2.43	0.51
32:Ay:75:C:HO2'	32:Ay:76:A:P	2.33	0.51
1:AA:702:C:OP1	1:AA:848:U:O2'	2.28	0.51
1:AA:818:C:OP2	103:AA:1870:HOH:O	2.18	0.51
1:AA:1598:G:O2'	28:A2:37:ARG:NH2	2.43	0.51
18:AR:162:SER:O	18:AR:170:ARG:NH1	2.41	0.51
33:A:2454:G:N7	103:A:3763:HOH:O	2.34	0.51
33:A:2987:U:O2'	33:A:2991:U:OP1	2.28	0.51
51:V:133:ILE:HD12	51:V:145:ARG:HB3	1.93	0.51
32:Ay:75:C:O2'	32:Ay:76:A:P	2.69	0.51
88:A5:482:ILE:HB	88:A5:483:PRO:HD3	1.93	0.51
8:AH:117:ARG:NH1	103:AH:304:HOH:O	2.38	0.51
24:AX:153:LEU:HD21	24:AX:244:LEU:CD2	2.40	0.51
37:F:212:TRP:O	37:F:258:THR:OG1	2.13	0.51
7:AG:299:ASP:OD2	7:AG:301:GLN:NE2	2.44	0.51
11:AK:56:SER:O	11:AK:60:ASN:ND2	2.44	0.51
1:AA:843:G:N2	1:AA:846:A:OP2	2.40	0.51
1:AA:1039:A:OP1	103:AA:1873:HOH:O	2.19	0.51
1:AA:1229:U:O2'	1:AA:1442:G:O4'	2.28	0.51
1:AA:947:U:OP1	12:AL:162:GLN:NE2	2.44	0.51
24:AX:151:LEU:CD2	24:AX:247:LEU:HD22	2.41	0.51
34:B:20:A:OP1	103:B:206:HOH:O	2.19	0.51
48:S:112:ASP:OD1	67:b:121:THR:OG1	2.24	0.51
1:AA:1583:MA6:N6	1:AA:1584:MA6:H103	2.26	0.50
27:A1:304:GLU:OE2	27:A1:309:ILE:HD11	2.11	0.50
28:A2:48:GLU:OE1	28:A2:48:GLU:N	2.39	0.50
1:AA:1151:C:OP2	12:AL:201:ARG:NH1	2.37	0.50
30:Aw:76:A:OP1	103:Aw:201:HOH:O	2.20	0.50
33:A:2512:A:O2'	33:A:2541:C:OP1	2.23	0.50
80:p:84:SER:OG	80:p:96:ASN:O	2.29	0.50
39:J:25:ARG:NH1	77:l:58:ASP:OD1	2.41	0.50
33:A:3190:A:OP2	82:r:120:LYS:NZ	2.44	0.50
88:A5:331:GLU:HG2	88:A5:332:ARG:H	1.75	0.50
38:I:148:VAL:HG23	38:I:148:VAL:O	2.11	0.50
1:AA:1490:U:O2'	103:AA:1804:HOH:O	1.99	0.50
33:A:1792:G:N7	58:2:87:ARG:NH2	2.50	0.50
36:E:129:VAL:CG1	36:E:145:LEU:HD11	2.41	0.50
33:A:3018:A:N3	33:A:3126:C:O2'	2.42	0.49
50:U:47:GLU:OE1	50:U:47:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:AY:202:SER:HB3	87:AY:205:ILE:HD13	1.93	0.49
4:AD:112:LYS:NZ	4:AD:235:GLU:O	2.45	0.49
33:A:2301:U:O2'	103:A:3635:HOH:O	2.18	0.49
33:A:2546:G:N7	103:A:3775:HOH:O	2.35	0.49
6:AF:174:LEU:O	6:AF:179:ARG:NH1	2.45	0.49
6:AF:242:TRP:O	28:A2:84:ARG:NH2	2.45	0.49
33:A:1882:A:N7	103:A:3769:HOH:O	2.35	0.49
50:U:71:ARG:NH2	103:U:202:HOH:O	2.34	0.49
88:A5:474:GLN:HB2	88:A5:506:MET:HE3	1.93	0.49
87:AY:244:LEU:HD13	89:A4:391:PHE:HD2	1.76	0.49
33:A:1822:U:O2	33:A:2707:A:O2'	2.29	0.49
33:A:1867:A:N1	33:A:2019:G:O2'	2.39	0.49
41:L:95:ARG:NH2	103:L:203:HOH:O	2.39	0.49
86:z:262:MET:SD	86:z:270:ASN:ND2	2.86	0.49
10:AJ:78:ARG:NH2	10:AJ:117:ASP:OD2	2.44	0.49
33:A:2535:A:N7	103:A:3768:HOH:O	2.34	0.49
33:A:2651:A:OP2	103:A:3644:HOH:O	2.20	0.48
33:A:3201:A:H2'	33:A:3202:U:O4'	2.13	0.48
63:7:87:THR:O	63:7:90:SER:OG	2.28	0.48
71:f:147:ASP:OD1	78:m:72:ARG:NH2	2.43	0.48
5:AE:50:ARG:NH2	103:AE:201:HOH:O	2.45	0.48
41:L:97:THR:O	103:L:202:HOH:O	2.20	0.48
1:AA:1119:U:OP2	19:AS:50:ARG:NH2	2.46	0.48
39:J:75:ASP:OD1	39:J:77:THR:HG22	2.13	0.48
33:A:2315:A:N6	103:A:3928:HOH:O	2.46	0.48
48:S:109:THR:N	48:S:112:ASP:OD2	2.46	0.48
69:d:89:VAL:HG23	69:d:89:VAL:O	2.13	0.48
26:A0:37:ASP:O	26:A0:41:LEU:N	2.46	0.48
88:A5:407:LEU:HD21	88:A5:429:ALA:HB3	1.94	0.48
1:AA:1372:C:OP2	103:AA:1877:HOH:O	2.20	0.48
33:A:2695:G:O6	103:A:3642:HOH:O	2.19	0.48
43:N:59:VAL:O	43:N:59:VAL:HG13	2.13	0.48
67:b:41:ARG:NE	103:b:308:HOH:O	2.47	0.48
1:AA:1271:C:OP2	103:AA:1878:HOH:O	2.20	0.48
3:AC:106:ASP:OD1	3:AC:107:GLN:N	2.42	0.48
89:A4:372:TYR:CE2	89:A4:400:LEU:HD21	2.48	0.48
33:A:3089:A:H3'	33:A:3090:G:C5'	2.44	0.48
1:AA:841:A:OP1	13:AM:39:ASN:ND2	2.43	0.48
14:AN:93:ASP:O	14:AN:97:GLY:N	2.43	0.48
68:c:263:GLY:N	103:c:402:HOH:O	2.35	0.48
1:AA:845:A:H4'	21:AU:60:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A2:15:ASN:OD1	28:A2:17:ARG:NH1	2.47	0.48
39:J:50:CYS:O	39:J:54:ASN:ND2	2.46	0.48
82:r:184:ASN:OD1	103:r:305:HOH:O	2.20	0.48
88:A5:305:LEU:HD23	88:A5:328:VAL:HG22	1.96	0.48
88:A5:349:LYS:O	88:A5:349:LYS:HG2	2.14	0.48
7:AG:102:GLU:OE1	7:AG:102:GLU:N	2.44	0.47
9:AI:125:GLY:N	103:AI:206:HOH:O	2.40	0.47
26:A0:13:GLU:OE2	26:A0:16:ARG:NH1	2.47	0.47
86:z:127:LEU:HD22	86:z:290:VAL:HG22	1.96	0.47
89:A4:632:GLU:O	89:A4:635:SER:OG	2.28	0.47
1:AA:1581:G:OP2	103:AA:1879:HOH:O	2.20	0.47
4:AD:340:ILE:HG22	4:AD:340:ILE:O	2.14	0.47
88:A5:309:ILE:HG23	88:A5:321:VAL:CG1	2.42	0.47
33:A:2449:G:OP2	83:s:225:ARG:NH2	2.45	0.47
33:A:2909:G:OP1	57:1:63:ARG:NH1	2.43	0.47
87:AY:204:ILE:O	87:AY:208:MET:N	2.46	0.47
88:A5:192:ASN:O	88:A5:192:ASN:CG	2.57	0.47
34:B:44:A:H2'	34:B:45:G:O4'	2.15	0.47
88:A5:397:LEU:HD23	88:A5:402:MET:HE3	1.96	0.47
34:B:32:C:N4	103:B:210:HOH:O	2.45	0.47
88:A5:368:GLY:O	88:A5:370:SER:N	2.45	0.47
88:A5:570:TYR:O	88:A5:572:GLN:N	2.47	0.47
3:AC:84:GLU:OE1	3:AC:84:GLU:N	2.45	0.47
7:AG:299:ASP:OD1	7:AG:300:TYR:N	2.47	0.47
36:E:111:THR:OG1	36:E:113:ASP:OD1	2.25	0.47
69:d:81:THR:HG22	69:d:82:ALA:N	2.30	0.47
82:r:154:TRP:NE1	103:r:307:HOH:O	2.43	0.47
1:AA:825:U:O2'	103:AA:1807:HOH:O	2.02	0.47
62:6:188:TYR:OH	103:6:403:HOH:O	2.07	0.47
62:6:252:CYS:SG	62:6:296:ARG:NH1	2.88	0.47
70:e:55:ARG:NH2	70:e:155:ARG:O	2.48	0.47
88:A5:420:THR:OG1	88:A5:449:ARG:NH2	2.48	0.47
5:AE:17:GLU:OE1	5:AE:17:GLU:N	2.47	0.47
33:A:1969:G:N7	103:A:3785:HOH:O	2.36	0.47
76:k:10:LEU:O	76:k:46:ASN:ND2	2.46	0.47
31:Ax:8:U:O2'	31:Ax:46:A:N3	2.45	0.47
33:A:2883:A:N3	33:A:2883:A:H2'	2.29	0.47
53:X:91:TYR:CE2	85:H:79:VAL:HG11	2.50	0.47
89:A4:501:ASP:OD1	89:A4:537:ARG:NH2	2.47	0.47
24:AX:81:HIS:CD2	24:AX:190:ASN:HB3	2.50	0.46
33:A:3004:C:O2'	103:A:3618:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:6:257:PRO:HB3	62:6:268:LEU:HD21	1.97	0.46
88:A5:529:LYS:NZ	88:A5:563:LEU:O	2.48	0.46
24:AX:208:TYR:OH	24:AX:246:GLU:OE2	2.28	0.46
46:Q:72:GLU:N	46:Q:72:GLU:OE1	2.48	0.46
6:AF:35:SER:N	103:AF:303:HOH:O	2.46	0.46
33:A:2135:A:N3	33:A:2135:A:H2'	2.31	0.46
33:A:2261:C:O2'	48:S:184:ARG:NH1	2.46	0.46
86:z:133:LYS:HG2	86:z:134:LYS:N	2.31	0.46
4:AD:264:ARG:NH1	91:Az:13:U:O2	2.49	0.46
26:A0:63:ARG:NH2	26:A0:110:ASP:OD2	2.48	0.46
33:A:1828:A:O2'	33:A:2684:C:N3	2.38	0.46
34:B:38:C:OP1	62:6:56:ARG:NH2	2.48	0.46
3:AC:109:VAL:CG2	27:A1:103:LEU:HD11	2.46	0.46
24:AX:153:LEU:HD21	24:AX:244:LEU:HD22	1.97	0.46
33:A:2810:G:OP2	103:A:3648:HOH:O	2.21	0.46
67:b:48:GLU:OE2	79:o:101:TRP:NE1	2.43	0.46
88:A5:69:GLN:O	88:A5:69:GLN:HG2	2.16	0.46
1:AA:1484:C:O2'	103:AA:1808:HOH:O	2.02	0.46
43:N:73:ARG:O	43:N:155:LYS:NZ	2.49	0.46
1:AA:878:G:O2'	103:AA:1816:HOH:O	2.05	0.46
69:d:84:ILE:HD13	69:d:265:ILE:HD11	1.98	0.46
88:A5:88:MET:HE3	88:A5:88:MET:HA	1.98	0.46
1:AA:1279:C:O2'	1:AA:1296:A:N1	2.40	0.46
38:I:45:GLN:NE2	79:o:25:ARG:O	2.44	0.46
87:AY:209:LYS:HG3	87:AY:210:VAL:HG23	1.97	0.46
33:A:3211:C:HO2'	33:A:3212:C:H5	1.60	0.46
7:AG:200:LEU:HD11	7:AG:204:GLU:HB3	1.98	0.46
88:A5:309:ILE:HD11	88:A5:324:ILE:HG22	1.98	0.46
33:A:2353:A:O2'	33:A:2355:A:OP2	2.27	0.45
85:H:223:VAL:N	85:H:231:VAL:O	2.45	0.45
1:AA:1004:G:O2'	9:AI:98:GLN:NE2	2.49	0.45
33:A:3089:A:H3'	33:A:3090:G:H5''	1.99	0.45
79:o:22:ARG:NH2	103:o:304:HOH:O	2.38	0.45
87:AY:210:VAL:HG12	87:AY:212:ARG:H	1.81	0.45
1:AA:746:A:N6	103:AA:1990:HOH:O	2.49	0.45
19:AS:106:LEU:HB2	19:AS:117:LEU:HD11	1.98	0.45
33:A:1735:A:H2'	33:A:1735:A:N3	2.31	0.45
33:A:2388:A:O2'	103:A:3531:HOH:O	2.04	0.45
33:A:2454:G:OP1	44:O:48:ARG:NH2	2.49	0.45
63:7:156:ARG:HG3	63:7:156:ARG:HH11	1.80	0.45
72:g:154:ASP:OD1	72:g:154:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:706:C:OP1	26:A0:43:ARG:NE	2.49	0.45
1:AA:783:A:N6	103:AA:1976:HOH:O	2.40	0.45
33:A:2757:A:N1	33:A:2789:C:O2'	2.46	0.45
68:c:267:LEU:N	68:c:268:PRO:HD3	2.32	0.45
86:z:133:LYS:HG2	86:z:134:LYS:H	1.81	0.45
88:A5:309:ILE:CG2	88:A5:321:VAL:HG13	2.44	0.45
7:AG:301:GLN:OE1	24:AX:385:ASN:ND2	2.46	0.45
18:AR:317:ALA:O	18:AR:321:ALA:N	2.49	0.45
42:M:250:ASP:OD1	42:M:251:GLU:N	2.50	0.45
1:AA:812:A:O2'	1:AA:814:A:N1	2.49	0.45
27:A1:166:PRO:O	27:A1:169:ARG:NH1	2.50	0.45
44:O:140:SER:O	44:O:146:ASN:ND2	2.45	0.45
70:e:55:ARG:NH1	70:e:149:LEU:O	2.48	0.45
81:q:168:VAL:HG12	81:q:168:VAL:O	2.17	0.45
88:A5:438:ARG:NH1	90:A6:34:GLN:OE1	2.50	0.45
48:S:130:LEU:O	103:S:304:HOH:O	2.21	0.45
63:7:276:PHE:HB2	63:7:304:VAL:HG22	1.97	0.45
68:c:161:THR:O	68:c:192:GLN:NE2	2.49	0.45
87:AY:244:LEU:HD12	87:AY:245:LYS:H	1.81	0.45
33:A:1752:U:OP1	59:3:94:LEU:N	2.50	0.45
33:A:2928:C:OP2	69:d:37:THR:N	2.50	0.45
7:AG:377:ARG:NH2	103:AG:405:HOH:O	2.43	0.44
12:AL:189:TYR:OH	103:AL:301:HOH:O	2.09	0.44
34:B:12:U:O2'	34:B:14:A:OP1	2.34	0.44
1:AA:706:C:O2	26:A0:210:LYS:NZ	2.46	0.44
10:AJ:43:LYS:N	103:AJ:205:HOH:O	2.49	0.44
22:AV:225:LEU:HD11	22:AV:283:LEU:HD22	1.98	0.44
24:AX:123:ARG:NH2	24:AX:337:LEU:O	2.50	0.44
33:A:2355:A:HO2'	33:A:2673:G:HO2'	1.54	0.44
51:V:169:THR:HG22	51:V:169:THR:O	2.16	0.44
33:A:2499:U:OP2	33:A:2504:A:N6	2.40	0.44
33:A:3219:G:O2'	33:A:3221:A:OP2	2.27	0.44
1:AA:1080:A:O2'	1:AA:1082:A:N7	2.43	0.44
18:AR:162:SER:HB2	18:AR:165:ILE:HD12	2.00	0.44
22:AV:52:ASP:OD1	46:Q:66:HIS:ND1	2.50	0.44
33:A:3039:OMU:OP2	103:A:3647:HOH:O	2.21	0.44
51:V:54:TRP:NE1	51:V:56:LEU:O	2.50	0.44
61:5:173:ARG:HA	61:5:176:TYR:CE2	2.53	0.44
62:6:207:GLU:O	103:6:405:HOH:O	2.21	0.44
33:A:1916:G:OP1	58:2:64:HIS:ND1	2.47	0.44
80:p:113:GLU:OE1	80:p:116:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:A:2595:A:H2'	33:A:2596:G:O4'	2.18	0.44
5:AE:67:ASP:OD2	5:AE:96:HIS:NE2	2.51	0.44
27:A1:198:TYR:OH	27:A1:203:ASP:OD1	2.21	0.44
83:s:174:LEU:HB3	83:s:175:PRO:HD3	1.99	0.44
91:Az:32:A:H5'	91:Az:33:U:H4'	1.98	0.44
33:A:2310:G:O2'	33:A:2675:G:O6	2.32	0.44
33:A:1943:A:O2'	103:A:3538:HOH:O	2.05	0.44
33:A:1980:A:OP1	58:2:56:SER:OG	2.29	0.44
33:A:2099:U:H2'	33:A:2100:C:C6	2.52	0.44
33:A:2954:C:OP1	60:4:73:LYS:NZ	2.40	0.44
35:D:257:ILE:O	35:D:262:ARG:NH1	2.47	0.44
1:AA:1065:C:H2'	1:AA:1066:C:O4'	2.18	0.43
33:A:3003:A:N7	103:A:3789:HOH:O	2.36	0.43
39:J:20:ILE:HD11	39:J:42:ARG:HD3	1.99	0.43
83:s:298:GLN:NE2	103:s:507:HOH:O	2.46	0.43
90:A6:25:ARG:N	90:A6:61:GLY:O	2.51	0.43
1:AA:1080:A:N6	103:AA:2012:HOH:O	2.50	0.43
1:AA:1264:C:H1'	8:AH:124:VAL:HG13	1.99	0.43
22:AV:35:VAL:O	22:AV:35:VAL:HG12	2.18	0.43
46:Q:237:ASN:OD1	46:Q:238:PHE:N	2.51	0.43
63:7:257:ILE:O	63:7:257:ILE:HG13	2.17	0.43
33:A:1795:A:N6	33:A:1796:A:N1	2.67	0.43
38:I:180:CYS:SG	38:I:184:THR:N	2.91	0.43
89:A4:381:GLN:N	89:A4:382:PRO:CD	2.81	0.43
89:A4:387:LYS:O	89:A4:388:ARG:HG2	2.19	0.43
8:AH:167:GLY:O	103:AH:303:HOH:O	2.21	0.43
24:AX:265:ILE:HD11	24:AX:297:MET:HE2	2.00	0.43
33:A:1672:C:O2'	49:T:143:ARG:O	2.34	0.43
83:s:153:GLU:OE1	83:s:153:GLU:HA	2.19	0.43
1:AA:1583:MA6:OP1	29:A3:145:LYS:NZ	2.51	0.43
40:K:178:LEU:HD13	82:r:35:PHE:CZ	2.53	0.43
4:AD:198:TRP:HA	4:AD:201:ILE:HD12	2.00	0.43
27:A1:217:GLN:NE2	87:AY:323:ASP:OD2	2.50	0.43
33:A:1902:C:OP2	103:A:3645:HOH:O	2.20	0.43
49:T:206:LEU:HA	67:b:119:PHE:HE1	1.82	0.43
73:h:69:ARG:NH2	73:h:107:ASP:OD1	2.51	0.43
86:z:129:MET:HG2	86:z:129:MET:O	2.17	0.43
1:AA:997:A:N6	103:AA:1969:HOH:O	2.39	0.43
1:AA:1035:U:O2'	103:AA:1817:HOH:O	2.05	0.43
1:AA:1057:G:H4'	1:AA:1578:A:H4'	2.00	0.43
27:A1:86:ARG:NH1	27:A1:96:PRO:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:D:86:ASP:OD1	35:D:88:THR:OG1	2.30	0.43
37:F:191:ASP:OD1	37:F:192:SER:N	2.52	0.43
88:A5:465:MET:O	88:A5:469:GLY:N	2.49	0.43
24:AX:159:HIS:NE2	24:AX:266:ASN:OD1	2.50	0.43
26:A0:158:GLU:O	26:A0:158:GLU:HG2	2.19	0.43
27:A1:299:LEU:HD21	27:A1:309:ILE:HD13	2.01	0.43
59:3:146:GLU:HA	59:3:146:GLU:OE1	2.19	0.43
1:AA:1458:A:OP1	6:AF:104:LYS:NZ	2.33	0.43
11:AK:102:ARG:NH2	103:AK:206:HOH:O	2.37	0.43
23:AW:92:MET:O	23:AW:98:LYS:NZ	2.52	0.43
70:e:151:ARG:NH2	70:e:259:GLU:OE2	2.37	0.43
88:A5:197:ARG:HA	88:A5:228:LEU:HD13	2.01	0.43
18:AR:169:GLU:OE1	26:A0:180:LYS:NZ	2.48	0.43
24:AX:108:LEU:HD23	24:AX:141:VAL:HG21	2.00	0.43
33:A:2227:A:N3	33:A:2227:A:H2'	2.33	0.43
33:A:3039:OMU:O3'	33:A:3039:OMU:HM22	2.18	0.43
46:Q:251:GLU:OE1	46:Q:251:GLU:HA	2.19	0.43
89:A4:384:ASP:CG	89:A4:385:PRO:HD2	2.43	0.43
3:AC:115:ASN:ND2	87:AY:309:LYS:O	2.52	0.42
7:AG:237:GLU:OE1	7:AG:237:GLU:N	2.51	0.42
44:O:16:ARG:NH2	44:O:50:ASP:OD2	2.46	0.42
86:z:250:GLU:O	86:z:250:GLU:HG2	2.19	0.42
87:AY:250:ILE:HB	89:A4:354:LEU:HD22	2.01	0.42
89:A4:303:CYS:SG	89:A4:344:ARG:NH2	2.92	0.42
1:AA:994:A:O2'	6:AF:166:ARG:NH1	2.52	0.42
37:F:220:ASP:O	37:F:245:ALA:N	2.52	0.42
88:A5:239:VAL:HG23	88:A5:254:ILE:HG21	2.02	0.42
88:A5:335:ILE:N	88:A5:336:PRO:HD2	2.35	0.42
1:AA:1582:G:N3	33:A:2582:A:O2'	2.48	0.42
10:AJ:38:ARG:NH2	103:AJ:206:HOH:O	2.51	0.42
23:AW:162:VAL:HG12	23:AW:162:VAL:O	2.19	0.42
31:Ax:48:U:OP1	31:Ax:48:U:H4'	2.17	0.42
42:M:177:ALA:HA	42:M:222:TYR:CD1	2.54	0.42
50:U:46:MET:HE1	50:U:72:VAL:HG13	1.99	0.42
33:A:2420:U:O2'	65:9:31:ARG:O	2.32	0.42
7:AG:200:LEU:HD13	7:AG:246:ARG:CZ	2.49	0.42
33:A:1851:G:H2'	33:A:2693:A:N7	2.34	0.42
55:Z:149:TRP:NE1	75:j:45:GLU:OE1	2.50	0.42
8:AH:184:ILE:O	8:AH:184:ILE:HG22	2.18	0.42
63:7:51:GLU:OE1	63:7:51:GLU:HA	2.20	0.42
86:z:250:GLU:O	86:z:251:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
91:Az:35:A:H2'	91:Az:36:C:C5	2.54	0.42
6:AF:159:VAL:HG23	6:AF:172:VAL:HG21	2.00	0.42
33:A:1950:U:OP1	103:A:3655:HOH:O	2.22	0.42
33:A:2231:A:N3	33:A:3003:A:O2'	2.47	0.42
37:F:175:LYS:NZ	37:F:277:ASP:OD2	2.53	0.42
42:M:276:ASN:O	42:M:280:LYS:N	2.53	0.42
27:A1:224:TYR:OH	78:m:115:HIS:ND1	2.46	0.42
51:V:188:VAL:O	51:V:188:VAL:CG2	2.68	0.42
56:0:166:SER:OG	56:0:167:GLU:N	2.53	0.42
61:5:105:TYR:CE1	61:5:262:ILE:HD12	2.55	0.42
63:7:114:ASP:OD1	63:7:268:LEU:N	2.53	0.42
4:AD:415:GLN:NE2	4:AD:417:MET:SD	2.92	0.42
5:AE:54:HIS:O	5:AE:55:SER:OG	2.37	0.42
28:A2:95:GLU:HG2	28:A2:95:GLU:O	2.20	0.42
33:A:2665:U:OP2	44:O:17:ARG:NE	2.50	0.42
33:A:2776:G:N2	85:H:179:ASN:OD1	2.52	0.42
33:A:2971:A:O2'	43:N:182:LYS:O	2.36	0.42
46:Q:96:ARG:HA	46:Q:99:MET:HE3	2.01	0.42
57:1:54:VAL:HG12	57:1:55:LEU:N	2.35	0.42
61:5:166:THR:O	83:s:287:LYS:NZ	2.44	0.42
66:a:142:ARG:O	66:a:142:ARG:HG3	2.19	0.42
70:e:108:GLU:O	70:e:108:GLU:HG3	2.20	0.42
1:AA:894:C:N4	10:AJ:117:ASP:OD2	2.52	0.41
4:AD:363:ALA:O	4:AD:367:GLY:N	2.52	0.41
8:AH:155:VAL:HG21	27:A1:129:PHE:CB	2.50	0.41
41:L:42:ASP:OD1	41:L:42:ASP:C	2.63	0.41
88:A5:119:GLY:O	88:A5:122:HIS:N	2.53	0.41
8:AH:95:ALA:HB3	8:AH:143:LEU:HD21	2.01	0.41
31:Ax:24:A:O2'	33:A:2586:U:OP1	2.33	0.41
33:A:1764:C:OP1	81:q:34:ARG:NH2	2.52	0.41
33:A:2419:C:OP1	103:A:3656:HOH:O	2.22	0.41
70:e:156:ASN:OD1	70:e:157:LEU:N	2.53	0.41
70:e:223:THR:HG22	70:e:224:GLU:N	2.35	0.41
1:AA:1308:U:O2'	3:AC:64:HIS:ND1	2.54	0.41
6:AF:155:MET:HE2	6:AF:155:MET:HA	2.01	0.41
33:A:1958:G:OP1	103:A:3657:HOH:O	2.22	0.41
33:A:2005:C:N4	103:A:3949:HOH:O	2.47	0.41
61:5:56:GLU:O	61:5:56:GLU:HG3	2.20	0.41
83:s:85:LYS:O	103:s:503:HOH:O	2.22	0.41
86:z:203:ILE:HG22	86:z:203:ILE:O	2.20	0.41
1:AA:875:U:O2'	1:AA:882:A:N1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:318:ASP:OD1	22:AV:319:ILE:N	2.53	0.41
33:A:2127:A:H4'	33:A:2251:A:C5	2.56	0.41
88:A5:208:CYS:O	88:A5:241:GLY:HA2	2.20	0.41
89:A4:58:VAL:O	89:A4:58:VAL:HG23	2.19	0.41
1:AA:952:A:N3	1:AA:954:C:N4	2.68	0.41
1:AA:1016:U:O2'	103:AA:1856:HOH:O	2.15	0.41
7:AG:198:ARG:NH1	7:AG:201:ILE:HG23	2.36	0.41
69:d:52:THR:O	103:d:402:HOH:O	2.22	0.41
69:d:109:THR:OG1	69:d:110:GLU:N	2.53	0.41
85:H:75:ARG:O	103:H:301:HOH:O	2.22	0.41
88:A5:210:VAL:O	88:A5:210:VAL:HG22	2.20	0.41
90:A6:24:ARG:NH1	91:Az:38:U:O4'	2.52	0.41
33:A:1823:A:OP2	66:a:127:GLY:N	2.51	0.41
33:A:2868:C:H2'	33:A:2869:A:O4'	2.21	0.41
67:b:15:LEU:HD11	68:c:172:ASN:HB2	2.02	0.41
87:AY:199:ILE:HG22	87:AY:200:SER:N	2.35	0.41
1:AA:1291:U:O2'	103:AA:1869:HOH:O	2.17	0.41
21:AU:49:ASP:OD1	21:AU:49:ASP:C	2.64	0.41
86:z:230:ILE:O	86:z:232:LYS:N	2.54	0.41
88:A5:69:GLN:O	88:A5:73:THR:N	2.44	0.41
13:AM:55:ASP:OD2	20:AT:146:GLN:NE2	2.49	0.41
40:K:7:ALA:HB3	40:K:8:PRO:HD3	2.02	0.41
50:U:66:ALA:HB2	50:U:100:ALA:HA	2.02	0.41
59:3:104:ARG:NH1	59:3:160:LYS:O	2.54	0.41
20:AT:47:PHE:CE2	20:AT:52:ILE:HD11	2.56	0.41
20:AT:92:THR:O	20:AT:92:THR:HG22	2.20	0.41
28:A2:22:LYS:NZ	103:A2:203:HOH:O	2.35	0.41
33:A:2651:A:H2'	33:A:2652:G:O4'	2.21	0.41
62:6:324:ASP:OD1	62:6:324:ASP:C	2.64	0.41
86:z:123:LEU:HB3	86:z:257:ILE:HG12	2.03	0.41
86:z:236:LEU:O	86:z:240:GLY:N	2.52	0.41
4:AD:278:HIS:O	103:AD:504:HOH:O	2.22	0.41
33:A:2870:G:OP1	59:3:140:ARG:NE	2.47	0.41
51:V:127:ASP:O	51:V:129:LYS:N	2.54	0.41
87:AY:264:VAL:HG12	87:AY:265:THR:N	2.36	0.41
88:A5:602:GLU:H	88:A5:602:GLU:CD	2.29	0.41
8:AH:155:VAL:HG21	27:A1:129:PHE:HB2	2.04	0.40
33:A:2999:C:H2'	33:A:3000:A:O4'	2.21	0.40
51:V:165:ILE:HG21	65:9:76:TYR:CD2	2.56	0.40
51:V:190:CYS:SG	51:V:191:LEU:N	2.94	0.40
70:e:177:GLU:O	70:e:190:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:r:35:PHE:N	82:r:56:THR:OG1	2.46	0.40
85:H:238:VAL:HG12	85:H:239:ASN:N	2.36	0.40
87:AY:205:ILE:HG22	87:AY:205:ILE:O	2.22	0.40
88:A5:90:LEU:C	88:A5:90:LEU:HD23	2.47	0.40
33:A:2398:A:H2'	33:A:2399:A:O4'	2.22	0.40
42:M:149:THR:O	42:M:149:THR:HG22	2.20	0.40
88:A5:531:ASN:O	88:A5:570:TYR:OH	2.37	0.40
7:AG:229:LEU:HD13	7:AG:241:VAL:HG11	2.03	0.40
33:A:1848:U:O2'	103:A:3653:HOH:O	2.21	0.40
79:o:22:ARG:NH1	103:o:305:HOH:O	2.44	0.40
88:A5:332:ARG:NH2	91:Az:31:C:N3	2.69	0.40
13:AM:24:GLY:N	13:AM:31:PHE:O	2.43	0.40
22:AV:39:LYS:NZ	22:AV:376:GLU:OE2	2.45	0.40
24:AX:265:ILE:CD1	24:AX:297:MET:HE2	2.51	0.40
68:c:173:LEU:O	103:c:401:HOH:O	2.22	0.40
81:q:169:ASP:N	81:q:170:PRO:CD	2.85	0.40
88:A5:375:PHE:CD1	88:A5:375:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
3	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
4	AD	341/430 (79%)	329 (96%)	12 (4%)	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%)	136 (99%)	1 (1%)	1 (1%)	18	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AI	134/194 (69%)	131 (98%)	3 (2%)	0	100	100
10	AJ	106/138 (77%)	106 (100%)	0	0	100	100
11	AK	99/128 (77%)	99 (100%)	0	0	100	100
12	AL	172/257 (67%)	169 (98%)	3 (2%)	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%)	187 (98%)	4 (2%)	0	100	100
16	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
17	AQ	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
18	AR	293/360 (81%)	283 (97%)	10 (3%)	0	100	100
19	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
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%)	343 (98%)	7 (2%)	0	100	100
25	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
26	A0	213/217 (98%)	209 (98%)	4 (2%)	0	100	100
27	A1	275/323 (85%)	271 (98%)	4 (2%)	0	100	100
28	A2	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
29	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
35	D	236/305 (77%)	232 (98%)	4 (2%)	0	100	100
36	E	303/348 (87%)	298 (98%)	4 (1%)	1 (0%)	36	54
37	F	250/311 (80%)	244 (98%)	6 (2%)	0	100	100
38	I	210/261 (80%)	201 (96%)	9 (4%)	0	100	100
39	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
40	K	175/178 (98%)	173 (99%)	2 (1%)	0	100	100
41	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
42	M	287/296 (97%)	284 (99%)	3 (1%)	0	100	100
43	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
44	O	152/175 (87%)	148 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
46	Q	236/292 (81%)	234 (99%)	2 (1%)	0	100	100
47	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
48	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
49	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
50	U	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
51	V	203/216 (94%)	198 (98%)	5 (2%)	0	100	100
52	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
53	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
54	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
55	Z	120/161 (74%)	120 (100%)	0	0	100	100
56	0	108/188 (57%)	108 (100%)	0	0	100	100
57	1	54/65 (83%)	54 (100%)	0	0	100	100
58	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
59	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
60	4	36/103 (35%)	36 (100%)	0	0	100	100
61	5	392/423 (93%)	383 (98%)	9 (2%)	0	100	100
62	6	352/380 (93%)	344 (98%)	8 (2%)	0	100	100
63	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
64	8	155/206 (75%)	153 (99%)	2 (1%)	0	100	100
65	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
66	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
67	b	149/215 (69%)	146 (98%)	3 (2%)	0	100	100
68	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
69	d	235/306 (77%)	231 (98%)	4 (2%)	0	100	100
70	e	236/279 (85%)	222 (94%)	13 (6%)	1 (0%)	30	48
71	f	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
72	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
73	h	108/158 (68%)	108 (100%)	0	0	100	100
74	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
75	j	92/123 (75%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	k	99/112 (88%)	99 (100%)	0	0	100	100
77	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
78	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
79	o	92/102 (90%)	92 (100%)	0	0	100	100
80	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
81	q	161/222 (72%)	160 (99%)	1 (1%)	0	100	100
82	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
83	s	382/439 (87%)	372 (97%)	10 (3%)	0	100	100
84	t	44/198 (22%)	44 (100%)	0	0	100	100
84	u	30/198 (15%)	30 (100%)	0	0	100	100
84	v	30/198 (15%)	30 (100%)	0	0	100	100
84	w	29/198 (15%)	29 (100%)	0	0	100	100
84	x	29/198 (15%)	29 (100%)	0	0	100	100
84	y	29/198 (15%)	29 (100%)	0	0	100	100
85	H	200/267 (75%)	194 (97%)	6 (3%)	0	100	100
86	z	250/325 (77%)	240 (96%)	9 (4%)	1 (0%)	30	48
87	AY	219/395 (55%)	207 (94%)	11 (5%)	1 (0%)	24	42
88	A5	579/1394 (42%)	561 (97%)	17 (3%)	1 (0%)	43	62
89	A4	591/689 (86%)	577 (98%)	13 (2%)	1 (0%)	43	62
90	A6	72/109 (66%)	69 (96%)	3 (4%)	0	100	100
All	All	15427/20987 (74%)	15135 (98%)	285 (2%)	7 (0%)	100	100

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AH	126	ILE
86	z	128	ASP
87	AY	233	ASP
36	E	150	LYS
70	e	109	GLU
88	A5	299	HIS
89	A4	385	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	198/249 (80%)	198 (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
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	AZ	90/95 (95%)	90 (100%)	0	100	100
26	A0	188/189 (100%)	188 (100%)	0	100	100
27	A1	255/291 (88%)	255 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	A2	100/101 (99%)	100 (100%)	0	100	100
29	A3	65/166 (39%)	65 (100%)	0	100	100
35	D	192/245 (78%)	192 (100%)	0	100	100
36	E	260/290 (90%)	260 (100%)	0	100	100
37	F	219/262 (84%)	219 (100%)	0	100	100
38	I	194/232 (84%)	194 (100%)	0	100	100
39	J	138/150 (92%)	138 (100%)	0	100	100
40	K	154/155 (99%)	154 (100%)	0	100	100
41	L	98/124 (79%)	98 (100%)	0	100	100
42	M	245/249 (98%)	245 (100%)	0	100	100
43	N	189/211 (90%)	189 (100%)	0	100	100
44	O	134/150 (89%)	134 (100%)	0	100	100
45	P	126/155 (81%)	126 (100%)	0	100	100
46	Q	220/256 (86%)	220 (100%)	0	100	100
47	R	118/126 (94%)	118 (100%)	0	100	100
48	S	146/180 (81%)	146 (100%)	0	100	100
49	T	146/176 (83%)	146 (100%)	0	100	100
50	U	134/135 (99%)	134 (100%)	0	100	100
51	V	183/191 (96%)	183 (100%)	0	100	100
52	W	94/119 (79%)	94 (100%)	0	100	100
53	X	220/229 (96%)	220 (100%)	0	100	100
54	Y	163/223 (73%)	163 (100%)	0	100	100
55	Z	113/147 (77%)	113 (100%)	0	100	100
56	0	99/164 (60%)	99 (100%)	0	100	100
57	1	53/60 (88%)	53 (100%)	0	100	100
58	2	40/72 (56%)	40 (100%)	0	100	100
59	3	88/166 (53%)	88 (100%)	0	100	100
60	4	37/89 (42%)	37 (100%)	0	100	100
61	5	353/368 (96%)	353 (100%)	0	100	100
62	6	313/332 (94%)	313 (100%)	0	100	100
63	7	270/303 (89%)	270 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	8	146/190 (77%)	146 (100%)	0	100	100
65	9	104/112 (93%)	104 (100%)	0	100	100
66	a	96/133 (72%)	96 (100%)	0	100	100
67	b	132/185 (71%)	132 (100%)	0	100	100
68	c	251/288 (87%)	251 (100%)	0	100	100
69	d	223/274 (81%)	223 (100%)	0	100	100
70	e	207/236 (88%)	207 (100%)	0	100	100
71	f	139/188 (74%)	139 (100%)	0	100	100
72	g	124/148 (84%)	124 (100%)	0	100	100
73	h	104/148 (70%)	104 (100%)	0	100	100
74	i	86/110 (78%)	86 (100%)	0	100	100
75	j	74/97 (76%)	74 (100%)	0	100	100
76	k	83/90 (92%)	83 (100%)	0	100	100
77	l	76/116 (66%)	76 (100%)	0	100	100
78	m	85/113 (75%)	85 (100%)	0	100	100
79	o	80/87 (92%)	80 (100%)	0	100	100
80	p	135/181 (75%)	135 (100%)	0	100	100
81	q	142/178 (80%)	142 (100%)	0	100	100
82	r	147/169 (87%)	147 (100%)	0	100	100
83	s	340/381 (89%)	340 (100%)	0	100	100
84	t	40/158 (25%)	40 (100%)	0	100	100
84	u	31/158 (20%)	31 (100%)	0	100	100
84	v	31/158 (20%)	31 (100%)	0	100	100
84	w	30/158 (19%)	30 (100%)	0	100	100
84	x	30/158 (19%)	30 (100%)	0	100	100
84	y	30/158 (19%)	30 (100%)	0	100	100
85	H	182/228 (80%)	182 (100%)	0	100	100
86	z	226/287 (79%)	226 (100%)	0	100	100
87	AY	202/357 (57%)	202 (100%)	0	100	100
88	A5	515/1219 (42%)	515 (100%)	0	100	100
89	A4	532/609 (87%)	532 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
90	A6	63/90 (70%)	63 (100%)	0	100	100
All	All	13813/18099 (76%)	13813 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	167	HIS
2	AB	216	ASN
4	AD	359	HIS
4	AD	361	GLN
4	AD	415	GLN
4	AD	424	ASN
5	AE	54	HIS
5	AE	56	GLN
6	AF	113	GLN
6	AF	127	HIS
6	AF	147	GLN
6	AF	214	HIS
6	AF	238	HIS
7	AG	288	HIS
7	AG	384	GLN
8	AH	109	HIS
8	AH	122	GLN
8	AH	183	HIS
9	AI	87	HIS
9	AI	146	HIS
10	AJ	105	HIS
10	AJ	134	HIS
11	AK	124	GLN
12	AL	174	ASN
13	AM	50	GLN
13	AM	61	HIS
15	AO	160	HIS
15	AO	169	GLN
16	AP	95	HIS
18	AR	88	GLN
18	AR	288	GLN
18	AR	299	ASN
18	AR	320	GLN

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Mol	Chain	Res	Type
20	AT	101	HIS
22	AV	78	ASN
22	AV	224	GLN
22	AV	338	HIS
22	AV	380	GLN
22	AV	383	HIS
25	AZ	55	HIS
25	AZ	56	HIS
25	AZ	76	GLN
26	A0	133	HIS
27	A1	122	HIS
27	A1	146	HIS
27	A1	185	HIS
28	A2	113	ASN
35	D	221	ASN
35	D	276	HIS
36	E	52	HIS
36	E	202	GLN
37	F	130	GLN
37	F	208	HIS
37	F	223	HIS
38	I	43	GLN
38	I	119	HIS
39	J	168	GLN
40	K	89	GLN
40	K	94	GLN
41	L	103	ASN
42	M	53	HIS
42	M	114	GLN
43	N	222	ASN
43	N	237	HIS
44	O	100	GLN
45	P	79	HIS
45	P	115	HIS
48	S	118	ASN
49	T	126	HIS
53	X	27	HIS
53	X	93	ASN
53	X	172	GLN
54	Y	179	HIS
54	Y	225	ASN
55	Z	64	HIS

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Mol	Chain	Res	Type
57	1	15	ASN
57	1	31	ASN
57	1	45	HIS
58	2	54	GLN
58	2	92	HIS
59	3	181	HIS
61	5	160	HIS
61	5	165	GLN
61	5	367	ASN
62	6	102	GLN
62	6	308	GLN
62	6	320	GLN
62	6	373	HIS
63	7	255	HIS
63	7	284	HIS
63	7	298	GLN
64	8	143	GLN
67	b	90	HIS
68	c	69	HIS
68	c	77	HIS
68	c	80	GLN
69	d	207	ASN
69	d	262	HIS
70	e	67	GLN
70	e	95	ASN
70	e	251	HIS
74	i	120	HIS
74	i	124	HIS
77	l	135	ASN
79	o	21	HIS
79	o	94	HIS
81	q	180	GLN
82	r	96	HIS
83	s	107	GLN
83	s	277	GLN
83	s	423	HIS
85	H	88	HIS
85	H	126	GLN
85	H	192	HIS
86	z	241	HIS
86	z	266	GLN
86	z	272	GLN

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Mol	Chain	Res	Type
86	z	276	ASN
87	AY	182	GLN
87	AY	234	ASN
87	AY	316	ASN
88	A5	174	GLN
88	A5	192	ASN
88	A5	201	GLN
88	A5	408	GLN
88	A5	466	GLN
88	A5	609	HIS
89	A4	175	GLN
89	A4	373	HIS
89	A4	381	GLN
89	A4	495	HIS
89	A4	504	ASN
90	A6	38	HIS
90	A6	92	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	953/954 (99%)	136 (14%)	1 (0%)
30	Aw	67/68 (98%)	18 (26%)	0
31	Ax	68/70 (97%)	12 (17%)	0
32	Ay	68/70 (97%)	13 (19%)	0
33	A	1556/1561 (99%)	224 (14%)	3 (0%)
34	B	71/72 (98%)	12 (16%)	0
91	Az	41/42 (97%)	21 (51%)	0
All	All	2824/2837 (99%)	436 (15%)	4 (0%)

All (436) 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

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Mol	Chain	Res	Type
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	890	C
1	AA	903	U
1	AA	904	C
1	AA	907	A
1	AA	919	A
1	AA	923	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	951	G
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

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Mol	Chain	Res	Type
1	AA	1019	A
1	AA	1031	G
1	AA	1042	U
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
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

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Mol	Chain	Res	Type
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	1463	G
1	AA	1469	G
1	AA	1474	G
1	AA	1481	C
1	AA	1503	G
1	AA	1519	A
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	1584	MA6
1	AA	1594	G

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Mol	Chain	Res	Type
1	AA	1595	G
1	AA	1599	A
30	Aw	3	G
30	Aw	7	A
30	Aw	9	A
30	Aw	16	A
30	Aw	21	A
30	Aw	22	A
30	Aw	30	G
30	Aw	46	A
30	Aw	49	U
30	Aw	50	A
30	Aw	55	A
30	Aw	56	A
30	Aw	61	U
30	Aw	65	A
30	Aw	68	U
30	Aw	71	C
30	Aw	73	U
30	Aw	74	C
31	Ax	2	A
31	Ax	3	G
31	Ax	8	U
31	Ax	9	A
31	Ax	25	C
31	Ax	44	A
31	Ax	45	G
31	Ax	46	A
31	Ax	48	U
31	Ax	49	G
31	Ax	59	U
31	Ax	76	A
32	Ay	3	G
32	Ay	4	G
32	Ay	28	C
32	Ay	29	U
32	Ay	30	G
32	Ay	37	A
32	Ay	44	A
32	Ay	45	G
32	Ay	48	U
32	Ay	49	G

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Mol	Chain	Res	Type
32	A _y	59	U
32	A _y	75	C
32	A _y	76	A
33	A	1681	G
33	A	1689	C
33	A	1692	A
33	A	1693	C
33	A	1694	U
33	A	1699	C
33	A	1700	U
33	A	1704	U
33	A	1708	A
33	A	1711	C
33	A	1724	A
33	A	1727	A
33	A	1728	U
33	A	1748	G
33	A	1765	C
33	A	1805	A
33	A	1807	U
33	A	1808	A
33	A	1809	U
33	A	1810	A
33	A	1821	A
33	A	1827	C
33	A	1828	A
33	A	1829	A
33	A	1832	A
33	A	1836	A
33	A	1844	A
33	A	1854	U
33	A	1856	A
33	A	1869	A
33	A	1882	A
33	A	1886	G
33	A	1887	A
33	A	1893	A
33	A	1901	C
33	A	1903	C
33	A	1918	G
33	A	1937	A
33	A	1940	A

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Mol	Chain	Res	Type
33	A	1958	G
33	A	1985	G
33	A	1992	C
33	A	1993	A
33	A	1994	A
33	A	2003	A
33	A	2015	G
33	A	2022	G
33	A	2030	U
33	A	2031	A
33	A	2036	C
33	A	2037	U
33	A	2039	A
33	A	2054	U
33	A	2060	A
33	A	2069	U
33	A	2070	C
33	A	2071	U
33	A	2079	C
33	A	2099	U
33	A	2113	G
33	A	2125	C
33	A	2126	U
33	A	2147	G
33	A	2159	U
33	A	2160	A
33	A	2163	A
33	A	2168	U
33	A	2181	A
33	A	2192	A
33	A	2198	A
33	A	2200	A
33	A	2214	A
33	A	2219	C
33	A	2220	A
33	A	2221	C
33	A	2222	U
33	A	2225	C
33	A	2226	U
33	A	2227	A
33	A	2228	A
33	A	2230	A

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Mol	Chain	Res	Type
33	A	2237	A
33	A	2239	A
33	A	2241	A
33	A	2243	A
33	A	2245	A
33	A	2246	A
33	A	2262	C
33	A	2263	C
33	A	2284	C
33	A	2285	U
33	A	2297	A
33	A	2300	G
33	A	2322	C
33	A	2331	C
33	A	2332	C
33	A	2345	G
33	A	2349	G
33	A	2350	A
33	A	2353	A
33	A	2357	C
33	A	2363	A
33	A	2372	U
33	A	2374	A
33	A	2390	A
33	A	2399	A
33	A	2401	A
33	A	2404	U
33	A	2407	U
33	A	2415	C
33	A	2444	A
33	A	2446	A
33	A	2451	A
33	A	2478	G
33	A	2484	C
33	A	2485	U
33	A	2493	C
33	A	2502	C
33	A	2520	C
33	A	2521	A
33	A	2527	A
33	A	2558	A
33	A	2570	C

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Mol	Chain	Res	Type
33	A	2587	G
33	A	2592	G
33	A	2593	G
33	A	2599	U
33	A	2600	A
33	A	2601	A
33	A	2603	C
33	A	2618	U
33	A	2627	G
33	A	2629	A
33	A	2630	U
33	A	2633	A
33	A	2635	G
33	A	2654	U
33	A	2656	U
33	A	2683	C
33	A	2686	G
33	A	2694	A
33	A	2696	A
33	A	2706	A
33	A	2718	C
33	A	2719	G
33	A	2723	A
33	A	2724	G
33	A	2725	A
33	A	2732	G
33	A	2745	A
33	A	2761	C
33	A	2762	C
33	A	2765	A
33	A	2767	A
33	A	2768	A
33	A	2775	A
33	A	2781	U
33	A	2782	A
33	A	2786	U
33	A	2787	A
33	A	2788	C
33	A	2791	A
33	A	2810	G
33	A	2832	A
33	A	2833	A

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Mol	Chain	Res	Type
33	A	2847	C
33	A	2864	U
33	A	2865	C
33	A	2882	U
33	A	2883	A
33	A	2884	C
33	A	2885	U
33	A	2887	U
33	A	2889	C
33	A	2893	A
33	A	2910	A
33	A	2911	C
33	A	2913	A
33	A	2917	G
33	A	2922	A
33	A	2928	C
33	A	2932	G
33	A	2935	A
33	A	2956	A
33	A	2989	G
33	A	2990	A
33	A	2992	G
33	A	3005	A
33	A	3007	C
33	A	3016	G
33	A	3041	U
33	A	3053	A
33	A	3054	G
33	A	3060	C
33	A	3090	G
33	A	3100	U
33	A	3102	U
33	A	3108	U
33	A	3109	U
33	A	3110	C
33	A	3111	A
33	A	3112	A
33	A	3113	A
33	A	3157	C
33	A	3158	A
33	A	3162	C
33	A	3169	C

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Mol	Chain	Res	Type
33	A	3172	C
33	A	3176	A
33	A	3183	U
33	A	3190	A
33	A	3199	U
33	A	3200	U
33	A	3207	A
33	A	3208	C
33	A	3209	A
33	A	3210	C
33	A	3212	C
33	A	3217	A
33	A	3218	A
33	A	3228	U
33	A	3229	U
33	A	3230	G
33	A	3231	U
34	B	8	U
34	B	16	C
34	B	21	A
34	B	45	G
34	B	48	U
34	B	54	C
34	B	55	U
34	B	56	U
34	B	58	A
34	B	64	A
34	B	69	U
34	B	76	A
91	Az	0	U
91	Az	1	U
91	Az	8	U
91	Az	11	U
91	Az	12	U
91	Az	13	U
91	Az	15	U
91	Az	18	A
91	Az	22	A
91	Az	25	U
91	Az	26	A
91	Az	27	C
91	Az	31	C

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Mol	Chain	Res	Type
91	Az	32	A
91	Az	34	C
91	Az	35	A
91	Az	36	C
91	Az	37	C
91	Az	38	U
91	Az	39	U
91	Az	40	C

All (4) RNA pucker outliers are listed below:

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

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

19 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	$\# Z > 2$
33	OMU	A	3039	33,96	19,22,23	0.29	0	26,31,34	0.43	0
1	5MU	AA	1076	1	19,22,23	0.63	0	28,32,35	1.21	3 (10%)
33	PSU	A	3067	33	18,21,22	0.79	0	22,30,33	2.55	5 (22%)
76	AYA	k	2	76	6,7,8	0.82	0	5,8,10	0.50	0
1	5MC	AA	1488	1	18,22,23	0.32	0	26,32,35	0.42	0
40	SAC	K	2	40	7,8,9	0.21	0	8,9,11	0.55	0
28	AYA	A2	2	28	6,7,8	0.80	0	5,8,10	0.58	0
1	MA6	AA	1583	1	23,26,27	0.30	0	34,38,41	0.59	1 (2%)
33	OMG	A	2815	33,96,31	23,26,27	0.30	0	33,38,41	0.38	0
1	MA6	AA	1584	1	23,26,27	0.33	0	34,38,41	0.61	1 (2%)
34	2MG	B	10	34	23,26,27	0.48	0	32,38,41	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	5F0	AI	184	9	8,8,9	0.59	0	7,9,11	1.17	1 (14%)
1	B8T	AA	1486	95,1	19,22,23	0.30	0	26,31,34	0.35	0
34	1MA	B	9	34	21,25,26	0.75	1 (4%)	31,37,40	0.64	1 (3%)
50	AYA	U	2	50	6,7,8	0.77	0	5,8,10	0.58	0
33	1MA	A	2617	33	21,25,26	0.76	1 (4%)	31,37,40	0.65	1 (3%)
17	AYA	AQ	2	17	6,7,8	0.78	0	5,8,10	0.43	0
34	PSU	B	39	34	18,21,22	0.77	0	22,30,33	2.55	4 (18%)
33	OMG	A	3040	33,30	23,26,27	0.29	0	33,38,41	0.38	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
33	OMU	A	3039	33,96	-	0/9/27/28	0/2/2/2
1	5MU	AA	1076	1	-	0/7/25/26	0/2/2/2
33	PSU	A	3067	33	-	0/7/25/26	0/2/2/2
76	AYA	k	2	76	-	1/4/6/8	-
1	5MC	AA	1488	1	-	0/7/25/26	0/2/2/2
40	SAC	K	2	40	-	0/7/8/10	-
28	AYA	A2	2	28	-	0/4/6/8	-
1	MA6	AA	1583	1	-	0/11/29/30	0/3/3/3
33	OMG	A	2815	33,96,31	-	0/9/27/28	0/3/3/3
1	MA6	AA	1584	1	-	2/11/29/30	0/3/3/3
34	2MG	B	10	34	-	0/9/27/28	0/3/3/3
9	5F0	AI	184	9	-	0/9/9/10	-
1	B8T	AA	1486	95,1	-	1/7/27/28	0/2/2/2
34	1MA	B	9	34	-	0/7/25/26	0/3/3/3
50	AYA	U	2	50	-	1/4/6/8	-
33	1MA	A	2617	33	-	0/7/25/26	0/3/3/3
17	AYA	AQ	2	17	-	0/4/6/8	-
34	PSU	B	39	34	-	0/7/25/26	0/2/2/2
33	OMG	A	3040	33,30	-	0/9/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	2617	1MA	C6-N6	3.02	1.35	1.28
34	B	9	1MA	C6-N6	2.98	1.35	1.28

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	39	PSU	N1-C2-N3	8.07	124.27	115.13
33	A	3067	PSU	N1-C2-N3	8.04	124.24	115.13
34	B	39	PSU	C4-N3-C2	-6.57	116.87	126.34
33	A	3067	PSU	C4-N3-C2	-6.53	116.93	126.34
1	AA	1076	5MU	C4-N3-C2	-4.83	121.11	127.35
33	A	3067	PSU	O2-C2-N1	-3.66	118.76	122.79
34	B	39	PSU	O2-C2-N1	-3.63	118.79	122.79
9	AI	184	5F0	O-C-CB	-2.76	117.39	125.43
1	AA	1076	5MU	C5-C4-N3	2.71	117.62	115.31
34	B	39	PSU	O2-C2-N3	-2.59	116.94	121.82
33	A	3067	PSU	O2-C2-N3	-2.55	117.00	121.82
1	AA	1584	MA6	C2-N1-C6	2.41	117.44	111.75
1	AA	1583	MA6	C2-N1-C6	2.38	117.37	111.75
1	AA	1076	5MU	N3-C2-N1	2.23	117.85	114.89
33	A	3067	PSU	O4'-C1'-C2'	2.16	108.19	105.14
34	B	9	1MA	N1-C6-N6	2.14	125.21	119.77
33	A	2617	1MA	N1-C6-N6	2.07	125.05	119.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1584	MA6	C5-C6-N6-C9
76	k	2	AYA	C-CA-N-CT
1	AA	1584	MA6	C4'-C5'-O5'-P
1	AA	1486	B8T	O4'-C4'-C5'-O5'
50	U	2	AYA	C-CA-N-CT

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	3039	OMU	2	0
1	AA	1583	MA6	2	0
1	AA	1584	MA6	1	0
33	A	3040	OMG	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 271 ligands modelled in this entry, 258 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
93	SPM	AA	1702	-	13,13,13	0.25	0	12,12,12	0.99	0
98	FES	r	201	38,82	0,4,4	-	-	-		
94	SPD	A	3301	-	9,9,9	0.22	0	8,8,8	1.24	0
94	SPD	AA	1703	-	9,9,9	0.24	0	8,8,8	1.34	2 (25%)
98	FES	AT	201	13,20	0,4,4	-	-	-		
99	ATP	AX	501	95	29,33,33	0.49	0	44,52,52	0.49	0
102	VAL	B	101	34	4,6,7	0.53	0	6,7,9	0.78	0
94	SPD	A	3303	-	9,9,9	0.26	0	8,8,8	1.18	0
101	PUT	A	3304	-	5,5,5	0.24	0	4,4,4	0.51	0
94	SPD	A	3302	-	9,9,9	0.25	0	8,8,8	1.15	0
98	FES	AP	201	16,5	0,4,4	-	-	-		
100	GDP	AX	503	-	28,30,30	0.42	0	44,47,47	0.40	0
92	NAD	AA	1701	95	45,48,48	0.38	0	63,73,73	0.38	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
93	SPM	AA	1702	-	-	0/11/11/11	-
98	FES	r	201	38,82	-	-	0/1/1/1
94	SPD	A	3301	-	-	1/7/7/7	-
98	FES	AP	201	16,5	-	-	0/1/1/1
94	SPD	AA	1703	-	-	0/7/7/7	-
98	FES	AT	201	13,20	-	-	0/1/1/1
99	ATP	AX	501	95	-	0/22/38/38	0/3/3/3
102	VAL	B	101	34	-	0/5/6/8	-
94	SPD	A	3303	-	-	2/7/7/7	-
101	PUT	A	3304	-	-	0/3/3/3	-
94	SPD	A	3302	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
100	GDP	AX	503	-	-	0/16/32/32	0/3/3/3
92	NAD	AA	1701	95	-	0/30/62/62	0/5/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
94	AA	1703	SPD	C4-C5-N6	-2.33	105.86	112.14
94	AA	1703	SPD	C8-C7-N6	-2.10	106.46	112.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
102	B	101	VAL	1	0

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
32	Ay	1
31	Ax	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	9.63
1	Ax	15:A	O3'	21:A	P	8.88

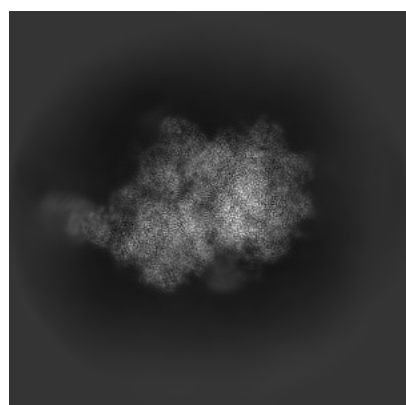
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15544. These allow visual inspection of the internal detail of the map and identification of artifacts.

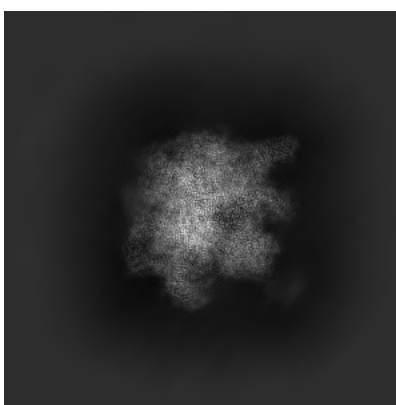
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

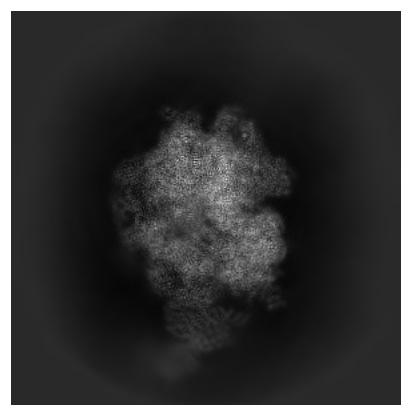
6.1.1 Primary map



X



Y

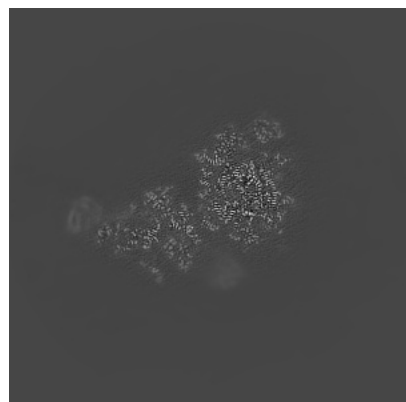


Z

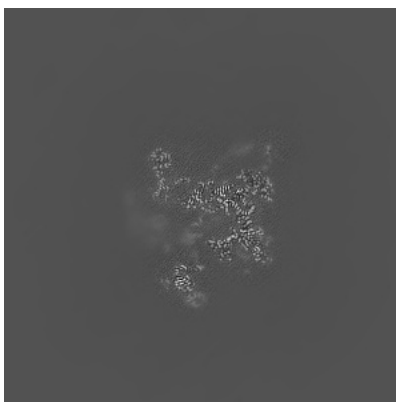
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 320



Y Index: 320

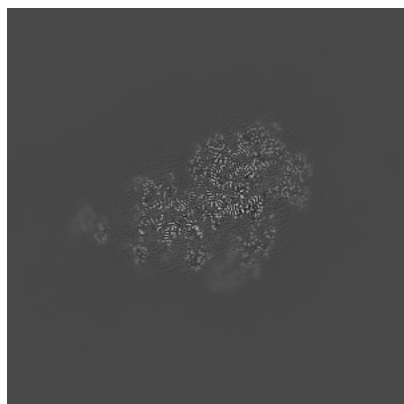


Z Index: 320

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

6.3 Largest variance slices [i](#)

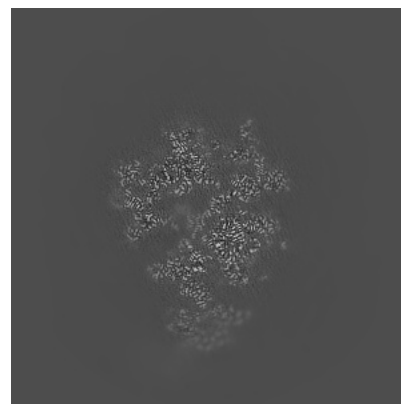
6.3.1 Primary map



X Index: 342



Y Index: 369

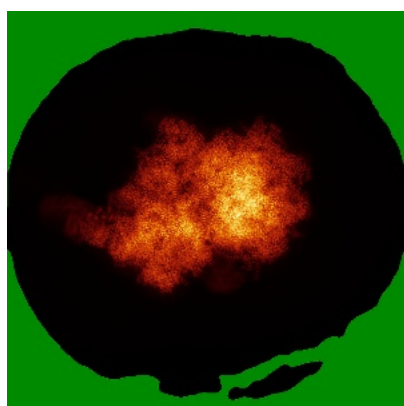


Z Index: 292

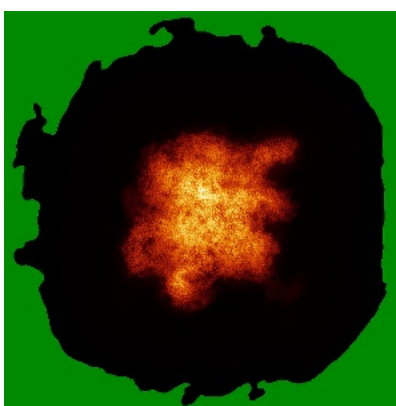
The images above show the largest variance slices of the map in three orthogonal directions.

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

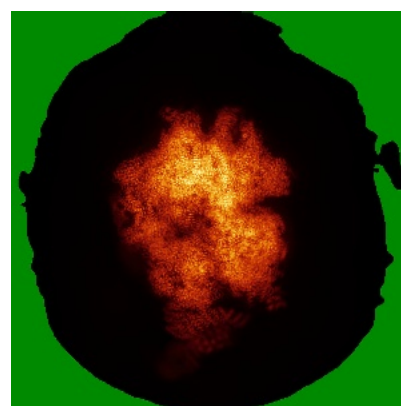
6.4.1 Primary map



X



Y

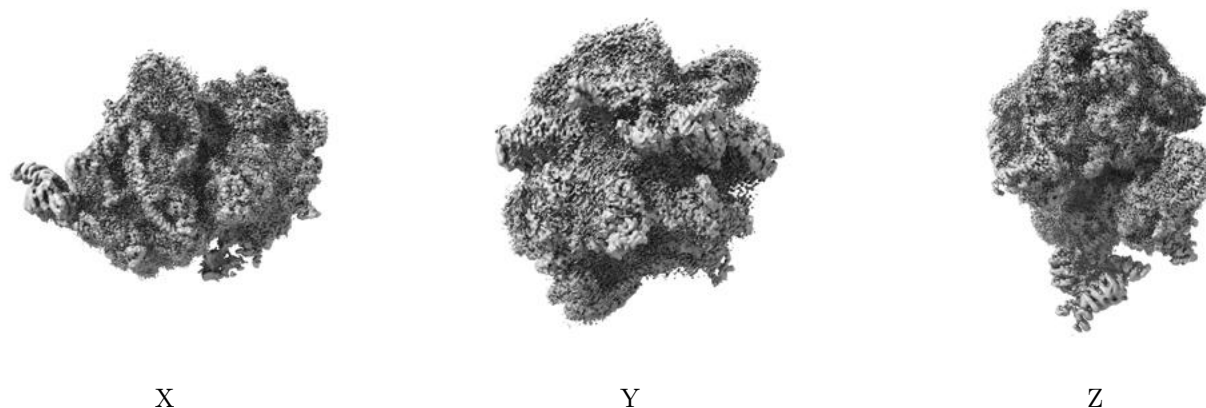


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

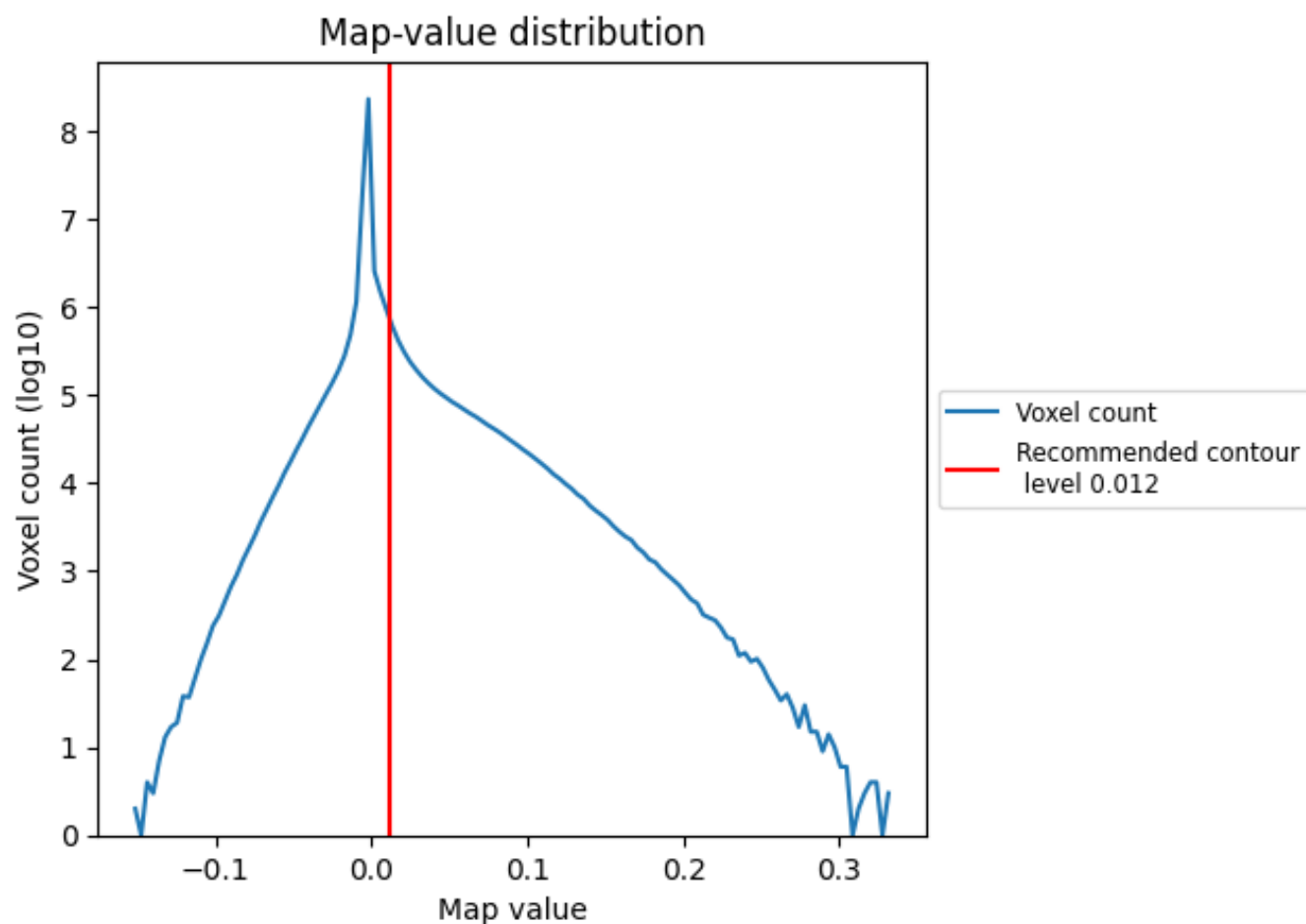
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

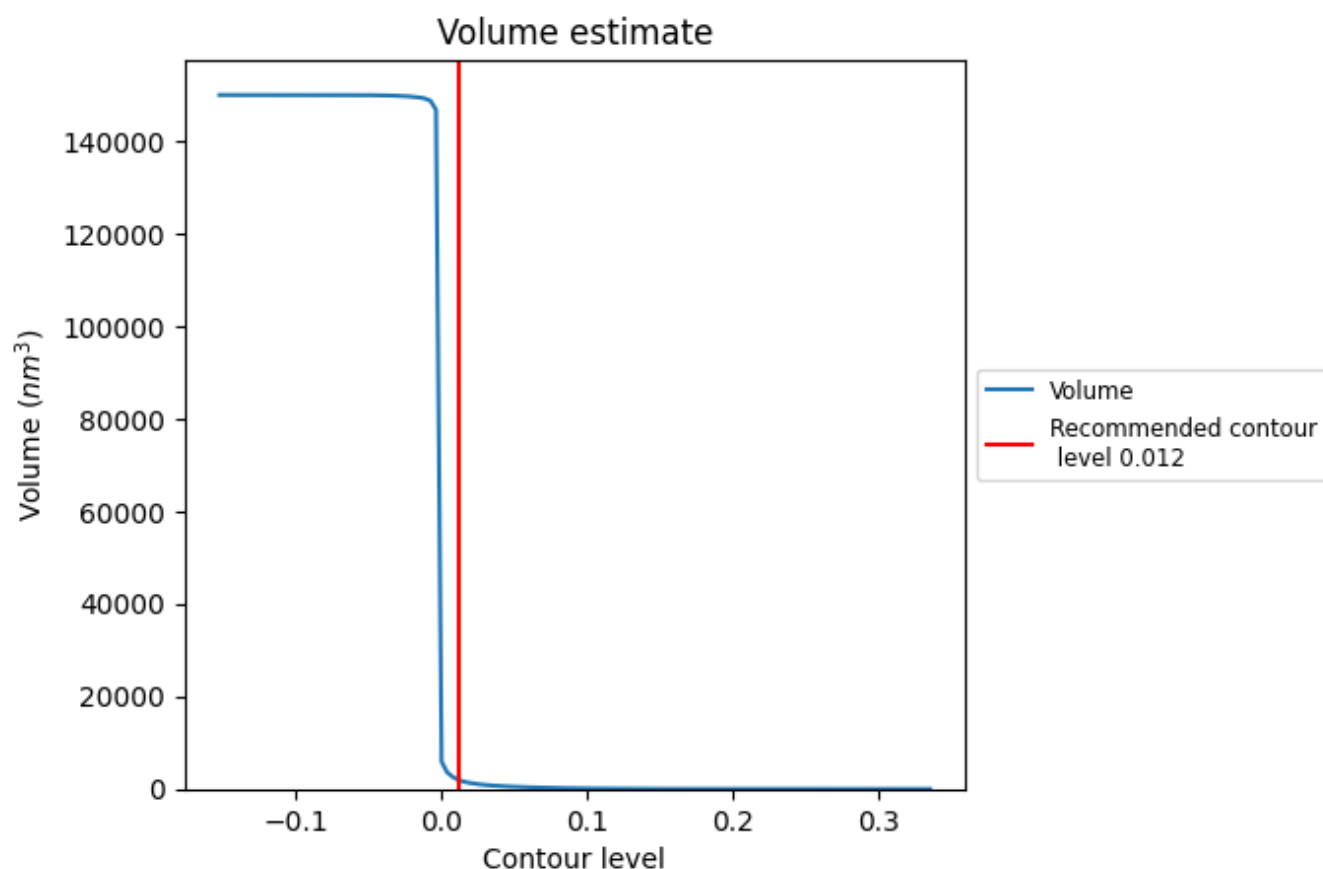
This section contains the results of statistical analysis of the map.

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.

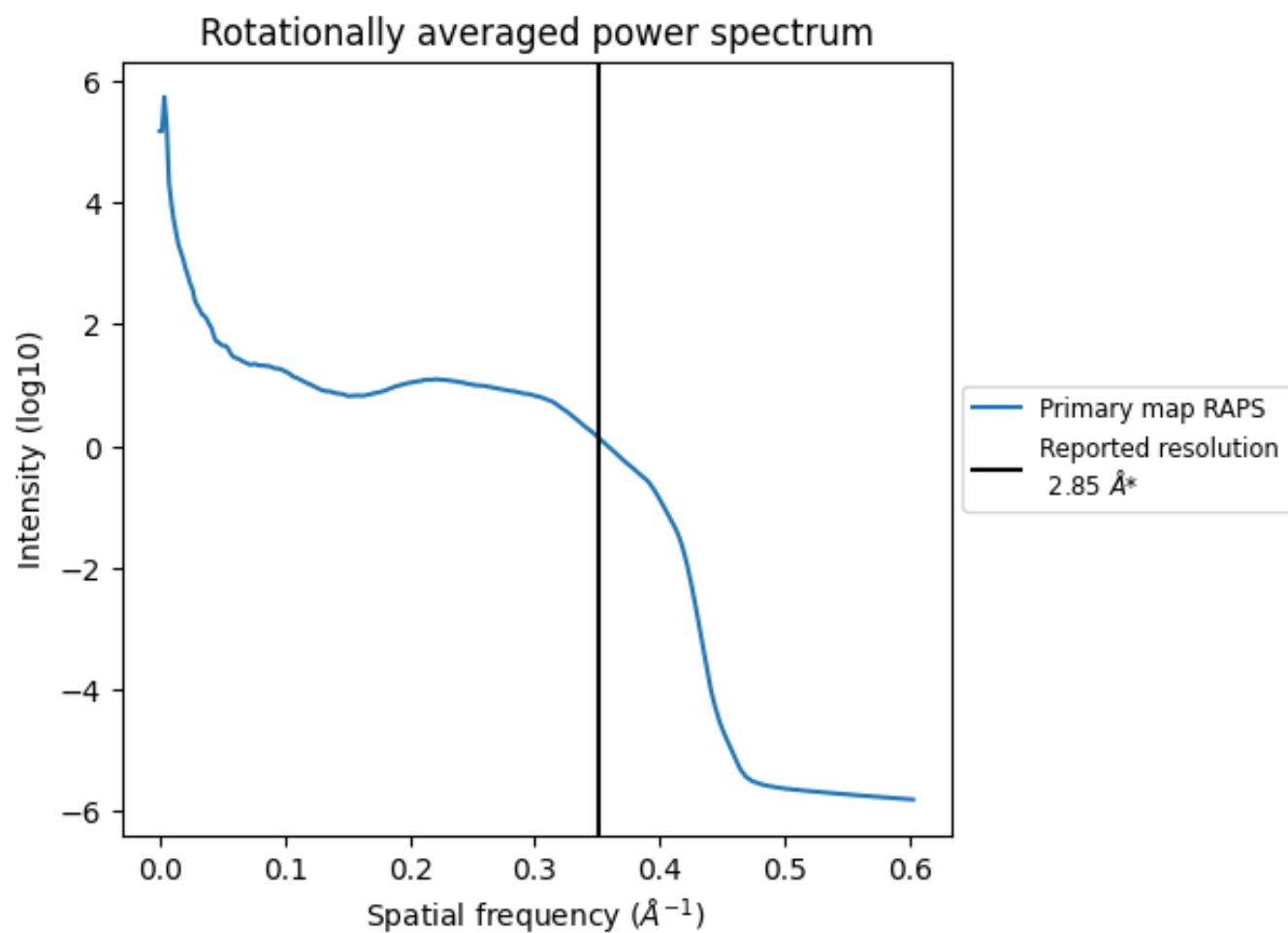
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1967 nm^3 ; this corresponds to an approximate mass of 1777 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

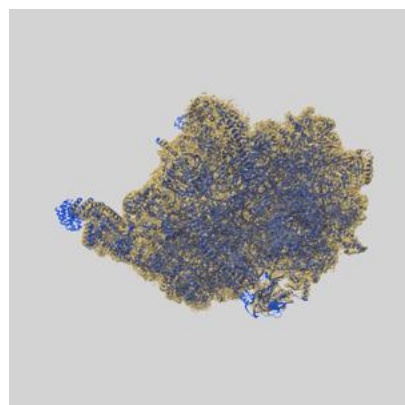
8 Fourier-Shell correlation ⓘ

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

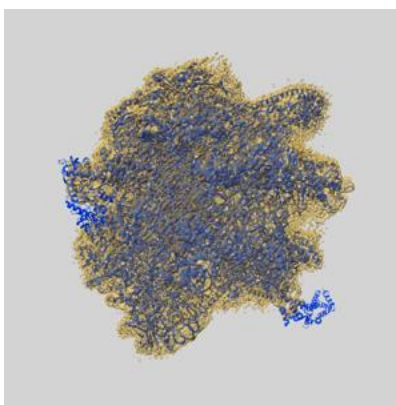
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15544 and PDB model 8ANY. Per-residue inclusion information can be found in section [3](#) on page [31](#).

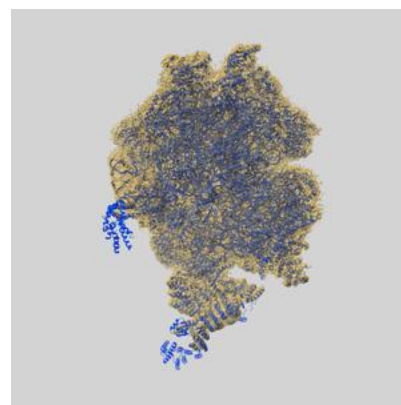
9.1 Map-model overlay [i](#)



X



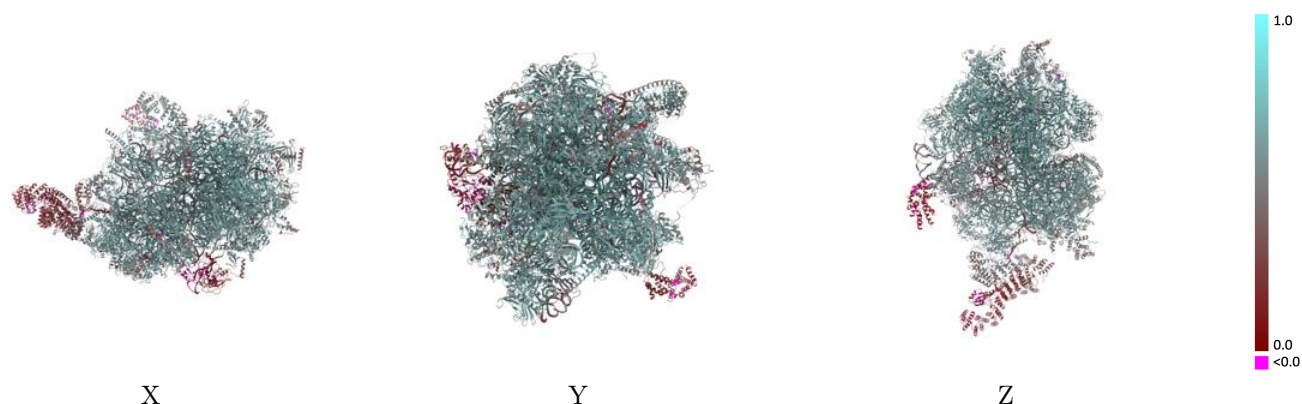
Y



Z

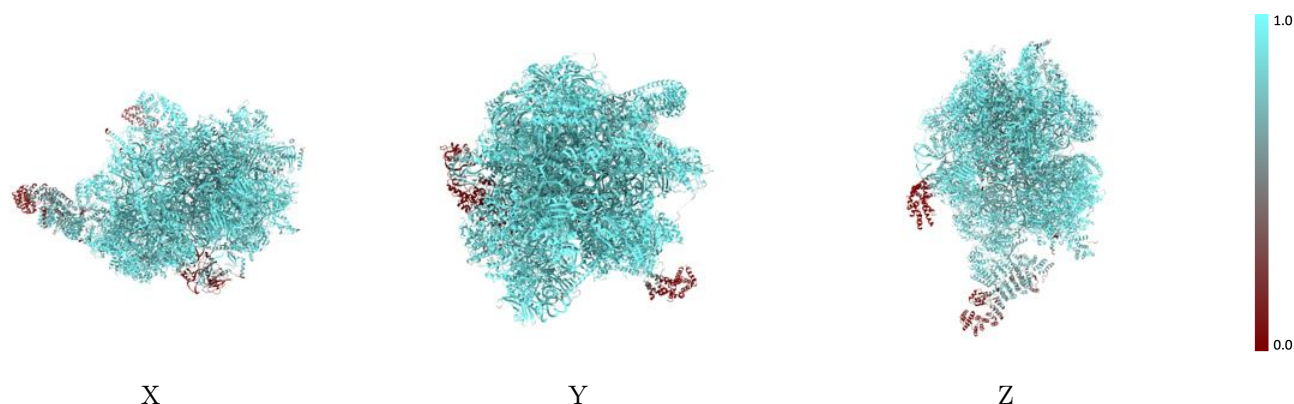
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



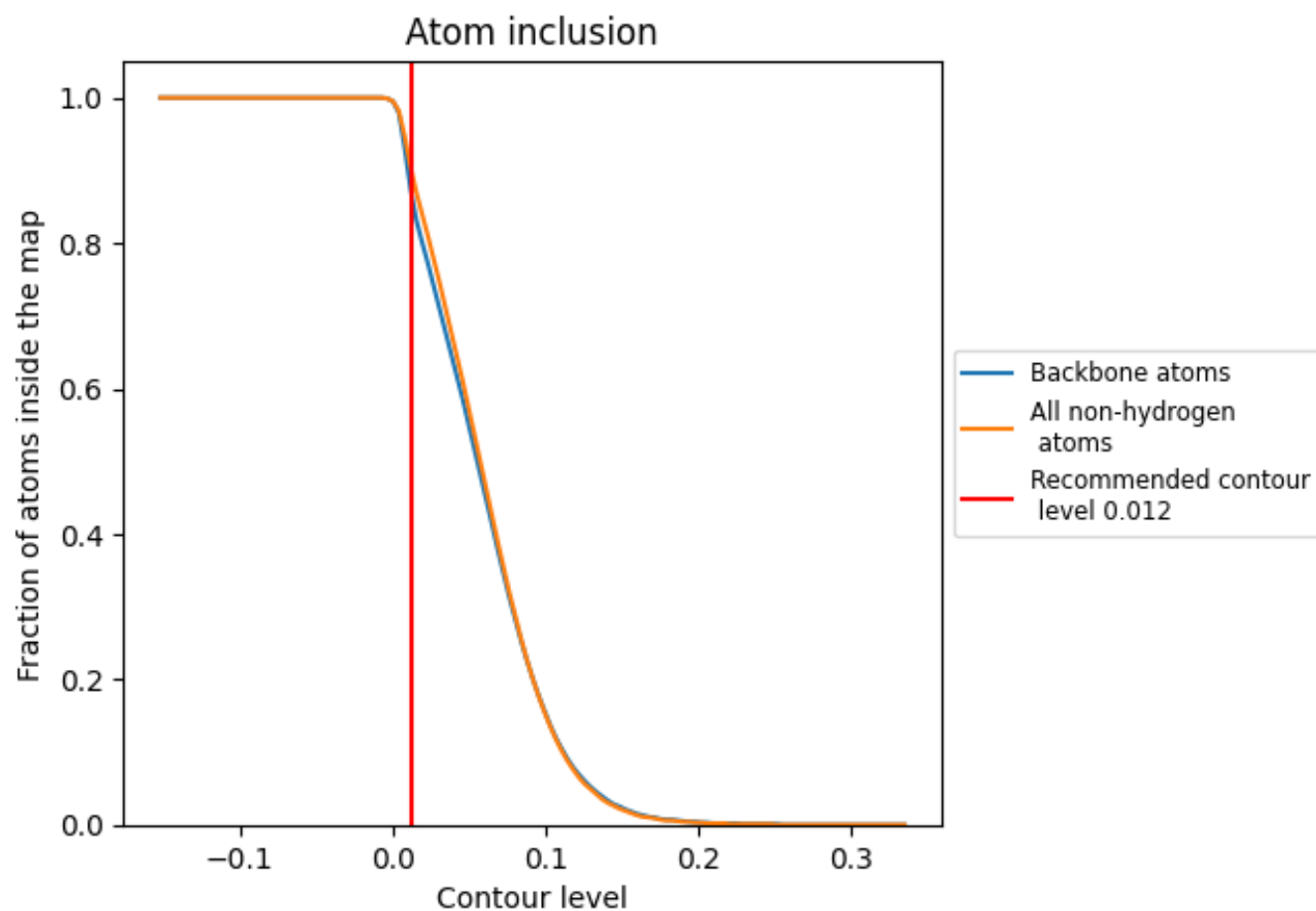
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.5540
0	 0.9620	 0.6050
1	 0.9450	 0.5770
2	 0.9950	 0.6820
3	 0.9910	 0.6710
4	 0.9880	 0.6420
5	 0.9640	 0.5810
6	 0.9650	 0.5940
7	 0.9410	 0.5410
8	 0.8720	 0.4880
9	 0.9310	 0.5690
A	 0.9810	 0.6290
A0	 0.9360	 0.5540
A1	 0.9340	 0.5680
A2	 0.9070	 0.5040
A3	 0.9610	 0.6000
A4	 0.8590	 0.4320
A5	 0.4750	 0.1750
A6	 0.2210	 0.1260
AA	 0.9930	 0.6240
AB	 0.9610	 0.5980
AC	 0.9860	 0.6490
AD	 0.9500	 0.5700
AE	 0.9520	 0.5800
AF	 0.9550	 0.5730
AG	 0.9270	 0.5530
AH	 0.9570	 0.5990
AI	 0.9700	 0.5910
AJ	 0.9570	 0.5740
AK	 0.9890	 0.6560
AL	 0.9240	 0.5440
AM	 0.9290	 0.5770
AN	 0.9590	 0.5930
AO	 0.9510	 0.5610
AP	 0.9620	 0.5930



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Chain	Atom inclusion	Q-score
AQ	 0.9790	 0.6240
AR	 0.9040	 0.4830
AS	 0.9170	 0.5270
AT	 0.9440	 0.5720
AU	 0.9060	 0.5090
AV	 0.9290	 0.5300
AW	 0.9490	 0.5580
AX	 0.9680	 0.5870
AY	 0.7040	 0.4040
AZ	 0.9400	 0.5880
Aw	 0.7730	 0.3380
Ax	 0.9390	 0.4600
Ay	 0.5110	 0.2100
Az	 0.7640	 0.2910
B	 0.9740	 0.5180
D	 0.9830	 0.6350
E	 0.9720	 0.6260
F	 0.9820	 0.6360
H	 0.5850	 0.3310
I	 0.7680	 0.4640
J	 0.8970	 0.4790
K	 0.9760	 0.6420
L	 0.9830	 0.6300
M	 0.9780	 0.6270
N	 0.9660	 0.6120
O	 0.9770	 0.6180
P	 0.9820	 0.6270
Q	 0.9350	 0.5810
R	 0.9810	 0.6560
S	 0.9720	 0.6220
T	 0.9800	 0.6390
U	 0.9160	 0.5650
V	 0.9320	 0.5310
W	 0.9810	 0.6490
X	 0.9460	 0.5770
Y	 0.9710	 0.6130
Z	 0.9630	 0.6260
a	 0.9150	 0.5520
b	 0.9840	 0.6320
c	 0.9440	 0.5700
d	 0.8920	 0.4830
e	 0.8790	 0.4870

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Chain	Atom inclusion	Q-score
f	 0.9100	 0.5390
g	 0.9610	 0.6090
h	 0.9450	 0.5290
i	 0.9890	 0.6640
j	 0.9330	 0.5710
k	 0.9420	 0.5240
l	 0.9220	 0.5190
m	 0.8500	 0.4660
o	 0.9870	 0.6520
p	 0.8840	 0.5060
q	 0.7490	 0.4140
r	 0.9590	 0.5940
s	 0.9620	 0.5980
t	 0.3910	 0.2650
u	 0.3360	 0.2270
v	 0.0000	 0.1330
w	 0.0000	 0.0430
x	 0.0000	 0.0870
y	 0.0000	 0.0560
z	 0.1860	 0.1010