



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 11:17 am GMT

PDB ID : 6ZSG
EMDB ID : EMD-11397
Title : Human mitochondrial ribosome in complex with mRNA, A-site tRNA, P-site tRNA and E-site tRNA
Authors : Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.
Deposited on : 2020-07-15
Resolution : 4.00 Å(reported)

This is a wwPDB EM Validation Summary 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

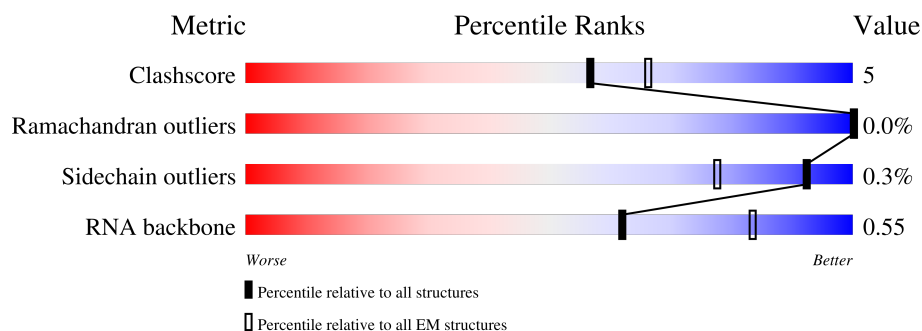
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	188	
2	1	65	
3	2	92	
4	3	188	
5	4	103	
6	5	423	
7	6	380	







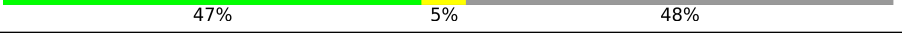

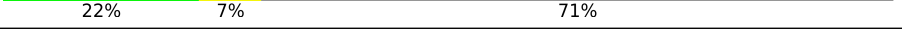

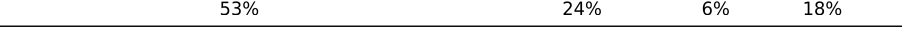
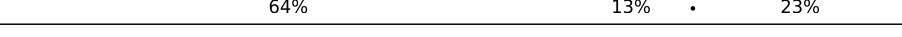

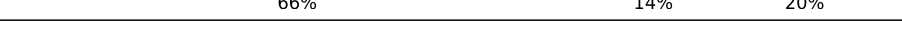


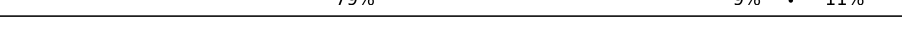

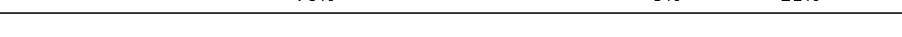






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Mol	Chain	Length	Quality of chain
8	7	338	
9	8	206	
10	9	137	
11	XA	1561	
12	A0	218	
13	A1	323	
14	A2	118	
15	A3	199	
16	A4	689	
17	AA	954	
18	AB	296	
19	AC	167	
20	AD	430	
21	AE	125	
22	AF	242	
23	AG	396	
24	AH	201	
25	AI	194	
26	AJ	138	
27	AK	128	
28	AL	257	
29	AM	137	
30	AN	130	
31	AO	258	
32	AP	142	

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Mol	Chain	Length	Quality of chain
33	AQ	86	
34	AR	360	
35	AS	190	
36	AT	173	
37	AU	205	
38	AV	414	
39	AW	187	
40	AX	398	
41	AY	395	
42	AZ	106	
43	XB	72	
44	XD	305	
45	XE	348	
46	XF	311	
47	XH	267	
48	XI	261	
49	XJ	192	
50	XK	178	
51	XL	145	
52	XM	296	
53	XN	251	
54	XO	175	
55	XP	180	
56	XQ	292	
57	XR	149	

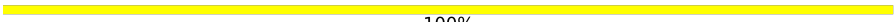
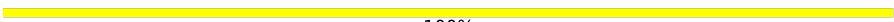









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Mol	Chain	Length	Quality of chain
58	XS	205	
59	XT	206	
60	XU	153	
61	XV	216	
62	XW	148	
63	XX	256	
64	XY	250	
65	XZ	161	
66	a	142	
67	b	215	
68	c	332	
69	d	306	
70	e	279	
71	f	212	
72	g	166	
73	h	158	
74	i	128	
75	j	123	
76	k	112	
77	l	138	
78	m	128	
79	o	102	
80	p	206	
81	q	222	
82	r	196	

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Mol	Chain	Length	Quality of chain
83	r1	14	 100%
84	r2	76	 100%
85	r3	75	 100%
86	r4	75	 100%
87	s	439	 84% 16%
88	t1	198	 23% 77%
88	t2	198	 15% 85%
88	t3	198	 15% 85%
88	t4	198	 15% 85%
88	t5	198	 15% 85%
88	t6	198	 14% 86%

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 315349 atoms, of which 143121 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	108	Total	C	H	N	O	S	0	0
			1783	545	903	172	157	6		

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	53	Total	C	H	N	O	S	0	0
			919	281	480	84	72	2		

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	46	Total	C	H	N	O	S	0	0
			783	233	407	83	59	1		

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	95	Total	C	H	N	O	S	0	0
			1714	539	883	162	127	3		

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	38	Total	C	H	N	O	S	0	0
			702	217	361	72	48	4		

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	393	Total	C	H	N	O	S	0	0
			6405	2070	3201	559	564	11		

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	354	Total	C	H	N	O	S	0	0
			5788	1881	2841	525	532	9		

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	291	Total	C	H	N	O	S	0	0
			4740	1514	2375	401	432	18		

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	8	139	Total	C	H	N	O	S	0	0
			2377	747	1202	208	218	2		

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	9	124	Total	C	H	N	O	S	0	0
			1983	644	987	170	180	2		

- Molecule 11 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	XA	1499	Total	C	H	N	O	P	0	0
			47993	14284	16160	5756	10294	1499		

- Molecule 12 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	A0	201	Total	C	H	N	O	S	0	0
			3369	1065	1685	322	292	5		

- Molecule 13 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	A1	275	Total	C	H	N	O	S	0	0
			4491	1414	2261	380	425	11		

- Molecule 14 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	A2	116	Total	C	H	N	O	S	0	0
			1889	574	964	181	162	8		

- Molecule 15 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	A3	69	Total	C	H	N	O	S	0	0
			1292	393	682	130	86	1		

- Molecule 16 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	A4	552	Total	C	H	N	O	S	0	0
			8955	2866	4485	756	820	28		

- Molecule 17 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AA	924	Total	C	H	N	O	P	0	0
			29593	8800	9965	3540	6364	924		

- Molecule 18 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AB	218	Total	C	H	N	O	S	0	0
			3545	1135	1769	322	309	10		

- Molecule 19 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AC	132	Total	C	H	N	O	S	0	0
			2170	699	1088	195	184	4		

- Molecule 20 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AD	343	Total	C	H	N	O	S	0	0
			5500	1706	2784	515	482	13		

- Molecule 21 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AE	122	Total	C	H	N	O	S	0	0
			1973	614	1001	177	177	4		

- Molecule 22 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AF	201	Total	C	H	N	O	S	0	0
			3384	1069	1716	305	283	11		

- Molecule 23 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AG	304	Total	C	H	N	O	S	0	0
			4996	1593	2491	444	454	14		

- Molecule 24 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AH	135	Total	C	H	N	O	S	0	0
			2241	712	1136	187	203	3		

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AI	136	Total	C	H	N	O	S	0	0
			2063	637	1052	192	178	4		

- Molecule 26 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AJ	108	Total	C	H	N	O	S	0	0
			1725	521	887	169	142	6		

- Molecule 27 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AK	101	Total	C	H	N	O	S	0	0
			1746	537	885	179	140	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AL	164	Total	C	H	N	O	S	0	0
			2854	883	1472	257	235	7		

- Molecule 29 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	AM	116	Total	C	H	N	O	S	0	0
			1871	582	951	182	150	6		

- Molecule 30 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	AN	107	Total	C	H	N	O	S	0	0
			1754	549	908	153	141	3		

- Molecule 31 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	AO	185	Total	C	H	N	O	S	0	0
			3017	970	1489	285	267	6		

- Molecule 32 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	AP	95	Total	C	H	N	O	S	0	0
			1561	493	796	132	132	8		

- Molecule 33 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	AQ	85	Total	C	H	N	O	S	0	0
			1483	455	749	149	123	7		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 34 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	AR	250	Total	C	H	N	O	S	0	0
			4134	1314	2074	353	385	8		

- Molecule 35 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	AS	133	Total	C	H	N	O	S	0	0
			2203	709	1103	196	194	1		

- Molecule 36 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	AT	162	Total	C	H	N	O	S	0	0
			2672	850	1342	231	238	11		

- Molecule 37 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	AU	173	Total	C	H	N	O	S	0	0
			2932	900	1471	294	263	4		

- Molecule 38 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	AV	349	Total	C	H	N	O	S	0	0
			5729	1841	2862	478	536	12		

- Molecule 39 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	AW	97	Total	C	H	N	O	S	0	0
			1551	486	785	137	139	4		

- Molecule 40 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	AX	348	Total	C	H	N	O	S	0	0
			5619	1802	2805	491	510	11		

- Molecule 41 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	AY	113	Total	C	H	N	O	S	0	0
			1868	621	912	157	176	2		

- Molecule 42 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	AZ	86	Total	C	H	N	O	S	0	0
			1465	467	734	131	129	4		

- Molecule 43 is a RNA chain called mitochondrial tRNA^{Val}.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	XB	59	Total	C	H	N	O	P	0	0
			1890	563	635	227	406	59		

- Molecule 44 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	XD	236	Total	C	H	N	O	S	0	0
			3739	1145	1897	373	315	9		

- Molecule 45 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	XE	304	Total	C	H	N	O	S	0	0
			4798	1539	2402	416	430	11		

- Molecule 46 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	XF	250	Total	C	H	N	O	S	0	0
			4058	1294	2045	365	348	6		

- Molecule 47 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	XH	95	Total	C	H	N	O		0	0
			1616	498	832	152	134			

- Molecule 48 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	XI	211	Total	C	H	N	O	S	0	0
			3474	1086	1783	303	291	11		

- Molecule 49 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	XJ	170	Total	C	H	N	O	S	0	0
			2657	825	1366	230	234	2		

- Molecule 50 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	XK	177	Total	C	H	N	O	S	0	0
			2899	934	1448	259	251	7		

- Molecule 51 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	XL	115	Total	C	H	N	O	S	0	0
			1830	559	941	171	154	5		

- Molecule 52 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	XM	287	Total	C	H	N	O	S	0	0
			4682	1472	2377	425	402	6		

- Molecule 53 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	XN	221	Total	C	H	N	O	S	0	0
			3586	1138	1808	325	305	10		

- Molecule 54 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	XO	152	Total	C	H	N	O	S	0	0
			2528	784	1283	239	215	7		

- Molecule 55 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
55	XP	143	Total	C	H	N	O	S	0	0
			2326	729	1162	223	207	5		

- Molecule 56 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	XQ	238	Total	C	H	N	O	S	0	0
			4000	1268	2022	352	349	9		

- Molecule 57 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
57	XR	140	Total	C	H	N	O	S	0	0
			2367	732	1214	231	186	4		

- Molecule 58 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
58	XS	160	Total	C	H	N	O	S	0	0
			2638	829	1354	226	225	4		

- Molecule 59 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	XT	166	Total	C	H	N	O	S	0	0
			2778	875	1410	254	232	7		

- Molecule 60 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	XU	141	Total	C	H	N	O	S	0	0
			2335	743	1164	222	203	3		

- Molecule 61 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	XV	202	Total	C	H	N	O	S	0	0
			3304	1051	1656	294	295	8		

- Molecule 62 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	XW	111	Total	C	H	N	O	S	0	0
			1769	558	898	164	146	3		

- Molecule 63 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	XX	243	Total	C	H	N	O	S	0	0
			4089	1317	2054	351	362	5		

- Molecule 64 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	XY	178	Total	C	H	N	O	S	0	0
			3109	981	1575	295	254	4		

- Molecule 65 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	XZ	120	Total	C	H	N	O	S	0	0
			2008	626	1030	183	166	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
66	a	97	Total	C	H	N	O	S	0	0
			1590	512	777	145	151	5		

- Molecule 67 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	b	148	Total	C	H	N	O	S	0	0
			2358	733	1180	229	213	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
68	c	275	Total	C	H	N	O	S	0	0
			4437	1415	2220	383	410	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
69	d	216	Total	C	H	N	O	S	0	0
			3501	1125	1743	305	315	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
70	e	217	Total	C	H	N	O	S	0	0
			3529	1124	1767	310	323	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
71	f	143	Total	C	H	N	O	S	0	0
			2314	737	1165	187	221	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
72	g	132	Total	C	H	N	O	S	0	0
			2183	710	1086	191	194	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
73	h	108	Total	C	H	N	O	S	0	0
			1748	560	866	154	165	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
			1684	532	857	165	126	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
75	j	86	Total	C	H	N	O	S	0	0
			1367	426	678	134	127	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
76	k	95	Total	C	H	N	O	S	0	0
			1477	456	745	139	132	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
77	l	80	Total	C	H	N	O	S	0	0
			1327	427	654	118	125	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
78	m	60	Total	C	H	N	O	S	0	0
			1025	309	525	104	85	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
			1601	501	804	165	128	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
80	p	127	Total	C	H	N	O	S	0	0
			2141	661	1083	201	192	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	164	Total	C	H	N	O	S	0	0
			2738	858	1359	267	249	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
82	r	161	Total	C	H	N	O	S	0	0
			2653	834	1341	250	220	8		

- Molecule 83 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	r1	14	Total	C	N	O	P	0	0
			252	126	28	84	14		

- Molecule 84 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	r2	76	Total	C	N	O	P	0	0
			1485	723	230	456	76		

- Molecule 85 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	r3	75	Total	C	N	O	P	0	0
			1459	711	222	451	75		

- Molecule 86 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	r4	75	Total	C	N	O	P	0	0
			1464	713	226	450	75		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
87	s	370	Total	C	H	N	O	S	
			6059	1946	3023	542	534	14	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
88	t1	46	Total	C	H	N	O	2	0
			733	228	379	56	70		
88	t2	30	Total	C	H	N	O	0	0
			506	154	268	38	46		
88	t3	30	Total	C	H	N	O	0	0
			506	154	268	38	46		
88	t4	29	Total	C	H	N	O	0	0
			484	148	255	36	45		
88	t5	29	Total	C	H	N	O	0	0
			484	148	255	36	45		
88	t6	27	Total	C	H	N	O	0	0
			450	137	236	34	43		

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

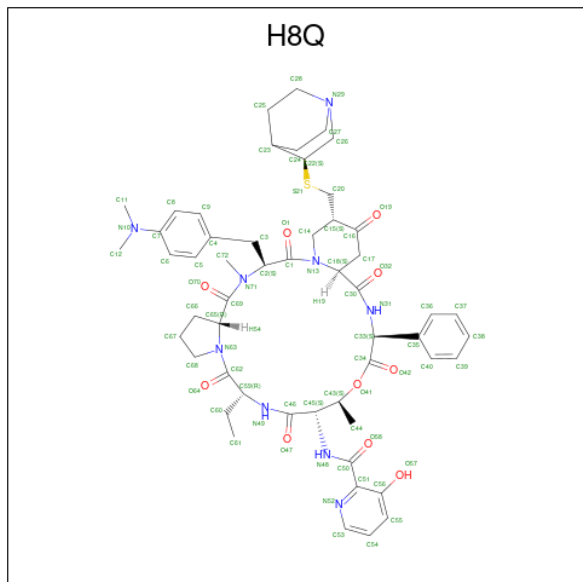
Mol	Chain	Residues	Atoms		AltConf
89	0	1	Total 1	Zn 1	0
89	4	1	Total 1	Zn 1	0
89	AB	1	Total 1	Zn 1	0
89	AO	1	Total 1	Zn 1	0
89	AP	1	Total 1	Zn 1	0
89	AT	1	Total 1	Zn 1	0
89	r	1	Total 1	Zn 1	0

- Molecule 90 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	2	1	Total 1	Mg 1	0
90	9	1	Total 1	Mg 1	0
90	XA	141	Total 141	Mg 141	0
90	AA	46	Total 46	Mg 46	0
90	XD	1	Total 1	Mg 1	0
90	XE	1	Total 1	Mg 1	0
90	XI	1	Total 1	Mg 1	0
90	XM	1	Total 1	Mg 1	0
90	XW	1	Total 1	Mg 1	0
90	g	1	Total 1	Mg 1	0

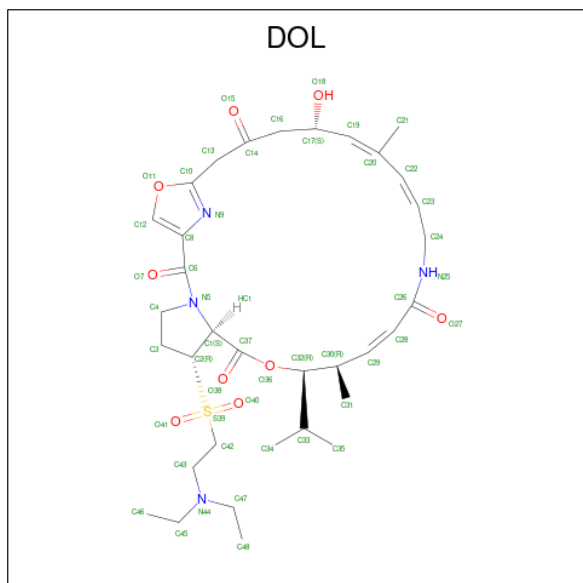
- Molecule 91 is {N}-[(3 {S},6 {R},12 {R},15 {S},16 {S},19 {S},22 {S},25 {S})-25-[[[3 {S}))-1-azabicyclo[2.2.2]octan-3-yl]sulfanylmethyl]-3-[[4-(dimethylamino)phenyl]methyl]-12-ethyl-4,16-dimethyl-2,5,11,14,18,21,24-heptakis(oxidanylidene)-19-phenyl-17-oxa-1,4,10,1

3,20-pentazatricyclo[20.4.0.0[^]{6,10}]hexacosan-15-yl]-3-oxidanyl-pyridine-2-carboxamide (three-letter code: H8Q) (formula: C₅₃H₆₇N₉O₁₀S).



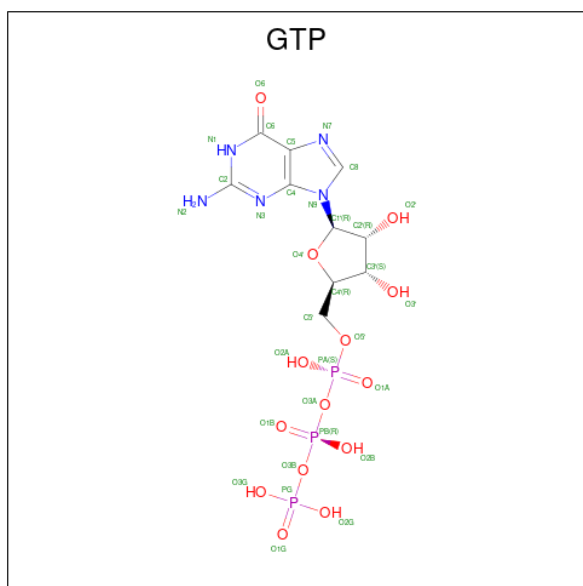
Mol	Chain	Residues	Atoms						AltConf
91	XA	1	Total	C	H	N	O	S	0
			140	53	67	9	10	1	

- Molecule 92 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C₃₄H₅₀N₄O₉S).



Mol	Chain	Residues	Atoms					AltConf	
92	XA	1	Total	C	H	N	O	S	0
			98	34	50	4	9	1	

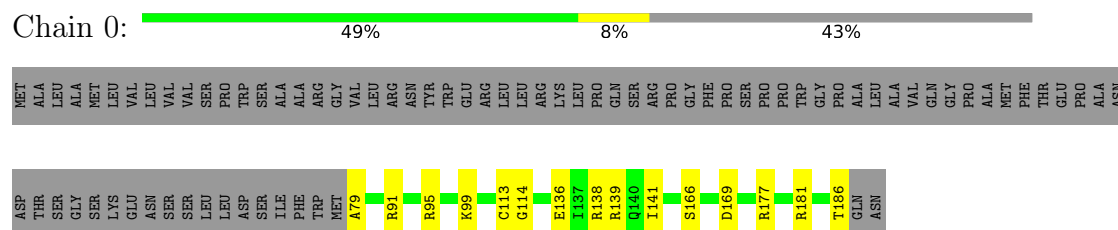
- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



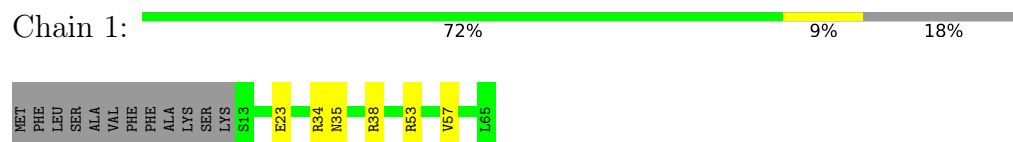
3 Residue-property plots

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. 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. 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.

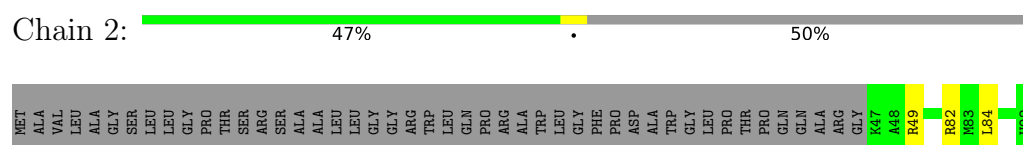
- Molecule 1: 39S ribosomal protein L32, mitochondrial



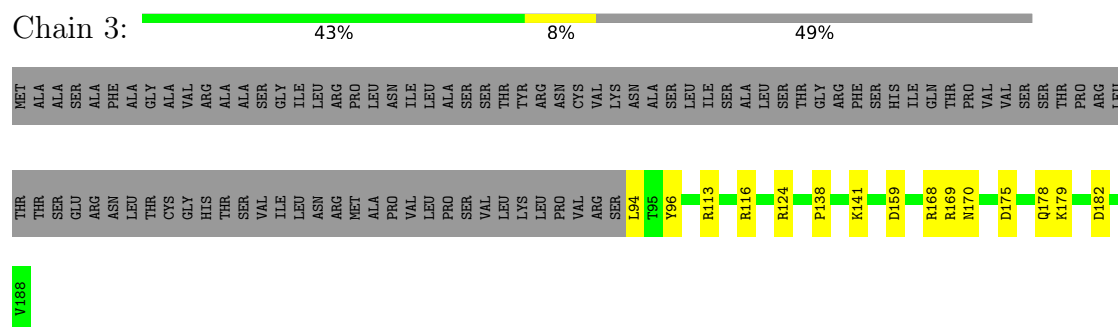
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial

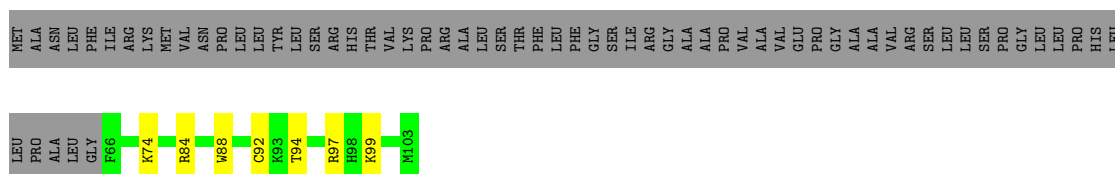


- Molecule 4: 39S ribosomal protein L35, mitochondrial



- Molecule 5: 39S ribosomal protein L36, mitochondrial





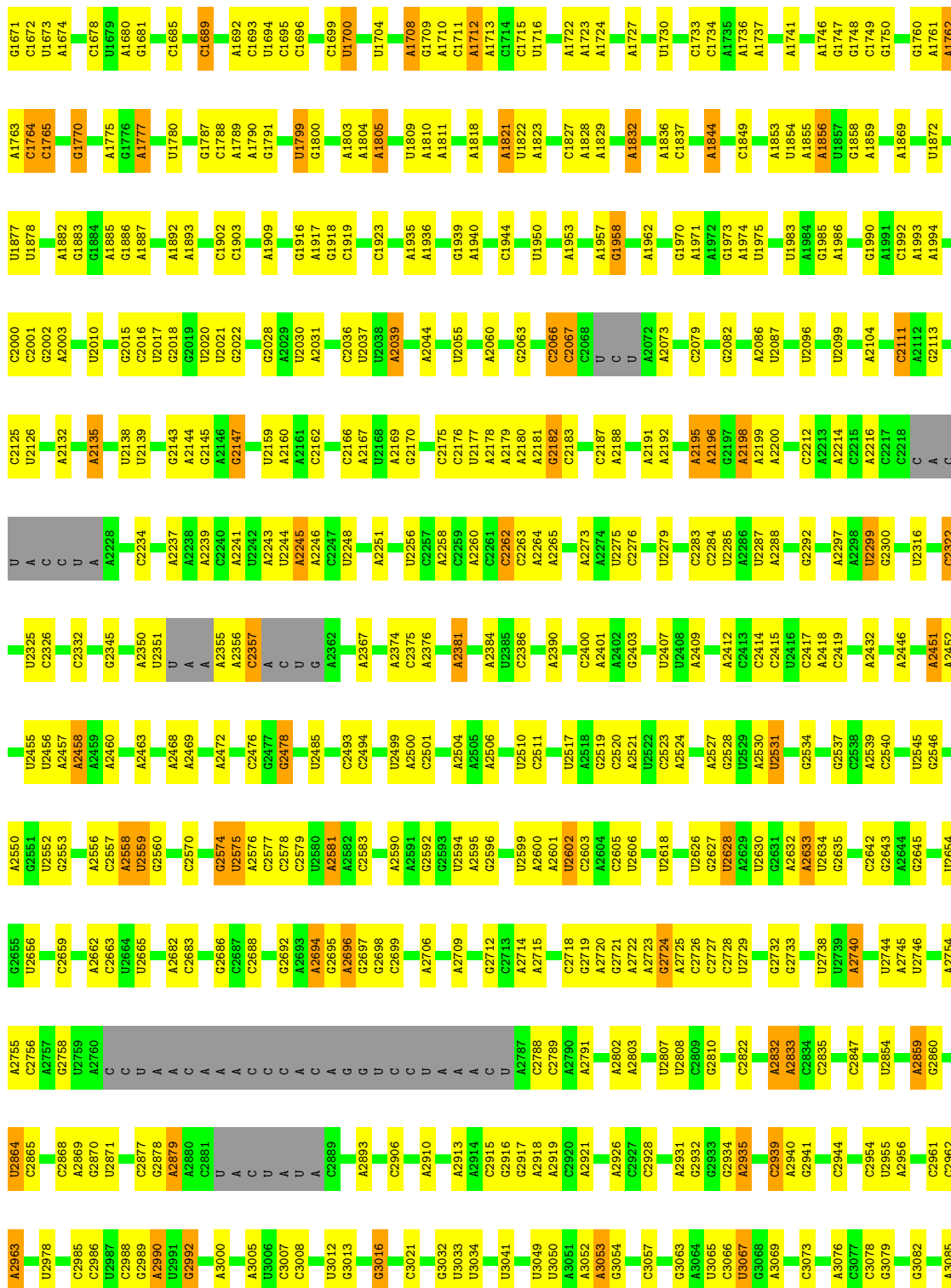
- Molecule 6: 39S ribosomal protein L37, mitochondrial

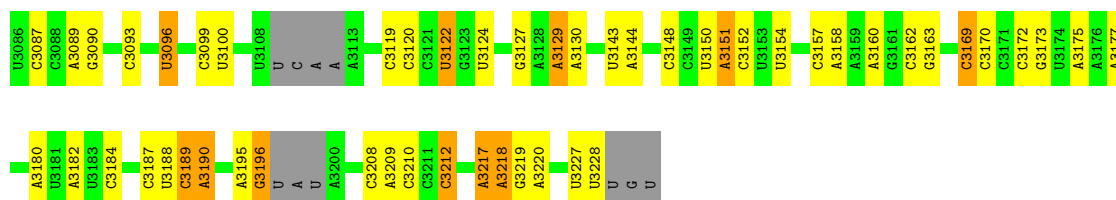
- Molecule 7: 39S ribosomal protein L38, mitochondrial

- Molecule 8: 39S ribosomal protein L39, mitochondrial

- Molecule 9: 39S ribosomal protein L40, mitochondrial

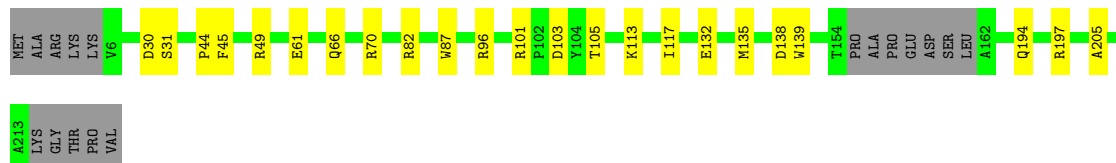
- Molecule 10: 39S ribosomal protein L41, mitochondrial





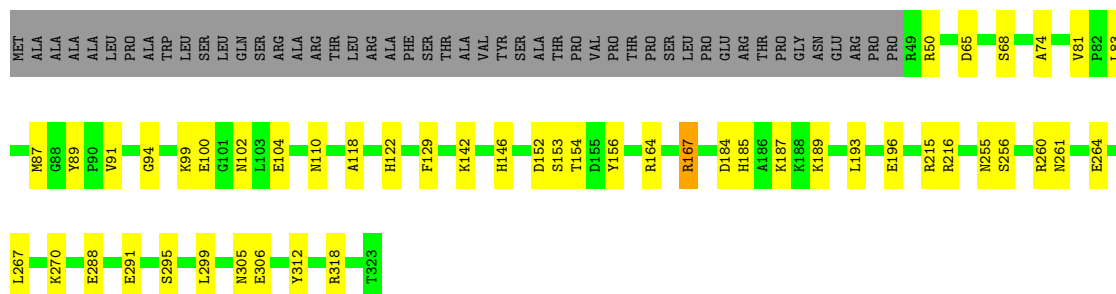
- Molecule 12: 28S ribosomal protein S34, mitochondrial

Chain A0: 82% 11% 8%



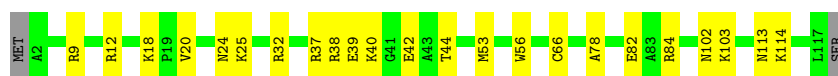
- Molecule 13: 28S ribosomal protein S35, mitochondrial

Chain A1: 70% 15% 15%



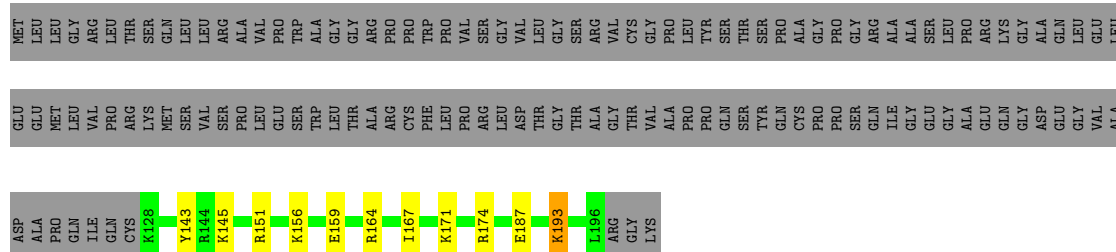
- Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2: 79% 19%



- Molecule 15: Aurora kinase A-interacting protein

Chain A3: 29% 5% 65%



- Molecule 16: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Response	Percentage
Yes	70%
No	10%
Don't know	20%

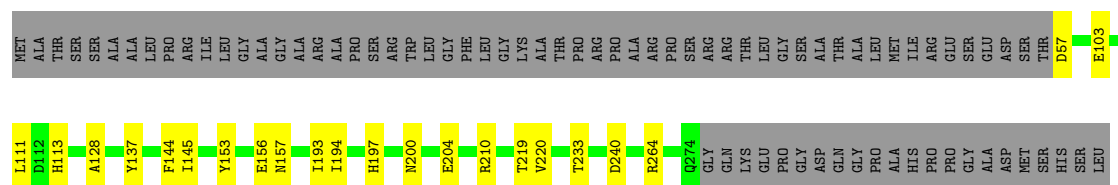


Device Type	Percentage
Smartphone	66%
Tablet	26%
Feature Phone	5%



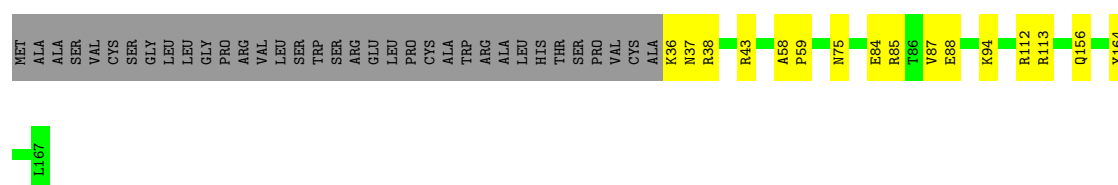
- Molecule 18: 28S ribosomal protein S2, mitochondrial

Chain AB:  66% 7% 26%



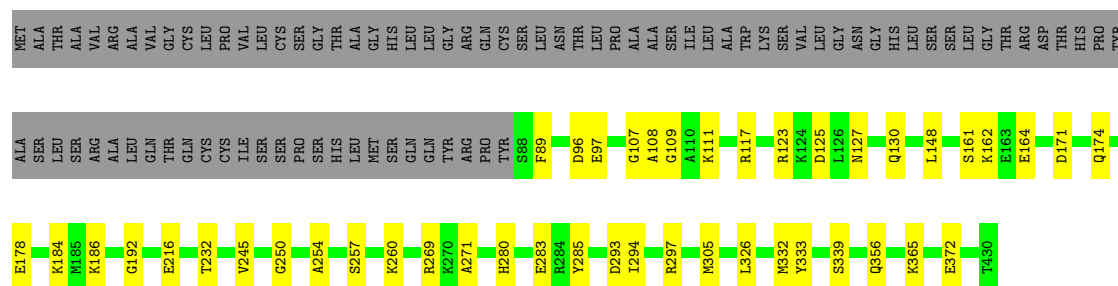
- Molecule 19: 28S ribosomal protein S24, mitochondrial

Chain AC:  69% 10% 21%




- Molecule 20: 28S ribosomal protein S5, mitochondrial

Chain AD:  69% 10% 20%



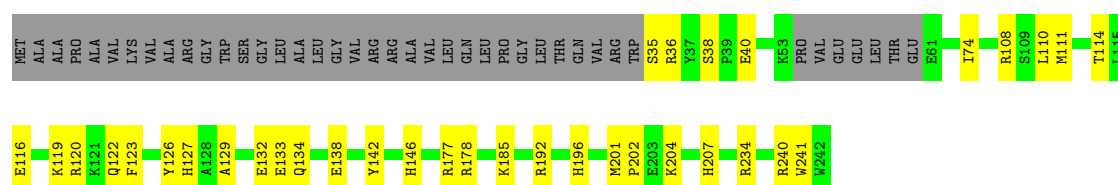
- Molecule 21: 28S ribosomal protein S6, mitochondrial

Chain AE:  82% 16% .

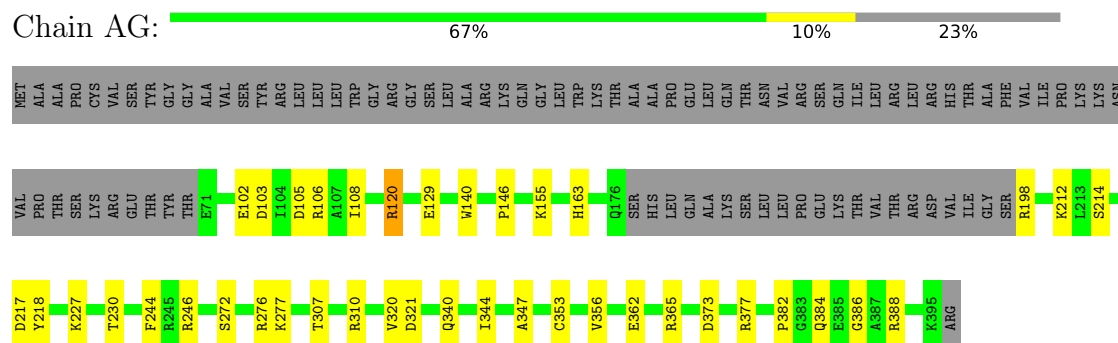


- Molecule 22: 28S ribosomal protein S7, mitochondrial

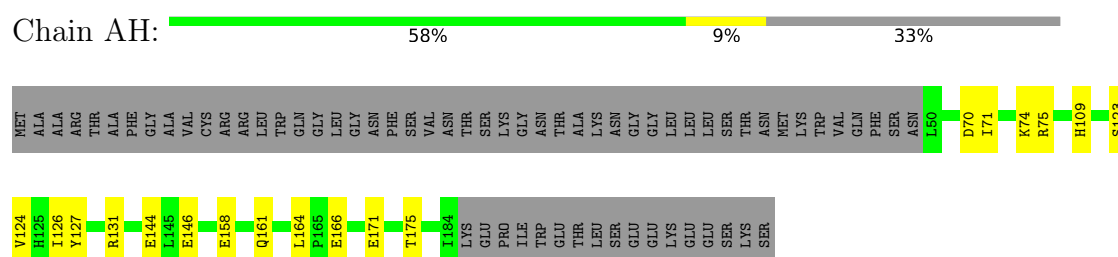
Chain AF:  69% 14% 17%



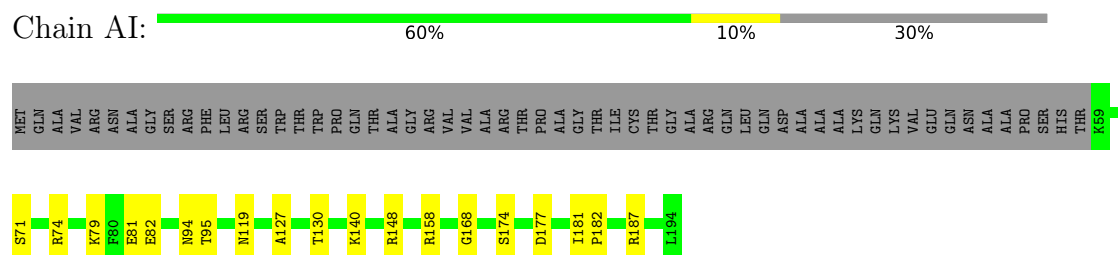
- Molecule 23: 28S ribosomal protein S9, mitochondrial



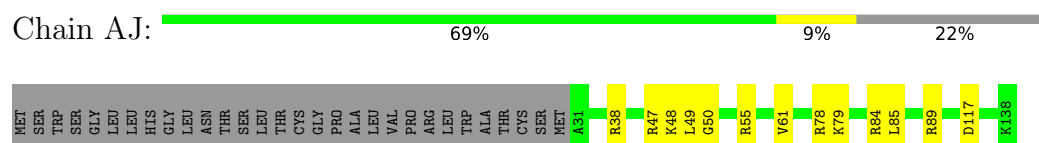
- Molecule 24: 28S ribosomal protein S10, mitochondrial



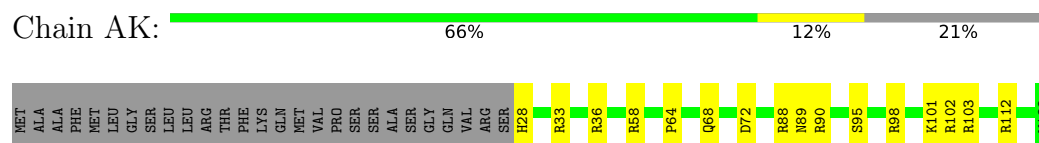
- Molecule 25: 28S ribosomal protein S11, mitochondrial



- Molecule 26: 28S ribosomal protein S12, mitochondrial

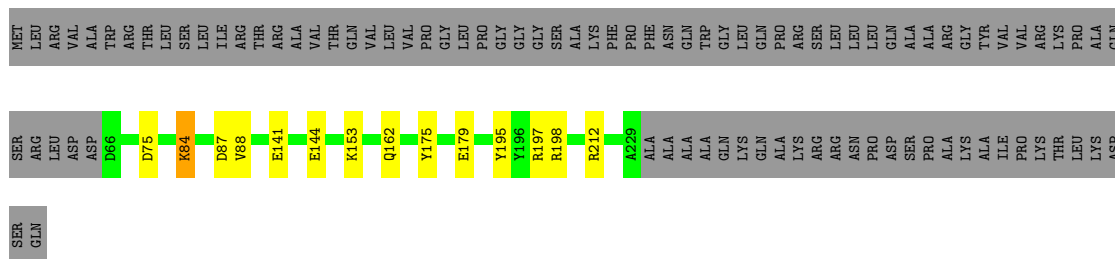


- Molecule 27: 28S ribosomal protein S14, mitochondrial

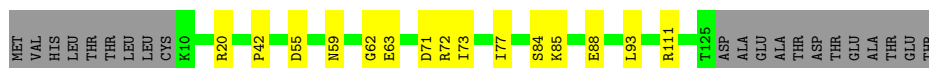
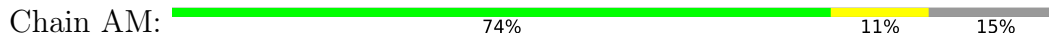


- Molecule 28: 28S ribosomal protein S15, mitochondrial





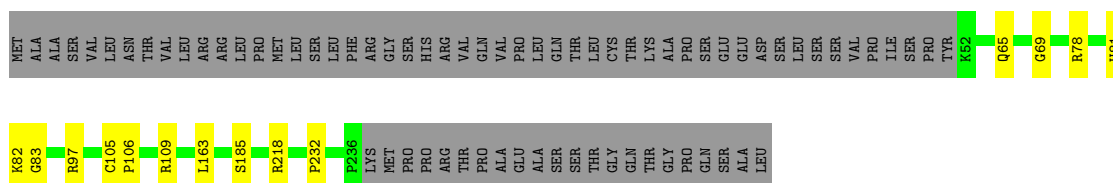
- Molecule 29: 28S ribosomal protein S16, mitochondrial



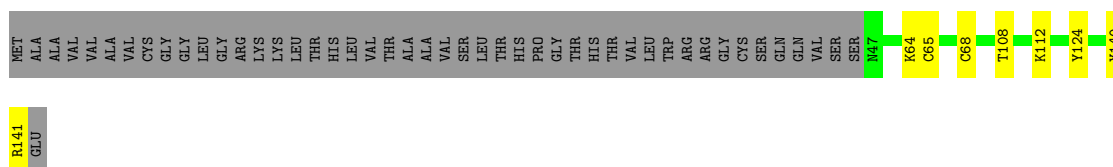
- Molecule 30: 28S ribosomal protein S17, mitochondrial



- Molecule 31: 28S ribosomal protein S18b, mitochondrial



- Molecule 32: 28S ribosomal protein S18c, mitochondrial

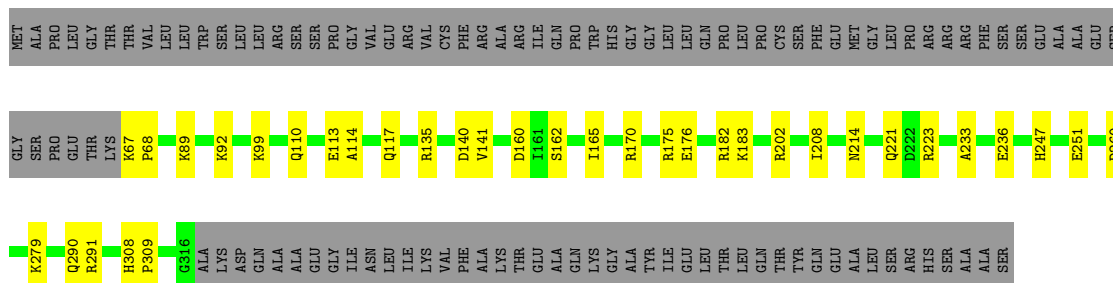


- Molecule 33: 28S ribosomal protein S21, mitochondrial



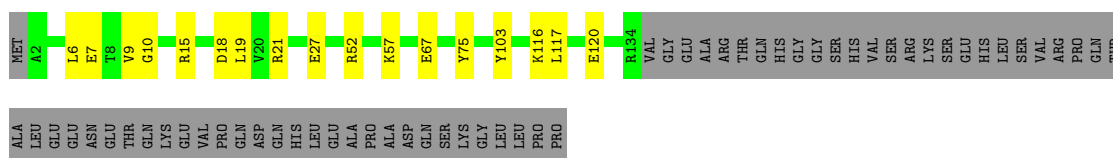
- Molecule 34: 28S ribosomal protein S22, mitochondrial

Chain AR:  60% 10% 31%




- Molecule 35: 28S ribosomal protein S23, mitochondrial

Chain AS:  61% 9% 30%



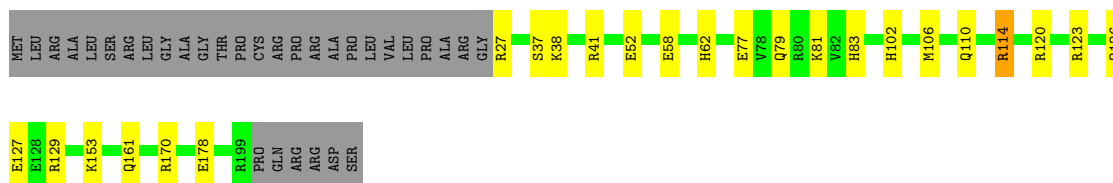
- Molecule 36: 28S ribosomal protein S25, mitochondrial

Chain AT:  83% 11% 6%



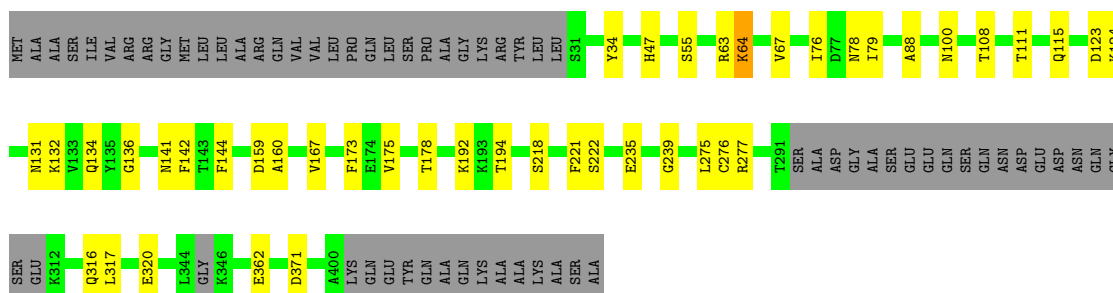
- Molecule 37: 28S ribosomal protein S26, mitochondrial

Chain AU:  73% 11% 16%



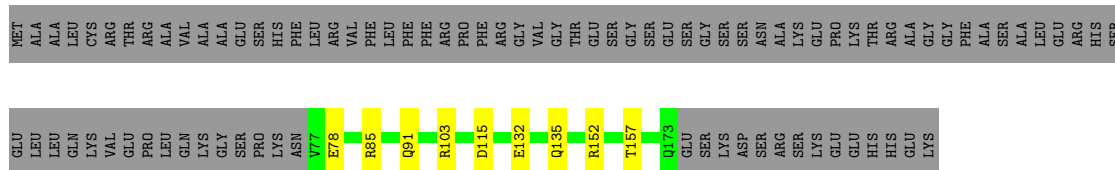
- Molecule 38: 28S ribosomal protein S27, mitochondrial

Chain AV:  74% 10% 16%




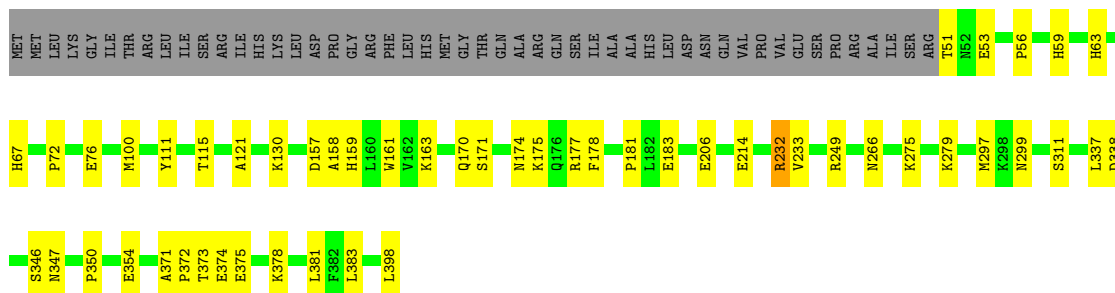
- Molecule 39: 28S ribosomal protein S28, mitochondrial

Chain AW:  47% 5% 48%



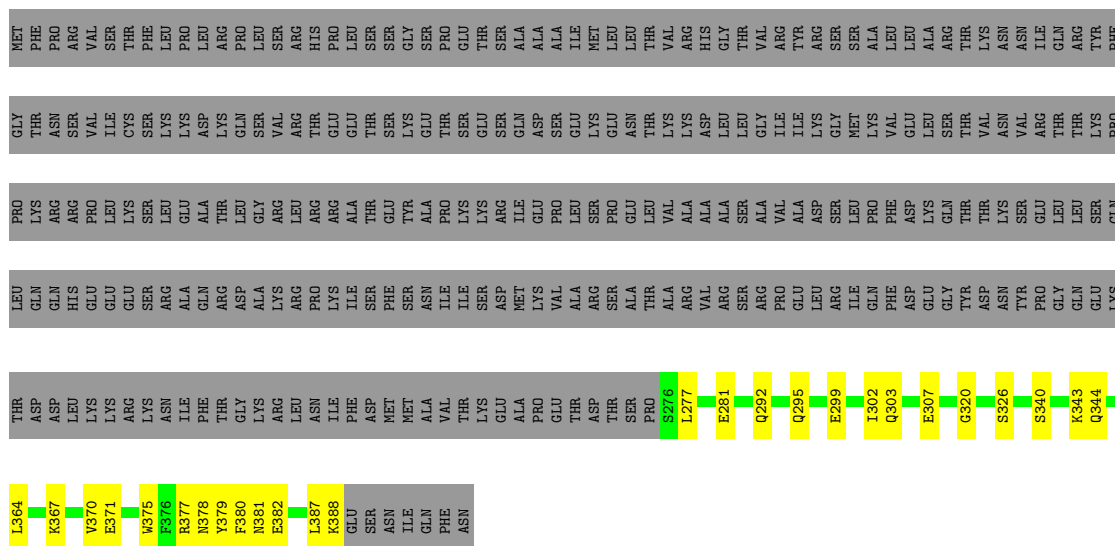
- Molecule 40: 28S ribosomal protein S29, mitochondrial

Chain AX:  74% 13% 13%



- Molecule 41: 28S ribosomal protein S31, mitochondrial

Chain AY:  22% 7% 71%

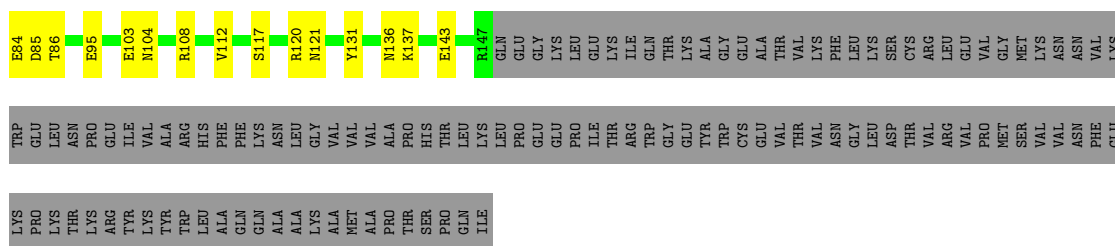


- Molecule 42: 28S ribosomal protein S33, mitochondrial

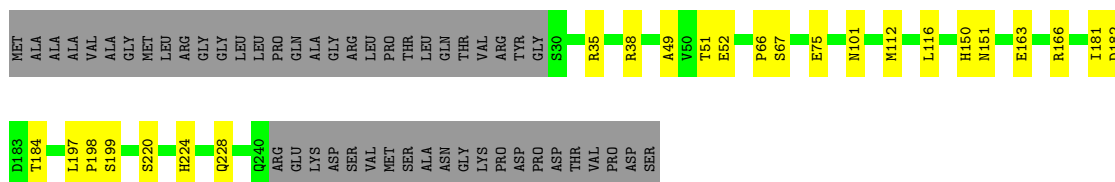
Chain AZ:  72% 9% 19%



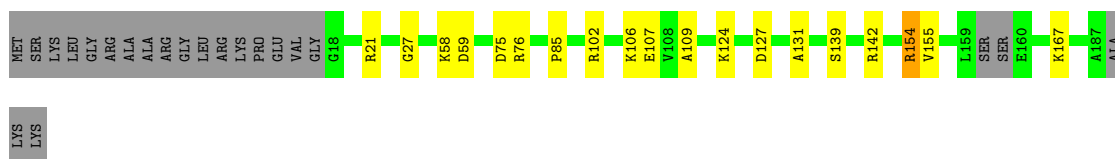
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | ALA | PRO | VAL | VAL | THR | ALA | ALA | GLY | ARG | ALA | ALA | LEU | LEU | ARG | GLY | GLY | VAL | GLN | GLU | LEU | LEU | ARG | PRO | HIS | ARG | GLU | GLY | ASN | ALA | ALA | ASP | LEU | ALA | CYS | ASN | PHE | SER | LEU | LEU | GLN | ASN | ARG | GLY | T63 | R58 | R75 | R76 | H77 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



- Molecule 48: 39S ribosomal protein L10, mitochondrial



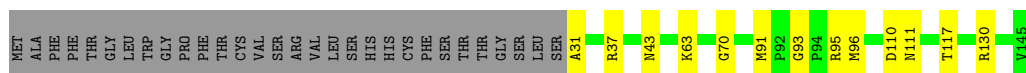
- Molecule 49: 39S ribosomal protein L11, mitochondrial



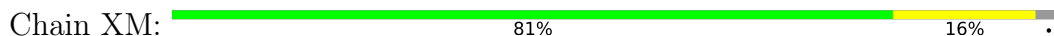
- Molecule 50: 39S ribosomal protein L13, mitochondrial



- Molecule 51: 39S ribosomal protein L14, mitochondrial



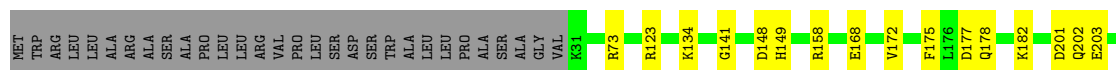
- Molecule 52: 39S ribosomal protein L15, mitochondrial





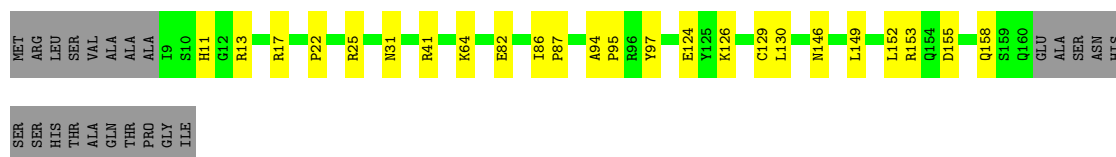
- Molecule 53: 39S ribosomal protein L16, mitochondrial

Chain XN: 79% 9% 12%



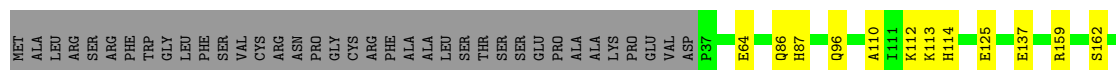
- Molecule 54: 39S ribosomal protein L17, mitochondrial

Chain XO: 73% 14% 13%



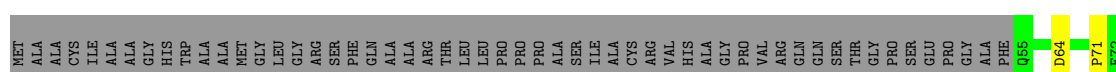
- Molecule 55: 39S ribosomal protein L18, mitochondrial

Chain XP: 72% 7% 21%



- Molecule 56: 39S ribosomal protein L19, mitochondrial

Chain XQ: 71% 11% 18%



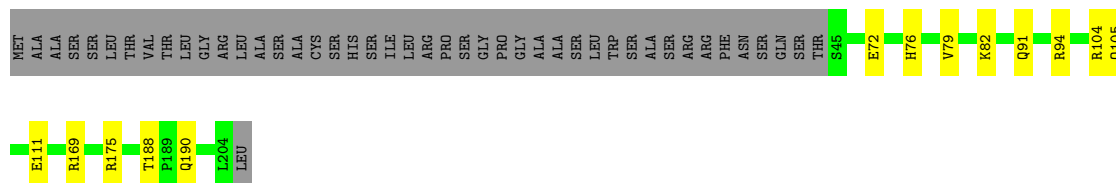
- Molecule 57: 39S ribosomal protein L20, mitochondrial

Chain XR: 80% 14% 6%




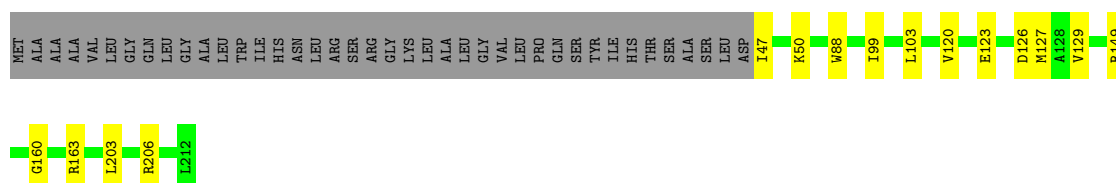
- Molecule 58: 39S ribosomal protein L21, mitochondrial

Chain XS:  72% 6% 22%



- Molecule 59: 39S ribosomal protein L22, mitochondrial

Chain XT:  73% 7% 19%




- Molecule 60: 39S ribosomal protein L23, mitochondrial

Chain XU:  86% 7% 8%



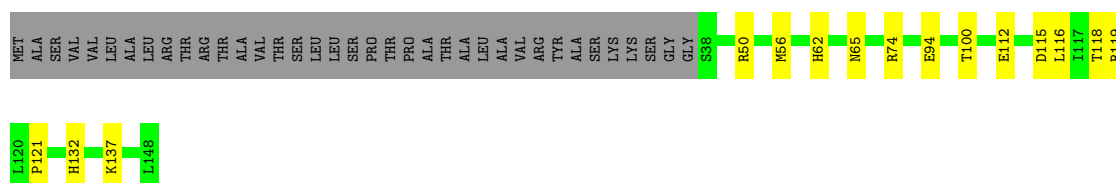
- Molecule 61: 39S ribosomal protein L24, mitochondrial

Chain XV:  83% 11% 6%




- Molecule 62: 39S ribosomal protein L27, mitochondrial

Chain XW:  65% 10% 25%

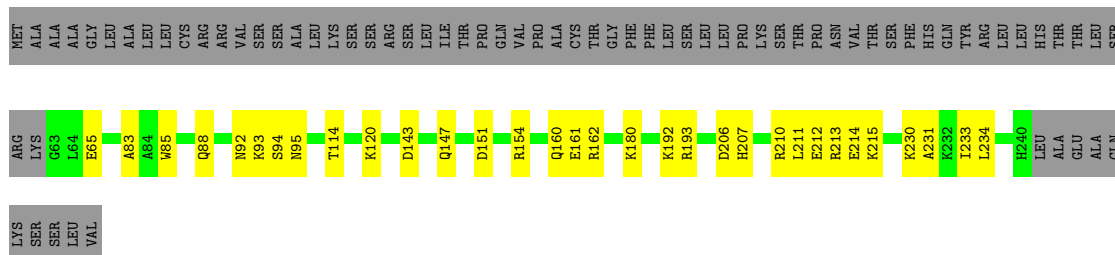


- Molecule 63: 39S ribosomal protein L28, mitochondrial

Chain XX:  81% 14% 5%

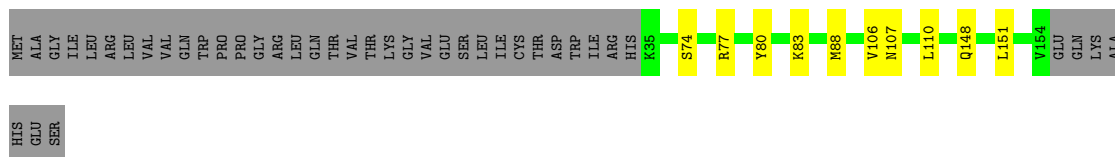
- Molecule 64: 39S ribosomal protein L47, mitochondrial

Chain XY: 58% 13% 29%



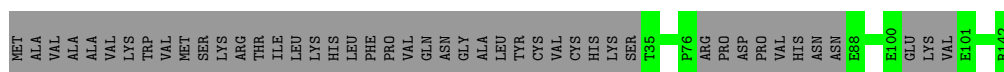
- Molecule 65: 39S ribosomal protein L30, mitochondrial

Chain XZ:  68% 6% 25%



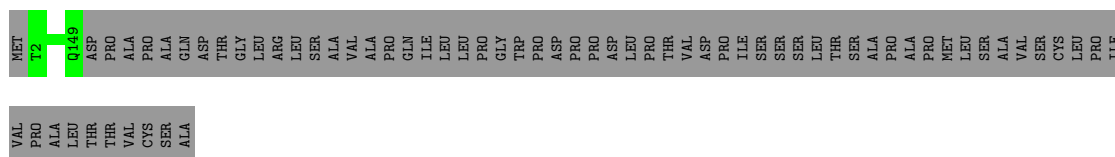
- Molecule 66: 39S ribosomal protein L42, mitochondrial

Chain a:  68% 32%



- Molecule 67: 39S ribosomal protein L43, mitochondrial

Chain b: 69% 31%



- Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c: 83% 17%



- Molecule 70: 39S ribosomal protein L46, mitochondrial

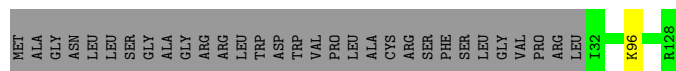
- Molecule 71: 39S ribosomal protein L48, mitochondrial

- Molecule 72: 39S ribosomal protein L49, mitochondrial

- Molecule 73: 39S ribosomal protein L50, mitochondrial

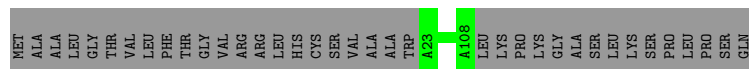
- Molecule 74: 39S ribosomal protein L51, mitochondrial

Chain i:  75% 24%



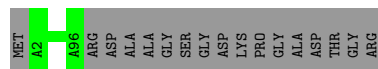
- Molecule 75: 39S ribosomal protein L52, mitochondrial

Chain j:  70% 30%



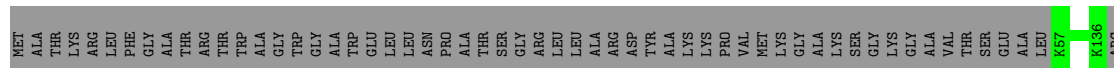
- Molecule 76: 39S ribosomal protein L53, mitochondrial

Chain k:  85% 15%



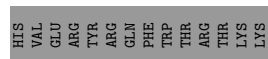
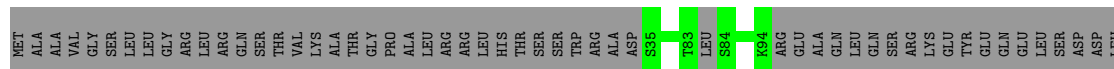
- Molecule 77: 39S ribosomal protein L54, mitochondrial

Chain l:  58% 42%



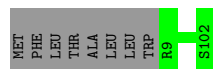
- Molecule 78: 39S ribosomal protein L55, mitochondrial

Chain m:  47% 53%



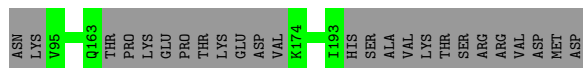
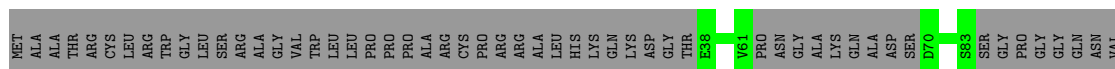
- Molecule 79: Ribosomal protein 63, mitochondrial

Chain o:  92% 8%



- Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:  62% 38%




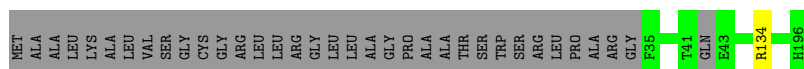
- Molecule 81: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:  73% 26%

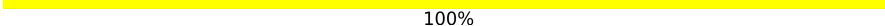


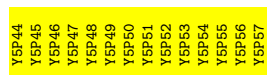
- Molecule 82: 39S ribosomal protein S18a, mitochondrial

Chain r:  82% 18%



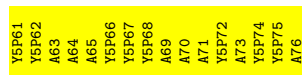
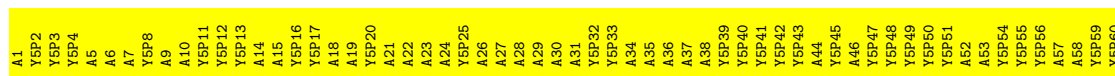
- Molecule 83: mRNA

Chain r1:  100%

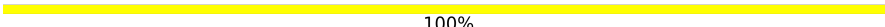


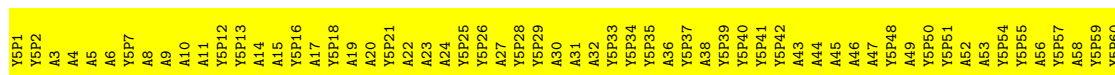
- Molecule 84: A-site tRNA

Chain r2:  100%



- Molecule 85: P-site tRNA

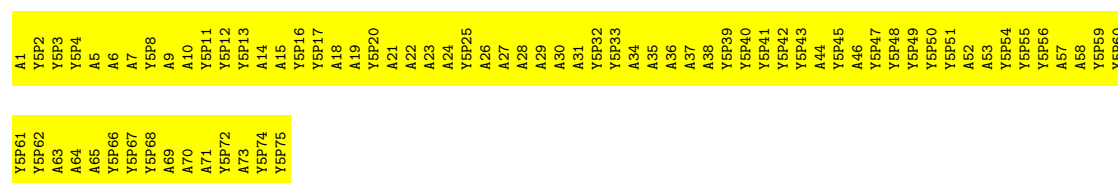
Chain r3:  100%



- Molecule 86: E-site tRNA

Chain r4:

100%

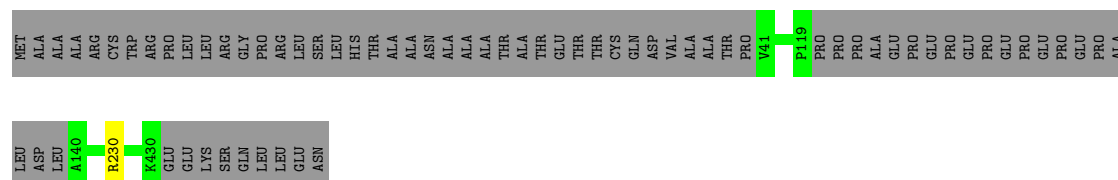


- Molecule 87: 39S ribosomal protein S30, mitochondrial

Chain s:

84%

16%

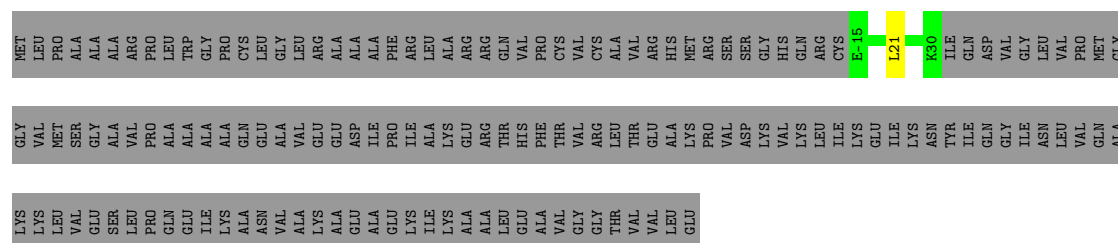


- Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain t1:

23%

77%

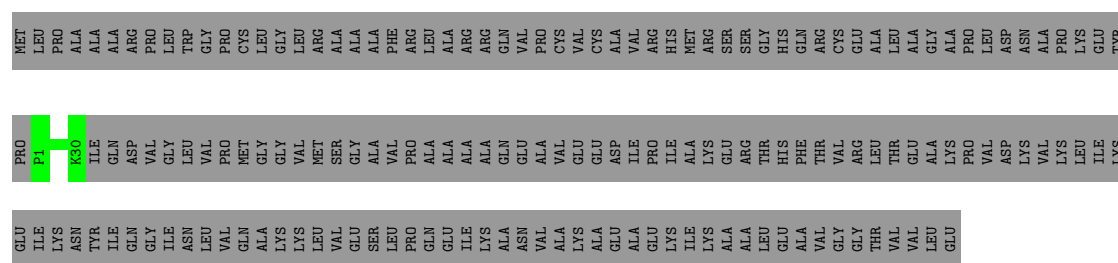


- Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain t2:

15%

85%

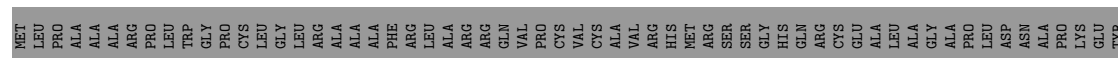


- Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain t3:

15%

85%



PRO	PI	K27	K30	ILE	GLN	ASP	VAL	GLY	LEU	VAL	PRO	MET	GLY	GLY	VAL	MET	SER	GLY	ALA	VAL	PRO	PRO	ALA	ALA	ALA	GLN	ASN	GLY	ALA	VAL	VAL	GLY	GLY	ASP	ILE	PRO	ILE	ALA	LYS	GLY	ALA	ARG	VAL	ARG	LEU	THR	THR	HIS	PHE	THR	VAL	ARG	LEU	THR	GLY	ALA	LYS	PRO	ASP	LYS	VAL	LYS	LEU
ILE	LYS	GLY	ILE	LYS	ASN	TYR	ILE	GLN	ILE	GLY	ASN	VAL	GLN	ALA	LYS	LEU	VAL	GLY	SER	LEU	GLN	GLY	ILE	LYS	ASN	VAL	ALA	VAL	ALA	LYS	ALA	GLY	ILE	LYS	ILE	ALA	LYS	LYS	ALA	ALA	LEU	GLY	GLY	THR	THR	VAL	VAL	LEU	GLY	GLY	THR	VAL	VAL	LEU	GLY								

• Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain t4: 15% 85%

LEU	PRO	ALA	ALA	ALA	ARG	PRO	LEU	TRP	GLY	LEU	VAL	CYS	LEU	GLY	ARG	ALA	ALA	ALA	PHE	GLY	VAL	PRO	ALA	ARG	ARG	GLN	VAL	ASN	CYS	VAL	CYS	ALA	VAL	ASP	VAL	ARG	HIS	MET	ARG	SER	GLY	GLY	HIS	ARG	CYS	THR	PHE	THR	VAL	GLY	ALA	LEU	ALA	GLY	VAL	ALA	PRO	LEU	ASP	ASN	ALA	PRO	LYS	GLU	TYR	
PRO	P1	L29	LYS	ILE	GLN	ASP	VAL	GLY	GLY	GLY	VAL	PRO	MET	GLY	GLY	VAL	MET	SER	GLY	GLY	ALA	VAL	VAL	PRO	ALA	ALA	ALA	GLN	GLU	ASN	VAL	VAL	GLU	ALA	GLU	ASP	VAL	ARG	ILE	PRO	ILE	ALA	LYS	GLY	GLY	ALA	THR	HIS	ARG	THR	THR	VAL	THR	THR	GLY	ALA	LYS	PRO	VAL	ASP	VAL	LYS	VAL	LYS	LEU	ILE
LYS	GLU	ILE	LYS	ASN	TYR	ILE	GLN	GLY	ILE	ASN	LEU	VAL	GLN	ALA	LYS	LEU	VAL	GLY	SER	LEU	VAL	PRO	GLN	ILE	LYS	ASN	VAL	VAL	ALA	LYS	ALA	GLU	GLU	VAL	ALA	ALA	GLY	LYS	LYS	ALA	ALA	LEU	GLN	ALA	VAL	THR	VAL	GLY	THR	VAL	VAL	LEU	GLU													

• Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain t5: 15% 85%

LEU	PRO	ALA	ALA	ARG	PRO	LEU	TRP	GLY	CYS	LEU	GLY	ARG	ALA	ALA	ALA	PHE	GLY	VAL	PRO	ALA	ARG	ARG	GLN	VAL	PRO	CYS	VAL	CYS	VAL	ALA	VAL	ARG	HIS	MET	ARG	SER	SER	GLY	HIS	GLN	GLN	ARG	CYS	GLU	ALA	ALA	LEU	PRO	ALA	ALA	PRO	LYS	GLU	TYR						
PRO	P1	L29	LYS	ILE	GLN	ASP	VAL	GLY	LEU	VAL	PRO	MET	GLY	GLY	VAL	MET	SER	GLY	ALA	VAL	PRO	ALA	ALA	ALA	ALA	GLN	GLU	ALA	VAL	VAL	GLU	ASP	ILE	PRO	ILE	ALA	LYS	GLU	ARG	THR	HIS	PHE	THR	VAL	ARG	LEU	THR	THR	GLU	ALA	LYS	PRO	VAL	ASP	ASN	ALA	PRO	LYS	LEU	ILE
LYS	GLU	ILE	LYS	ASN	TYR	ILE	GLN	GLY	ILE	ASN	LEU	VAL	GLN	ALA	LYS	LEU	VAL	SER	LEU	VAL	PRO	GLN	ILE	LYS	ASN	VAL	VAL	ALA	LYS	ALA	GLU	GLU	VAL	ALA	ALA	GLY	LYS	ALA	ALA	LEU	GLN	ALA	VAL	THR	VAL	VAL	LEU	GLU												

• Molecule 88: 39S ribosomal protein L12, mitochondrial

Chain t6: 14% 86%

LEU	ILE	LYS	GLU	ILE	LYS	ASN	TYR	ILE	GLN	GLY	ILE	ASN	LEU	VAL	GLN	ALA	LYS	LEU	VAL	VAL	SER	GLY	SER	LEU	VAL	PRO	GLN	GLY	ILE	LYS	ALA	ASN	VAL	VAL	LYS	GLU	ALA	GLY	LYS	ALA	LEU	GLU	ALA	VAL	THR	THR	VAL	VAL	GLY	THR	VAL	VAL	LEU	GLU	GLY					
PRO	PRO	K2	T28	LEU	LYS	ILE	GLN	ASP	VAL	GLY	LEU	VAL	VAL	PRO	MET	GLY	VAL	MET	SER	GLY	VAL	VAL	PRO	ALA	ALA	VAL	GLU	GLU	GLU	ASN	GLU	VAL	ASP	ILE	PRO	ILE	ALA	LYS	LYS	GLY	GLY	ALA	THR	HIS	PHE	THR	VAL	VAL	ARG	THR	THR	GLU	ALA	LYS	PRO	VAL	ASP	LYS	VAL	LYS
MET	PRO	ALA	ALA	ALA	ARG	PRO	LEU	TRP	GLY	GLY	CYS	LEU	GLY	LEU	GLY	ARG	ALA	ALA	ALA	PHE	LEU	ARG	VAL	PRO	CYS	VAL	VAL	GLN	CYS	VAL	GLN	ASN	VAL	GLY	SER	SER	GLY	HIS	MET	ARG	SER	GLY	HIS	GLN	ARG	CYS	GLU	ALA	LEU	ALA	PRO	LYS	GLY	ALA	PRO	TYR				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13350	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, DOL, Y5P, ZN, H8Q, P5P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.28	0/895	0.44	0/1201
2	1	0.26	0/444	0.48	0/591
3	2	0.33	0/382	0.42	0/507
4	3	0.33	0/852	0.45	0/1136
5	4	0.28	0/349	0.46	0/461
6	5	0.27	0/3299	0.43	0/4495
7	6	0.28	0/3042	0.42	0/4140
8	7	0.26	0/2422	0.41	0/3276
9	8	1.80	1/1199 (0.1%)	0.45	2/1612 (0.1%)
10	9	0.28	0/1024	0.41	0/1379
11	XA	0.37	0/35615	0.79	0/55429
12	A0	0.23	0/1727	0.41	0/2338
13	A1	0.25	0/2276	0.39	0/3079
14	A2	0.25	0/939	0.42	0/1256
15	A3	0.30	0/621	0.46	0/820
16	A4	0.25	0/4559	0.41	0/6149
17	AA	0.27	0/21952	0.77	1/34164 (0.0%)
18	AB	0.26	0/1819	0.40	0/2462
19	AC	0.28	0/1112	0.42	0/1505
20	AD	0.26	0/2768	0.44	0/3707
21	AE	0.26	0/989	0.45	0/1335
22	AF	0.24	0/1708	0.40	0/2291
23	AG	0.26	0/2559	0.42	0/3429
24	AH	0.27	0/1128	0.44	0/1529
25	AI	0.26	0/1031	0.42	0/1390
26	AJ	0.26	0/854	0.45	0/1148
27	AK	0.25	0/879	0.42	0/1182
28	AL	0.26	0/1406	0.40	0/1878
29	AM	0.25	0/941	0.42	0/1265
30	AN	0.26	0/864	0.44	0/1169
31	AO	0.24	0/1580	0.39	0/2150
32	AP	0.27	0/782	0.41	0/1050

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AQ	0.27	0/746	0.42	0/993
34	AR	0.36	1/2103 (0.0%)	0.43	0/2842
35	AS	0.26	0/1127	0.39	0/1518
36	AT	0.26	0/1361	0.42	0/1829
37	AU	0.24	0/1482	0.39	0/1987
38	AV	0.24	0/2925	0.39	0/3948
39	AW	0.26	0/778	0.44	0/1048
40	AX	0.25	0/2886	0.43	0/3909
41	AY	0.26	0/985	0.40	0/1329
42	AZ	0.26	0/748	0.38	0/1000
43	XB	0.20	0/1400	0.73	0/2168
44	XD	0.29	0/1879	0.47	0/2527
45	XE	0.29	0/2465	0.44	0/3344
46	XF	0.33	0/2071	0.45	0/2817
47	XH	0.26	0/798	0.43	0/1073
48	XI	0.25	0/1727	0.43	0/2340
49	XJ	0.24	0/1309	0.40	0/1764
50	XK	0.30	0/1495	0.41	0/2029
51	XL	0.27	0/904	0.44	0/1218
52	XM	0.31	0/2359	0.44	0/3185
53	XN	0.29	0/1825	0.45	0/2458
54	XO	0.27	0/1269	0.42	0/1708
55	XP	0.27	0/1190	0.44	0/1611
56	XQ	0.26	0/2026	0.43	0/2734
57	XR	0.32	0/1174	0.45	0/1572
58	XS	0.30	0/1311	0.47	0/1778
59	XT	0.31	0/1402	0.44	0/1886
60	XU	0.29	0/1200	0.42	0/1623
61	XV	0.27	0/1693	0.43	0/2297
62	XW	0.32	0/893	0.47	0/1204
63	XX	0.28	0/2090	0.41	0/2825
64	XY	0.28	0/1571	0.41	0/2106
65	XZ	0.29	0/1003	0.45	0/1354
66	a	0.28	0/838	0.45	0/1138
67	b	0.30	0/1202	0.45	0/1626
68	c	0.27	0/2264	0.40	0/3059
69	d	0.26	0/1807	0.42	0/2450
70	e	1.43	6/1797 (0.3%)	0.42	0/2422
71	f	0.28	0/1169	0.43	0/1576
72	g	0.34	1/1134 (0.1%)	0.44	0/1547
73	h	0.25	0/905	0.41	0/1233
74	i	0.32	0/849	0.45	0/1135
75	j	0.27	0/703	0.42	0/947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	k	0.24	0/743	0.43	0/1003
77	l	0.24	0/692	0.37	0/939
78	m	0.23	0/508	0.45	0/682
79	o	0.31	0/818	0.45	0/1097
80	p	0.24	0/1071	0.43	0/1433
81	q	0.25	0/1413	0.42	0/1906
82	r	0.27	0/1351	0.43	0/1831
87	s	0.27	0/3114	0.44	0/4225
88	t1	0.25	0/366	0.38	0/497
88	t2	0.22	0/238	0.39	0/319
88	t3	0.22	0/238	0.39	0/319
88	t4	0.23	0/229	0.41	0/308
88	t5	0.22	0/229	0.36	0/308
88	t6	0.25	0/213	0.46	0/286
All	All	0.36	9/176103 (0.0%)	0.58	3/249833 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
44	XD	0	1
48	XI	0	1
55	XP	0	1
71	f	0	1
73	h	0	1
All	All	0	5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	99	ARG	CG-CD	61.72	3.06	1.51
70	e	84	TYR	CD2-CE2	31.52	1.86	1.39
70	e	84	TYR	CD1-CE1	31.26	1.86	1.39
70	e	84	TYR	CE2-CZ	22.29	1.67	1.38
70	e	84	TYR	CE1-CZ	21.16	1.66	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	99	ARG	CB-CG-CD	5.74	126.51	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	99	ARG	CG-CD-NE	5.64	123.64	111.80
17	AA	765	C	C2-N1-C1'	5.44	124.78	118.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	XD	206	TYR	Peptide
48	XI	197	LEU	Peptide
55	XP	114	HIS	Peptide
71	f	138	GLN	Peptide
73	h	78	PHE	Peptide

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	0	880	903	903	13	0
2	1	439	480	480	5	0
3	2	376	407	406	4	0
4	3	831	883	883	12	0
5	4	341	361	361	6	0
6	5	3204	3201	3201	27	0
7	6	2947	2841	2841	34	0
8	7	2365	2375	2374	21	0
9	8	1175	1202	1202	7	0
10	9	996	987	987	13	0
11	XA	31833	16160	16169	258	0
12	A0	1684	1685	1685	13	0
13	A1	2230	2261	2261	34	0
14	A2	925	964	964	16	0
15	A3	610	682	682	8	0
16	A4	4470	4485	4486	43	0
17	AA	19628	9965	9972	146	0
18	AB	1776	1769	1769	13	0
19	AC	1082	1088	1088	14	0
20	AD	2716	2784	2785	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	AE	972	1001	1001	15	0
22	AF	1668	1716	1716	30	0
23	AG	2505	2491	2490	31	0
24	AH	1105	1136	1136	15	0
25	AI	1011	1052	1052	12	0
26	AJ	838	887	887	11	0
27	AK	861	885	885	13	0
28	AL	1382	1472	1472	11	0
29	AM	920	951	951	10	0
30	AN	846	908	908	12	0
31	AO	1528	1489	1489	12	0
32	AP	765	796	796	5	0
33	AQ	734	749	749	11	0
34	AR	2060	2074	2074	24	0
35	AS	1100	1103	1103	13	0
36	AT	1330	1342	1342	13	0
37	AU	1461	1471	1471	18	0
38	AV	2867	2862	2862	24	0
39	AW	766	785	785	6	0
40	AX	2814	2805	2804	31	0
41	AY	956	912	911	19	0
42	AZ	731	734	734	8	0
43	XB	1255	635	640	12	0
44	XD	1842	1897	1896	29	0
45	XE	2396	2402	2402	23	0
46	XF	2013	2045	2044	29	0
47	XH	784	832	832	13	0
48	XI	1691	1783	1783	15	0
49	XJ	1291	1366	1364	12	0
50	XK	1451	1448	1448	13	0
51	XL	889	941	941	8	0
52	XM	2305	2377	2377	34	0
53	XN	1778	1808	1808	16	0
54	XO	1245	1283	1283	19	0
55	XP	1164	1162	1162	11	0
56	XQ	1978	2022	2022	22	0
57	XR	1153	1214	1214	17	0
58	XS	1284	1354	1354	12	0
59	XT	1368	1410	1410	15	0
60	XU	1171	1164	1164	8	0
61	XV	1648	1656	1654	15	0
62	XW	871	898	898	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	XX	2035	2054	2054	25	0
64	XY	1534	1575	1575	29	0
65	XZ	978	1030	1030	9	0
66	a	813	777	777	0	0
67	b	1178	1180	1180	0	0
68	c	2217	2220	2220	0	0
69	d	1758	1743	1742	0	0
70	e	1762	1767	1767	0	0
71	f	1149	1165	1165	0	0
72	g	1097	1086	1085	0	0
73	h	882	866	867	0	0
74	i	827	857	857	0	0
75	j	689	678	678	0	0
76	k	732	745	745	0	0
77	l	673	654	653	0	0
78	m	500	525	525	0	0
79	o	797	804	804	0	0
80	p	1058	1083	1083	0	0
81	q	1379	1359	1359	0	0
82	r	1312	1341	1341	0	0
83	r1	252	0	169	0	0
84	r2	1485	0	835	0	0
85	r3	1459	0	830	0	0
86	r4	1464	0	825	0	0
87	s	3036	3023	3022	0	0
88	t1	354	379	374	0	0
88	t2	238	268	270	0	0
88	t3	238	268	270	0	0
88	t4	229	255	257	0	0
88	t5	229	255	257	0	0
88	t6	214	236	236	0	0
89	0	1	0	0	0	0
89	4	1	0	0	0	0
89	AB	1	0	0	0	0
89	AO	1	0	0	0	0
89	AP	1	0	0	0	0
89	AT	1	0	0	0	0
89	r	1	0	0	0	0
90	2	1	0	0	0	0
90	9	1	0	0	0	0
90	AA	46	0	0	0	0
90	XA	141	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	XD	1	0	0	0	0
90	XE	1	0	0	0	0
90	XI	1	0	0	0	0
90	XM	1	0	0	0	0
90	XW	1	0	0	0	0
90	g	1	0	0	0	0
91	XA	73	67	0	5	0
92	XA	48	50	50	2	0
93	AX	32	10	12	1	0
All	All	172228	143121	145727	1169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1169 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)
23:AG:155:LYS:NZ	23:AG:212:LYS:O	1.98	0.97
43:XB:1621:A:OP1	55:XP:112:LYS:NZ	2.00	0.94
11:XA:2039:A:N6	11:XA:2729:U:O2	2.03	0.92
23:AG:310:ARG:NH1	40:AX:383:LEU:O	2.05	0.90
11:XA:1680:A:OP1	64:XY:230:LYS:NZ	2.06	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
2	1	51/65 (78%)	49 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	93 (100%)	0	0	100	100
5	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
6	5	391/423 (92%)	371 (95%)	20 (5%)	0	100	100
7	6	352/380 (93%)	330 (94%)	22 (6%)	0	100	100
8	7	289/338 (86%)	270 (93%)	19 (7%)	0	100	100
9	8	137/206 (66%)	132 (96%)	5 (4%)	0	100	100
10	9	122/137 (89%)	115 (94%)	7 (6%)	0	100	100
12	A0	197/218 (90%)	187 (95%)	10 (5%)	0	100	100
13	A1	273/323 (84%)	259 (95%)	14 (5%)	0	100	100
14	A2	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
15	A3	67/199 (34%)	66 (98%)	1 (2%)	0	100	100
16	A4	526/689 (76%)	493 (94%)	33 (6%)	0	100	100
18	AB	216/296 (73%)	211 (98%)	5 (2%)	0	100	100
19	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
20	AD	341/430 (79%)	321 (94%)	20 (6%)	0	100	100
21	AE	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
22	AF	197/242 (81%)	192 (98%)	5 (2%)	0	100	100
23	AG	300/396 (76%)	283 (94%)	17 (6%)	0	100	100
24	AH	133/201 (66%)	125 (94%)	8 (6%)	0	100	100
25	AI	134/194 (69%)	128 (96%)	6 (4%)	0	100	100
26	AJ	106/138 (77%)	98 (92%)	8 (8%)	0	100	100
27	AK	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
28	AL	162/257 (63%)	157 (97%)	5 (3%)	0	100	100
29	AM	114/137 (83%)	112 (98%)	2 (2%)	0	100	100
30	AN	105/130 (81%)	101 (96%)	4 (4%)	0	100	100
31	AO	183/258 (71%)	180 (98%)	3 (2%)	0	100	100
32	AP	93/142 (66%)	87 (94%)	6 (6%)	0	100	100
33	AQ	83/86 (96%)	79 (95%)	4 (5%)	0	100	100
34	AR	248/360 (69%)	234 (94%)	14 (6%)	0	100	100
35	AS	131/190 (69%)	121 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	AT	160/173 (92%)	151 (94%)	9 (6%)	0	100	100
37	AU	171/205 (83%)	169 (99%)	2 (1%)	0	100	100
38	AV	341/414 (82%)	320 (94%)	21 (6%)	0	100	100
39	AW	95/187 (51%)	90 (95%)	5 (5%)	0	100	100
40	AX	346/398 (87%)	328 (95%)	18 (5%)	0	100	100
41	AY	111/395 (28%)	103 (93%)	8 (7%)	0	100	100
42	AZ	84/106 (79%)	84 (100%)	0	0	100	100
44	XD	234/305 (77%)	220 (94%)	12 (5%)	2 (1%)	17	55
45	XE	302/348 (87%)	285 (94%)	17 (6%)	0	100	100
46	XF	248/311 (80%)	238 (96%)	10 (4%)	0	100	100
47	XH	93/267 (35%)	86 (92%)	7 (8%)	0	100	100
48	XI	209/261 (80%)	196 (94%)	13 (6%)	0	100	100
49	XJ	168/192 (88%)	156 (93%)	12 (7%)	0	100	100
50	XK	175/178 (98%)	167 (95%)	8 (5%)	0	100	100
51	XL	113/145 (78%)	107 (95%)	6 (5%)	0	100	100
52	XM	285/296 (96%)	271 (95%)	14 (5%)	0	100	100
53	XN	219/251 (87%)	210 (96%)	9 (4%)	0	100	100
54	XO	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
55	XP	141/180 (78%)	132 (94%)	9 (6%)	0	100	100
56	XQ	236/292 (81%)	224 (95%)	12 (5%)	0	100	100
57	XR	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
58	XS	158/205 (77%)	152 (96%)	6 (4%)	0	100	100
59	XT	164/206 (80%)	160 (98%)	4 (2%)	0	100	100
60	XU	137/153 (90%)	132 (96%)	5 (4%)	0	100	100
61	XV	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
62	XW	109/148 (74%)	106 (97%)	3 (3%)	0	100	100
63	XX	241/256 (94%)	234 (97%)	7 (3%)	0	100	100
64	XY	176/250 (70%)	168 (96%)	8 (4%)	0	100	100
65	XZ	118/161 (73%)	114 (97%)	4 (3%)	0	100	100
66	a	93/142 (66%)	87 (94%)	6 (6%)	0	100	100
67	b	146/215 (68%)	136 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	c	271/332 (82%)	261 (96%)	10 (4%)	0	100	100
69	d	212/306 (69%)	200 (94%)	11 (5%)	1 (0%)	29	67
70	e	211/279 (76%)	203 (96%)	8 (4%)	0	100	100
71	f	139/212 (66%)	132 (95%)	7 (5%)	0	100	100
72	g	130/166 (78%)	125 (96%)	5 (4%)	0	100	100
73	h	106/158 (67%)	100 (94%)	6 (6%)	0	100	100
74	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
75	j	84/123 (68%)	83 (99%)	1 (1%)	0	100	100
76	k	93/112 (83%)	86 (92%)	7 (8%)	0	100	100
77	l	78/138 (56%)	72 (92%)	6 (8%)	0	100	100
78	m	58/128 (45%)	54 (93%)	4 (7%)	0	100	100
79	o	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
80	p	119/206 (58%)	113 (95%)	6 (5%)	0	100	100
81	q	162/222 (73%)	160 (99%)	2 (1%)	0	100	100
82	r	157/196 (80%)	148 (94%)	9 (6%)	0	100	100
87	s	366/439 (83%)	349 (95%)	17 (5%)	0	100	100
88	t1	45/198 (23%)	42 (93%)	3 (7%)	0	100	100
88	t2	28/198 (14%)	28 (100%)	0	0	100	100
88	t3	28/198 (14%)	27 (96%)	1 (4%)	0	100	100
88	t4	27/198 (14%)	25 (93%)	2 (7%)	0	100	100
88	t5	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
88	t6	25/198 (13%)	25 (100%)	0	0	100	100
All	All	13807/19159 (72%)	13157 (95%)	647 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	XD	207	ILE
44	XD	208	ARG
69	d	289	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	
1	0	97/164 (59%)	97 (100%)	0	100	100
2	1	50/60 (83%)	50 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	352 (100%)	1 (0%)	92	95
7	6	313/332 (94%)	311 (99%)	2 (1%)	86	92
8	7	267/303 (88%)	267 (100%)	0	100	100
9	8	128/190 (67%)	127 (99%)	1 (1%)	81	89
10	9	104/112 (93%)	104 (100%)	0	100	100
12	A0	176/190 (93%)	175 (99%)	1 (1%)	86	92
13	A1	253/291 (87%)	251 (99%)	2 (1%)	81	89
14	A2	99/101 (98%)	97 (98%)	2 (2%)	55	73
15	A3	63/166 (38%)	62 (98%)	1 (2%)	62	79
16	A4	494/609 (81%)	490 (99%)	4 (1%)	81	89
18	AB	192/249 (77%)	192 (100%)	0	100	100
19	AC	115/143 (80%)	115 (100%)	0	100	100
20	AD	283/357 (79%)	280 (99%)	3 (1%)	73	85
21	AE	104/107 (97%)	103 (99%)	1 (1%)	76	86
22	AF	178/209 (85%)	178 (100%)	0	100	100
23	AG	264/342 (77%)	263 (100%)	1 (0%)	91	94
24	AH	125/180 (69%)	125 (100%)	0	100	100
25	AI	104/147 (71%)	104 (100%)	0	100	100
26	AJ	93/118 (79%)	93 (100%)	0	100	100
27	AK	91/113 (80%)	91 (100%)	0	100	100
28	AL	152/226 (67%)	151 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	AM	95/113 (84%)	95 (100%)	0	100	100
30	AN	93/115 (81%)	93 (100%)	0	100	100
31	AO	166/230 (72%)	166 (100%)	0	100	100
32	AP	86/123 (70%)	86 (100%)	0	100	100
33	AQ	77/78 (99%)	77 (100%)	0	100	100
34	AR	229/318 (72%)	228 (100%)	1 (0%)	91	94
35	AS	115/164 (70%)	115 (100%)	0	100	100
36	AT	150/157 (96%)	150 (100%)	0	100	100
37	AU	149/174 (86%)	148 (99%)	1 (1%)	84	90
38	AV	315/364 (86%)	314 (100%)	1 (0%)	92	95
39	AW	84/158 (53%)	84 (100%)	0	100	100
40	AX	307/351 (88%)	304 (99%)	3 (1%)	76	86
41	AY	104/357 (29%)	103 (99%)	1 (1%)	76	86
42	AZ	79/95 (83%)	79 (100%)	0	100	100
44	XD	190/245 (78%)	190 (100%)	0	100	100
45	XE	259/290 (89%)	259 (100%)	0	100	100
46	XF	217/262 (83%)	217 (100%)	0	100	100
47	XH	86/228 (38%)	85 (99%)	1 (1%)	71	84
48	XI	194/232 (84%)	194 (100%)	0	100	100
49	XJ	133/150 (89%)	131 (98%)	2 (2%)	65	80
50	XK	155/156 (99%)	155 (100%)	0	100	100
51	XL	98/124 (79%)	98 (100%)	0	100	100
52	XM	245/249 (98%)	244 (100%)	1 (0%)	91	94
53	XN	188/211 (89%)	188 (100%)	0	100	100
54	XO	133/150 (89%)	133 (100%)	0	100	100
55	XP	125/155 (81%)	125 (100%)	0	100	100
56	XQ	220/256 (86%)	220 (100%)	0	100	100
57	XR	118/126 (94%)	117 (99%)	1 (1%)	81	89
58	XS	145/180 (81%)	145 (100%)	0	100	100
59	XT	146/176 (83%)	146 (100%)	0	100	100
60	XU	126/135 (93%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	XV	179/191 (94%)	179 (100%)	0	100	100
62	XW	91/119 (76%)	89 (98%)	2 (2%)	52	71
63	XX	219/229 (96%)	219 (100%)	0	100	100
64	XY	161/223 (72%)	161 (100%)	0	100	100
65	XZ	111/147 (76%)	111 (100%)	0	100	100
66	a	93/133 (70%)	93 (100%)	0	100	100
67	b	130/186 (70%)	130 (100%)	0	100	100
68	c	241/288 (84%)	240 (100%)	1 (0%)	91	94
69	d	196/274 (72%)	196 (100%)	0	100	100
70	e	188/236 (80%)	187 (100%)	1 (0%)	88	93
71	f	128/188 (68%)	128 (100%)	0	100	100
72	g	122/148 (82%)	122 (100%)	0	100	100
73	h	103/148 (70%)	103 (100%)	0	100	100
74	i	86/110 (78%)	85 (99%)	1 (1%)	71	84
75	j	68/97 (70%)	68 (100%)	0	100	100
76	k	80/90 (89%)	80 (100%)	0	100	100
77	l	74/116 (64%)	74 (100%)	0	100	100
78	m	54/113 (48%)	54 (100%)	0	100	100
79	o	80/87 (92%)	80 (100%)	0	100	100
80	p	117/181 (65%)	117 (100%)	0	100	100
81	q	141/178 (79%)	140 (99%)	1 (1%)	84	90
82	r	146/169 (86%)	145 (99%)	1 (1%)	84	90
87	s	326/381 (86%)	325 (100%)	1 (0%)	92	95
88	t1	41/158 (26%)	40 (98%)	1 (2%)	49	69
88	t2	29/158 (18%)	29 (100%)	0	100	100
88	t3	29/158 (18%)	28 (97%)	1 (3%)	37	61
88	t4	28/158 (18%)	28 (100%)	0	100	100
88	t5	28/158 (18%)	28 (100%)	0	100	100
88	t6	26/158 (16%)	26 (100%)	0	100	100
All	All	12405/16506 (75%)	12363 (100%)	42 (0%)	92	95

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	XJ	154	ARG
70	e	273	ARG
49	XJ	167	LYS
62	XW	119	ARG
81	q	140	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
76	k	15	GLN
88	t4	5	GLN
24	AH	163	ASN
42	AZ	76	GLN
45	XE	174	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	XA	1490/1561 (95%)	266 (17%)	7 (0%)
17	AA	916/954 (96%)	158 (17%)	4 (0%)
43	XB	54/72 (75%)	11 (20%)	0
83	r1	0/14	-	-
84	r2	0/76	-	-
85	r3	0/75	-	-
86	r4	0/75	-	-
All	All	2460/2827 (87%)	435 (17%)	11 (0%)

5 of 435 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	XA	1685	C
11	XA	1689	C
11	XA	1692	A
11	XA	1693	C
11	XA	1695	C

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	AA	770	C
17	AA	1048	C

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Mol	Chain	Res	Type
17	AA	1558	A
17	AA	1234	C
11	XA	2574	G

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

240 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	$\# Z > 2$
86	Y5P	r4	2	86	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	16	85	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	11	84	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
86	P5P	r4	52	86	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r2	12	84	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
84	P5P	r2	18	84	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r2	9	84	16,23,24	0.95	1 (6%)	14,33,36	2.02	3 (21%)
84	P5P	r2	7	84	16,23,24	0.96	1 (6%)	14,33,36	2.01	3 (21%)
86	Y5P	r4	75	86	14,19,20	3.15	3 (21%)	18,26,29	0.59	0
85	Y5P	r3	7	85	14,19,20	3.14	3 (21%)	18,26,29	0.61	0
86	P5P	r4	15	86	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r2	66	84	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
83	Y5P	r1	47	83	14,19,20	3.09	3 (21%)	18,26,29	0.65	0
84	Y5P	r2	41	84	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
84	P5P	r2	64	84	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
85	P5P	r3	36	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
86	P5P	r4	34	86	16,23,24	0.97	1 (6%)	14,33,36	2.00	3 (21%)
86	Y5P	r4	54	86	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	16	84	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
85	P5P	r3	67	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	P5P	r3	17	85	16,23,24	0.95	1 (6%)	14,33,36	2.01	3 (21%)
84	P5P	r2	30	84	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	P5P	r3	56	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
84	Y5P	r2	59	84	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
86	P5P	r4	19	86	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r3	54	85	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
86	Y5P	r4	51	86	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
86	P5P	r4	70	86	16,23,24	0.94	1 (6%)	14,33,36	1.97	3 (21%)
85	P5P	r3	4	85	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
84	Y5P	r2	45	84	14,19,20	3.13	3 (21%)	18,26,29	0.53	0
85	P5P	r3	22	85	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r1	50	83	14,19,20	3.11	3 (21%)	18,26,29	0.61	0
86	P5P	r4	35	86	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
86	Y5P	r4	59	86	14,19,20	3.12	3 (21%)	18,26,29	0.60	0
85	Y5P	r3	34	85	14,19,20	3.11	3 (21%)	18,26,29	0.56	0
85	P5P	r3	19	85	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r3	42	85	14,19,20	3.12	3 (21%)	18,26,29	0.60	0
85	Y5P	r3	63	85	14,19,20	3.12	3 (21%)	18,26,29	0.63	0
86	P5P	r4	38	86	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
86	Y5P	r4	49	86	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	P5P	r3	58	85	16,23,24	0.93	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	11	85	16,23,24	0.97	1 (6%)	14,33,36	1.96	3 (21%)
83	Y5P	r1	45	83	14,19,20	3.14	4 (28%)	18,26,29	0.60	0
85	Y5P	r3	61	85	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
86	Y5P	r4	8	86	14,19,20	3.15	3 (21%)	18,26,29	0.58	0
86	Y5P	r4	20	86	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
85	P5P	r3	20	85	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r1	49	83	14,19,20	3.11	3 (21%)	18,26,29	0.56	0
84	P5P	r2	65	84	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
84	Y5P	r2	13	84	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
84	P5P	r2	38	84	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	P5P	r3	24	85	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r3	29	85	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
86	P5P	r4	10	86	16,23,24	0.95	1 (6%)	14,33,36	2.01	3 (21%)
84	P5P	r2	22	84	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	Y5P	r2	48	84	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	67	84	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	2	84	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
84	P5P	r2	27	84	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
85	P5P	r3	47	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
85	Y5P	r3	59	85	14,19,20	3.13	3 (21%)	18,26,29	0.62	0
86	Y5P	r4	55	86	14,19,20	3.15	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	65	85	14,19,20	3.12	3 (21%)	18,26,29	0.57	0
86	P5P	r4	22	86	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r2	62	84	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
84	Y5P	r2	61	84	14,19,20	3.14	4 (28%)	18,26,29	0.58	0
84	P5P	r2	6	84	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r2	63	84	16,23,24	0.97	1 (6%)	14,33,36	2.01	3 (21%)
85	P5P	r3	10	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r3	71	85	14,19,20	3.14	3 (21%)	18,26,29	0.60	0
86	P5P	r4	64	86	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r2	15	84	16,23,24	0.95	1 (6%)	14,33,36	2.01	3 (21%)
85	P5P	r3	49	85	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
86	Y5P	r4	50	86	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
86	P5P	r4	30	86	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r3	41	85	14,19,20	3.09	3 (21%)	18,26,29	0.63	0
85	P5P	r3	72	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
86	Y5P	r4	62	86	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r1	44	83	14,19,20	3.14	3 (21%)	18,26,29	0.60	0
86	Y5P	r4	25	86	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
86	P5P	r4	69	86	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r3	55	85	14,19,20	3.15	3 (21%)	18,26,29	0.54	0
84	Y5P	r2	49	84	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
85	P5P	r3	69	85	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
86	P5P	r4	65	86	16,23,24	0.97	1 (6%)	14,33,36	1.96	3 (21%)
85	Y5P	r3	62	85	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
86	Y5P	r4	66	86	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	21	85	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
86	P5P	r4	1	86	16,23,24	0.95	1 (6%)	14,33,36	2.01	3 (21%)
85	Y5P	r3	40	85	14,19,20	3.14	3 (21%)	18,26,29	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	Y5P	r4	3	86	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	17	84	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
86	P5P	r4	9	86	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
83	Y5P	r1	55	83	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
85	P5P	r3	14	85	16,23,24	0.94	1 (6%)	14,33,36	2.02	3 (21%)
86	P5P	r4	63	86	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
86	Y5P	r4	39	86	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
85	P5P	r3	45	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
86	P5P	r4	53	86	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r2	50	84	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
84	P5P	r2	71	84	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
84	Y5P	r2	40	84	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
85	Y5P	r3	68	85	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
83	Y5P	r1	56	83	14,19,20	3.13	3 (21%)	18,26,29	0.62	0
84	P5P	r2	36	84	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
86	Y5P	r4	32	86	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r1	48	83	14,19,20	3.10	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	26	85	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
84	Y5P	r2	33	84	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
84	P5P	r2	73	84	16,23,24	0.98	1 (6%)	14,33,36	2.01	3 (21%)
85	P5P	r3	9	85	16,23,24	0.97	1 (6%)	14,33,36	2.01	3 (21%)
84	P5P	r2	57	84	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	P5P	r3	8	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
84	P5P	r2	26	84	16,23,24	0.94	1 (6%)	14,33,36	2.00	3 (21%)
85	P5P	r3	15	85	16,23,24	0.98	1 (6%)	14,33,36	1.97	3 (21%)
86	P5P	r4	27	86	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
84	Y5P	r2	42	84	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
84	Y5P	r2	25	84	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	P5P	r3	52	85	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
84	P5P	r2	37	84	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	27	85	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	53	85	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
86	Y5P	r4	4	86	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
86	Y5P	r4	33	86	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
86	Y5P	r4	48	86	14,19,20	3.14	3 (21%)	18,26,29	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	Y5P	r4	74	86	14,19,20	3.16	3 (21%)	18,26,29	0.56	0
86	P5P	r4	37	86	16,23,24	0.96	1 (6%)	14,33,36	1.96	3 (21%)
86	Y5P	r4	16	86	14,19,20	3.12	3 (21%)	18,26,29	0.63	0
83	Y5P	r1	46	83	14,19,20	3.10	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	8	84	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
83	Y5P	r1	53	83	14,19,20	3.10	3 (21%)	18,26,29	0.66	0
85	Y5P	r3	1	85	18,20,20	2.76	3 (16%)	25,29,29	0.69	0
86	P5P	r4	71	86	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r3	48	85	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
86	Y5P	r4	45	86	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
84	Y5P	r2	43	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
86	P5P	r4	18	86	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
86	P5P	r4	7	86	16,23,24	0.96	1 (6%)	14,33,36	2.01	3 (21%)
83	Y5P	r1	51	83	14,19,20	3.11	3 (21%)	18,26,29	0.62	0
86	Y5P	r4	47	86	14,19,20	3.16	3 (21%)	18,26,29	0.57	0
84	P5P	r2	53	84	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	74	85	14,19,20	3.10	3 (21%)	18,26,29	0.54	0
85	Y5P	r3	50	85	14,19,20	3.15	3 (21%)	18,26,29	0.57	0
86	P5P	r4	26	86	16,23,24	0.95	1 (6%)	14,33,36	2.01	3 (21%)
86	P5P	r4	57	86	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
86	P5P	r4	58	86	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
86	Y5P	r4	13	86	14,19,20	3.15	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	70	85	14,19,20	3.13	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	35	85	14,19,20	3.11	3 (21%)	18,26,29	0.58	0
86	Y5P	r4	60	86	14,19,20	3.12	3 (21%)	18,26,29	0.58	0
83	Y5P	r1	54	83	14,19,20	3.16	4 (28%)	18,26,29	0.56	0
86	P5P	r4	14	86	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
85	Y5P	r3	12	85	14,19,20	3.10	3 (21%)	18,26,29	0.59	0
84	P5P	r2	23	84	16,23,24	0.97	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r3	13	85	14,19,20	3.13	3 (21%)	18,26,29	0.62	0
85	Y5P	r3	33	85	14,19,20	3.12	3 (21%)	18,26,29	0.56	0
86	Y5P	r4	68	86	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	51	85	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
86	Y5P	r4	61	86	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	32	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	Y5P	r3	28	85	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	60	85	14,19,20	3.12	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	54	84	14,19,20	3.15	3 (21%)	18,26,29	0.56	0
84	P5P	r2	5	84	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
85	P5P	r3	75	85	16,23,24	0.95	1 (6%)	14,33,36	2.02	3 (21%)
84	P5P	r2	21	84	16,23,24	0.94	1 (6%)	14,33,36	1.98	3 (21%)
84	Y5P	r2	47	84	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	55	84	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
84	P5P	r2	19	84	16,23,24	0.96	1 (6%)	14,33,36	2.01	3 (21%)
84	P5P	r2	44	84	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
84	P5P	r2	14	84	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r3	25	85	14,19,20	3.11	3 (21%)	18,26,29	0.65	0
85	Y5P	r3	66	85	14,19,20	3.13	3 (21%)	18,26,29	0.65	0
86	P5P	r4	21	86	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
86	Y5P	r4	12	86	14,19,20	3.14	3 (21%)	18,26,29	0.60	0
85	P5P	r3	3	85	16,23,24	0.95	1 (6%)	14,33,36	2.05	3 (21%)
86	P5P	r4	24	86	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	46	85	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
85	P5P	r3	38	85	16,23,24	0.96	1 (6%)	14,33,36	1.96	3 (21%)
86	Y5P	r4	42	86	14,19,20	3.15	3 (21%)	18,26,29	0.56	0
86	P5P	r4	73	86	16,23,24	0.97	1 (6%)	14,33,36	2.01	3 (21%)
84	P5P	r2	28	84	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r3	37	85	14,19,20	3.11	3 (21%)	18,26,29	0.65	0
86	P5P	r4	6	86	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r2	31	84	16,23,24	0.93	1 (6%)	14,33,36	2.01	3 (21%)
84	Y5P	r2	3	84	14,19,20	3.14	4 (28%)	18,26,29	0.59	0
85	Y5P	r3	2	85	14,19,20	3.13	3 (21%)	18,26,29	0.55	0
86	P5P	r4	5	86	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	P5P	r3	23	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
86	P5P	r4	29	86	16,23,24	0.95	1 (6%)	14,33,36	2.01	3 (21%)
84	Y5P	r2	51	84	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	P5P	r3	6	85	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	44	85	16,23,24	0.94	1 (6%)	14,33,36	1.98	3 (21%)
85	P5P	r3	32	85	16,23,24	0.94	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r3	39	85	14,19,20	3.12	3 (21%)	18,26,29	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	Y5P	r3	57	85	14,19,20	3.13	4 (28%)	18,26,29	0.64	0
84	P5P	r2	46	84	16,23,24	0.97	1 (6%)	14,33,36	2.00	3 (21%)
85	Y5P	r3	18	85	14,19,20	3.15	3 (21%)	18,26,29	0.56	0
84	P5P	r2	58	84	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
86	Y5P	r4	40	86	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
84	P5P	r2	35	84	16,23,24	0.94	1 (6%)	14,33,36	2.04	3 (21%)
84	P5P	r2	70	84	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r2	76	84	16,23,24	0.94	1 (6%)	14,33,36	1.97	3 (21%)
84	Y5P	r2	72	84	14,19,20	3.13	3 (21%)	18,26,29	0.55	0
86	Y5P	r4	11	86	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	39	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	68	84	14,19,20	3.12	3 (21%)	18,26,29	0.55	0
84	P5P	r2	69	84	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
86	Y5P	r4	43	86	14,19,20	3.15	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	56	84	14,19,20	3.15	3 (21%)	18,26,29	0.58	0
86	Y5P	r4	41	86	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
85	P5P	r3	43	85	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r2	52	84	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
86	P5P	r4	28	86	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
83	Y5P	r1	57	83	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
85	P5P	r3	5	85	16,23,24	0.97	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r2	10	84	16,23,24	0.94	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r2	1	84	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
84	Y5P	r2	20	84	14,19,20	3.14	3 (21%)	18,26,29	0.61	0
84	Y5P	r2	74	84	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
86	P5P	r4	31	86	16,23,24	0.95	1 (6%)	14,33,36	2.03	3 (21%)
85	P5P	r3	30	85	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
86	P5P	r4	46	86	16,23,24	0.96	1 (6%)	14,33,36	1.96	3 (21%)
84	P5P	r2	34	84	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
86	Y5P	r4	56	86	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
84	P5P	r2	29	84	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
86	Y5P	r4	72	86	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	4	84	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
85	P5P	r3	31	85	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r3	73	85	14,19,20	3.09	3 (21%)	18,26,29	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	P5P	r4	44	86	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r2	75	84	14,19,20	3.11	3 (21%)	18,26,29	0.58	0
86	P5P	r4	23	86	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r2	24	84	16,23,24	0.95	1 (6%)	14,33,36	2.01	3 (21%)
85	Y5P	r3	64	85	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
86	Y5P	r4	17	86	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	52	83	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
84	Y5P	r2	60	84	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
86	Y5P	r4	67	86	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
86	P5P	r4	36	86	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)

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
86	Y5P	r4	2	86	-	1/7/33/34	0/2/2/2
85	Y5P	r3	16	85	-	2/7/33/34	0/2/2/2
84	Y5P	r2	11	84	-	1/7/33/34	0/2/2/2
86	P5P	r4	52	86	-	2/3/25/26	0/3/3/3
84	Y5P	r2	12	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	18	84	-	1/3/25/26	0/3/3/3
84	P5P	r2	9	84	-	3/3/25/26	0/3/3/3
84	P5P	r2	7	84	-	2/3/25/26	0/3/3/3
86	Y5P	r4	75	86	-	5/7/33/34	0/2/2/2
85	Y5P	r3	7	85	-	3/7/33/34	0/2/2/2
86	P5P	r4	15	86	-	0/3/25/26	0/3/3/3
84	Y5P	r2	66	84	-	3/7/33/34	0/2/2/2
83	Y5P	r1	47	83	-	3/7/33/34	0/2/2/2
84	Y5P	r2	41	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	64	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	36	85	-	0/3/25/26	0/3/3/3
86	P5P	r4	34	86	-	2/3/25/26	0/3/3/3
86	Y5P	r4	54	86	-	1/7/33/34	0/2/2/2
84	Y5P	r2	16	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	67	85	-	1/3/25/26	0/3/3/3
85	P5P	r3	17	85	-	3/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	P5P	r2	30	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	56	85	-	2/3/25/26	0/3/3/3
84	Y5P	r2	59	84	-	2/7/33/34	0/2/2/2
86	P5P	r4	19	86	-	0/3/25/26	0/3/3/3
85	Y5P	r3	54	85	-	3/7/33/34	0/2/2/2
86	Y5P	r4	51	86	-	1/7/33/34	0/2/2/2
86	P5P	r4	70	86	-	0/3/25/26	0/3/3/3
85	P5P	r3	4	85	-	3/3/25/26	0/3/3/3
84	Y5P	r2	45	84	-	3/7/33/34	0/2/2/2
85	P5P	r3	22	85	-	3/3/25/26	0/3/3/3
83	Y5P	r1	50	83	-	2/7/33/34	0/2/2/2
86	P5P	r4	35	86	-	0/3/25/26	0/3/3/3
86	Y5P	r4	59	86	-	2/7/33/34	0/2/2/2
85	Y5P	r3	34	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	19	85	-	3/3/25/26	0/3/3/3
85	Y5P	r3	42	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	63	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	38	86	-	2/3/25/26	0/3/3/3
86	Y5P	r4	49	86	-	3/7/33/34	0/2/2/2
85	P5P	r3	58	85	-	2/3/25/26	0/3/3/3
85	P5P	r3	11	85	-	0/3/25/26	0/3/3/3
83	Y5P	r1	45	83	-	3/7/33/34	0/2/2/2
85	Y5P	r3	61	85	-	2/7/33/34	0/2/2/2
86	Y5P	r4	8	86	-	1/7/33/34	0/2/2/2
86	Y5P	r4	20	86	-	2/7/33/34	0/2/2/2
85	P5P	r3	20	85	-	2/3/25/26	0/3/3/3
83	Y5P	r1	49	83	-	3/7/33/34	0/2/2/2
84	P5P	r2	65	84	-	0/3/25/26	0/3/3/3
84	Y5P	r2	13	84	-	3/7/33/34	0/2/2/2
84	P5P	r2	38	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	24	85	-	2/3/25/26	0/3/3/3
85	Y5P	r3	29	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	10	86	-	0/3/25/26	0/3/3/3
84	P5P	r2	22	84	-	1/3/25/26	0/3/3/3
84	Y5P	r2	48	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	67	84	-	3/7/33/34	0/2/2/2
84	Y5P	r2	2	84	-	2/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	P5P	r2	27	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	47	85	-	1/3/25/26	0/3/3/3
85	Y5P	r3	59	85	-	1/7/33/34	0/2/2/2
86	Y5P	r4	55	86	-	1/7/33/34	0/2/2/2
85	Y5P	r3	65	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	22	86	-	3/3/25/26	0/3/3/3
84	Y5P	r2	62	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	61	84	-	2/7/33/34	0/2/2/2
84	P5P	r2	6	84	-	1/3/25/26	0/3/3/3
84	P5P	r2	63	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	10	85	-	0/3/25/26	0/3/3/3
85	Y5P	r3	71	85	-	3/7/33/34	0/2/2/2
86	P5P	r4	64	86	-	2/3/25/26	0/3/3/3
84	P5P	r2	15	84	-	2/3/25/26	0/3/3/3
85	P5P	r3	49	85	-	1/3/25/26	0/3/3/3
86	Y5P	r4	50	86	-	2/7/33/34	0/2/2/2
86	P5P	r4	30	86	-	1/3/25/26	0/3/3/3
85	Y5P	r3	41	85	-	3/7/33/34	0/2/2/2
85	P5P	r3	72	85	-	0/3/25/26	0/3/3/3
86	Y5P	r4	62	86	-	1/7/33/34	0/2/2/2
83	Y5P	r1	44	83	-	1/7/33/34	0/2/2/2
86	Y5P	r4	25	86	-	1/7/33/34	0/2/2/2
86	P5P	r4	69	86	-	0/3/25/26	0/3/3/3
85	Y5P	r3	55	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	49	84	-	3/7/33/34	0/2/2/2
85	P5P	r3	69	85	-	0/3/25/26	0/3/3/3
86	P5P	r4	65	86	-	0/3/25/26	0/3/3/3
85	Y5P	r3	62	85	-	1/7/33/34	0/2/2/2
86	Y5P	r4	66	86	-	3/7/33/34	0/2/2/2
85	Y5P	r3	21	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	1	86	-	3/3/25/26	0/3/3/3
85	Y5P	r3	40	85	-	1/7/33/34	0/2/2/2
86	Y5P	r4	3	86	-	1/7/33/34	0/2/2/2
84	Y5P	r2	17	84	-	4/7/33/34	0/2/2/2
86	P5P	r4	9	86	-	2/3/25/26	0/3/3/3
83	Y5P	r1	55	83	-	3/7/33/34	0/2/2/2
85	P5P	r3	14	85	-	1/3/25/26	0/3/3/3
86	P5P	r4	63	86	-	0/3/25/26	0/3/3/3
86	Y5P	r4	39	86	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	P5P	r3	45	85	-	0/3/25/26	0/3/3/3
86	P5P	r4	53	86	-	3/3/25/26	0/3/3/3
84	Y5P	r2	50	84	-	3/7/33/34	0/2/2/2
84	P5P	r2	71	84	-	0/3/25/26	0/3/3/3
84	Y5P	r2	40	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	68	85	-	1/7/33/34	0/2/2/2
83	Y5P	r1	56	83	-	5/7/33/34	0/2/2/2
84	P5P	r2	36	84	-	3/3/25/26	0/3/3/3
86	Y5P	r4	32	86	-	3/7/33/34	0/2/2/2
83	Y5P	r1	48	83	-	1/7/33/34	0/2/2/2
85	Y5P	r3	26	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	33	84	-	6/7/33/34	0/2/2/2
84	P5P	r2	73	84	-	3/3/25/26	0/3/3/3
85	P5P	r3	9	85	-	1/3/25/26	0/3/3/3
84	P5P	r2	57	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	8	85	-	0/3/25/26	0/3/3/3
84	P5P	r2	26	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	15	85	-	0/3/25/26	0/3/3/3
86	P5P	r4	27	86	-	0/3/25/26	0/3/3/3
84	Y5P	r2	42	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	25	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	52	85	-	2/3/25/26	0/3/3/3
84	P5P	r2	37	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	27	85	-	0/3/25/26	0/3/3/3
85	P5P	r3	53	85	-	0/3/25/26	0/3/3/3
86	Y5P	r4	4	86	-	1/7/33/34	0/2/2/2
86	Y5P	r4	33	86	-	2/7/33/34	0/2/2/2
86	Y5P	r4	48	86	-	3/7/33/34	0/2/2/2
86	Y5P	r4	74	86	-	4/7/33/34	0/2/2/2
86	P5P	r4	37	86	-	0/3/25/26	0/3/3/3
86	Y5P	r4	16	86	-	1/7/33/34	0/2/2/2
83	Y5P	r1	46	83	-	2/7/33/34	0/2/2/2
84	Y5P	r2	8	84	-	1/7/33/34	0/2/2/2
83	Y5P	r1	53	83	-	6/7/33/34	0/2/2/2
85	Y5P	r3	1	85	-	1/10/34/34	0/2/2/2
86	P5P	r4	71	86	-	0/3/25/26	0/3/3/3
85	Y5P	r3	48	85	-	4/7/33/34	0/2/2/2
86	Y5P	r4	45	86	-	4/7/33/34	0/2/2/2
84	Y5P	r2	43	84	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	P5P	r4	18	86	-	2/3/25/26	0/3/3/3
86	P5P	r4	7	86	-	2/3/25/26	0/3/3/3
83	Y5P	r1	51	83	-	2/7/33/34	0/2/2/2
86	Y5P	r4	47	86	-	4/7/33/34	0/2/2/2
84	P5P	r2	53	84	-	0/3/25/26	0/3/3/3
85	Y5P	r3	74	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	50	85	-	4/7/33/34	0/2/2/2
86	P5P	r4	26	86	-	2/3/25/26	0/3/3/3
86	P5P	r4	57	86	-	0/3/25/26	0/3/3/3
86	P5P	r4	58	86	-	0/3/25/26	0/3/3/3
86	Y5P	r4	13	86	-	3/7/33/34	0/2/2/2
85	Y5P	r3	70	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	35	85	-	3/7/33/34	0/2/2/2
86	Y5P	r4	60	86	-	1/7/33/34	0/2/2/2
83	Y5P	r1	54	83	-	1/7/33/34	0/2/2/2
86	P5P	r4	14	86	-	0/3/25/26	0/3/3/3
85	Y5P	r3	12	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	23	84	-	2/3/25/26	0/3/3/3
85	Y5P	r3	13	85	-	5/7/33/34	0/2/2/2
85	Y5P	r3	33	85	-	1/7/33/34	0/2/2/2
86	Y5P	r4	68	86	-	1/7/33/34	0/2/2/2
85	Y5P	r3	51	85	-	4/7/33/34	0/2/2/2
86	Y5P	r4	61	86	-	2/7/33/34	0/2/2/2
84	Y5P	r2	32	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	28	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	60	85	-	2/7/33/34	0/2/2/2
84	Y5P	r2	54	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	5	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	75	85	-	0/3/25/26	0/3/3/3
84	P5P	r2	21	84	-	2/3/25/26	0/3/3/3
84	Y5P	r2	47	84	-	2/7/33/34	0/2/2/2
84	Y5P	r2	55	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	19	84	-	3/3/25/26	0/3/3/3
84	P5P	r2	44	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	14	84	-	3/3/25/26	0/3/3/3
85	Y5P	r3	25	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	66	85	-	3/7/33/34	0/2/2/2
86	P5P	r4	21	86	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	Y5P	r4	12	86	-	2/7/33/34	0/2/2/2
85	P5P	r3	3	85	-	3/3/25/26	0/3/3/3
86	P5P	r4	24	86	-	2/3/25/26	0/3/3/3
85	P5P	r3	46	85	-	0/3/25/26	0/3/3/3
85	P5P	r3	38	85	-	2/3/25/26	0/3/3/3
86	Y5P	r4	42	86	-	1/7/33/34	0/2/2/2
86	P5P	r4	73	86	-	3/3/25/26	0/3/3/3
84	P5P	r2	28	84	-	0/3/25/26	0/3/3/3
85	Y5P	r3	37	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	6	86	-	2/3/25/26	0/3/3/3
84	P5P	r2	31	84	-	0/3/25/26	0/3/3/3
84	Y5P	r2	3	84	-	3/7/33/34	0/2/2/2
85	Y5P	r3	2	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	5	86	-	0/3/25/26	0/3/3/3
85	P5P	r3	23	85	-	0/3/25/26	0/3/3/3
86	P5P	r4	29	86	-	2/3/25/26	0/3/3/3
84	Y5P	r2	51	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	6	85	-	0/3/25/26	0/3/3/3
85	P5P	r3	44	85	-	1/3/25/26	0/3/3/3
85	P5P	r3	32	85	-	0/3/25/26	0/3/3/3
85	Y5P	r3	39	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	57	85	-	3/7/33/34	0/2/2/2
84	P5P	r2	46	84	-	3/3/25/26	0/3/3/3
85	Y5P	r3	18	85	-	4/7/33/34	0/2/2/2
84	P5P	r2	58	84	-	0/3/25/26	0/3/3/3
86	Y5P	r4	40	86	-	1/7/33/34	0/2/2/2
84	P5P	r2	35	84	-	2/3/25/26	0/3/3/3
84	P5P	r2	70	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	76	84	-	1/3/25/26	0/3/3/3
84	Y5P	r2	72	84	-	3/7/33/34	0/2/2/2
86	Y5P	r4	11	86	-	1/7/33/34	0/2/2/2
84	Y5P	r2	39	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	68	84	-	3/7/33/34	0/2/2/2
84	P5P	r2	69	84	-	3/3/25/26	0/3/3/3
86	Y5P	r4	43	86	-	1/7/33/34	0/2/2/2
84	Y5P	r2	56	84	-	1/7/33/34	0/2/2/2
86	Y5P	r4	41	86	-	3/7/33/34	0/2/2/2
85	P5P	r3	43	85	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	P5P	r2	52	84	-	1/3/25/26	0/3/3/3
86	P5P	r4	28	86	-	2/3/25/26	0/3/3/3
83	Y5P	r1	57	83	-	1/7/33/34	0/2/2/2
85	P5P	r3	5	85	-	2/3/25/26	0/3/3/3
84	P5P	r2	10	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	1	84	-	3/3/25/26	0/3/3/3
84	Y5P	r2	20	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	74	84	-	3/7/33/34	0/2/2/2
86	P5P	r4	31	86	-	0/3/25/26	0/3/3/3
85	P5P	r3	30	85	-	2/3/25/26	0/3/3/3
86	P5P	r4	46	86	-	0/3/25/26	0/3/3/3
84	P5P	r2	34	84	-	0/3/25/26	0/3/3/3
86	Y5P	r4	56	86	-	3/7/33/34	0/2/2/2
84	P5P	r2	29	84	-	0/3/25/26	0/3/3/3
86	Y5P	r4	72	86	-	3/7/33/34	0/2/2/2
84	Y5P	r2	4	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	31	85	-	1/3/25/26	0/3/3/3
85	Y5P	r3	73	85	-	3/7/33/34	0/2/2/2
86	P5P	r4	44	86	-	0/3/25/26	0/3/3/3
84	Y5P	r2	75	84	-	4/7/33/34	0/2/2/2
86	P5P	r4	23	86	-	3/3/25/26	0/3/3/3
84	P5P	r2	24	84	-	0/3/25/26	0/3/3/3
85	Y5P	r3	64	85	-	3/7/33/34	0/2/2/2
86	Y5P	r4	17	86	-	3/7/33/34	0/2/2/2
83	Y5P	r1	52	83	-	1/7/33/34	0/2/2/2
84	Y5P	r2	60	84	-	1/7/33/34	0/2/2/2
86	Y5P	r4	67	86	-	5/7/33/34	0/2/2/2
86	P5P	r4	36	86	-	0/3/25/26	0/3/3/3

The worst 5 of 499 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	r4	75	Y5P	C6-C5	10.60	1.52	1.33
86	r4	74	Y5P	C6-C5	10.59	1.52	1.33
85	r3	18	Y5P	C6-C5	10.59	1.52	1.33
85	r3	40	Y5P	C6-C5	10.59	1.52	1.33
86	r4	66	Y5P	C6-C5	10.58	1.52	1.33

The worst 5 of 339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r3	3	P5P	N1-C2-N3	-6.12	119.82	127.65
86	r4	15	P5P	N1-C2-N3	-6.03	119.94	127.65
84	r2	63	P5P	N1-C2-N3	-6.02	119.95	127.65
85	r3	24	P5P	N1-C2-N3	-6.01	119.96	127.65
84	r2	70	P5P	N1-C2-N3	-6.00	119.97	127.65

There are no chirality outliers.

5 of 378 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	r1	51	Y5P	O4'-C1'-N1-C2
83	r1	53	Y5P	O4'-C4'-C5'-O5'
84	r2	12	Y5P	O4'-C1'-N1-C2
84	r2	13	Y5P	O4'-C4'-C5'-O5'
84	r2	13	Y5P	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 205 ligands modelled in this entry, 202 are monoatomic - leaving 3 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	GTP	AX	500	-	26,34,34	1.14	2 (7%)	32,54,54	1.53	6 (18%)
91	H8Q	XA	5142	-	77,80,80	1.08	5 (6%)	103,115,115	1.34	15 (14%)
92	DOL	XA	5143	-	43,50,50	3.53	17 (39%)	51,70,70	2.78	11 (21%)

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	GTP	AX	500	-	-	8/18/38/38	0/3/3/3
91	H8Q	XA	5142	-	-	31/83/127/127	0/8/8/8
92	DOL	XA	5143	-	-	16/58/77/77	0/2/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	XA	5143	DOL	C28-C29	9.95	1.55	1.32
92	XA	5143	DOL	C22-C23	9.60	1.57	1.32
92	XA	5143	DOL	C19-C20	7.39	1.57	1.34
92	XA	5143	DOL	C6-N5	6.53	1.49	1.34
92	XA	5143	DOL	C26-N25	6.52	1.48	1.34

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	XA	5143	DOL	O40-S39-O41	-15.71	100.27	118.19
92	XA	5143	DOL	C24-N25-C26	-5.47	113.18	122.03
92	XA	5143	DOL	C23-C22-C20	-4.11	119.68	125.89
93	AX	500	GTP	PA-O3A-PB	-3.94	119.31	132.83
91	XA	5142	H8Q	O41-C34-C33	3.84	122.03	110.83

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	XA	5142	H8Q	C2-C1-N13-C14
91	XA	5142	H8Q	C2-C1-N13-C18
91	XA	5142	H8Q	O1-C1-N13-C14
91	XA	5142	H8Q	O1-C1-N13-C18
91	XA	5142	H8Q	C33-C34-O41-C43

There are no ring outliers.

3 monomers are involved in 8 short contacts:

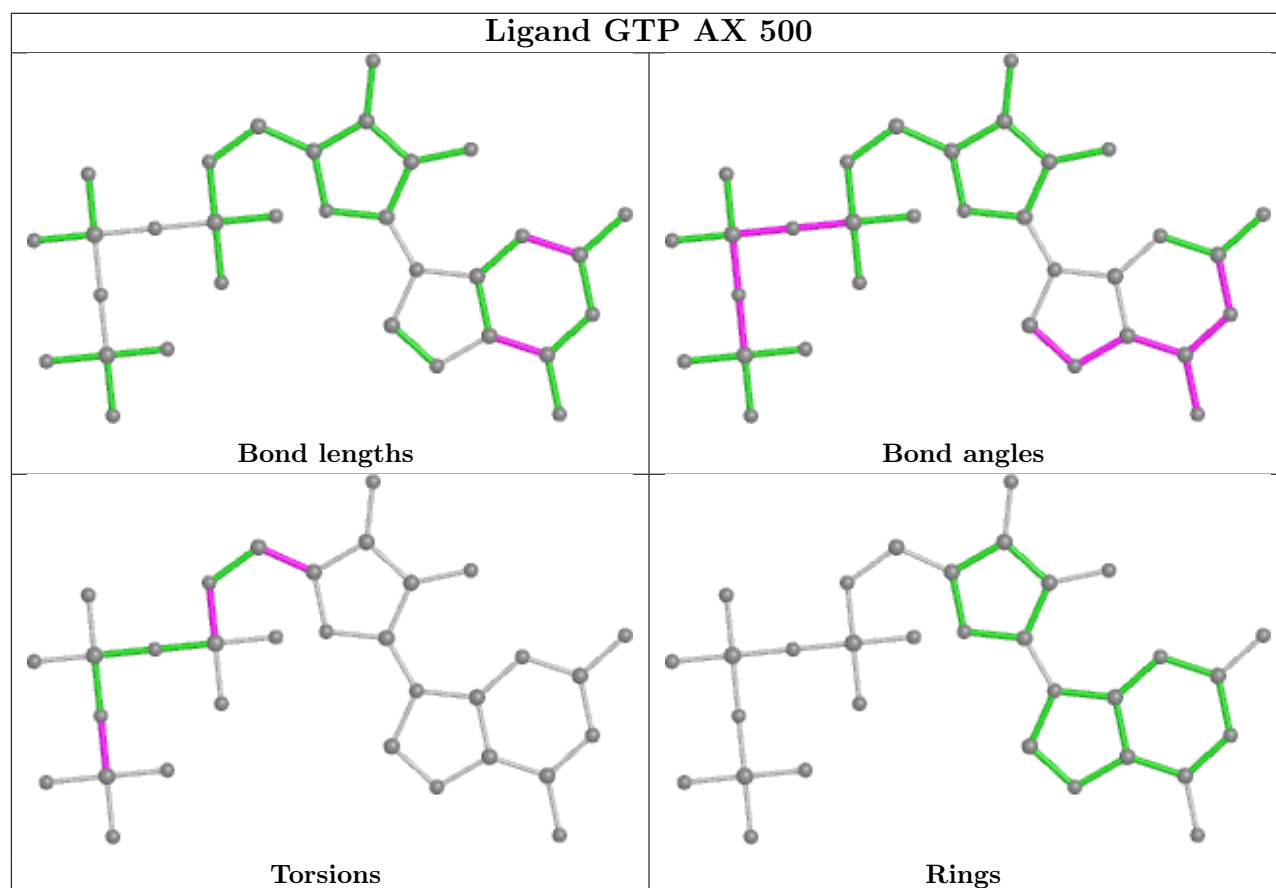
Mol	Chain	Res	Type	Clashes	Symm-Clashes
93	AX	500	GTP	1	0

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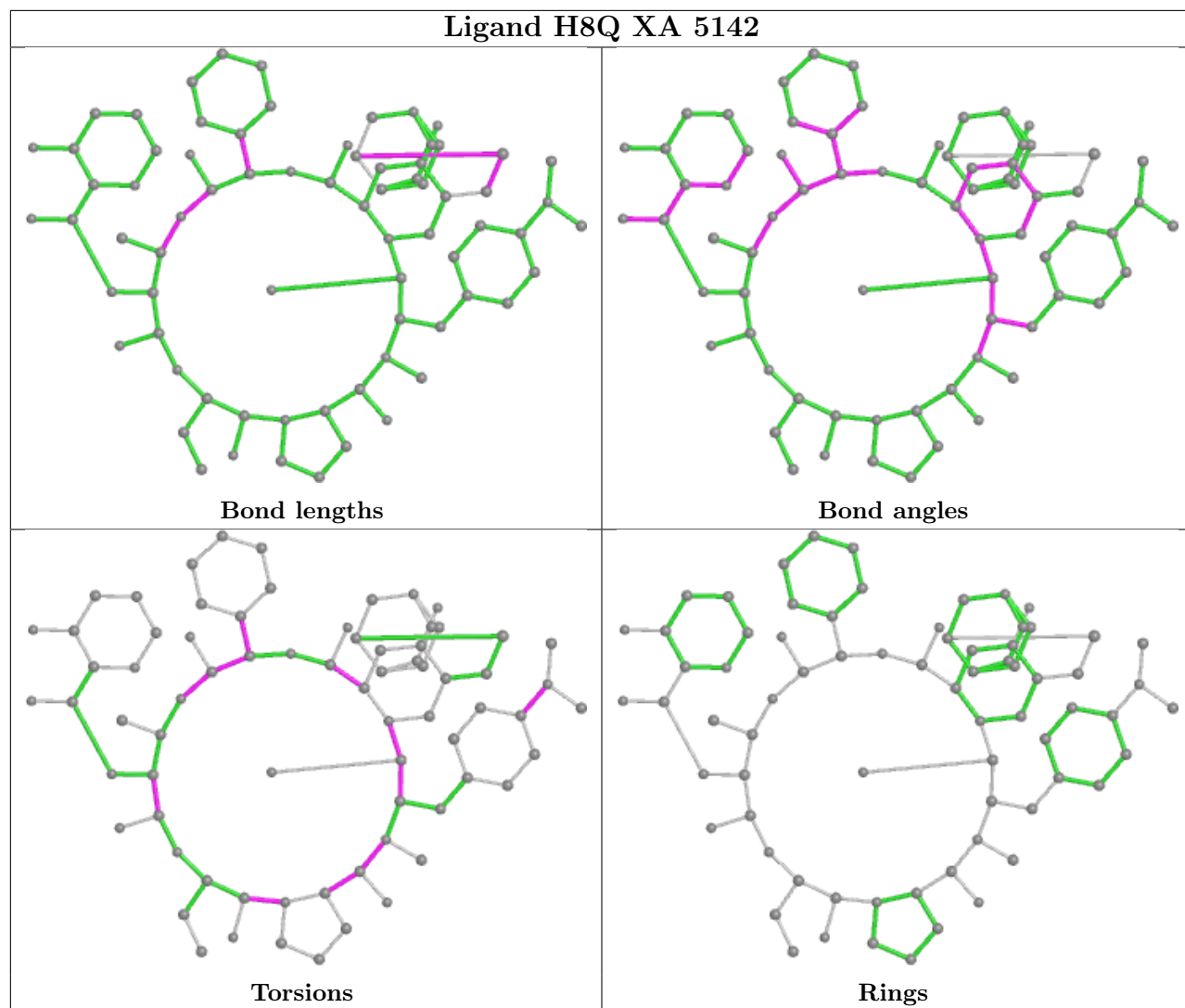
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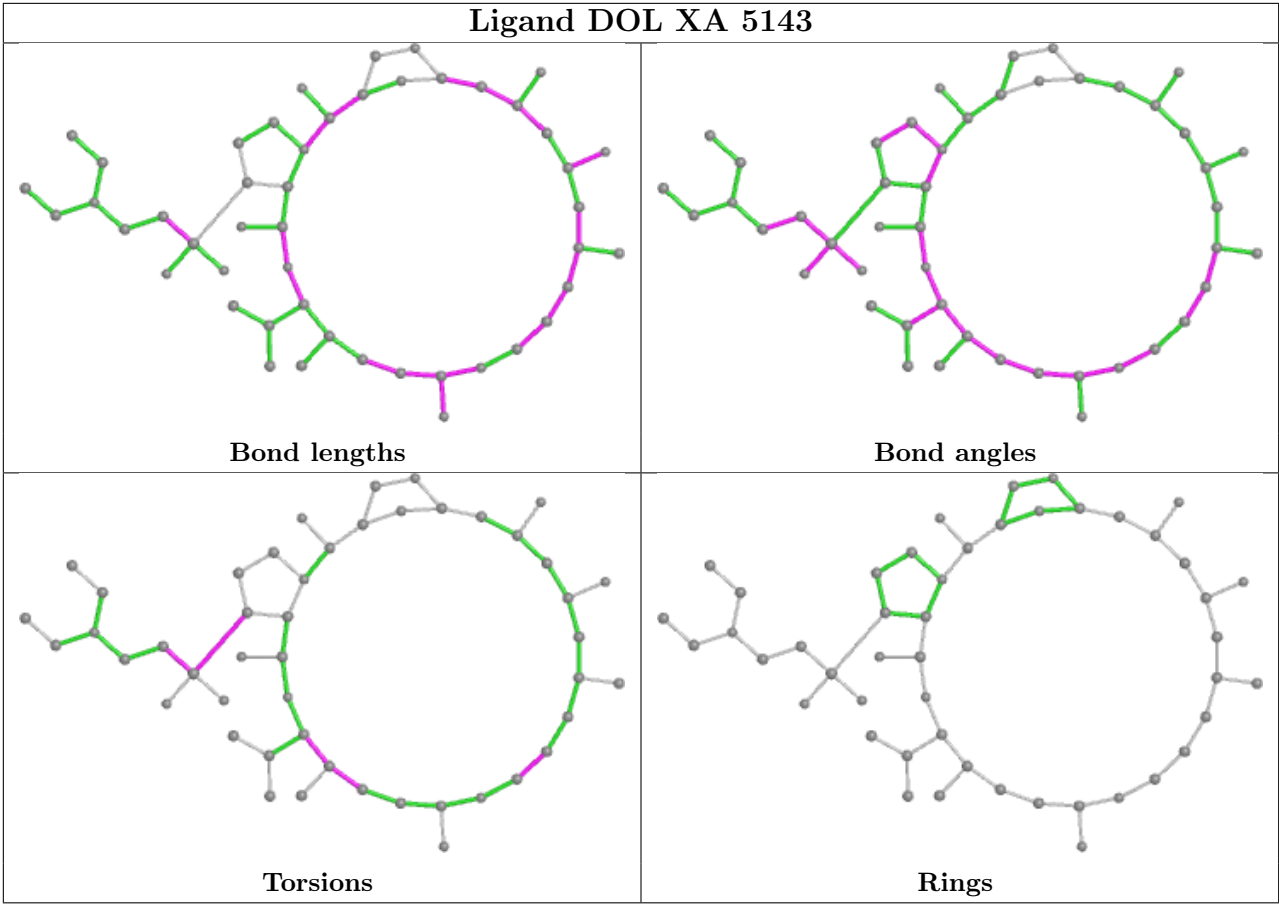
Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	XA	5142	H8Q	5	0
92	XA	5143	DOL	2	0

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



Ligand H8Q XA 5142





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
85	r3	3
16	A4	2
38	AV	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r3	18:Y5P	O3'	19:P5P	P	6.45
1	A4	537:ARG	C	538:ASP	N	6.17
1	r3	17:P5P	O3'	18:Y5P	P	5.79
1	r3	16:Y5P	O3'	17:P5P	P	5.56

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AV	269:SER	C	270:PRO	N	4.72

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11397. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.