



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 05:33 PM UTC

PDB ID : 9OLF / pdb_00009olf
EMDB ID : EMD-70592
Title : Membrane-associated human mitoribosome in complex with TACO1
Authors : Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on : 2025-05-12
Resolution : 2.46 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

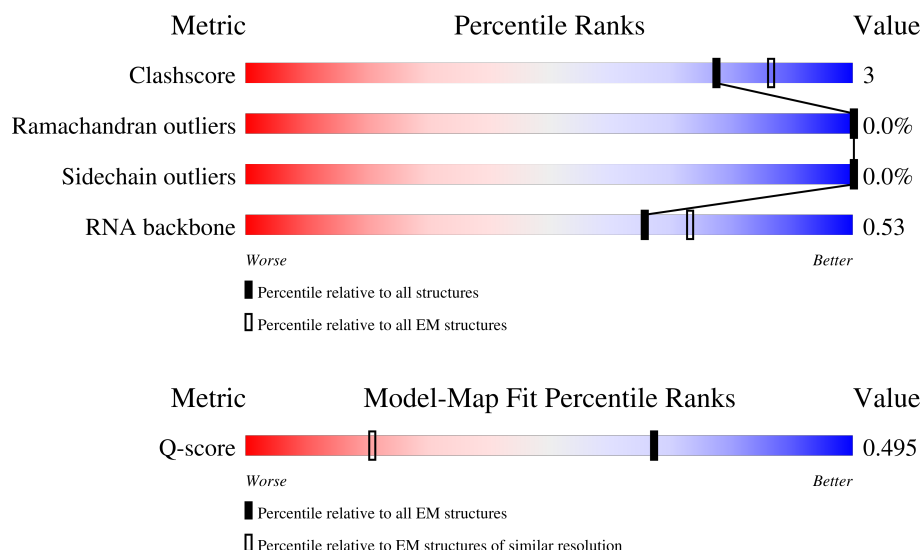
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.46 Å.

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











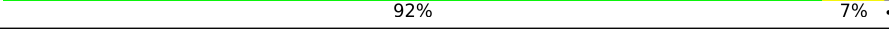

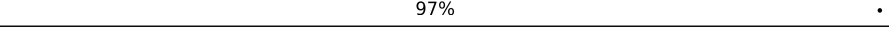
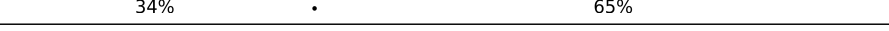







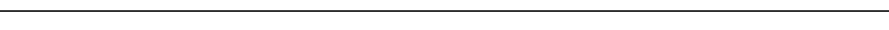

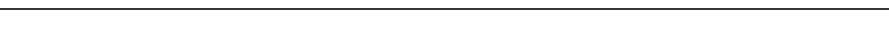
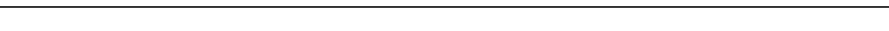


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6014 (1.96 - 2.96)

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

Mol	Chain	Length	Quality of chain
1	0	188	
2	1	65	
3	2	92	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1558	
12	A0	217	
13	A1	323	
14	A2	118	
15	A3	199	
16	A4	689	
17	A5	1394	
18	A6	109	
19	AA	954	
20	AB	296	
21	AC	167	
22	AD	430	
23	AE	125	
24	AF	242	
25	AG	396	
26	AH	201	
27	AI	194	
28	AJ	138	






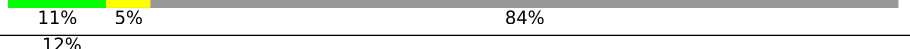

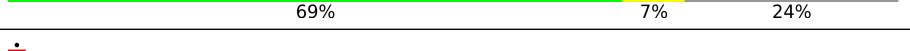
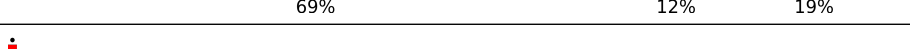
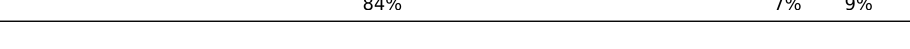
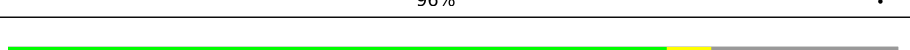

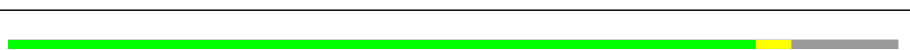

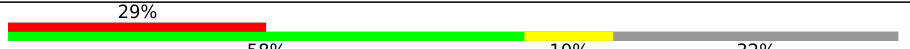





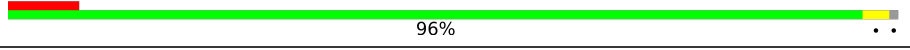
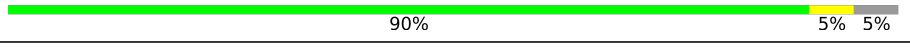

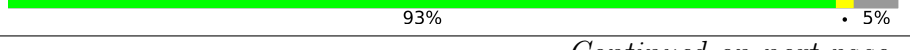

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	AK	128	
30	AL	257	
31	AM	137	
32	AN	130	
33	AO	258	
34	AP	142	
35	AQ	87	
36	AR	360	
37	AS	190	
38	AT	173	
39	AU	205	
40	AV	414	
41	AW	187	
42	AX	398	
43	AY	395	
44	AZ	106	
45	Aw	76	
46	Ax	71	
47	Ay	76	
48	Az	34	
49	B	72	
50	C	297	
51	D	305	
52	E	348	
53	F	311	











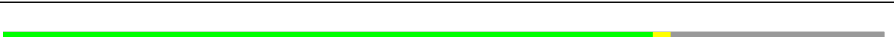


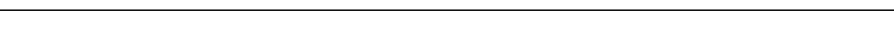
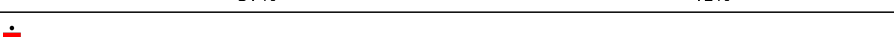
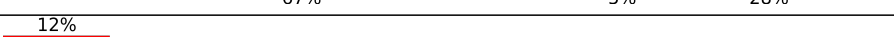
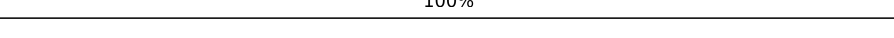





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	G	198	
54	t	198	
54	u	198	
54	v	198	
54	w	198	
54	x	198	
54	y	198	
55	H	267	
56	I	261	
57	J	192	
58	K	178	
59	L	145	
60	M	296	
61	N	251	
62	O	175	
63	OX	435	
64	P	180	
65	Q	292	
66	R	149	
67	S	205	
68	T	206	
69	U	153	
70	V	216	
71	W	148	
72	X	256	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
73	Y	250	
74	Z	161	
75	a	142	
76	b	215	
77	c	332	
78	d	306	
79	e	279	
80	f	212	
81	g	166	
82	h	158	
83	i	128	
84	j	123	
85	k	112	
86	l	138	
87	m	128	
88	n	43	
89	o	102	
90	p	206	
91	q	222	
92	r	196	
93	s	439	
94	z	325	

2 Entry composition

There are 105 unique types of molecules in this entry. The entry contains 192936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	56	Total	C	N	O	S	0	0
			464	296	89	77	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	157	Total	C	N	O	S	0	0
			1327	844	235	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1558	Total	C	N	O	P	0	0
			33070	14843	5963	10706	1558		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	A	deletion	GB 2756414513
A	?	-	C	deletion	GB 2756414513
A	?	-	U	deletion	GB 2756414513

- Molecule 12 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A0	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	279	Total	C	N	O	S	0	0
			2265	1435	387	432	11		

- Molecule 14 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A2	118	Total	C	N	O	S	0	0
			935	579	182	166	8		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A3	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A4	588	Total	C	N	O	S	0	0
			4768	3053	808	879	28		

- Molecule 17 is a protein called Leucine-rich PPR motif-containing protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A5	581	Total	C	N	O	S	0	0
			4646	2959	790	871	26		

- Molecule 18 is a protein called SRA stem-loop-interacting RNA-binding protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A6	74	Total	C	N	O	S	0	0
			603	384	115	103	1		

- Molecule 19 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AA	954	Total	C	N	O	P	0	0
			20260	9088	3647	6571	954		

- Molecule 20 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AB	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 21 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AC	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 22 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AD	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 23 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AE	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 24 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AF	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 25 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AG	327	Total	C	N	O	S	0	0
			2688	1710	477	487	14		

- Molecule 26 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AH	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 27 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AI	137	Total	C	N	O	S	0	0
			1019	641	193	181	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AJ	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 29 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AK	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 30 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AL	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 31 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 32 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AN	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 33 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AO	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

- Molecule 34 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AP	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 35 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AQ	87	Total	C	N	O	S	0	0
			744	460	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	1	ACE	-	acetylation	UNP P82921
AQ	50	ARG	CYS	variant	UNP P82921

- Molecule 36 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AR	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 37 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AS	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 38 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AT	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 39 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AU	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 40 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AV	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 41 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AW	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 42 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AX	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 43 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AY	221	Total	C	N	O	S	0	0
			1835	1159	319	352	5		

- Molecule 44 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AZ	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 45 is a RNA chain called A/A-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Aw	68	Total	C	N	O	P	0	0
			1434	646	248	472	68		

- Molecule 46 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ax	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

- Molecule 47 is a RNA chain called E/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ay	70	Total	C	N	O	P	0	0
			1483	665	261	487	70		

- Molecule 48 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Az	34	Total	C	N	O	P	0	0
			719	324	123	238	34		

- Molecule 49 is a RNA chain called RNA (73-MER)mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B	72	Total	C	N	O	P	0	0
			1524	685	269	498	72		

- Molecule 50 is a protein called Translational activator of cytochrome c oxidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C	223	Total	C	N	O	S	0	0
			1732	1072	310	340	10		

- Molecule 51 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	D	238	Total	C	N	O	S	0	0
			1859	1157	376	317	9		

- Molecule 52 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	E	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

- Molecule 53 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	F	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

- Molecule 54 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	G	72	Total	C	N	O		0	0
			558	358	97	103			
54	t	46	Total	C	N	O		0	0
			354	228	56	70			
54	u	32	Total	C	N	O		0	0
			257	168	40	49			
54	v	32	Total	C	N	O		0	0
			257	168	40	49			
54	w	31	Total	C	N	O		0	0
			245	159	39	47			
54	x	31	Total	C	N	O		0	0
			245	159	39	47			
54	y	31	Total	C	N	O		0	0
			245	159	39	47			

- Molecule 55 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	H	202	Total	C	N	O	S	0	0
			1661	1067	304	286	4		

- Molecule 56 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	I	212	Total	C	N	O	S	0	0
			1695	1088	304	292	11		

- Molecule 57 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	J	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 58 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	K	178	Total	C	N	O	S	0	0
			1455	936	259	253	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP H2QWN0
K	132	TYR	ASP	conflict	UNP H2QWN0

- Molecule 59 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	L	115	Total	C	N	O	S	0	0
			890	559	171	155	5		

- Molecule 60 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	M	291	Total	C	N	O	S	0	0
			2327	1483	430	408	6		

- Molecule 61 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	N	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 62 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	O	154	Total	C	N	O	S	0	0
			1259	792	241	219	7		

- Molecule 63 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	OX	297	Total	C	N	O	S	0	0
			2404	1568	417	405	14		

- Molecule 64 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	P	144	Total	C	N	O	S	0	0
			1173	733	224	211	5		

- Molecule 65 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Q	239	Total	C	N	O	S	0	0
			1990	1277	353	351	9		

- Molecule 66 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	R	140	Total	C	N	O	S	0	0
			1154	732	231	187	4		

- Molecule 67 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	S	161	Total	C	N	O	S	0	0
			1293	835	227	227	4		

- Molecule 68 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	T	166	Total	C	N	O	S	0	0
			1369	875	254	233	7		

- Molecule 69 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	U	152	Total	C	N	O	S	0	0
			1248	786	234	225	3		

- Molecule 70 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	V	205	Total	C	N	O	S	0	0
			1676	1068	298	302	8		

- Molecule 71 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	W	116	Total	C	N	O	S	0	0
			904	577	171	153	3		

- Molecule 72 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	X	244	Total	C	N	O	S	0	0
			2044	1322	352	365	5		

- Molecule 73 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Y	181	Total	C	N	O	S	0	0
			1556	995	298	259	4		

- Molecule 74 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Z	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 75 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	a	103	Total	C	N	O	S	0	0
			865	543	155	162	5		

- Molecule 76 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	b	150	Total	C	N	O	S	0	0
			1193	742	231	217	3		

- Molecule 77 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	c	286	Total	C	N	O	S	0	0
			2299	1470	397	423	9		

- Molecule 78 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	d	259	Total	C	N	O	S	0	0
			2124	1357	369	384	14		

- Molecule 79 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	e	238	Total	C	N	O	S	0	0
			1931	1222	339	364	6		

- Molecule 80 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	f	157	Total	C	N	O	S	0	0
			1252	799	207	242	4		

- Molecule 81 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	g	134	Total	C	N	O	S	0	0
			1113	719	193	199	2		

- Molecule 82 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	h	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 83 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	i	97	Total	C	N	O	S	0	0
			828	532	165	127	4		

- Molecule 84 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	j	94	Total	C	N	O	S	0	0
			745	463	144	136	2		

- Molecule 85 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	k	102	Total	C	N	O	S	0	0
			774	479	148	142	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 86 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	l	82	Total	C	N	O	S	0	0
			688	437	120	128	3		

- Molecule 87 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	m	92	Total	C	N	O	S	0	0
			791	488	159	142	2		

- Molecule 88 is a protein called Nascent polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
88	n	43	Total	C	N	O	0	0
			215	129	43	43		

- Molecule 89 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	o	94	Total	C	N	O	S	0	0
			798	501	165	129	3		

- Molecule 90 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	p	147	Total	C	N	O	S	0	0
			1205	748	228	225	4		

- Molecule 91 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	q	177	Total	C	N	O	S	0	0
			1495	929	292	269	5		

- Molecule 92 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

- Molecule 93 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	s	385	Total	C	N	O	S	0	0
			3148	2018	558	558	14		

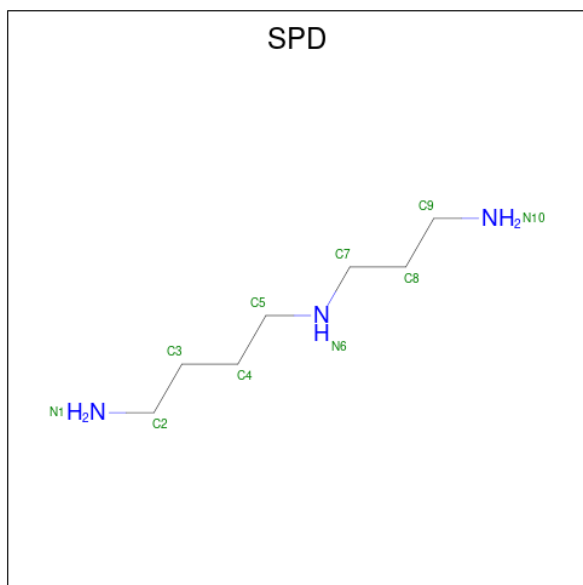
- Molecule 94 is a protein called Large ribosomal subunit protein uL1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	z	252	Total	C	N	O	S	0	0
			2027	1304	336	381	6		

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

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

- Molecule 96 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
96	A	1	Total	C	N	0
			10	7	3	
96	A	1	Total	C	N	0
			10	7	3	
96	A	1	Total	C	N	0
			10	7	3	
96	A	1	Total	C	N	0
			10	7	3	
96	AA	1	Total	C	N	0
			10	7	3	
96	AA	1	Total	C	N	0
			10	7	3	
96	O	1	Total	C	N	0
			10	7	3	

- Molecule 97 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

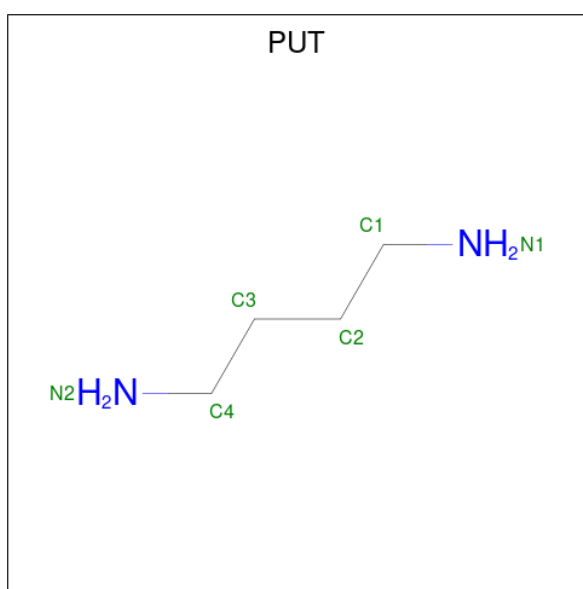
Mol	Chain	Residues	Atoms		AltConf
97	A	137	Total	Mg	0
			137	137	
97	A3	1	Total	Mg	0
			1	1	
97	AA	60	Total	Mg	0
			60	60	
97	AB	1	Total	Mg	0
			1	1	
97	AX	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
97	Az	1	Total	Mg	0
			1	1	
97	D	2	Total	Mg	0
			2	2	
97	E	1	Total	Mg	0
			1	1	
97	g	1	Total	Mg	0
			1	1	

- Molecule 98 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
98	A	1	Total	C	N	0
			6	4	2	

- Molecule 99 is POTASSIUM ION (CCD ID: K) (formula: K).

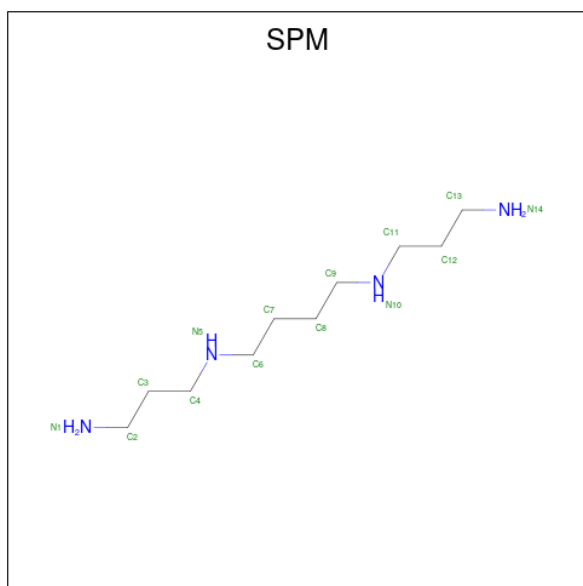
Mol	Chain	Residues	Atoms		AltConf
99	A	29	Total	K	0
			29	29	
99	AA	18	Total	K	0
			18	18	
99	D	1	Total	K	0
			1	1	
99	M	2	Total	K	0
			2	2	

Continued on next page...

Continued from previous page...

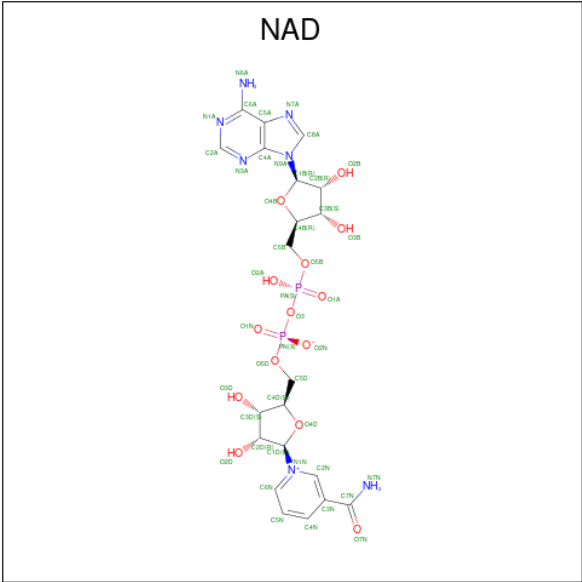
Mol	Chain	Residues	Atoms		AltConf
99	N	1	Total	K	0
			1	1	
99	P	1	Total	K	0
			1	1	
99	W	1	Total	K	0
			1	1	
99	o	1	Total	K	0
			1	1	

- Molecule 100 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



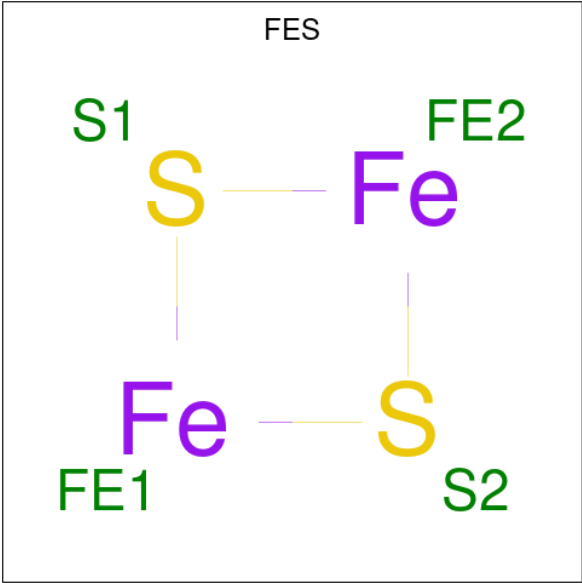
Mol	Chain	Residues	Atoms			AltConf
100	AA	1	Total	C	N	0
			14	10	4	
100	AA	1	Total	C	N	0
			14	10	4	

- Molecule 101 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 102 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



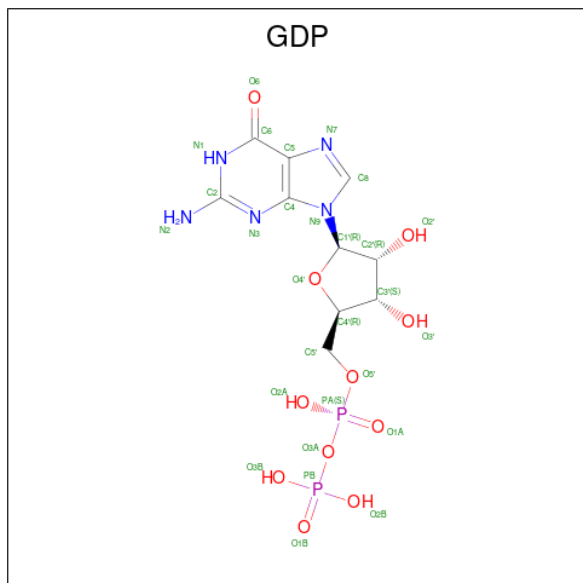
Mol	Chain	Residues	Atoms			AltConf
102	AP	1	Total	Fe	S	0
			4	2	2	
102	AT	1	Total	Fe	S	0
			4	2	2	

Continued on next page...

Continued from previous page...

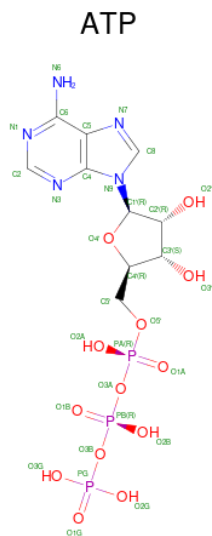
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
102	r	1	4	2	2	0

- Molecule 103 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



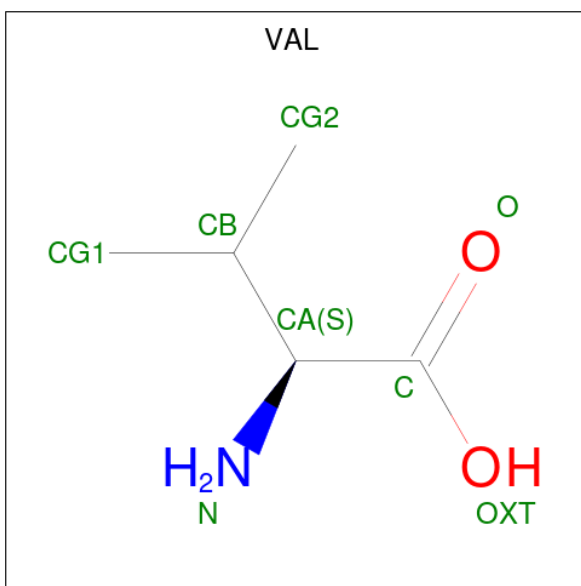
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
103	AX	1	28	10	5	11	2	0

- Molecule 104 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 105 is VALINE (CCD ID: VAL) (formula: $\text{C}_5\text{H}_{11}\text{NO}_2$).

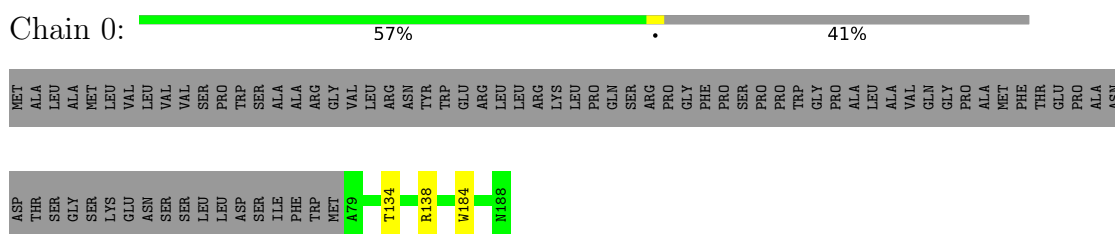


Mol	Chain	Residues	Atoms				AltConf
105	B	1	Total	C	N	O	0
			7	5	1	1	

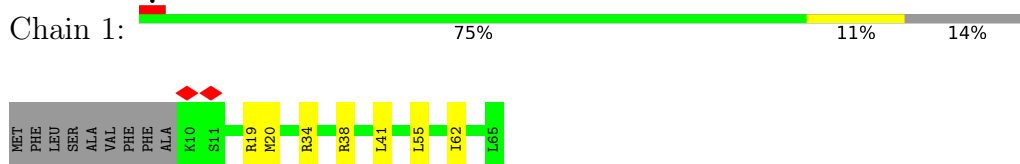
3 Residue-property plots [i](#)

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

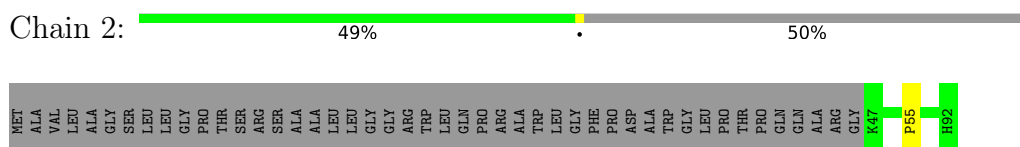
- Molecule 1: 39S ribosomal protein L32, mitochondrial



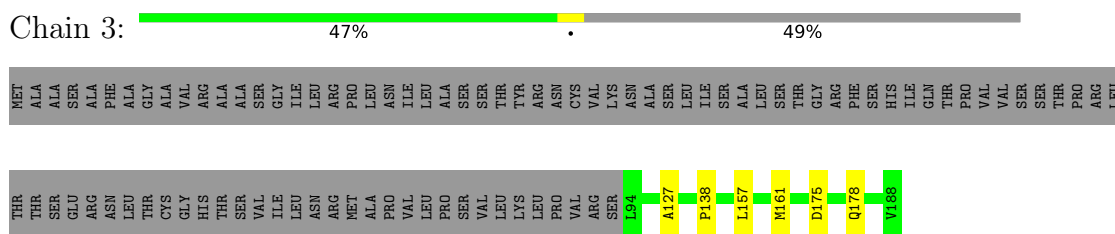
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial

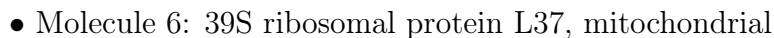


- Molecule 4: 39S ribosomal protein L35, mitochondrial

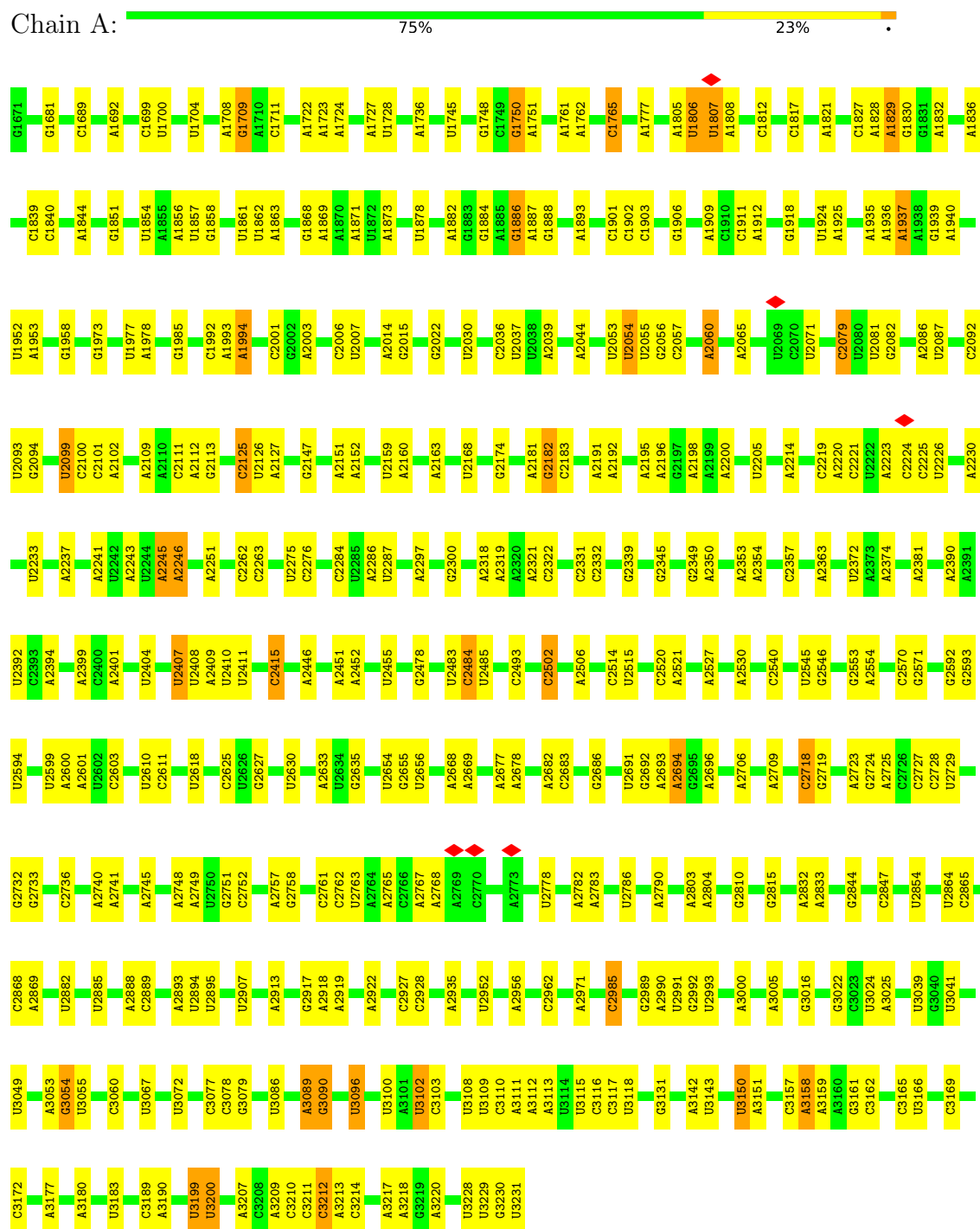


- Molecule 5: 39S ribosomal protein L36, mitochondrial

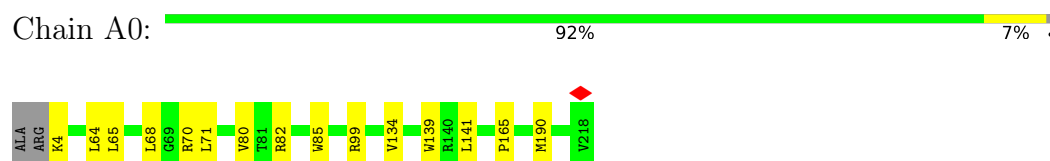




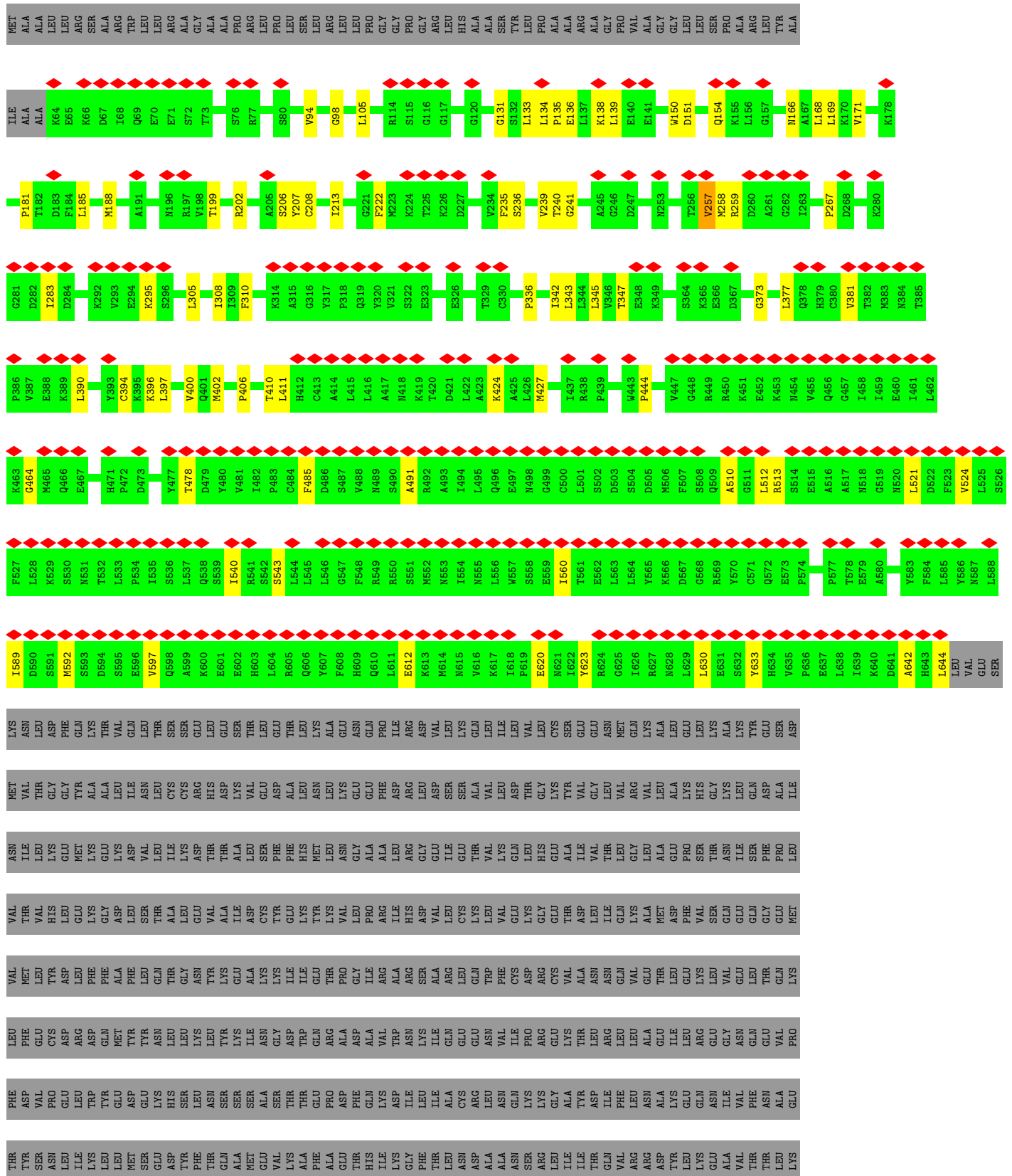
• Molecule 11: 16S mitochondrial rRNA



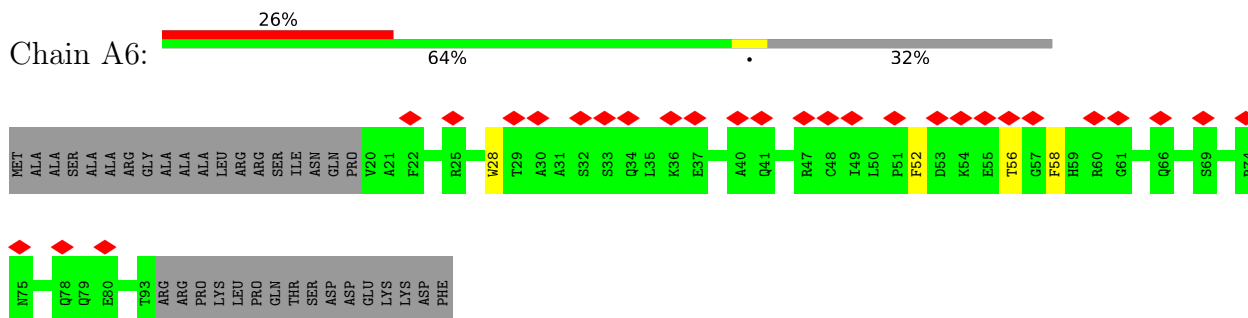
• Molecule 12: Small ribosomal subunit protein mS34



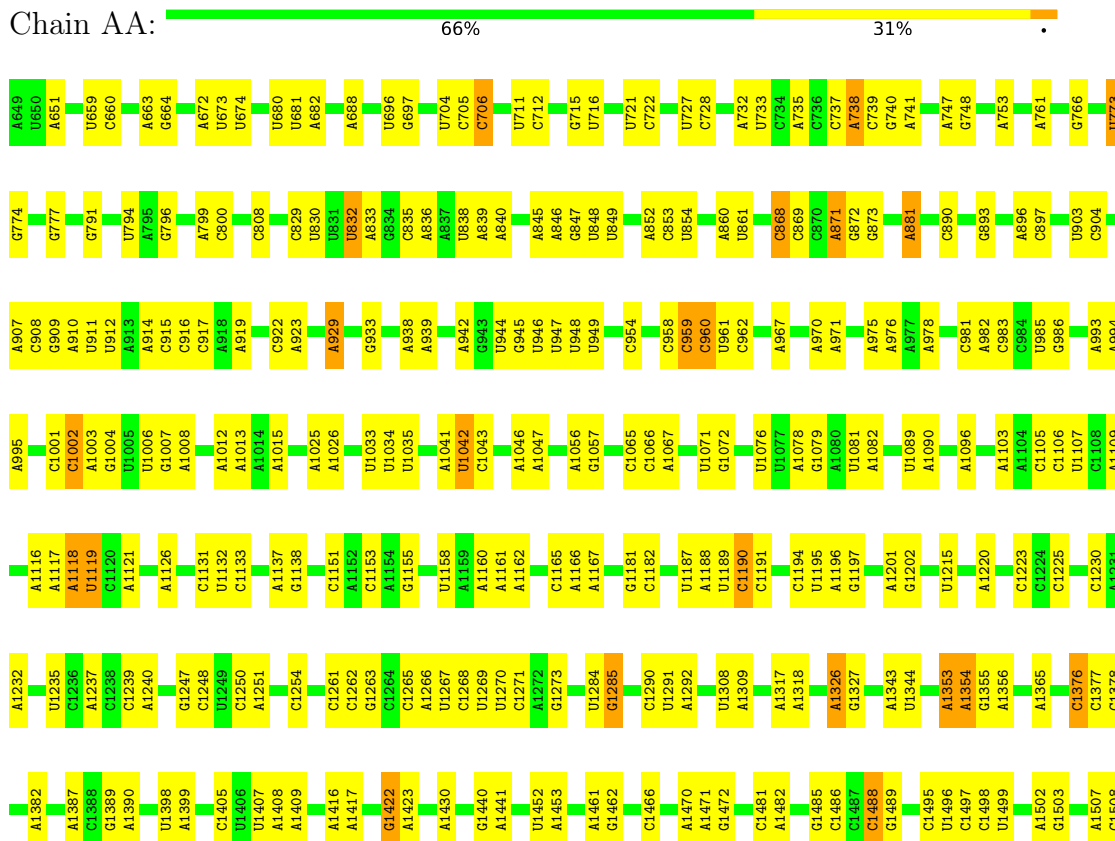
Chain A5:



- Molecule 18: SRA stem-loop-interacting RNA-binding protein, mitochondrial



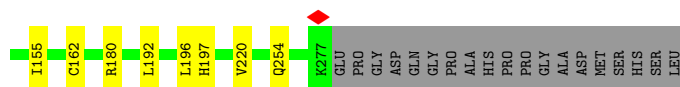
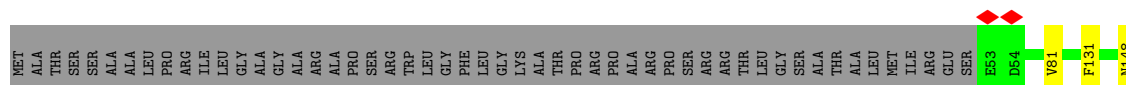
- Molecule 19: 12S mitochondrial rRNA





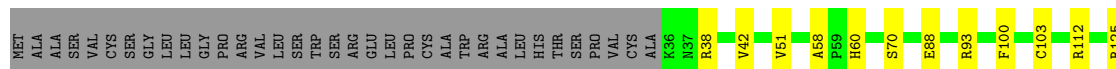
- Molecule 20: 28S ribosomal protein S2, mitochondrial

Chain AB: 72% 24%



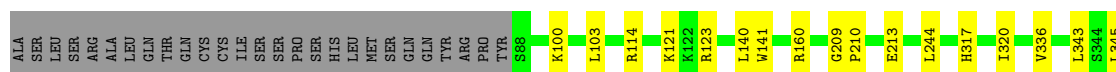
- Molecule 21: 28S ribosomal protein S24, mitochondrial

Chain AC: 69% 10% 21%



- Molecule 22: 28S ribosomal protein S5, mitochondrial

Chain AD: 75% 5% 20%



- Molecule 23: 28S ribosomal protein S6, mitochondrial

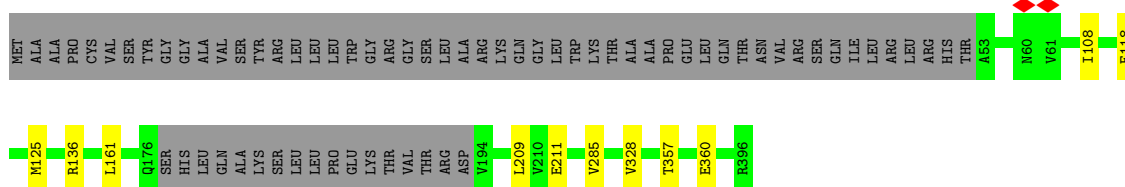
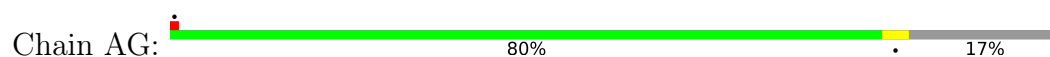
Chain AE: 91% 6%



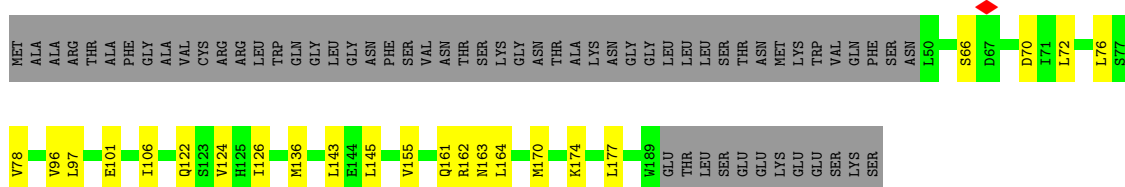
- Molecule 24: 28S ribosomal protein S7, mitochondrial

Chain AF: 81% 5% 14%

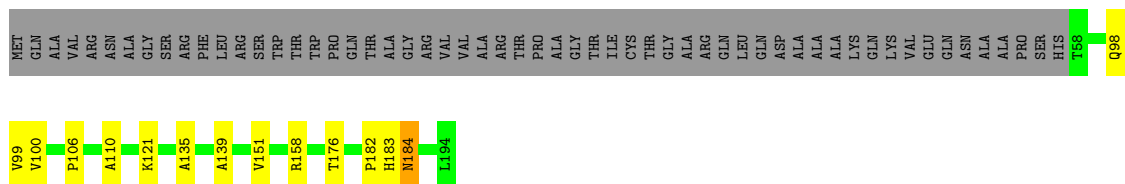
- Molecule 25: 28S ribosomal protein S9, mitochondrial



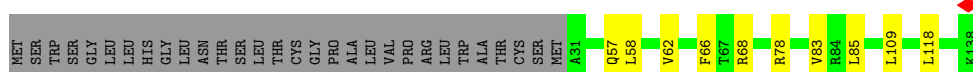
- Molecule 26: 28S ribosomal protein S10, mitochondrial



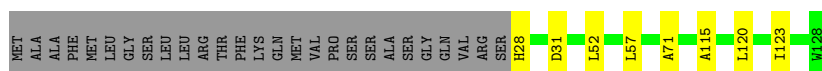
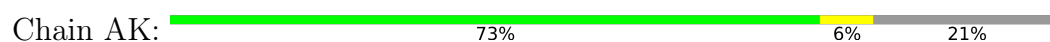
- Molecule 27: 28S ribosomal protein S11, mitochondrial



- Molecule 28: 28S ribosomal protein S12, mitochondrial

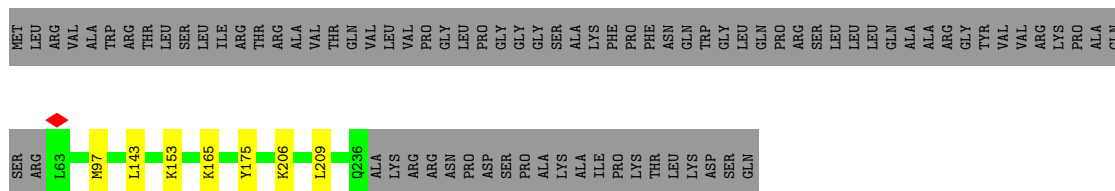


- Molecule 29: 28S ribosomal protein S14, mitochondrial




- Molecule 30: 28S ribosomal protein S15, mitochondrial

Chain AL:  65% 32%




- Molecule 31: 28S ribosomal protein S16, mitochondrial

Chain AM:  75% 12% 13%



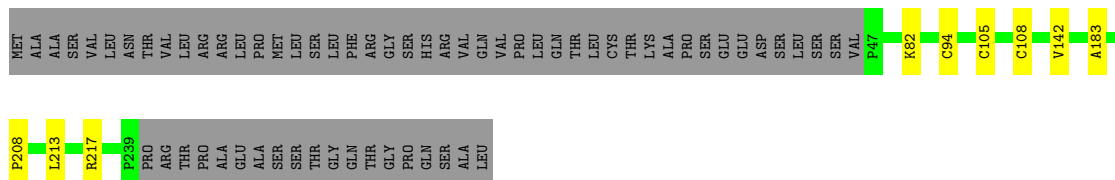
- Molecule 32: 28S ribosomal protein S17, mitochondrial

Chain AN:  78% 6% 15%



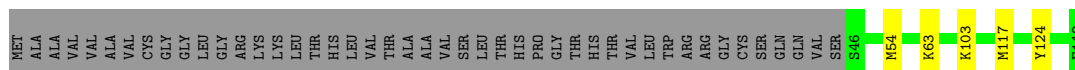
- Molecule 33: 28S ribosomal protein S18b, mitochondrial

Chain AO:  71% 25%



- Molecule 34: 28S ribosomal protein S18c, mitochondrial

Chain AP:  65% 32%




- Molecule 35: Small ribosomal subunit protein bS21m

Chain AQ:  94% 6%



- Molecule 36: 28S ribosomal protein S22, mitochondrial

Chain AR:  77% 5% 18%

MET ALA PRO LEU GLY THR THR VAL LEU LEU TRP SER LEU LEU ARG SER SER PRO PRO GLY VAL GLU ARG VAL CYS PHE ARG ALA ARG ILE ILE GLN LYS PRO TRP HIS HIS GLY GLY LEU LEU LEU GLN PRO CYS SER PHE GLU MET GLY LEU PRO ARG ARG ARG PHE SER SER SER GLU ALA ALA SER

GLY SER PRO E84 M62 M128 L142 K155 Y156 Y157 V174 P177 K183 Q194 K199 I204 P207 I208 I209 D254 F275 Q288 L300 A358 ALA SER

- Molecule 37: 28S ribosomal protein S23, mitochondrial

Chain AS:  67% 29%

MET A2 R48 V51 W64 L106 E120 R134 V135 G136 GLU ALA ARG THR GLN HIS GLY SER HIS VAL SER ARG LYS SER GLU HIS LEU SER VAL ARG PRO GLN THR ALA LEU LEU GLU ASN GLU GLU THR GLN LYS VAL VAL PRO GLN ASP ASP HIS LEU GLU ALA PRO


ALA ASP GLN SER LYS GLY LEU LEU PRO PRO

- Molecule 38: 28S ribosomal protein S25, mitochondrial

Chain AT:  93% . .


MET P2 L76 L80 E84 V88 I140 G161 K164 L167 K168 A169 ASP ALA GLN ASP

- Molecule 39: 28S ribosomal protein S26, mitochondrial

Chain AU:  84% 14%

MET LEU ARG ALA ALA SER ARG LEU LEU ALA ALA THR PRO CYS ARG PRO ARG ALA ALA LEU LEU PRO ALA ARG ARG GLY E27 R64 V67 K183 F167 F202 ARG ASP SER

- Molecule 40: 28S ribosomal protein S27, mitochondrial

Chain AV:  79% 9% 13%

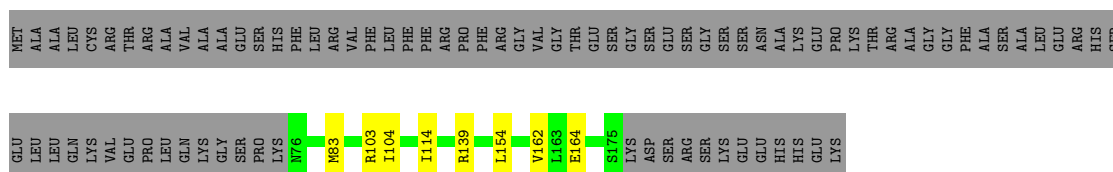
MET ALA ALA SER ILE VAL ARG ARG GLY MET LEU LEU ALA ALA ARG GLN VAL VAL LEU PRO GLN LEU LEU SER PRO PRO ALA ALA GLY LYS ARG TYR L29 P66 V67 S68 S69 L70 L76 R96 C101 V112 V113 R114 L117 D120 A121 Q122 M148 D149 I152 V163 V167

V175 P176 S177 V185 A206 Y228 A229 K233 K246 L249 A259 V262 M263 E264 K265 V286 A293 ASP GLY ALA SER GLU GLU GLN SER GLN ASN ASP ASP ASP ASN GLN GLY SER E311 T322 S325 L331 F334 K335 I389 I390 A407

LYS ALA ALA LYS LYS SER ALA ALA

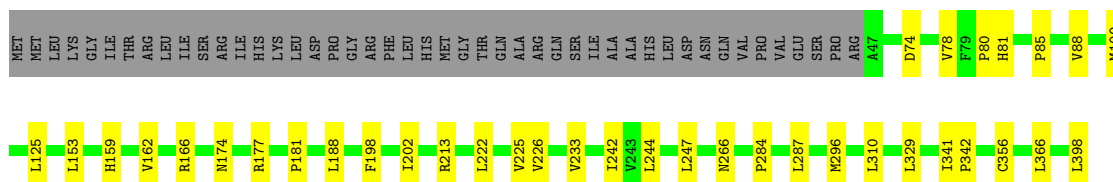
- Molecule 41: 28S ribosomal protein S28, mitochondrial

Chain AW:  49% 47%



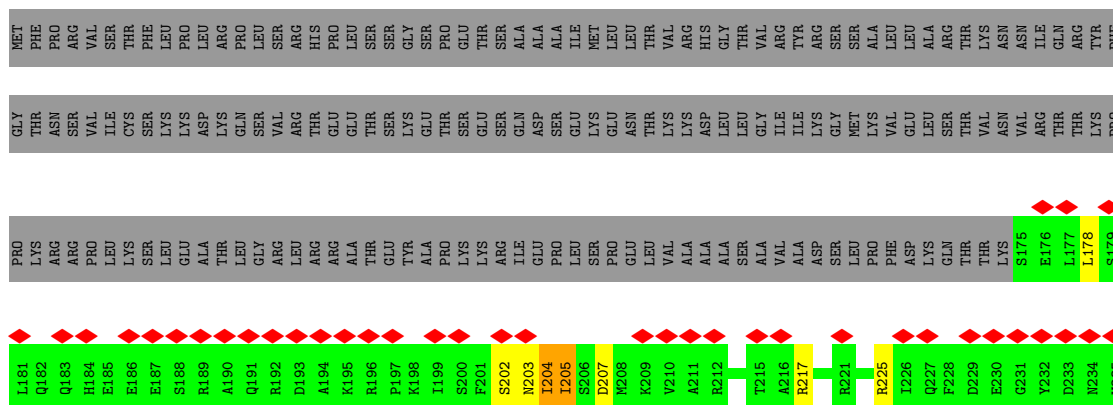
- Molecule 42: 28S ribosomal protein S29, mitochondrial

Chain AX:



- Molecule 43: 28S ribosomal protein S31, mitochondrial

Chain AY:



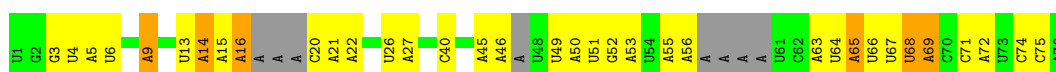
- Molecule 44: 28S ribosomal protein S33, mitochondrial

Chain AZ:



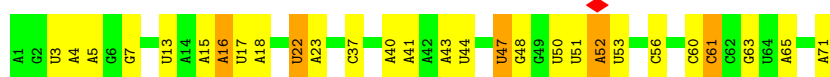
- Molecule 45: A/A-tRNA

Chain Aw:



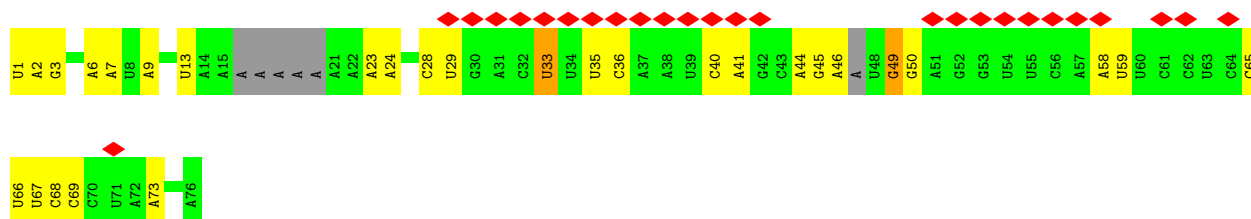
- Molecule 46: P/P-tRNA

Chain Ax: 



- Molecule 47: E/E-tRNA

Chain Ay: 



- Molecule 48: mRNA

Chain Az: 



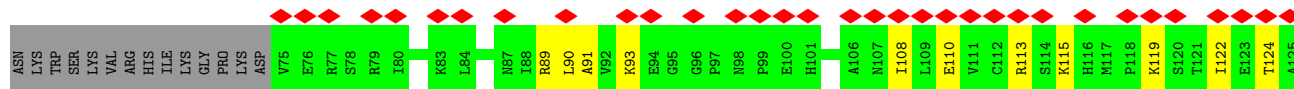
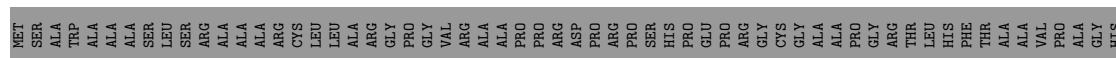
- Molecule 49: RNA (73-MER)mitochondrial tRNAVal

Chain B: 



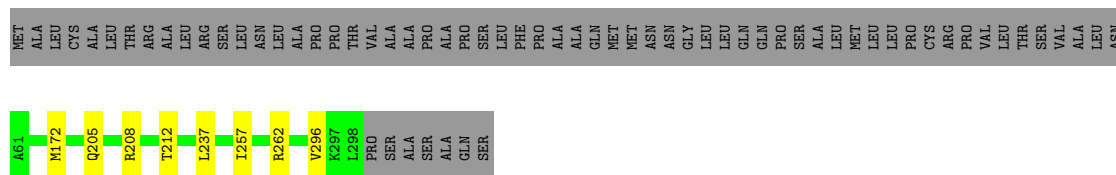
- Molecule 50: Translational activator of cytochrome c oxidase 1

Chain C: 




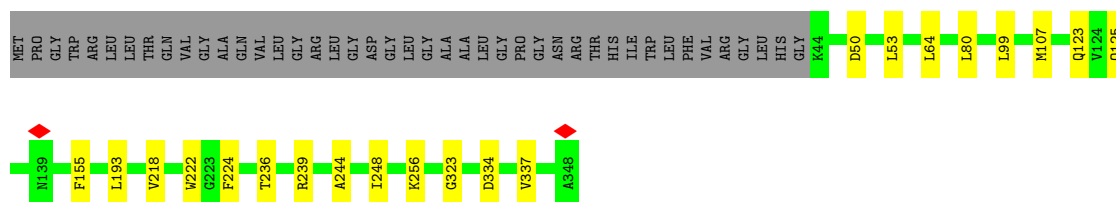
- Molecule 51: 39S ribosomal protein L2, mitochondrial

Chain D:  75% 22%



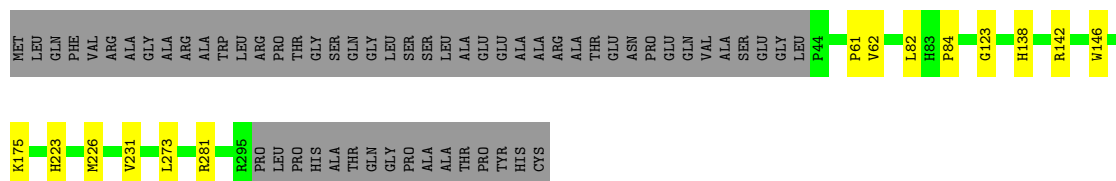
- Molecule 52: 39S ribosomal protein L3, mitochondrial

Chain E:  82% 6% 12%



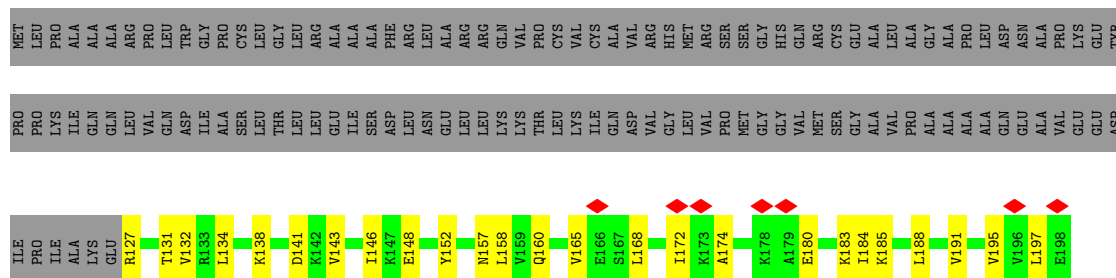
- Molecule 53: 39S ribosomal protein L4, mitochondrial

Chain F:  77% 5% 19%



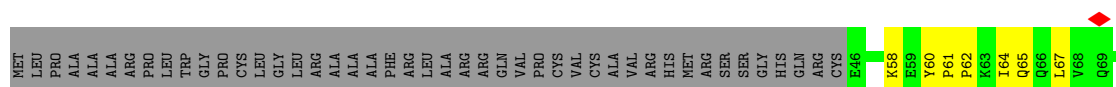
- Molecule 54: 39S ribosomal protein L12, mitochondrial

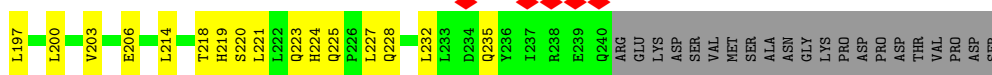
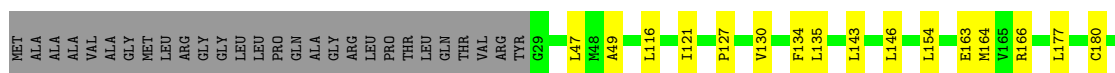
Chain G:  24% 13% 64%



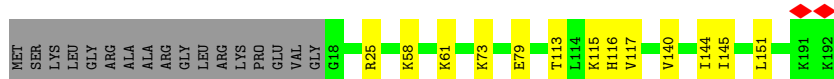
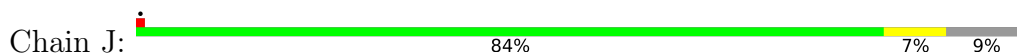
- Molecule 54: 39S ribosomal protein L12, mitochondrial

Chain t:  17% 7% 77%

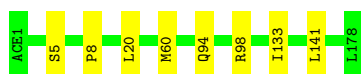




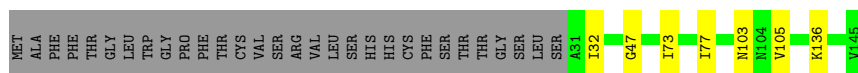
- Molecule 57: 39S ribosomal protein L11, mitochondrial



- Molecule 58: Large ribosomal subunit protein uL13m



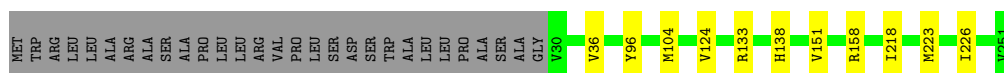
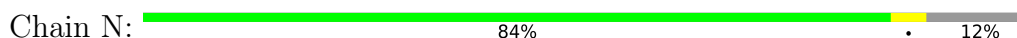
- Molecule 59: 39S ribosomal protein L14, mitochondrial



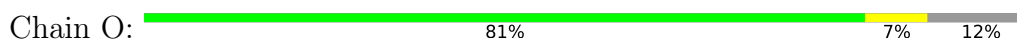
- Molecule 60: 39S ribosomal protein L15, mitochondrial



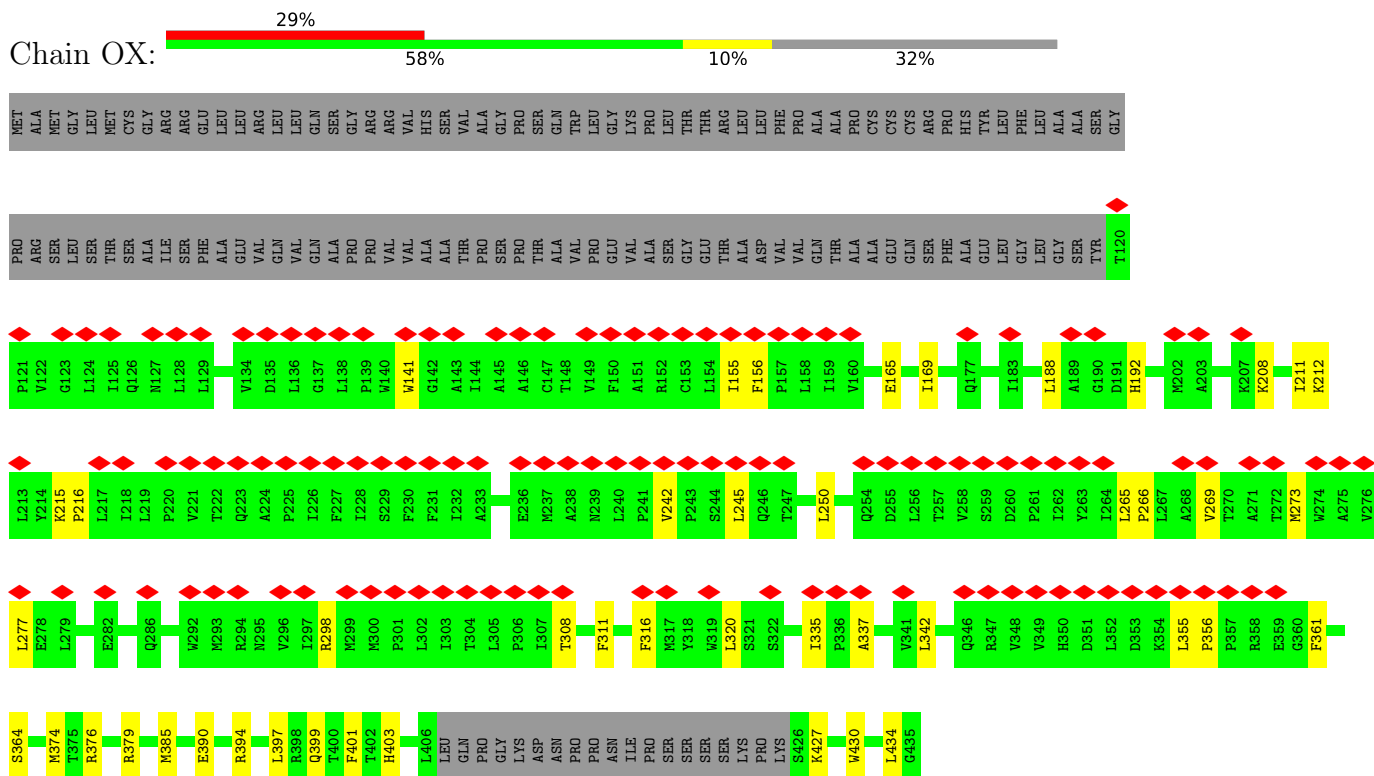
- Molecule 61: 39S ribosomal protein L16, mitochondrial



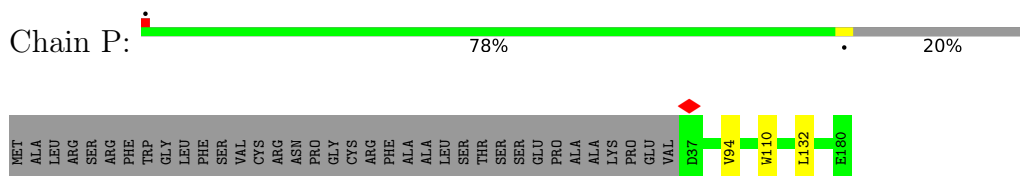
- Molecule 62: 39S ribosomal protein L17, mitochondrial



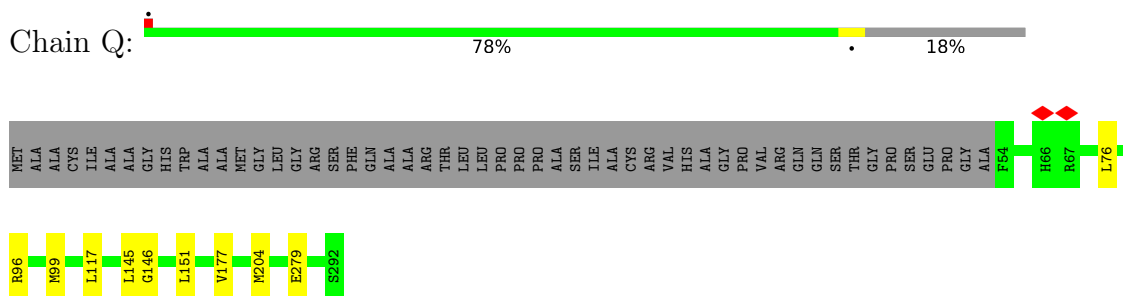
- Molecule 63: Mitochondrial inner membrane protein OXA1L



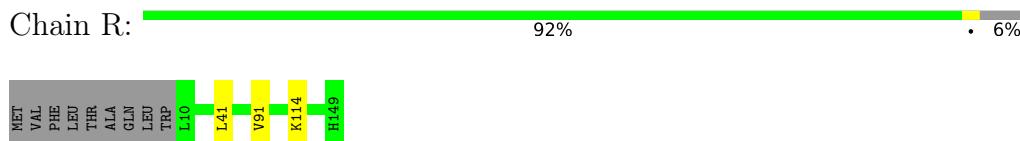
- Molecule 64: 39S ribosomal protein L18, mitochondrial



- Molecule 65: 39S ribosomal protein L19, mitochondrial

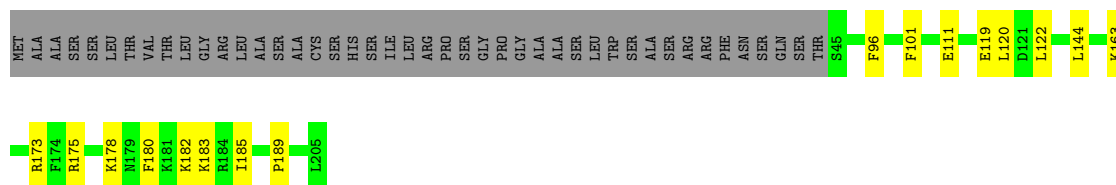


- Molecule 66: 39S ribosomal protein L20, mitochondrial



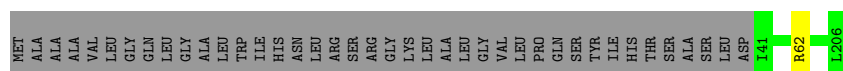
- Molecule 67: 39S ribosomal protein L21, mitochondrial

Chain S:  71% 8% 21%



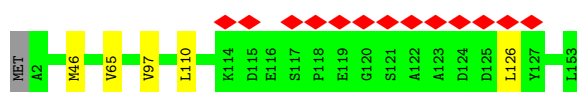
- Molecule 68: 39S ribosomal protein L22, mitochondrial

Chain T:  80% 19%



- Molecule 69: 39S ribosomal protein L23, mitochondrial

Chain U:  8% 96%




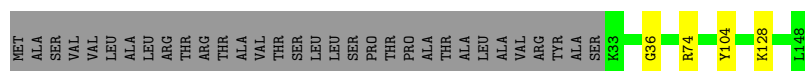
- Molecule 70: 39S ribosomal protein L24, mitochondrial

Chain V:  90% 5% 5%



- Molecule 71: 39S ribosomal protein L27, mitochondrial

Chain W:  76% 22%



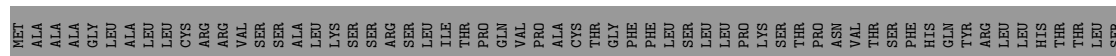
- Molecule 72: 39S ribosomal protein L28, mitochondrial

Chain X:  93% 5%



- Molecule 73: 39S ribosomal protein L47, mitochondrial

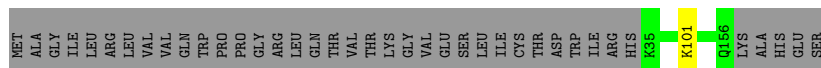
Chain Y:  70% 28%





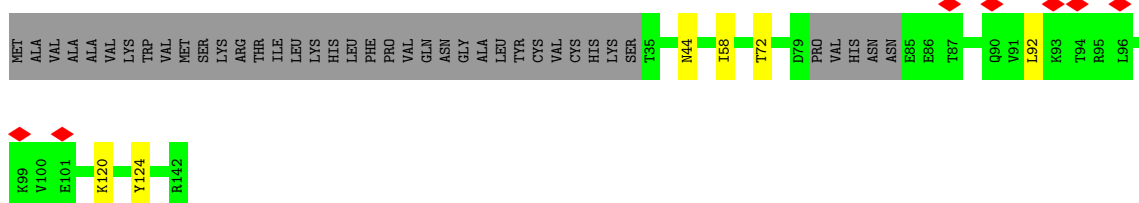
- Molecule 74: 39S ribosomal protein L30, mitochondrial

Chain Z: 75% 24%



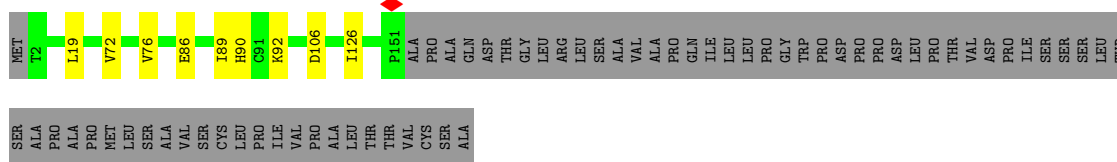
- Molecule 75: 39S ribosomal protein L42, mitochondrial

Chain a: 5% 68% 27%



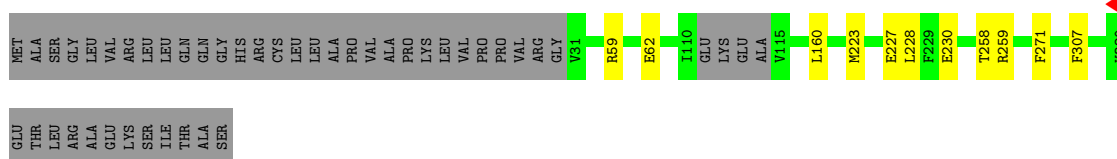
- Molecule 76: 39S ribosomal protein L43, mitochondrial

Chain b: 66% 30%



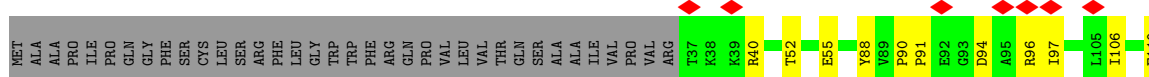
- Molecule 77: 39S ribosomal protein L44, mitochondrial

Chain c: 83% 14%



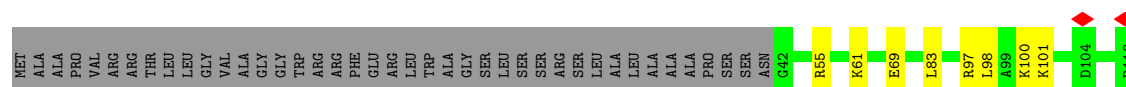
- Molecule 78: 39S ribosomal protein L45, mitochondrial

Chain d: 75% 10% 15%

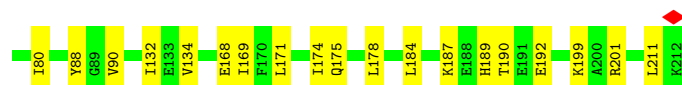
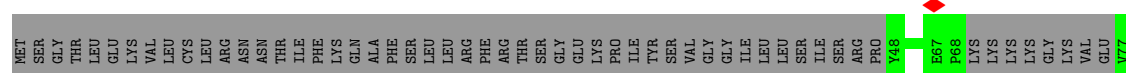




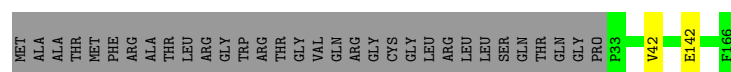
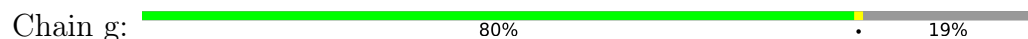
- Molecule 79: 39S ribosomal protein L46, mitochondrial



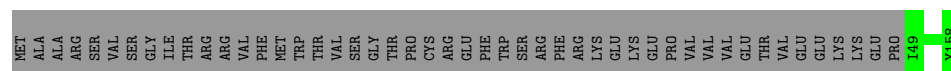
- Molecule 80: 39S ribosomal protein L48, mitochondrial



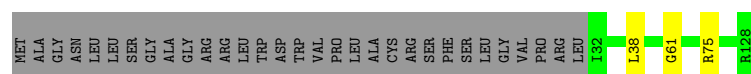
- Molecule 81: 39S ribosomal protein L49, mitochondrial



- Molecule 82: 39S ribosomal protein L50, mitochondrial

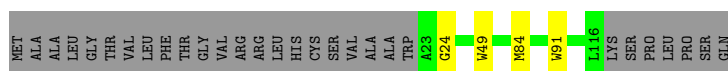


- Molecule 83: 39S ribosomal protein L51, mitochondrial

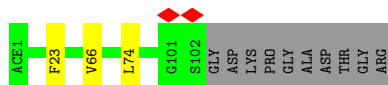
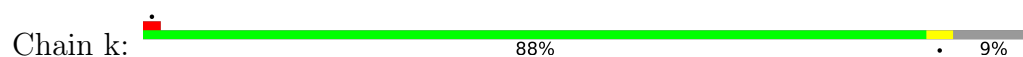


- Molecule 84: 39S ribosomal protein L52, mitochondrial

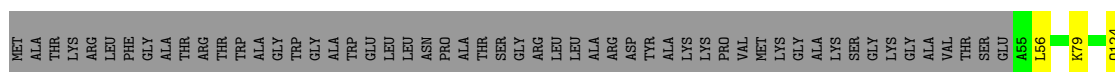




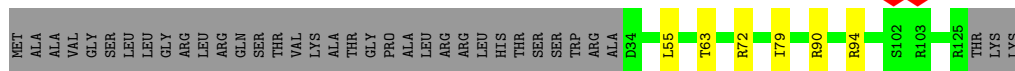
- Molecule 85: Large ribosomal subunit protein mL53



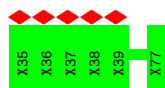
- Molecule 86: 39S ribosomal protein L54, mitochondrial



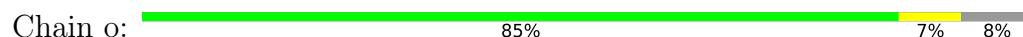
- Molecule 87: 39S ribosomal protein L55, mitochondrial



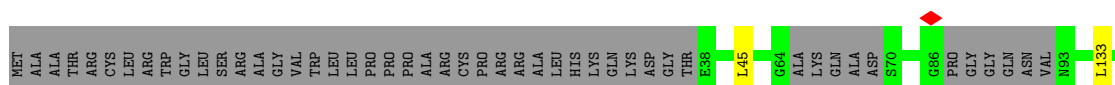
- Molecule 88: Nascent polypeptide

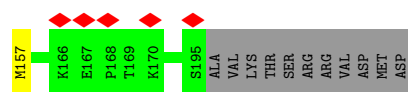


- Molecule 89: Ribosomal protein 63, mitochondrial

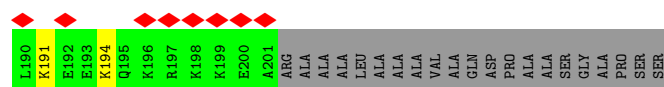
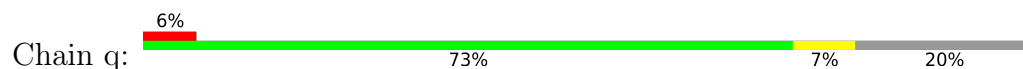


- Molecule 90: Peptidyl-tRNA hydrolase ICT1, mitochondrial

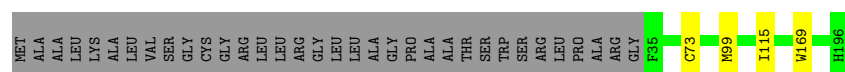
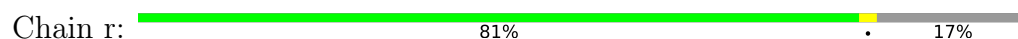




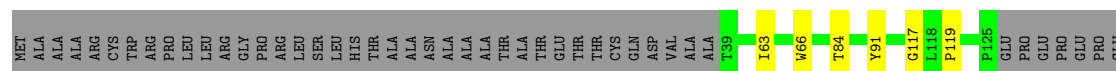
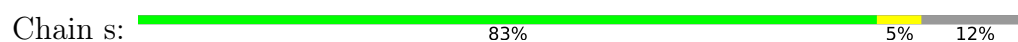
- Molecule 91: Growth arrest and DNA damage-inducible proteins-interacting protein 1



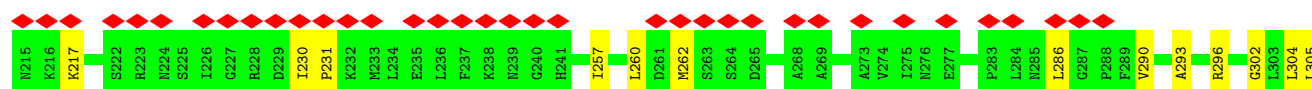
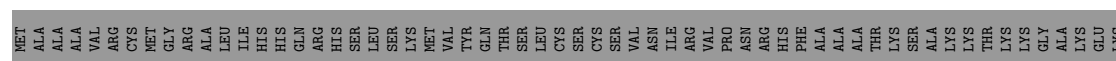
- Molecule 92: 39S ribosomal protein S18a, mitochondrial



- Molecule 93: 39S ribosomal protein S30, mitochondrial



- Molecule 94: Large ribosomal subunit protein uL1m



K306	I307	D308	P309	L310	L311	P312	LYS	GLU	VAL	LYS	ASN	GLU	SER	GLU	LYS	GLU	ASP	ALA
------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	526704	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.651	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.016	Depositor
Map size (\AA)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.24	0/913	0.24	0/1224
2	1	0.22	0/469	0.28	0/621
3	2	0.31	0/383	0.28	0/507
4	3	0.30	0/853	0.29	0/1136
5	4	0.29	0/350	0.27	0/461
6	5	0.22	0/3305	0.27	0/4502
7	6	0.18	0/3043	0.26	0/4140
8	7	0.18	0/2447	0.24	0/3310
9	8	0.13	0/1354	0.30	0/1819
10	9	0.22	0/1025	0.25	0/1379
11	A	0.31	0/36876	0.31	0/57402
12	A0	0.12	0/1834	0.27	0/2484
13	A1	0.17	0/2313	0.26	0/3129
14	A2	0.18	0/947	0.27	0/1266
15	A3	0.21	0/636	0.24	0/839
16	A4	0.13	0/4877	0.28	0/6598
17	A5	0.12	0/4737	0.33	0/6398
18	A6	0.11	0/619	0.30	0/835
19	AA	0.25	0/22537	0.27	0/35085
20	AB	0.21	0/1871	0.25	0/2531
21	AC	0.22	0/1113	0.29	0/1505
22	AD	0.19	0/2783	0.24	0/3724
23	AE	0.20	0/989	0.25	0/1335
24	AF	0.17	0/1767	0.23	0/2373
25	AG	0.18	0/2746	0.24	0/3681
26	AH	0.23	0/1178	0.30	0/1598
27	AI	0.21	0/1039	0.28	0/1400
28	AJ	0.20	0/855	0.27	0/1148
29	AK	0.22	0/880	0.23	0/1182
30	AL	0.20	0/1477	0.21	0/1974
31	AM	0.16	0/963	0.28	0/1295

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AN	0.20	0/886	0.26	0/1199
33	AO	0.16	0/1648	0.27	0/2243
34	AP	0.22	0/798	0.25	0/1070
35	AQ	0.22	0/754	0.22	0/1003
36	AR	0.13	0/2456	0.24	0/3317
37	AS	0.15	0/1138	0.18	0/1533
38	AT	0.18	0/1402	0.26	0/1883
39	AU	0.12	0/1510	0.21	0/2025
40	AV	0.11	0/3030	0.29	0/4093
41	AW	0.18	0/801	0.25	0/1079
42	AX	0.15	0/2921	0.29	0/3954
43	AY	0.16	0/1877	0.33	0/2524
44	AZ	0.19	0/857	0.29	0/1141
45	Aw	0.14	0/1600	0.28	0/2476
46	Ax	0.18	0/1673	0.33	0/2602
47	Ay	0.12	0/1655	0.24	0/2567
48	Az	0.17	0/804	0.33	0/1248
49	B	0.17	0/1626	0.26	0/2523
50	C	0.12	0/1754	0.28	0/2357
51	D	0.24	0/1896	0.27	0/2549
52	E	0.25	0/2475	0.30	0/3355
53	F	0.26	0/2090	0.28	0/2842
54	G	0.16	0/562	0.48	0/754
54	t	0.20	0/358	0.44	0/486
54	u	0.21	0/259	0.39	0/350
54	v	0.17	0/259	0.33	0/350
54	w	0.22	0/246	0.51	0/331
54	x	0.15	0/246	0.34	0/331
54	y	0.18	0/246	0.42	0/331
55	H	0.15	0/1698	0.26	0/2292
56	I	0.20	0/1731	0.32	0/2345
57	J	0.12	0/1348	0.26	0/1813
58	K	0.27	0/1497	0.28	0/2031
59	L	0.23	0/905	0.28	0/1218
60	M	0.26	0/2381	0.28	0/3212
61	N	0.24	0/1833	0.27	0/2468
62	O	0.25	0/1283	0.27	0/1727
63	OX	0.15	0/2471	0.36	1/3360 (0.0%)
64	P	0.20	0/1199	0.25	0/1623
65	Q	0.23	0/2039	0.28	0/2750
66	R	0.28	0/1175	0.24	0/1572
67	S	0.27	0/1320	0.30	0/1789
68	T	0.26	0/1403	0.26	0/1886

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
69	U	0.25	0/1279	0.33	0/1730
70	V	0.21	0/1721	0.26	0/2333
71	W	0.27	0/926	0.26	0/1244
72	X	0.22	0/2099	0.24	0/2837
73	Y	0.25	0/1593	0.24	0/2136
74	Z	0.25	0/1021	0.29	0/1378
75	a	0.22	0/891	0.31	0/1208
76	b	0.25	0/1218	0.28	0/1649
77	c	0.21	0/2347	0.24	0/3171
78	d	0.17	0/2181	0.30	0/2949
79	e	0.11	0/1970	0.27	0/2658
80	f	0.15	0/1273	0.31	0/1716
81	g	0.24	0/1151	0.27	0/1569
82	h	0.17	0/918	0.22	0/1249
83	i	0.29	0/850	0.28	0/1135
84	j	0.22	0/760	0.23	0/1023
85	k	0.15	0/783	0.22	0/1057
86	l	0.12	0/707	0.25	0/960
87	m	0.11	0/805	0.29	0/1081
89	o	0.26	0/819	0.28	0/1097
90	p	0.17	0/1223	0.25	0/1641
91	q	0.16	0/1529	0.26	0/2055
92	r	0.23	0/1362	0.29	0/1846
93	s	0.24	0/3231	0.27	0/4389
94	z	0.13	0/2067	0.33	0/2793
All	All	0.23	0/202013	0.28	1/286387 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	OX	155	ILE	N-CA-C	-5.68	106.95	112.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	898	0	916	3	0
2	1	464	0	511	5	0
3	2	377	0	406	1	0
4	3	832	0	883	4	0
5	4	342	0	361	3	0
6	5	3210	0	3206	12	0
7	6	2948	0	2841	8	0
8	7	2390	0	2397	15	0
9	8	1327	0	1368	15	0
10	9	997	0	987	4	0
11	A	33070	0	16793	117	0
12	A0	1787	0	1796	10	0
13	A1	2265	0	2294	20	0
14	A2	935	0	971	3	0
15	A3	625	0	699	3	0
16	A4	4768	0	4766	56	0
17	A5	4646	0	4674	51	0
18	A6	603	0	588	3	0
19	AA	20260	0	10284	157	0
20	AB	1828	0	1815	7	0
21	AC	1083	0	1088	10	0
22	AD	2731	0	2804	15	0
23	AE	972	0	1000	6	0
24	AF	1725	0	1769	7	0
25	AG	2688	0	2687	6	0
26	AH	1152	0	1183	17	0
27	AI	1019	0	1059	10	0
28	AJ	839	0	887	5	0
29	AK	862	0	885	6	0
30	AL	1453	0	1540	6	0
31	AM	942	0	965	11	0
32	AN	868	0	928	5	0
33	AO	1592	0	1557	6	0
34	AP	781	0	806	5	0
35	AQ	744	0	758	6	0
36	AR	2409	0	2428	14	0
37	AS	1111	0	1115	5	0
38	AT	1371	0	1393	4	0
39	AU	1488	0	1499	3	0
40	AV	2969	0	2961	22	0
41	AW	789	0	802	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	AX	2849	0	2844	21	0
43	AY	1835	0	1780	18	0
44	AZ	839	0	858	6	0
45	Aw	1434	0	728	11	0
46	Ax	1498	0	766	9	0
47	Ay	1483	0	754	18	0
48	Az	719	0	359	2	0
49	B	1524	0	779	9	0
50	C	1732	0	1740	29	0
51	D	1859	0	1920	5	0
52	E	2406	0	2415	12	0
53	F	2031	0	2065	8	0
54	G	558	0	612	18	0
54	t	354	0	377	15	0
54	u	257	0	283	12	0
54	v	257	0	283	8	0
54	w	245	0	275	22	0
54	x	245	0	275	6	0
54	y	245	0	275	7	0
55	H	1661	0	1734	11	0
56	I	1695	0	1785	25	0
57	J	1330	0	1407	9	0
58	K	1455	0	1452	4	0
59	L	890	0	941	4	0
60	M	2327	0	2395	8	0
61	N	1786	0	1817	9	0
62	O	1259	0	1294	9	0
63	OX	2404	0	2464	30	0
64	P	1173	0	1165	2	0
65	Q	1990	0	2031	6	0
66	R	1154	0	1214	3	0
67	S	1293	0	1365	12	0
68	T	1369	0	1410	1	0
69	U	1248	0	1228	4	0
70	V	1676	0	1687	8	0
71	W	904	0	934	3	0
72	X	2044	0	2060	4	0
73	Y	1556	0	1597	5	0
74	Z	996	0	1044	1	0
75	a	865	0	829	5	0
76	b	1193	0	1191	6	0
77	c	2299	0	2320	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
78	d	2124	0	2125	19	0
79	e	1931	0	1916	26	0
80	f	1252	0	1269	15	0
81	g	1113	0	1097	2	0
82	h	895	0	881	0	0
83	i	828	0	857	3	0
84	j	745	0	746	4	0
85	k	774	0	784	2	0
86	l	688	0	673	3	0
87	m	791	0	796	5	0
88	n	215	0	54	0	0
89	o	798	0	804	6	0
90	p	1205	0	1223	2	0
91	q	1495	0	1492	10	0
92	r	1322	0	1348	3	0
93	s	3148	0	3131	14	0
94	z	2027	0	2076	30	0
95	0	1	0	0	0	0
95	4	1	0	0	0	0
95	AO	1	0	0	0	0
96	A	40	0	76	0	0
96	AA	20	0	38	1	0
96	O	10	0	19	0	0
97	A	137	0	0	0	0
97	A3	1	0	0	0	0
97	AA	60	0	0	0	0
97	AB	1	0	0	0	0
97	AX	1	0	0	0	0
97	Az	1	0	0	0	0
97	D	2	0	0	0	0
97	E	1	0	0	0	0
97	g	1	0	0	0	0
98	A	6	0	12	0	0
99	A	29	0	0	0	0
99	AA	18	0	0	0	0
99	D	1	0	0	0	0
99	M	2	0	0	0	0
99	N	1	0	0	0	0
99	P	1	0	0	0	0
99	W	1	0	0	0	0
99	o	1	0	0	0	0
100	AA	28	0	52	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
101	AA	44	0	26	1	0
102	AP	4	0	0	0	0
102	AT	4	0	0	0	0
102	r	4	0	0	1	0
103	AX	28	0	12	0	0
104	AX	31	0	12	0	0
105	B	7	0	8	2	0
All	All	192936	0	164949	1030	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (1030) 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)
56:I:220:SER:HA	56:I:223:GLN:HG2	1.61	0.81
17:A5:98:GLY:HA3	17:A5:336:PRO:HB3	1.64	0.78
50:C:268:LEU:HD23	50:C:272:ASP:HB3	1.66	0.78
79:e:219:GLN:HA	79:e:222:ARG:HB2	1.66	0.76
54:t:76:LEU:HB3	54:w:71:ILE:HG21	1.68	0.73
54:y:79:ILE:HA	54:y:82:LEU:HB2	1.70	0.72
54:x:64:ILE:HG21	54:y:82:LEU:HD21	1.71	0.72
68:T:62:ARG:HE	78:d:230:ARG:HD2	1.55	0.71
79:e:183:THR:HG23	79:e:186:GLY:H	1.55	0.71
91:q:164:LEU:HB3	91:q:168:VAL:HG21	1.72	0.70
63:OX:434:LEU:HD23	72:X:20:ILE:HG22	1.71	0.70
54:w:76:LEU:HA	54:w:79:ILE:HD12	1.74	0.70
23:AE:26:ILE:HG23	23:AE:36:VAL:HG21	1.74	0.69
16:A4:321:ARG:HH21	43:AY:258:ILE:HG23	1.57	0.69
11:A:2545:U:H5''	11:A:2546:G:H5'	1.75	0.68
16:A4:429:LEU:HA	16:A4:464:LEU:HD21	1.74	0.67
9:8:187:PRO:HG2	87:m:79:ILE:HD11	1.77	0.67
50:C:211:ILE:HD12	54:G:143:VAL:HG12	1.76	0.67
94:z:127:LEU:HD22	94:z:290:VAL:HG13	1.78	0.66
94:z:181:THR:HA	94:z:184:ILE:HD12	1.76	0.66
54:t:73:SER:HA	54:w:73:SER:HA	1.78	0.65
17:A5:342:ILE:HA	17:A5:345:LEU:HD12	1.78	0.65
63:OX:208:LYS:HE2	69:U:126:LEU:HD22	1.77	0.65
54:v:82:LEU:HG	54:w:63:LYS:HE2	1.79	0.65
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.79	0.64
63:OX:399:GLN:HE22	63:OX:401:PHE:HD1	1.45	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:AX:366:LEU:HD22	42:AX:398:LEU:HD22	1.80	0.64
8:7:143:TRP:HE1	8:7:172:VAL:HG23	1.62	0.64
17:A5:513:ARG:HD2	17:A5:543:SER:HB3	1.79	0.63
17:A5:305:LEU:HA	17:A5:308:ILE:HD12	1.79	0.63
31:AM:64:LYS:HD2	36:AR:156:TYR:CE1	2.34	0.63
79:e:205:LEU:HB3	80:f:168:GLU:HB2	1.81	0.63
63:OX:269:VAL:HG21	63:OX:316:PHE:HB3	1.79	0.62
54:t:75:THR:OG1	54:w:68:VAL:HG12	1.99	0.62
13:A1:126:LEU:HD11	16:A4:70:VAL:HG13	1.82	0.62
54:t:64:ILE:HD12	54:u:78:GLU:HG3	1.80	0.62
54:t:76:LEU:HD23	54:w:68:VAL:HG13	1.81	0.62
94:z:161:THR:HB	94:z:167:VAL:HG22	1.80	0.62
19:AA:1089:U:H2'	19:AA:1090:A:H8	1.62	0.62
19:AA:929:A:H4'	22:AD:420:SER:HA	1.81	0.62
54:u:91:LYS:HG2	54:w:76:LEU:HD11	1.81	0.62
16:A4:266:MET:HG2	16:A4:271:ALA:HB3	1.81	0.62
17:A5:381:VAL:HG22	17:A5:410:THR:HG22	1.81	0.62
43:AY:202:SER:HB3	43:AY:205:ILE:HG13	1.82	0.62
54:G:165:VAL:HA	54:G:168:LEU:HG	1.81	0.62
96:AA:1779:SPD:HN12	29:AK:31:ASP:HB3	1.65	0.61
63:OX:277:LEU:HB2	63:OX:298:ARG:HG2	1.81	0.61
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.82	0.61
32:AN:95:VAL:HG23	32:AN:96:THR:HG23	1.83	0.61
60:M:177:ALA:HB1	60:M:203:ARG:HH12	1.65	0.61
19:AA:1562:G:H1'	19:AA:1583:MA6:H2	1.80	0.61
20:AB:180:ARG:HH21	22:AD:210:PRO:HB2	1.65	0.61
61:N:218:ILE:HG23	61:N:223:MET:HB2	1.83	0.61
42:AX:181:PRO:HB2	42:AX:233:VAL:HG22	1.82	0.61
21:AC:136:VAL:HG22	21:AC:153:LEU:HD22	1.83	0.61
19:AA:960:C:H42	19:AA:1041:A:H2	1.50	0.60
19:AA:1002:C:H2'	19:AA:1003:A:H8	1.65	0.60
61:N:124:VAL:HG12	61:N:158:ARG:HE	1.66	0.60
92:r:73:CYS:HB3	102:r:201:FES:S2	2.40	0.60
17:A5:630:LEU:HD12	17:A5:642:ALA:HB2	1.82	0.60
17:A5:169:LEU:HD13	17:A5:202:ARG:HB3	1.83	0.60
50:C:90:LEU:HG	50:C:153:LEU:HD22	1.83	0.60
13:A1:239:TRP:CD1	44:AZ:10:ARG:HH12	2.20	0.60
19:AA:922:C:H2'	19:AA:923:A:C8	2.36	0.60
28:AJ:78:ARG:HG3	28:AJ:118:LEU:HD21	1.83	0.60
11:A:2099:U:H2'	11:A:2100:C:C6	2.37	0.60
16:A4:397:MET:HG3	16:A4:431:LEU:HD11	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A4:446:LYS:HD3	43:AY:290:ASN:HA	1.84	0.60
19:AA:1440:G:H2'	19:AA:1441:A:C8	2.37	0.60
11:A:2174:G:H4'	57:J:151:LEU:HD23	1.82	0.60
70:V:79:VAL:HG12	70:V:86:VAL:HG12	1.84	0.60
16:A4:343:ARG:HA	16:A4:378:LEU:HD13	1.83	0.60
43:AY:338:LEU:HD11	43:AY:351:MET:HB3	1.82	0.60
13:A1:126:LEU:HD12	26:AH:155:VAL:HG13	1.84	0.59
94:z:184:ILE:HD13	94:z:206:GLU:HB2	1.84	0.59
16:A4:62:LYS:HE3	26:AH:70:ASP:HA	1.83	0.59
22:AD:140:LEU:HD11	22:AD:160:ARG:HE	1.67	0.59
19:AA:1201:A:H2'	19:AA:1202:G:C8	2.37	0.59
19:AA:663:A:H2'	19:AA:664:G:C8	2.37	0.59
19:AA:1201:A:H2'	19:AA:1202:G:H8	1.68	0.59
26:AH:164:LEU:HD13	26:AH:170:MET:HE3	1.82	0.59
56:I:143:LEU:HD11	56:I:180:CYS:HB2	1.85	0.59
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.83	0.59
94:z:184:ILE:HG22	94:z:209:ARG:HH21	1.67	0.59
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.84	0.59
13:A1:134:PRO:HB2	13:A1:137:LEU:HD23	1.84	0.59
26:AH:78:VAL:HB	26:AH:143:LEU:HB2	1.85	0.59
50:C:110:GLU:HA	50:C:113:ARG:HD3	1.84	0.59
34:AP:54:MET:HE2	37:AS:64:TRP:HB3	1.84	0.58
16:A4:358:ARG:HH11	43:AY:255:ARG:HB3	1.67	0.58
19:AA:1117:A:H2'	19:AA:1118:A:H8	1.69	0.58
54:x:74:LEU:HD22	54:x:78:GLU:HG2	1.85	0.58
16:A4:532:LEU:HD11	16:A4:555:ILE:HG21	1.86	0.58
31:AM:34:ILE:HG12	31:AM:87:MET:HE1	1.86	0.58
90:p:133:LEU:HD21	90:p:157:MET:HE1	1.86	0.58
49:B:30:A:H2'	49:B:31:A:H8	1.68	0.58
50:C:217:ASP:HB2	50:C:233:ILE:HB	1.85	0.58
16:A4:324:VAL:HG11	43:AY:258:ILE:HG22	1.85	0.58
24:AF:172:VAL:HG12	24:AF:240:ARG:HD3	1.86	0.58
93:s:271:LEU:HD23	93:s:273:LEU:HD13	1.85	0.58
40:AV:70:LEU:HD22	40:AV:389:LEU:HG	1.85	0.58
54:G:143:VAL:HA	54:G:146:ILE:HG12	1.86	0.58
11:A:2740:A:H2'	11:A:2741:A:C8	2.39	0.57
63:OX:361:PHE:HA	63:OX:364:SER:HB2	1.85	0.57
19:AA:1528:A:H2'	19:AA:1529:A:H8	1.69	0.57
50:C:119:LYS:HD3	50:C:122:ILE:HD11	1.86	0.57
11:A:2055:U:H2'	11:A:2056:G:H8	1.69	0.57
19:AA:1239:C:H2'	19:AA:1240:A:H8	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:OX:390:GLU:HB3	63:OX:394:ARG:HH21	1.69	0.57
12:A0:71:LEU:HD11	12:A0:141:LEU:HD11	1.85	0.57
50:C:207:LEU:HD22	54:G:158:LEU:HD13	1.85	0.57
19:AA:777:G:H5''	32:AN:21:LYS:HB3	1.86	0.57
78:d:52:THR:HG23	78:d:55:GLU:H	1.70	0.57
42:AX:153:LEU:HD21	42:AX:247:LEU:HD13	1.86	0.56
16:A4:170:VAL:HG23	16:A4:247:ILE:HD11	1.86	0.56
63:OX:376:ARG:HG2	63:OX:379:ARG:HH22	1.70	0.56
19:AA:773:U:H2'	19:AA:774:G:H8	1.71	0.56
40:AV:76:ILE:HD12	40:AV:112:TRP:HD1	1.70	0.56
56:I:224:HIS:H	54:w:87:LYS:HZ1	1.53	0.56
63:OX:269:VAL:HG22	63:OX:320:LEU:HB2	1.86	0.56
11:A:1952:U:H2'	11:A:1953:A:C8	2.41	0.56
78:d:208:VAL:HG22	78:d:253:THR:HG23	1.88	0.56
54:w:67:LEU:HA	54:w:70:ASP:HB2	1.87	0.56
12:A0:99:ARG:HD3	19:AA:1526:U:H2'	1.87	0.56
5:4:103:MET:HE1	11:A:2952:U:H5'	1.86	0.56
50:C:239:LEU:HD11	50:C:256:CYS:HB2	1.87	0.56
79:e:217:PHE:H	79:e:228:GLY:HA2	1.70	0.56
94:z:198:VAL:HB	94:z:230:ILE:HG23	1.88	0.56
9:8:68:LEU:HD21	80:f:211:LEU:HB2	1.87	0.55
56:I:116:LEU:HG	56:I:121:ILE:HB	1.88	0.55
78:d:138:PRO:HG3	78:d:194:VAL:HG23	1.88	0.55
9:8:192:TYR:HE1	80:f:134:VAL:HG22	1.71	0.55
16:A4:556:LYS:HE3	16:A4:579:ILE:HD13	1.88	0.55
17:A5:411:LEU:HD22	17:A5:427:MET:HE3	1.87	0.55
11:A:3211:C:H4'	11:A:3212:C:H5	1.71	0.55
27:AI:184:ASN:H	35:AQ:42:ARG:HH12	1.53	0.55
49:B:29:C:H2'	49:B:30:A:H8	1.72	0.55
78:d:106:ILE:O	78:d:110:GLU:HG2	2.07	0.55
16:A4:316:ILE:HA	16:A4:319:LEU:HD12	1.88	0.55
16:A4:571:TRP:HE3	16:A4:576:LEU:HD21	1.72	0.55
19:AA:1003:A:H2'	19:AA:1004:G:H8	1.71	0.55
54:w:64:ILE:O	54:w:68:VAL:HG23	2.06	0.55
19:AA:1529:A:H1'	40:AV:66:PRO:HD3	1.89	0.55
11:A:1857:U:H2'	11:A:1858:G:C8	2.42	0.55
19:AA:1382:A:H5''	42:AX:166:ARG:HH21	1.71	0.55
33:AO:183:ALA:HA	36:AR:183:LYS:HE2	1.88	0.55
56:I:154:LEU:HD12	56:I:164:MET:HE3	1.88	0.55
54:x:86:LEU:HD23	54:x:90:LEU:HD12	1.88	0.55
11:A:2409:A:H2'	11:A:2410:U:C6	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:1239:C:H2'	19:AA:1240:A:C8	2.42	0.55
25:AG:161:LEU:HD22	25:AG:209:LEU:HD21	1.89	0.55
42:AX:244:LEU:HD22	42:AX:296:MET:HG3	1.89	0.55
36:AR:157:VAL:HG22	36:AR:174:VAL:HG22	1.89	0.54
50:C:93:LYS:HD3	50:C:133:ASP:HB2	1.89	0.54
15:A3:173:LEU:HD12	30:AL:209:LEU:HD13	1.89	0.54
17:A5:424:LYS:HG3	17:A5:464:GLY:HA3	1.89	0.54
19:AA:1470:A:H2'	19:AA:1471:A:H8	1.73	0.54
54:t:76:LEU:HA	54:t:79:ILE:HB	1.88	0.54
93:s:145:VAL:HG21	93:s:187:LEU:HD11	1.90	0.54
11:A:2761:C:H42	94:z:90:ARG:HE	1.54	0.54
17:A5:235:PHE:CE1	17:A5:258:MET:HG3	2.43	0.54
27:AI:151:VAL:HG21	27:AI:158:ARG:HG3	1.90	0.54
41:AW:103:ARG:HE	41:AW:139:ARG:HH21	1.56	0.54
56:I:224:HIS:HA	56:I:227:LEU:HD12	1.90	0.54
42:AX:188:LEU:HD22	42:AX:226:VAL:HG23	1.88	0.54
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.90	0.54
16:A4:593:TRP:HA	16:A4:596:LEU:HD23	1.89	0.54
11:A:2318:A:H2'	11:A:2319:A:C8	2.44	0.53
19:AA:1002:C:H2'	19:AA:1003:A:C8	2.42	0.53
25:AG:136:ARG:HH22	25:AG:211:GLU:HG2	1.72	0.53
43:AY:204:ILE:HD12	43:AY:207:ASP:HA	1.90	0.53
79:e:257:LYS:HE2	79:e:273:ARG:HE	1.74	0.53
11:A:2093:U:H2'	11:A:2094:G:C8	2.43	0.53
19:AA:705:C:H3'	19:AA:706:C:H6	1.74	0.53
17:A5:512:LEU:HD22	17:A5:540:ILE:HG12	1.89	0.53
36:AR:155:LYS:HB3	36:AR:177:PRO:HD3	1.91	0.53
54:t:62:PRO:HA	54:t:65:GLN:HG2	1.90	0.53
17:A5:267:PRO:HG2	43:AY:225:ARG:HH21	1.72	0.53
45:Aw:68:U:H2'	45:Aw:69:A:C8	2.44	0.53
19:AA:976:A:H5''	35:AQ:1:ACE:H1	1.90	0.53
52:E:50:ASP:HA	52:E:53:LEU:HG	1.91	0.53
16:A4:166:VAL:HG12	16:A4:194:LEU:HG	1.91	0.53
17:A5:136:GLU:HA	17:A5:343:LEU:HD22	1.91	0.53
80:f:90:VAL:HG13	80:f:189:HIS:HB3	1.89	0.53
13:A1:159:SER:HB2	21:AC:112:ARG:HB3	1.91	0.53
19:AA:872:G:H2'	19:AA:873:G:C8	2.44	0.53
39:AU:64:ARG:HA	39:AU:67:VAL:HG12	1.90	0.53
7:6:255:LEU:HD12	7:6:256:PRO:HD2	1.91	0.52
49:B:23:A:H2'	49:B:24:G:C8	2.44	0.52
55:H:201:VAL:HG11	55:H:206:LEU:HG	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:K:60:MET:HE2	58:K:133:ILE:HD11	1.91	0.52
92:r:99:MET:HE1	92:r:115:ILE:HG22	1.91	0.52
2:1:19:ARG:HB2	2:1:62:ILE:HD11	1.91	0.52
6:5:143:PRO:HA	6:5:146:HIS:HD1	1.73	0.52
94:z:119:GLN:HB2	94:z:260:LEU:HD12	1.91	0.52
17:A5:310:PHE:HD1	17:A5:345:LEU:HD23	1.74	0.52
31:AM:114:ARG:HA	31:AM:117:GLU:HB3	1.91	0.52
54:G:132:VAL:HG23	54:G:172:ILE:HB	1.90	0.52
4:3:157:LEU:HG	4:3:161:MET:HE2	1.90	0.52
19:AA:1365:A:H4'	19:AA:1389:G:H4'	1.91	0.52
79:e:97:ARG:HH11	79:e:112:GLN:HE22	1.57	0.52
19:AA:847:G:H2'	19:AA:848:U:C6	2.45	0.52
19:AA:1589:C:H2'	19:AA:1590:A:C8	2.44	0.52
46:Ax:40:A:H2'	46:Ax:41:A:C8	2.44	0.52
56:I:221:LEU:HD11	54:w:79:ILE:HG23	1.92	0.52
87:m:55:LEU:HD23	87:m:63:THR:HG21	1.92	0.52
54:t:64:ILE:HD11	54:u:82:LEU:HB2	1.91	0.52
78:d:90:PRO:HB2	78:d:269:TRP:HZ2	1.75	0.52
6:5:409:GLU:HG3	6:5:412:ARG:HH21	1.75	0.52
16:A4:308:LYS:HE3	16:A4:310:GLU:HB2	1.92	0.52
19:AA:947:U:H5''	30:AL:165:LYS:HE3	1.92	0.52
50:C:192:GLU:HA	50:C:227:ARG:HH12	1.75	0.52
52:E:334:ASP:HB3	52:E:337:VAL:HG23	1.91	0.52
1:0:138:ARG:HB3	11:A:2321:A:C8	2.44	0.52
12:A0:68:LEU:HD21	12:A0:80:VAL:HG21	1.92	0.52
19:AA:1398:U:H2'	19:AA:1399:A:H8	1.75	0.52
78:d:96:ARG:HG2	78:d:97:ILE:H	1.75	0.52
93:s:84:THR:HB	93:s:280:ASN:HB2	1.91	0.52
11:A:3089:A:H3'	11:A:3090:G:C5'	2.41	0.52
14:A2:29:LEU:HG	41:AW:154:LEU:HB3	1.92	0.52
17:A5:94:VAL:HA	17:A5:98:GLY:HA2	1.92	0.52
37:AS:106:LEU:HD13	37:AS:120:GLU:HG3	1.92	0.52
52:E:236:THR:HG23	52:E:239:ARG:HD3	1.91	0.52
54:G:138:LYS:HB2	54:G:141:ASP:HB2	1.92	0.52
16:A4:605:ILE:HD13	43:AY:203:ASN:HB2	1.90	0.51
50:C:191:VAL:HG11	50:C:251:LEU:HD23	1.90	0.51
9:8:170:PRO:HB3	80:f:187:LYS:NZ	2.25	0.51
11:A:2778:U:H5''	94:z:115:THR:HG22	1.92	0.51
19:AA:1025:A:H2'	19:AA:1026:A:C8	2.44	0.51
23:AE:92:ASN:HB2	34:AP:117:MET:HE3	1.91	0.51
55:H:174:VAL:HG12	55:H:192:HIS:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:e:183:THR:HG23	79:e:186:GLY:N	2.22	0.51
13:A1:67:PRO:HG3	13:A1:118:ALA:HB2	1.92	0.51
16:A4:397:MET:HA	16:A4:400:LEU:HG	1.93	0.51
17:A5:521:LEU:HD23	17:A5:560:ILE:HD12	1.92	0.51
19:AA:838:U:H2'	19:AA:839:A:H8	1.76	0.51
28:AJ:62:VAL:HA	28:AJ:83:VAL:HG12	1.91	0.51
41:AW:162:VAL:HG12	41:AW:164:GLU:HG2	1.92	0.51
60:M:44:ARG:HG3	60:M:45:ARG:HG3	1.92	0.51
54:G:185:LYS:HD2	54:G:188:LEU:HD11	1.93	0.51
19:AA:1578:A:H2'	19:AA:1579:C:C6	2.46	0.51
28:AJ:66:PHE:HE2	28:AJ:68:ARG:HE	1.57	0.51
54:G:132:VAL:HG12	54:G:197:LEU:HB3	1.92	0.51
12:A0:70:ARG:HH12	40:AV:246:ASN:HB2	1.74	0.51
28:AJ:58:LEU:HB3	28:AJ:85:LEU:HD12	1.93	0.51
43:AY:217:ARG:HH12	43:AY:225:ARG:HG3	1.76	0.51
55:H:98:LEU:HD11	55:H:105:VAL:HG23	1.92	0.51
59:L:32:ILE:HD11	59:L:103:ASN:HB3	1.93	0.51
78:d:164:VAL:HG12	78:d:261:MET:HB3	1.92	0.51
11:A:2718:C:H2'	11:A:2991:U:H4'	1.93	0.51
11:A:2727:C:H2'	11:A:2728:C:H6	1.76	0.51
22:AD:244:LEU:HD22	22:AD:343:LEU:HD23	1.92	0.51
33:AO:208:PRO:HG2	33:AO:213:LEU:HD21	1.93	0.51
52:E:99:LEU:HD22	52:E:193:LEU:HB3	1.93	0.51
57:J:117:VAL:HG21	57:J:145:ILE:HG13	1.92	0.51
94:z:78:MET:HE1	94:z:93:PRO:HD2	1.93	0.51
63:OX:212:LYS:HD2	63:OX:215:LYS:HZ2	1.75	0.51
9:8:117:LEU:HD11	79:e:69:GLU:HB3	1.93	0.50
14:A2:117:LEU:HD11	37:AS:51:VAL:HG13	1.92	0.50
56:I:221:LEU:HB3	54:w:86:LEU:HD12	1.93	0.50
67:S:163:LYS:HB2	76:b:106:ASP:HB3	1.91	0.50
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.91	0.50
9:8:173:LYS:HB3	80:f:184:LEU:HB3	1.93	0.50
11:A:2727:C:H2'	11:A:2728:C:C6	2.46	0.50
60:M:226:PRO:HG3	90:p:45:LEU:HD23	1.92	0.50
11:A:3150:U:H2'	11:A:3151:A:C8	2.47	0.50
55:H:106:GLY:HA2	55:H:158:LYS:HB2	1.93	0.50
11:A:2081:U:H2'	11:A:2082:G:C8	2.47	0.50
40:AV:70:LEU:HD21	40:AV:390:ILE:HD13	1.94	0.50
57:J:140:VAL:O	57:J:144:ILE:HG12	2.11	0.50
94:z:76:PRO:HB2	94:z:93:PRO:HG2	1.94	0.50
17:A5:377:LEU:HG	17:A5:397:LEU:HD13	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A5:139:LEU:HG	17:A5:347:THR:HG21	1.94	0.50
30:AL:175:TYR:HB2	32:AN:89:GLY:HA3	1.94	0.50
18:A6:28:TRP:HB2	18:A6:58:PHE:HB3	1.94	0.50
19:AA:1089:U:H2'	19:AA:1090:A:C8	2.46	0.50
27:AI:176:THR:HB	35:AQ:11:THR:HG23	1.94	0.50
54:w:79:ILE:HA	54:w:82:LEU:HD12	1.94	0.50
11:A:2151:A:H2'	11:A:2152:A:C8	2.47	0.49
16:A4:494:ILE:HD11	16:A4:527:LEU:HA	1.94	0.49
17:A5:181:PRO:HB3	17:A5:206:SER:HB2	1.94	0.49
17:A5:390:LEU:HD21	17:A5:410:THR:HG21	1.94	0.49
40:AV:149:ASP:HA	40:AV:152:ILE:HG22	1.94	0.49
53:F:123:GLY:HA3	53:F:142:ARG:HG2	1.94	0.49
54:v:85:LEU:HD13	54:w:61:PRO:HG3	1.94	0.49
8:7:204:LYS:HE3	75:a:92:LEU:HD22	1.93	0.49
11:A:2006:C:H2'	11:A:2007:U:C6	2.48	0.49
11:A:2086:A:H2'	11:A:2087:U:C6	2.46	0.49
19:AA:922:C:H2'	19:AA:923:A:H8	1.76	0.49
19:AA:1007:G:H2'	19:AA:1008:A:C8	2.47	0.49
50:C:89:ARG:HD2	50:C:153:LEU:HG	1.93	0.49
54:x:70:ASP:O	54:x:74:LEU:HG	2.12	0.49
94:z:214:LEU:HB3	94:z:217:LYS:HB3	1.94	0.49
11:A:2868:C:H2'	11:A:2869:A:O4'	2.12	0.49
45:Aw:9:A:H1'	45:Aw:45:A:H2'	1.94	0.49
47:Ay:33:U:H2'	47:Ay:36:C:H41	1.76	0.49
51:D:205:GLN:HA	51:D:208:ARG:HH21	1.76	0.49
11:A:1851:G:H2'	11:A:2693:A:N7	2.28	0.49
11:A:2415:C:H3'	93:s:165:ARG:NH2	2.27	0.49
21:AC:100:PHE:HB3	21:AC:103:CYS:HB2	1.95	0.49
42:AX:159:HIS:HA	42:AX:162:VAL:HG12	1.95	0.49
56:I:224:HIS:H	54:w:87:LYS:NZ	2.10	0.49
17:A5:105:LEU:HD22	17:A5:134:LEU:HD21	1.95	0.49
19:AA:832:U:H2'	19:AA:833:A:H8	1.76	0.49
19:AA:1308:U:H2'	19:AA:1309:A:H8	1.77	0.49
19:AA:1317:A:H3'	19:AA:1318:A:H8	1.77	0.49
11:A:1936:A:H4'	11:A:1937:A:C8	2.47	0.49
25:AG:357:THR:HG23	25:AG:360:GLU:H	1.78	0.49
40:AV:117:LEU:HA	40:AV:122:GLN:HE22	1.77	0.49
11:A:2677:A:H2'	11:A:2678:A:C8	2.48	0.49
16:A4:335:PHE:CG	16:A4:360:MET:HE2	2.48	0.49
50:C:124:THR:HA	50:C:127:LYS:HG2	1.95	0.49
7:6:175:VAL:HG22	7:6:204:VAL:HG22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:156:ARG:HH12	8:7:260:PHE:HB2	1.78	0.49
12:A0:64:LEU:HD12	12:A0:139:TRP:CD2	2.47	0.49
49:B:25:C:H2'	49:B:26:A:H8	1.78	0.49
53:F:175:LYS:HG2	53:F:273:LEU:HD13	1.94	0.49
19:AA:845:A:H2'	19:AA:846:A:C8	2.48	0.49
19:AA:1470:A:H2'	19:AA:1471:A:C8	2.48	0.49
40:AV:322:THR:HG23	40:AV:325:SER:H	1.78	0.49
45:Aw:66:U:H2'	45:Aw:67:U:C6	2.48	0.49
16:A4:302:VAL:HG21	16:A4:341:CYS:HB3	1.94	0.49
16:A4:513:TRP:CD1	16:A4:551:CYS:HG	2.30	0.49
79:e:98:LEU:HG	79:e:101:LYS:HE3	1.94	0.49
15:A3:193:LYS:HB3	15:A3:196:LEU:HD23	1.94	0.48
16:A4:236:VAL:HG22	16:A4:270:ARG:HG3	1.94	0.48
19:AA:1006:U:H5''	35:AQ:6:LYS:HZ3	1.78	0.48
19:AA:1071:U:H2'	19:AA:1072:G:H8	1.77	0.48
27:AI:99:VAL:HG11	27:AI:139:ALA:HB2	1.95	0.48
48:Az:30:A:H2'	48:Az:31:A:C4	2.48	0.48
50:C:201:VAL:HG22	50:C:205:ARG:HH22	1.78	0.48
54:G:188:LEU:HA	54:G:191:VAL:HG12	1.94	0.48
11:A:2125:C:P	67:S:178:LYS:HE2	2.53	0.48
11:A:3054:G:H2'	11:A:3055:U:C6	2.49	0.48
17:A5:213:ILE:HD11	17:A5:241:GLY:HA3	1.94	0.48
19:AA:672:A:H2'	19:AA:673:U:C6	2.48	0.48
19:AA:872:G:H2'	19:AA:873:G:H8	1.77	0.48
19:AA:1042:U:H2'	19:AA:1043:C:C6	2.48	0.48
19:AA:1042:U:H2'	19:AA:1043:C:H6	1.77	0.48
73:Y:191:ASN:HB3	73:Y:194:TYR:HB3	1.95	0.48
11:A:1886:G:H1	83:i:61:GLY:HA3	1.78	0.48
19:AA:916:C:H2'	19:AA:917:C:C6	2.49	0.48
29:AK:57:LEU:HD23	29:AK:71:ALA:HB2	1.95	0.48
50:C:207:LEU:HG	50:C:218:VAL:HG21	1.96	0.48
13:A1:71:PRO:HB3	16:A4:78:VAL:HG21	1.95	0.48
19:AA:1528:A:H2'	19:AA:1529:A:C8	2.49	0.48
40:AV:233:LYS:HD3	40:AV:286:VAL:HG23	1.94	0.48
54:G:131:THR:HA	54:G:174:ALA:HA	1.95	0.48
63:OX:355:LEU:HD12	63:OX:356:PRO:HD2	1.95	0.48
19:AA:705:C:H3'	19:AA:706:C:C6	2.49	0.48
19:AA:1326:A:C8	22:AD:114:ARG:HD3	2.49	0.48
21:AC:70:SER:HB2	21:AC:93:ARG:HH22	1.79	0.48
47:Ay:6:A:H2'	47:Ay:7:A:C8	2.49	0.48
54:G:134:LEU:HA	54:G:195:VAL:HA	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:v:82:LEU:HD11	54:w:61:PRO:HB2	1.95	0.48
11:A:1935:A:C2	11:A:1936:A:H1'	2.49	0.48
17:A5:512:LEU:HG	17:A5:524:VAL:HG22	1.95	0.48
19:AA:947:U:H2'	19:AA:948:U:H6	1.77	0.48
22:AD:140:LEU:HD11	22:AD:160:ARG:NE	2.29	0.48
22:AD:317:HIS:HB3	22:AD:320:ILE:HG13	1.96	0.48
40:AV:228:TYR:HB3	40:AV:259:ALA:HB2	1.96	0.48
17:A5:589:ILE:HA	17:A5:592:MET:HE2	1.96	0.48
38:AT:80:LEU:HD12	38:AT:84:GLU:HB3	1.94	0.48
42:AX:225:VAL:HG21	42:AX:242:ILE:HG21	1.95	0.48
47:Ay:23:A:H2'	47:Ay:24:A:C8	2.48	0.48
6:5:336:LEU:HD21	6:5:362:THR:HG23	1.96	0.48
9:8:136:ILE:HD11	80:f:169:ILE:HG23	1.94	0.48
9:8:160:GLU:HA	9:8:163:LYS:HE3	1.96	0.48
11:A:3150:U:H2'	11:A:3151:A:H8	1.78	0.48
17:A5:222:PHE:CG	43:AY:178:LEU:HD21	2.49	0.48
19:AA:747:A:H2'	19:AA:748:G:H8	1.77	0.48
19:AA:1488:5MC:H2'	19:AA:1489:G:C8	2.49	0.48
26:AH:136:MET:HG2	29:AK:123:ILE:HD13	1.95	0.48
49:B:21:A:H61	49:B:46:A:H2'	1.78	0.48
19:AA:1267:U:H2'	19:AA:1268:C:C6	2.48	0.48
65:Q:76:LEU:HD23	65:Q:279:GLU:HG2	1.95	0.48
77:c:227:GLU:HB3	77:c:230:GLU:HG3	1.96	0.48
47:Ay:67:U:H2'	47:Ay:68:C:C6	2.49	0.48
94:z:160:PHE:HD2	94:z:199:ALA:HB2	1.79	0.48
12:A0:65:LEU:HD23	12:A0:68:LEU:HB2	1.96	0.47
19:AA:1033:U:H2'	19:AA:1034:U:C6	2.49	0.47
19:AA:1440:G:H2'	19:AA:1441:A:H8	1.78	0.47
63:OX:169:ILE:HG22	63:OX:211:ILE:HG23	1.95	0.47
63:OX:265:LEU:O	63:OX:269:VAL:HG23	2.13	0.47
94:z:133:LYS:HE3	94:z:286:LEU:HD13	1.96	0.47
94:z:170:ALA:HA	94:z:231:PRO:HG3	1.96	0.47
11:A:2514:C:H2'	11:A:2515:U:H6	1.80	0.47
17:A5:131:GLY:HA2	17:A5:171:VAL:HA	1.95	0.47
17:A5:166:ASN:HA	17:A5:169:LEU:HD12	1.94	0.47
3:2:55:PRO:HB2	11:A:2339:G:H4'	1.96	0.47
11:A:1906:G:H2'	11:A:2014:A:H61	1.79	0.47
13:A1:134:PRO:HG3	16:A4:60:PRO:HD3	1.95	0.47
19:AA:839:A:H2'	19:AA:840:A:H8	1.79	0.47
79:e:265:LYS:HE3	79:e:268:TYR:HB2	1.94	0.47
19:AA:1057:G:H4'	19:AA:1578:A:H4'	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:I:47:LEU:HD22	61:N:226:ILE:HG12	1.96	0.47
63:OX:374:MET:HE1	70:V:168:GLU:HB3	1.97	0.47
9:8:201:GLN:HB2	80:f:199:LYS:HE2	1.97	0.47
28:AJ:57:GLN:HB3	28:AJ:109:LEU:HD11	1.96	0.47
29:AK:28:HIS:HB2	44:AZ:56:HIS:HD2	1.79	0.47
34:AP:124:TYR:HB3	35:AQ:9:ALA:HB2	1.96	0.47
62:O:38:ARG:HB2	62:O:85:LEU:HD11	1.97	0.47
10:9:118:GLY:HA3	70:V:191:LEU:HD12	1.96	0.47
11:A:2392:U:H2'	11:A:2394:A:H62	1.80	0.47
11:A:2668:A:H2'	11:A:2669:A:C8	2.50	0.47
60:M:261:ASP:HB3	60:M:264:GLN:HB2	1.95	0.47
72:X:34:GLU:OE2	72:X:36:ARG:HB2	2.14	0.47
79:e:55:ARG:HG3	79:e:149:LEU:HD22	1.96	0.47
89:o:15:ARG:HB3	89:o:18:ILE:HG12	1.97	0.47
11:A:1750:G:H2'	11:A:1751:A:C8	2.49	0.47
11:A:1839:C:H2'	11:A:1840:C:C6	2.50	0.47
11:A:1868:G:H2'	60:M:40:PRO:HG3	1.97	0.47
11:A:2748:A:H2'	11:A:2749:A:C8	2.50	0.47
16:A4:524:ARG:HB2	16:A4:527:LEU:HB3	1.96	0.47
19:AA:958:C:H4'	19:AA:959:C:O4'	2.15	0.47
19:AA:1269:U:H4'	19:AA:1270:U:H3'	1.96	0.47
26:AH:96:VAL:HA	26:AH:106:ILE:HD13	1.96	0.47
40:AV:114:ARG:HA	40:AV:117:LEU:HD12	1.96	0.47
47:Ay:23:A:H2'	47:Ay:24:A:H8	1.80	0.47
63:OX:165:GLU:HG2	63:OX:216:PRO:HG3	1.95	0.47
67:S:119:GLU:HG2	67:S:189:PRO:HB2	1.95	0.47
79:e:124:TRP:CD2	87:m:72:ARG:HG2	2.50	0.47
11:A:3078:C:H2'	11:A:3079:G:H8	1.80	0.47
11:A:3158:A:H2'	11:A:3159:A:C8	2.50	0.47
16:A4:236:VAL:HA	16:A4:270:ARG:HB3	1.97	0.47
19:AA:799:A:H2'	19:AA:800:C:C6	2.49	0.47
19:AA:832:U:H2'	19:AA:833:A:C8	2.49	0.47
24:AF:88:ASP:HB3	24:AF:91:ILE:HB	1.96	0.47
45:Aw:66:U:H4'	50:C:159:LYS:HE3	1.96	0.47
50:C:213:ALA:HA	50:C:245:LYS:HE3	1.96	0.47
81:g:142:GLU:HB3	89:o:88:ILE:HG13	1.96	0.47
11:A:3078:C:H2'	11:A:3079:G:C8	2.49	0.47
13:A1:60:MET:HE1	13:A1:66:TRP:HZ3	1.79	0.47
16:A4:489:HIS:HB3	16:A4:492:THR:HG23	1.96	0.47
17:A5:478:THR:HG22	17:A5:510:ALA:HA	1.96	0.47
31:AM:93:LEU:HD13	36:AR:156:TYR:CE2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2748:A:H2'	11:A:2749:A:H8	1.80	0.46
19:AA:1132:U:H2'	19:AA:1133:C:C6	2.50	0.46
58:K:94:GLN:O	58:K:98:ARG:HG2	2.16	0.46
63:OX:403:HIS:HB2	70:V:136:ARG:NH2	2.30	0.46
2:1:34:ARG:HD3	2:1:41:LEU:HD13	1.96	0.46
11:A:1709:G:H4'	73:Y:192:LYS:HZ2	1.79	0.46
16:A4:646:THR:HG23	16:A4:650:MET:HE3	1.97	0.46
19:AA:949:U:O2	101:AA:1781:NAD:H6N	2.16	0.46
49:B:43:G:H2'	49:B:44:A:C8	2.49	0.46
61:N:36:VAL:HG11	86:l:124:GLN:HB3	1.96	0.46
94:z:69:ILE:HA	94:z:72:ILE:HG12	1.96	0.46
10:9:36:ARG:HD2	69:U:46:MET:SD	2.54	0.46
11:A:1806:U:H4'	11:A:1807:U:H5'	1.97	0.46
11:A:2056:G:H2'	11:A:2057:C:H6	1.80	0.46
17:A5:406:PRO:O	17:A5:410:THR:HG23	2.15	0.46
17:A5:411:LEU:HD13	17:A5:427:MET:HG2	1.96	0.46
19:AA:852:A:H3'	19:AA:853:C:H6	1.81	0.46
24:AF:235:ALA:HB3	27:AI:121:LYS:HD2	1.97	0.46
78:d:91:PRO:HB2	78:d:94:ASP:HB2	1.97	0.46
2:1:38:ARG:HH12	2:1:41:LEU:HD11	1.80	0.46
11:A:1952:U:H2'	11:A:1953:A:H8	1.78	0.46
13:A1:114:LEU:HD11	26:AH:163:ASN:HB3	1.97	0.46
19:AA:868:C:H2'	19:AA:869:C:H6	1.79	0.46
20:AB:148:ASN:HD22	20:AB:197:HIS:CD2	2.34	0.46
31:AM:54:TYR:CD1	31:AM:66:VAL:HG22	2.51	0.46
53:F:231:VAL:HG13	91:q:26:ARG:HD2	1.96	0.46
71:W:104:TYR:HB2	71:W:128:LYS:HG3	1.98	0.46
13:A1:53:LEU:HD12	16:A4:518:GLU:HG2	1.97	0.46
19:AA:1194:C:H2'	19:AA:1195:U:C6	2.50	0.46
19:AA:1523:A:H5''	40:AV:68:SER:N	2.30	0.46
54:v:82:LEU:HD12	54:w:63:LYS:HB2	1.96	0.46
19:AA:681:U:H2'	19:AA:682:A:H8	1.80	0.46
19:AA:944:U:H2'	19:AA:945:G:C8	2.50	0.46
19:AA:1003:A:H2'	19:AA:1004:G:C8	2.48	0.46
19:AA:1452:U:H2'	19:AA:1453:A:H8	1.80	0.46
47:Ay:67:U:H2'	47:Ay:68:C:H6	1.81	0.46
50:C:243:ARG:HD2	50:C:256:CYS:HB3	1.97	0.46
65:Q:177:VAL:HG11	65:Q:204:MET:HG3	1.97	0.46
66:R:114:LYS:HD3	75:a:44:ASN:HB3	1.96	0.46
11:A:2740:A:H2'	11:A:2741:A:H8	1.80	0.46
47:Ay:68:C:H2'	47:Ay:69:C:H6	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
105:B:101:VAL:HB	79:e:166:GLY:HA3	1.98	0.46
8:7:276:PHE:HB2	8:7:304:VAL:HG22	1.97	0.46
46:Ax:47:U:H2'	46:Ax:48:G:C8	2.51	0.46
59:L:73:ILE:HD11	59:L:105:VAL:HG11	1.98	0.46
63:OX:266:PRO:HB3	63:OX:308:THR:HG22	1.97	0.46
78:d:204:ASN:O	78:d:205:GLN:HG2	2.16	0.46
16:A4:448:ILE:HG21	16:A4:454:ARG:HD3	1.97	0.46
19:AA:773:U:H2'	19:AA:774:G:C8	2.49	0.46
19:AA:914:A:H2'	19:AA:915:C:H6	1.81	0.46
33:AO:94:CYS:HB2	33:AO:108:CYS:SG	2.55	0.46
55:H:176:MET:HE1	55:H:188:ILE:HD11	1.98	0.46
61:N:124:VAL:HA	61:N:158:ARG:HH21	1.81	0.46
63:OX:156:PHE:HZ	63:OX:342:LEU:HD11	1.81	0.46
54:y:65:GLN:HA	54:y:68:VAL:HG12	1.96	0.46
11:A:1745:U:H5''	72:X:55:LYS:HD3	1.97	0.46
11:A:1994:A:H61	11:A:2736:C:H4'	1.80	0.46
12:A0:64:LEU:HD13	12:A0:134:VAL:HG12	1.98	0.46
40:AV:175:VAL:HG12	40:AV:177:SER:H	1.81	0.46
53:F:62:VAL:HG23	53:F:82:LEU:HB2	1.98	0.46
19:AA:1262:C:H4'	22:AD:100:LYS:HG2	1.97	0.45
36:AR:194:GLN:HE22	36:AR:199:LYS:H	1.64	0.45
42:AX:266:ASN:HA	42:AX:329:LEU:HD23	1.98	0.45
76:b:72:VAL:HG13	76:b:90:HIS:HB2	1.98	0.45
93:s:137:LEU:HD21	93:s:422:VAL:HG11	1.97	0.45
11:A:1761:A:H2'	11:A:1762:A:C8	2.52	0.45
11:A:2101:C:H2'	11:A:2102:A:H8	1.81	0.45
11:A:2483:U:H2'	11:A:2484:C:O4'	2.16	0.45
11:A:3024:U:H2'	11:A:3025:A:H8	1.81	0.45
17:A5:208:CYS:HB3	17:A5:240:THR:HG21	1.98	0.45
19:AA:970:A:H2'	19:AA:971:A:C8	2.51	0.45
19:AA:1495:C:H2'	19:AA:1496:U:C6	2.51	0.45
19:AA:1577:U:H2'	19:AA:1578:A:C8	2.51	0.45
25:AG:108:ILE:HG13	25:AG:125:MET:HB2	1.98	0.45
40:AV:120:ASP:HA	40:AV:122:GLN:HE21	1.82	0.45
52:E:123:GLN:HG2	52:E:125:GLN:HG3	1.97	0.45
79:e:213:TYR:HB3	79:e:231:VAL:HB	1.98	0.45
54:v:86:LEU:HB2	54:w:64:ILE:HG12	1.97	0.45
6:5:165:GLN:NE2	6:5:175:THR:HG22	2.31	0.45
13:A1:189:LYS:HG3	44:AZ:11:MET:HE1	1.98	0.45
15:A3:173:LEU:HD11	30:AL:206:LYS:HA	1.98	0.45
24:AF:167:PHE:HB2	47:Ay:33:U:H4'	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AI:100:VAL:HG12	27:AI:106:PRO:HA	1.98	0.45
37:AS:134:ARG:HG2	37:AS:136:GLY:H	1.81	0.45
40:AV:229:ALA:HB1	40:AV:286:VAL:HG11	1.98	0.45
47:Ay:1:U:H2'	47:Ay:2:A:C8	2.51	0.45
75:a:120:LYS:HG3	75:a:124:TYR:HE2	1.81	0.45
7:6:217:LEU:HB3	7:6:236:LEU:HD13	1.98	0.45
11:A:2111:C:H2'	11:A:2112:A:C8	2.51	0.45
11:A:3115:U:H2'	11:A:3116:C:C6	2.52	0.45
19:AA:673:U:H2'	19:AA:674:U:C6	2.52	0.45
62:O:46:TRP:CD1	62:O:121:ALA:HB2	2.51	0.45
69:U:110:LEU:HD12	73:Y:118:GLU:HG2	1.99	0.45
93:s:63:ILE:HA	93:s:66:TRP:CD1	2.51	0.45
94:z:184:ILE:HG12	94:z:207:LEU:HD13	1.99	0.45
7:6:106:ARG:HG2	64:P:110:TRP:CE2	2.51	0.45
11:A:2803:A:H2'	11:A:2804:A:O4'	2.16	0.45
17:A5:235:PHE:HZ	17:A5:259:ARG:HB2	1.81	0.45
67:S:96:PHE:HB3	76:b:126:ILE:HD13	1.99	0.45
94:z:108:LYS:O	94:z:112:LEU:HB2	2.16	0.45
9:8:129:ARG:HE	9:8:133:ARG:HH21	1.63	0.45
11:A:2778:U:O2'	94:z:116:SER:HB2	2.17	0.45
21:AC:88:GLU:HG2	21:AC:147:TYR:CE1	2.52	0.45
23:AE:86:ILE:HG12	51:D:172:MET:HE1	1.97	0.45
53:F:223:HIS:HA	53:F:226:MET:HE2	1.99	0.45
56:I:127:PRO:HG2	56:I:130:VAL:HG22	1.99	0.45
54:u:64:ILE:O	54:u:68:VAL:HG23	2.17	0.45
6:5:167:THR:HG21	93:s:281:HIS:CE1	2.51	0.45
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.51	0.45
19:AA:1071:U:H2'	19:AA:1072:G:C8	2.51	0.45
19:AA:1161:A:H2'	19:AA:1162:A:C8	2.52	0.45
19:AA:1471:A:H2'	19:AA:1472:G:C8	2.51	0.45
19:AA:1577:U:H2'	19:AA:1578:A:H8	1.82	0.45
50:C:284:SER:HA	50:C:289:VAL:HG11	1.99	0.45
80:f:171:LEU:HD13	80:f:174:ILE:HD11	1.99	0.45
80:f:190:THR:HG23	80:f:192:GLU:HG3	1.99	0.45
8:7:286:LEU:HD11	8:7:296:ARG:HB2	1.99	0.45
8:7:302:LEU:HD23	62:O:144:LEU:HD23	1.99	0.45
9:8:201:GLN:HB3	80:f:201:ARG:HG3	1.98	0.45
17:A5:236:SER:HA	17:A5:239:VAL:HG12	1.98	0.45
19:AA:1165:C:H2'	19:AA:1166:A:C8	2.52	0.45
41:AW:103:ARG:HE	41:AW:139:ARG:NH2	2.14	0.45
49:B:68:C:H2'	49:B:69:U:C6	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:H:163:THR:HG21	94:z:86:VAL:HG23	1.98	0.45
56:I:235:GLN:OE1	54:y:91:LYS:HA	2.16	0.45
11:A:2245:A:H4'	11:A:2246:A:OP1	2.17	0.45
19:AA:911:U:H2'	19:AA:912:U:C6	2.52	0.45
47:Ay:2:A:H2'	47:Ay:3:G:H8	1.82	0.45
54:G:127:ARG:HD2	54:G:127:ARG:HA	1.78	0.45
61:N:138:HIS:CD2	71:W:36:GLY:HA2	2.52	0.45
67:S:173:ARG:HB3	67:S:180:PHE:HE2	1.82	0.45
9:8:99:ARG:HG2	79:e:83:LEU:HB3	1.97	0.45
11:A:3151:A:H4'	65:Q:146:GLY:O	2.17	0.45
19:AA:1408:A:H2'	19:AA:1409:A:H8	1.82	0.45
51:D:237:LEU:HG	51:D:296:VAL:HG12	1.99	0.45
56:I:219:HIS:HB2	54:v:91:LYS:HZ1	1.82	0.45
11:A:2757:A:H2'	11:A:2758:G:O4'	2.16	0.44
17:A5:257:VAL:HG13	43:AY:203:ASN:HA	1.99	0.44
19:AA:1181:G:H2'	19:AA:1182:C:C6	2.52	0.44
22:AD:209:GLY:HA3	22:AD:213:GLU:HB2	2.00	0.44
45:Aw:16:A:H3'	45:Aw:20:C:H5'	1.99	0.44
54:G:134:LEU:HB2	54:G:195:VAL:HG22	1.99	0.44
56:I:203:VAL:HA	56:I:206:GLU:HB2	1.99	0.44
58:K:5:SER:HB2	58:K:8:PRO:HD2	1.99	0.44
67:S:144:LEU:HB2	75:a:58:ILE:HB	1.98	0.44
16:A4:236:VAL:HG13	16:A4:270:ARG:HB3	2.00	0.44
23:AE:35:ILE:HD12	30:AL:97:MET:HE2	1.99	0.44
38:AT:76:LEU:HB2	38:AT:88:VAL:HB	1.99	0.44
50:C:185:LYS:HD2	50:C:258:LEU:HB3	1.99	0.44
19:AA:732:A:H2'	19:AA:733:U:C6	2.52	0.44
19:AA:1416:A:H2'	19:AA:1417:A:C8	2.53	0.44
50:C:216:GLU:HB3	50:C:234:CYS:HA	1.98	0.44
59:L:47:GLY:HA2	59:L:77:ILE:HD11	1.98	0.44
11:A:1765:C:H5'	83:i:75:ARG:HH22	1.83	0.44
11:A:1977:U:H2'	11:A:1978:A:H8	1.82	0.44
19:AA:715:G:H2'	19:AA:716:U:C6	2.52	0.44
19:AA:1422:G:H2'	19:AA:1423:A:C8	2.52	0.44
19:AA:1502:A:H2'	19:AA:1503:G:O4'	2.17	0.44
57:J:25:ARG:HD2	86:l:56:LEU:HB3	1.99	0.44
11:A:3116:C:H2'	11:A:3117:C:H6	1.83	0.44
16:A4:94:TYR:HB2	21:AC:125:ARG:NH1	2.32	0.44
21:AC:58:ALA:HB3	21:AC:60:HIS:CE1	2.52	0.44
40:AV:148:MET:HE2	40:AV:185:VAL:HG21	2.00	0.44
57:J:113:THR:HG23	57:J:115:LYS:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:P:94:VAL:HG23	64:P:132:LEU:HD21	2.00	0.44
8:7:315:LYS:HD2	52:E:64:LEU:HD21	2.00	0.44
11:A:2407:U:H2'	11:A:2408:U:C6	2.52	0.44
11:A:2410:U:H2'	11:A:2411:U:H6	1.81	0.44
19:AA:1131:C:H2'	19:AA:1132:U:C6	2.52	0.44
19:AA:1510:U:H2'	19:AA:1511:C:C6	2.52	0.44
39:AU:153:LYS:HA	39:AU:153:LYS:HD3	1.81	0.44
50:C:180:ARG:NH1	50:C:181:HIS:HB3	2.32	0.44
56:I:146:LEU:HD11	85:k:23:PHE:CE2	2.53	0.44
57:J:73:LYS:NZ	57:J:79:GLU:HB2	2.33	0.44
62:O:44:ALA:HB3	62:O:49:VAL:HG23	2.00	0.44
8:7:166:LEU:HB3	8:7:181:TYR:HE1	1.81	0.44
11:A:1862:U:H2'	11:A:1863:A:C8	2.53	0.44
11:A:2694:A:C6	11:A:2985:C:H1'	2.52	0.44
11:A:3165:C:H2'	11:A:3166:U:C6	2.52	0.44
19:AA:1265:C:H2'	19:AA:1266:A:H8	1.82	0.44
19:AA:1376:C:H4'	19:AA:1377:C:H5'	1.99	0.44
32:AN:57:GLN:HG3	32:AN:84:ILE:HD11	2.00	0.44
54:w:84:GLU:O	54:w:88:LYS:HG2	2.17	0.44
19:AA:1353:A:H5'	19:AA:1354:A:H5'	2.00	0.44
61:N:104:MET:HE3	61:N:104:MET:HB3	1.81	0.44
13:A1:194:VAL:HG12	13:A1:229:LEU:HD21	2.00	0.44
17:A5:597:VAL:HG21	17:A5:633:TYR:CZ	2.52	0.44
19:AA:739:C:H2'	19:AA:740:G:O4'	2.18	0.44
19:AA:853:C:H2'	19:AA:854:U:C6	2.53	0.44
19:AA:1065:C:H2'	19:AA:1066:C:O4'	2.18	0.44
75:a:72:THR:HG22	77:c:258:THR:HA	1.99	0.44
77:c:259:ARG:HB2	77:c:271:PHE:HB2	1.99	0.44
94:z:123:LEU:HD23	94:z:257:ILE:HD11	2.00	0.44
11:A:2502:C:H1'	11:A:3096:U:H5'	2.00	0.43
11:A:2728:C:H2'	11:A:2729:U:H6	1.82	0.43
42:AX:284:PRO:HA	42:AX:287:LEU:HD23	2.00	0.43
52:E:107:MET:HE3	65:Q:145:LEU:HD12	2.00	0.43
56:I:225:GLN:HA	56:I:228:GLN:HE21	1.83	0.43
77:c:160:LEU:HD21	77:c:223:MET:HG3	1.99	0.43
94:z:296:ARG:HB3	94:z:302:GLY:HA2	1.99	0.43
16:A4:414:LYS:HE3	16:A4:453:HIS:HE1	1.83	0.43
17:A5:138:LYS:HD2	17:A5:347:THR:HG23	1.99	0.43
19:AA:838:U:H2'	19:AA:839:A:C8	2.51	0.43
36:AR:207:PRO:HB2	36:AR:209:ILE:HG22	1.99	0.43
40:AV:206:ALA:HB2	40:AV:249:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ax:37:C:H5''	47:Ay:35:U:H1'	1.99	0.43
47:Ay:68:C:H2'	47:Ay:69:C:C6	2.53	0.43
63:OX:242:VAL:HB	63:OX:245:LEU:HD12	1.99	0.43
63:OX:311:PHE:HB3	63:OX:316:PHE:CZ	2.53	0.43
67:S:173:ARG:HB2	67:S:182:LYS:HG3	2.01	0.43
85:k:66:VAL:HB	85:k:74:LEU:HB3	1.99	0.43
6:5:165:GLN:NE2	6:5:179:VAL:HG21	2.33	0.43
11:A:2092:C:H2'	11:A:2093:U:C6	2.53	0.43
11:A:3024:U:H2'	11:A:3025:A:C8	2.54	0.43
17:A5:258:MET:HB3	43:AY:204:ILE:HD11	2.00	0.43
19:AA:982:A:H2'	19:AA:983:C:C6	2.53	0.43
19:AA:1195:U:H2'	19:AA:1196:A:C8	2.53	0.43
32:AN:13:ILE:HG13	32:AN:66:LEU:HB2	2.00	0.43
47:Ay:65:C:H2'	47:Ay:66:U:C6	2.54	0.43
55:H:247:ARG:HG2	55:H:251:TRP:HE1	1.83	0.43
56:I:146:LEU:HD23	56:I:177:LEU:HB2	2.00	0.43
66:R:91:VAL:HG11	84:j:24:GLY:HA3	2.00	0.43
11:A:3116:C:H2'	11:A:3117:C:C6	2.52	0.43
13:A1:313:LYS:HG3	42:AX:341:ILE:HG23	2.00	0.43
19:AA:981:C:H2'	19:AA:982:A:H8	1.82	0.43
105:B:101:VAL:N	79:e:165:PHE:O	2.51	0.43
55:H:193:PHE:HZ	55:H:233:VAL:HG21	1.83	0.43
56:I:134:PHE:HD2	56:I:135:LEU:HD22	1.83	0.43
56:I:214:LEU:O	56:I:218:THR:HG23	2.18	0.43
67:S:120:LEU:HB3	67:S:122:LEU:HD12	1.99	0.43
91:q:168:VAL:HG12	91:q:175:PHE:HB2	1.99	0.43
54:t:87:LYS:HG3	54:t:91:LYS:NZ	2.33	0.43
11:A:1862:U:H2'	11:A:1863:A:H8	1.83	0.43
11:A:1939:G:O2'	11:A:1973:G:H4'	2.19	0.43
19:AA:738:A:H3'	19:AA:739:C:H6	1.83	0.43
24:AF:159:VAL:HG13	24:AF:172:VAL:HG21	2.00	0.43
50:C:163:ASP:CB	50:C:286:HIS:HE2	2.32	0.43
89:o:24:PRO:HG2	92:r:169:TRP:HB2	2.01	0.43
6:5:91:PRO:HG2	6:5:96:HIS:CD2	2.54	0.43
11:A:1924:U:H2'	11:A:1925:A:C8	2.53	0.43
11:A:2751:G:H2'	11:A:2752:C:C6	2.53	0.43
11:A:2894:U:H5''	11:A:2895:U:O4'	2.19	0.43
19:AA:659:U:H2'	19:AA:660:C:C6	2.54	0.43
19:AA:1004:G:H21	27:AI:98:GLN:HE22	1.67	0.43
20:AB:155:ILE:HG12	20:AB:196:LEU:HD13	1.99	0.43
46:Ax:15:A:O2'	46:Ax:16:A:H5'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C:115:LYS:HA	50:C:115:LYS:HD3	1.76	0.43
76:b:76:VAL:HG22	76:b:86:GLU:HG3	1.99	0.43
54:y:71:ILE:HD12	54:y:74:LEU:HD13	2.00	0.43
94:z:98:GLU:HB3	94:z:101:LYS:HB2	2.01	0.43
11:A:1861:U:H2'	11:A:1862:U:C6	2.53	0.43
11:A:3117:C:H2'	11:A:3118:U:H6	1.82	0.43
16:A4:414:LYS:HG2	48:Az:28:U:H1'	2.00	0.43
19:AA:1041:A:H8	19:AA:1041:A:P	2.42	0.43
24:AF:200:LEU:HB3	24:AF:202:PRO:HD2	2.01	0.43
27:AI:110:ALA:HB3	27:AI:135:ALA:HB2	1.99	0.43
31:AM:115:ALA:HA	31:AM:118:VAL:HG12	2.01	0.43
40:AV:163:VAL:O	40:AV:167:VAL:HG23	2.19	0.43
46:Ax:4:A:H2'	46:Ax:5:A:H8	1.83	0.43
50:C:154:SER:HB3	50:C:288:ASP:OD1	2.18	0.43
55:H:216:TRP:HA	55:H:237:VAL:HB	2.01	0.43
78:d:160:LEU:O	78:d:164:VAL:HG22	2.18	0.43
91:q:191:LYS:HA	91:q:194:LYS:HG2	2.01	0.43
6:5:115:GLU:HB2	6:5:119:GLN:HB2	1.99	0.43
12:A0:4:LYS:HA	12:A0:4:LYS:HD2	1.80	0.43
22:AD:336:VAL:HG11	22:AD:345:LEU:HD12	2.01	0.43
42:AX:222:LEU:HA	42:AX:225:VAL:HG12	2.00	0.43
46:Ax:22:U:C2	46:Ax:23:A:C8	3.06	0.43
54:G:148:GLU:O	54:G:152:TYR:HB3	2.19	0.43
57:J:61:LYS:HD3	86:l:79:LYS:HG2	1.99	0.43
79:e:97:ARG:HA	79:e:100:LYS:HG2	2.01	0.43
6:5:98:LEU:HD22	6:5:272:ASP:HB3	2.01	0.43
11:A:2053:U:HO2'	11:A:2054:U:H6	1.64	0.43
11:A:2815:OMG:HM23	11:A:2815:OMG:H1'	1.68	0.43
16:A4:393:ILE:HA	16:A4:396:ILE:HG22	2.01	0.43
16:A4:397:MET:HE3	16:A4:397:MET:HB3	1.83	0.43
17:A5:612:GLU:HB3	17:A5:644:LEU:HB3	2.00	0.43
18:A6:52:PHE:HD2	18:A6:58:PHE:HA	1.84	0.43
19:AA:914:A:H2'	19:AA:915:C:C6	2.54	0.43
19:AA:1485:G:H2'	19:AA:1486:B8T:O4'	2.18	0.43
19:AA:1498:C:H2'	19:AA:1499:U:H6	1.83	0.43
19:AA:1507:A:H2'	19:AA:1508:C:H6	1.84	0.43
33:AO:105:CYS:HB2	33:AO:142:VAL:HA	2.00	0.43
42:AX:85:PRO:HA	42:AX:88:VAL:HG12	2.01	0.43
43:AY:217:ARG:NH1	43:AY:225:ARG:HG3	2.34	0.43
63:OX:430:TRP:CG	73:Y:176:ILE:HG21	2.54	0.43
70:V:80:ILE:HB	70:V:85:TRP:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:e:159:LEU:HD12	79:e:254:TRP:CH2	2.54	0.43
93:s:91:TYR:HE2	93:s:229:LEU:HD22	1.84	0.43
54:w:61:PRO:O	54:w:65:GLN:HB3	2.18	0.43
94:z:64:GLU:HG2	94:z:65:LYS:N	2.34	0.43
19:AA:908:C:H2'	19:AA:909:G:C8	2.54	0.43
19:AA:1119:U:P	37:AS:48:ARG:HH22	2.42	0.43
53:F:138:HIS:CD2	53:F:146:TRP:HE1	2.37	0.43
56:I:197:LEU:HD22	54:u:76:LEU:HD12	1.99	0.43
56:I:232:LEU:HD23	54:y:91:LYS:NZ	2.34	0.43
77:c:228:LEU:HD22	77:c:307:PHE:HB3	2.00	0.43
13:A1:147:PHE:HB2	26:AH:177:LEU:HB3	1.99	0.42
13:A1:313:LYS:HB2	42:AX:342:PRO:HD2	2.01	0.42
38:AT:161:GLY:HA2	38:AT:164:LYS:HE2	1.99	0.42
91:q:138:GLN:O	91:q:141:GLU:HG3	2.19	0.42
6:5:204:VAL:HG13	93:s:152:GLN:HE21	1.85	0.42
11:A:2682:A:H4'	66:R:41:LEU:HD13	2.00	0.42
11:A:2728:C:H2'	11:A:2729:U:C6	2.53	0.42
12:A0:165:PRO:HG3	12:A0:190:MET:HE2	2.01	0.42
14:A2:43:ALA:HB1	14:A2:46:ILE:HD11	2.01	0.42
19:AA:1523:A:H2'	19:AA:1524:A:C8	2.54	0.42
25:AG:285:VAL:HG22	25:AG:328:VAL:HG22	2.02	0.42
31:AM:21:LEU:HB3	31:AM:32:TYR:HB3	2.01	0.42
49:B:74:C:H5''	79:e:219:GLN:HE22	1.84	0.42
50:C:91:ALA:HB2	50:C:108:ILE:HD12	2.01	0.42
52:E:222:TRP:CD1	52:E:256:LYS:HB3	2.55	0.42
56:I:163:GLU:HG3	56:I:166:ARG:HH22	1.84	0.42
57:J:58:LYS:HA	57:J:58:LYS:HD2	1.71	0.42
67:S:111:GLU:HG2	76:b:19:LEU:HD11	2.01	0.42
78:d:152:LEU:HD22	78:d:176:ILE:HD11	2.01	0.42
1:0:134:THR:HG23	62:O:130:LEU:HD22	2.02	0.42
13:A1:133:TRP:CZ3	26:AH:72:LEU:HD12	2.54	0.42
20:AB:81:VAL:HG12	41:AW:83:MET:HE1	2.02	0.42
31:AM:73:ILE:O	31:AM:77:ILE:HG12	2.19	0.42
40:AV:263:MET:HE1	40:AV:334:PHE:HD1	1.83	0.42
42:AX:80:PRO:HG2	42:AX:81:HIS:HD2	1.84	0.42
47:Ay:49:G:H2'	47:Ay:50:G:H8	1.84	0.42
49:B:49:U:H2'	49:B:50:U:C6	2.54	0.42
69:U:65:VAL:HG13	69:U:97:VAL:HG13	2.01	0.42
94:z:62:PRO:HG2	94:z:65:LYS:HB2	2.01	0.42
11:A:1911:C:H2'	11:A:1912:A:C8	2.54	0.42
19:AA:747:A:H2'	19:AA:748:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:985:U:H2'	19:AA:986:G:C8	2.54	0.42
19:AA:1265:C:H4'	26:AH:122:GLN:HG3	2.01	0.42
19:AA:1561:C:H2'	19:AA:1562:G:C8	2.55	0.42
19:AA:1578:A:H2'	19:AA:1579:C:H6	1.83	0.42
22:AD:141:TRP:HZ2	44:AZ:68:LEU:HB3	1.85	0.42
22:AD:380:LEU:HD12	22:AD:381:PRO:HD2	2.01	0.42
26:AH:76:LEU:HD23	26:AH:174:LYS:HA	2.00	0.42
26:AH:161:GLN:HG2	26:AH:170:MET:SD	2.59	0.42
47:Ay:66:U:H2'	47:Ay:67:U:C6	2.55	0.42
56:I:200:LEU:HD13	54:u:76:LEU:HB3	2.01	0.42
65:Q:117:LEU:HD12	65:Q:151:LEU:HD21	2.00	0.42
11:A:2127:A:H4'	11:A:2251:A:C5	2.55	0.42
11:A:2610:U:H2'	11:A:2611:C:C6	2.55	0.42
11:A:3199:U:H5''	11:A:3200:U:H4'	2.01	0.42
16:A4:392:ILE:HG13	16:A4:393:ILE:N	2.34	0.42
19:AA:696:U:H2'	19:AA:697:G:C8	2.54	0.42
19:AA:1034:U:H2'	19:AA:1035:U:C6	2.55	0.42
19:AA:1047:A:C5	19:AA:1158:U:H4'	2.55	0.42
19:AA:1407:U:H2'	19:AA:1408:A:C8	2.54	0.42
42:AX:74:ASP:O	42:AX:78:VAL:HG12	2.19	0.42
11:A:3142:A:H2'	11:A:3143:U:C6	2.54	0.42
16:A4:332:LEU:HD23	16:A4:368:SER:HB3	2.02	0.42
16:A4:427:ARG:HH22	43:AY:237:GLY:H	1.66	0.42
19:AA:1066:C:H2'	19:AA:1067:A:C8	2.55	0.42
24:AF:44:PRO:HD3	24:AF:75:LYS:HB2	2.01	0.42
27:AI:183:HIS:O	27:AI:184:ASN:HB2	2.20	0.42
42:AX:213:ARG:HH12	79:e:118:GLN:HG2	1.85	0.42
70:V:48:PRO:HD3	73:Y:234:LEU:HD22	2.02	0.42
54:t:58:LYS:HA	54:t:58:LYS:HD2	1.78	0.42
54:u:75:THR:O	54:u:79:ILE:HG13	2.19	0.42
8:7:317:LEU:HD23	8:7:317:LEU:HA	1.88	0.42
19:AA:1471:A:H2'	19:AA:1472:G:H8	1.85	0.42
63:OX:141:TRP:CD2	63:OX:250:LEU:HD11	2.55	0.42
63:OX:192:HIS:ND1	78:d:204:ASN:HB3	2.35	0.42
63:OX:269:VAL:O	63:OX:273:MET:HG2	2.19	0.42
67:S:183:LYS:HE2	67:S:185:ILE:HD11	2.02	0.42
54:t:58:LYS:HG3	54:t:60:TYR:CE1	2.54	0.42
11:A:2053:U:OP2	89:o:79:THR:HG23	2.20	0.42
11:A:2182:G:H2'	11:A:2183:C:C6	2.55	0.42
19:AA:1452:U:H2'	19:AA:1453:A:C8	2.54	0.42
46:Ax:3:U:H2'	46:Ax:4:A:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:K:20:LEU:HD22	58:K:141:LEU:HD13	2.01	0.42
84:j:91:TRP:CD2	89:o:58:GLN:HG2	2.54	0.42
2:1:20:MET:HE3	2:1:20:MET:HB3	1.98	0.42
11:A:1911:C:H2'	11:A:1912:A:H8	1.84	0.42
52:E:244:ALA:HB1	52:E:248:ILE:HD11	2.01	0.42
60:M:281:LYS:HG2	81:g:42:VAL:HG22	2.02	0.42
65:Q:96:ARG:HA	65:Q:99:MET:HE3	2.01	0.42
79:e:61:LYS:HE2	79:e:155:ARG:HD2	2.01	0.42
80:f:175:GLN:HA	80:f:178:LEU:HD23	2.01	0.42
94:z:99:VAL:HG22	94:z:305:LEU:HD22	2.02	0.42
8:7:309:HIS:CE1	52:E:155:PHE:HA	2.55	0.42
11:A:3102:U:H2'	11:A:3103:C:H6	1.84	0.42
16:A4:446:LYS:HB3	16:A4:446:LYS:HE3	1.82	0.42
16:A4:529:GLU:HB3	16:A4:533:MET:HE3	2.01	0.42
17:A5:620:GLU:HA	17:A5:623:TYR:HB3	2.01	0.42
19:AA:839:A:H5''	31:AM:20:ARG:HB2	2.01	0.42
19:AA:1190:C:H2'	19:AA:1191:C:H6	1.84	0.42
19:AA:1408:A:H2'	19:AA:1409:A:C8	2.55	0.42
21:AC:38:ARG:HE	21:AC:38:ARG:HB3	1.71	0.42
29:AK:52:LEU:HD22	44:AZ:41:PRO:HG3	2.02	0.42
57:J:113:THR:HG22	57:J:116:HIS:ND1	2.34	0.42
62:O:52:MET:HE3	62:O:52:MET:HB3	1.91	0.42
4:3:127:ALA:HA	60:M:79:PRO:HD3	2.02	0.41
4:3:175:ASP:HB3	4:3:178:GLN:HB2	2.01	0.41
16:A4:513:TRP:HE1	16:A4:554:ASP:HB2	1.84	0.41
17:A5:185:LEU:HD12	17:A5:207:TYR:CZ	2.54	0.41
17:A5:396:LYS:O	17:A5:400:VAL:HG23	2.20	0.41
36:AR:204:ILE:HD13	36:AR:204:ILE:HA	1.89	0.41
47:Ay:2:A:H2'	47:Ay:3:G:C8	2.55	0.41
91:q:188:LYS:O	91:q:191:LYS:HG2	2.20	0.41
54:u:74:LEU:HD12	54:u:74:LEU:HA	1.83	0.41
6:5:129:ILE:HD11	6:5:373:LEU:HD22	2.02	0.41
9:8:164:ARG:HG3	80:f:88:TYR:CE1	2.54	0.41
17:A5:150:TRP:CE3	17:A5:168:LEU:HD22	2.55	0.41
17:A5:295:LYS:HE3	17:A5:295:LYS:HB3	1.94	0.41
19:AA:659:U:O2'	19:AA:1285:G:H1'	2.19	0.41
19:AA:881:A:N6	33:AO:82:LYS:HB3	2.35	0.41
19:AA:1237:A:H1'	19:AA:1254:C:O2	2.21	0.41
19:AA:1308:U:H4'	25:AG:118:GLU:HG2	2.02	0.41
19:AA:1461:A:H4'	19:AA:1462:G:C8	2.55	0.41
42:AX:174:ASN:HB3	42:AX:177:ARG:HG3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:G:165:VAL:HG22	54:G:168:LEU:HD11	2.01	0.41
62:O:50:ASP:HB2	62:O:107:MET:HE1	2.00	0.41
79:e:217:PHE:HB3	79:e:221:MET:HG3	2.00	0.41
87:m:90:ARG:HE	87:m:94:ARG:HG3	1.84	0.41
54:t:60:TYR:CG	54:u:85:LEU:HD21	2.54	0.41
10:9:68:PHE:CE2	10:9:70:LEU:HB2	2.55	0.41
22:AD:103:LEU:HD11	22:AD:123:ARG:HB2	2.02	0.41
29:AK:115:ALA:HB2	29:AK:120:LEU:HD12	2.01	0.41
93:s:119:PRO:HG3	93:s:394:TRP:CD2	2.54	0.41
93:s:142:LEU:HD13	93:s:422:VAL:HG21	2.01	0.41
54:u:74:LEU:HD23	54:u:79:ILE:HG12	2.03	0.41
11:A:2455:U:H5''	62:O:47:ALA:HB3	2.03	0.41
11:A:3077:C:H2'	11:A:3078:C:H6	1.85	0.41
16:A4:126:LYS:HA	16:A4:129:GLN:HG2	2.02	0.41
19:AA:711:U:H5'	19:AA:712:C:C5	2.55	0.41
19:AA:839:A:H2'	19:AA:840:A:C8	2.56	0.41
19:AA:1034:U:H2'	19:AA:1035:U:H6	1.85	0.41
40:AV:262:VAL:HG23	40:AV:265:LYS:HE3	2.03	0.41
46:Ax:60:C:H2'	46:Ax:61:C:C6	2.55	0.41
77:c:59:ARG:HB2	77:c:62:GLU:HG2	2.03	0.41
54:y:83:ASN:HA	54:y:86:LEU:HB2	2.03	0.41
1:0:184:TRP:CD1	1:0:184:TRP:H	2.38	0.41
2:1:55:LEU:H	91:q:128:MET:HE2	1.85	0.41
7:6:327:VAL:HA	7:6:330:ILE:HD12	2.02	0.41
8:7:316:LEU:HD21	62:O:149:LEU:HD23	2.02	0.41
11:A:2109:A:H5'	61:N:133:ARG:HD3	2.02	0.41
11:A:2205:U:H4'	50:C:177:VAL:HG13	2.03	0.41
13:A1:319:LEU:HD23	13:A1:319:LEU:HA	1.89	0.41
17:A5:373:GLY:HA3	17:A5:402:MET:HG3	2.02	0.41
19:AA:1078:A:H2'	19:AA:1079:G:C8	2.56	0.41
19:AA:1496:U:H2'	19:AA:1497:C:C6	2.56	0.41
36:AR:142:LEU:HD21	36:AR:183:LYS:HE3	2.02	0.41
42:AX:100:MET:HE1	42:AX:356:CYS:HB2	2.03	0.41
56:I:49:ALA:HB1	89:o:32:LYS:HE3	2.03	0.41
59:L:136:LYS:HE2	59:L:136:LYS:HB2	1.91	0.41
93:s:119:PRO:HG3	93:s:394:TRP:CE3	2.56	0.41
9:8:53:LYS:NZ	45:Aw:40:C:H5''	2.35	0.41
11:A:1884:G:N7	53:F:281:ARG:HD2	2.35	0.41
11:A:1977:U:H2'	11:A:1978:A:C8	2.56	0.41
16:A4:61:LYS:HA	16:A4:61:LYS:HD3	1.69	0.41
17:A5:222:PHE:CD2	43:AY:178:LEU:HD21	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:848:U:H2'	19:AA:849:U:C6	2.55	0.41
19:AA:1181:G:H2'	19:AA:1182:C:H6	1.86	0.41
19:AA:1542:U:H2'	19:AA:1543:U:C6	2.55	0.41
26:AH:97:LEU:O	26:AH:101:GLU:HG3	2.20	0.41
42:AX:198:PHE:O	42:AX:202:ILE:HG22	2.21	0.41
51:D:257:ILE:O	51:D:262:ARG:HD2	2.21	0.41
55:H:118:LEU:HD11	55:H:122:ARG:HE	1.84	0.41
63:OX:188:LEU:HD12	70:V:169:THR:HG23	2.03	0.41
74:Z:101:LYS:HD3	84:j:84:MET:HG3	2.03	0.41
78:d:197:VAL:HG13	78:d:212:ILE:HG12	2.03	0.41
54:t:67:LEU:HD23	54:t:67:LEU:HA	1.88	0.41
54:x:82:LEU:O	54:x:86:LEU:HG	2.21	0.41
11:A:2065:A:C5	71:W:74:ARG:HD2	2.56	0.41
13:A1:268:GLN:HE21	13:A1:268:GLN:HB2	1.70	0.41
17:A5:151:ASP:O	17:A5:154:GLN:HG3	2.21	0.41
19:AA:1572:A:H2'	19:AA:1573:A:C8	2.55	0.41
22:AD:103:LEU:HD23	22:AD:121:LYS:HB3	2.01	0.41
23:AE:6:LEU:HB3	23:AE:66:VAL:HB	2.03	0.41
45:Aw:5:A:H2'	45:Aw:6:U:H6	1.86	0.41
50:C:163:ASP:HB3	50:C:286:HIS:HE2	1.84	0.41
52:E:218:VAL:HB	52:E:224:PHE:CD2	2.56	0.41
53:F:61:PRO:HA	53:F:84:PRO:HD3	2.03	0.41
77:c:228:LEU:HB2	77:c:307:PHE:CD1	2.56	0.41
79:e:124:TRP:CE2	87:m:72:ARG:HG2	2.56	0.41
79:e:164:LYS:HE2	79:e:164:LYS:HB2	1.91	0.41
94:z:262:MET:H	94:z:262:MET:HG3	1.74	0.41
17:A5:188:MET:HE2	17:A5:199:THR:HG21	2.03	0.41
19:AA:672:A:H2'	19:AA:673:U:H6	1.85	0.41
19:AA:871:A:H4'	19:AA:872:G:H5'	2.03	0.41
23:AE:37:ARG:HG3	39:AU:167:PHE:CE1	2.56	0.41
31:AM:29:ARG:HH22	38:AT:140:ILE:HG23	1.85	0.41
41:AW:104:ILE:HG13	41:AW:114:ILE:HG13	2.02	0.41
44:AZ:61:LEU:HG	44:AZ:62:MET:HE2	2.03	0.41
61:N:96:TYR:HB3	61:N:151:VAL:HB	2.02	0.41
63:OX:211:ILE:H	63:OX:211:ILE:HG13	1.72	0.41
63:OX:427:LYS:HD2	63:OX:427:LYS:HA	1.87	0.41
70:V:16:PRO:HD2	70:V:19:TYR:HB2	2.01	0.41
5:4:69:LYS:HB2	5:4:72:LEU:HD23	2.03	0.41
5:4:103:MET:HB3	5:4:103:MET:HE2	1.87	0.41
6:5:201:ARG:HB3	6:5:232:THR:HG22	2.03	0.41
11:A:2060:A:C8	11:A:2079:C:C4	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2408:U:H2'	11:A:2409:A:H8	1.86	0.41
11:A:3115:U:H2'	11:A:3116:C:H6	1.86	0.41
11:A:3213:A:H2'	11:A:3214:C:C6	2.56	0.41
13:A1:50:ARG:NE	21:AC:129:PRO:HG3	2.36	0.41
16:A4:377:ARG:HD3	16:A4:377:ARG:HA	1.93	0.41
16:A4:646:THR:O	16:A4:650:MET:HG2	2.21	0.41
17:A5:133:LEU:C	17:A5:135:PRO:HD3	2.46	0.41
19:AA:896:A:H2'	19:AA:897:C:C6	2.56	0.41
19:AA:1012:A:H2'	19:AA:1013:A:C8	2.56	0.41
20:AB:192:LEU:HD11	20:AB:220:VAL:HG23	2.03	0.41
34:AP:63:LYS:HD2	34:AP:63:LYS:HA	1.92	0.41
34:AP:103:LYS:HA	34:AP:103:LYS:HD3	1.81	0.41
36:AR:82:MET:HE2	36:AR:82:MET:HB3	1.94	0.41
47:Ay:65:C:H2'	47:Ay:66:U:H6	1.86	0.41
54:G:157:ASN:O	54:G:160:GLN:HG3	2.21	0.41
55:H:201:VAL:HA	94:z:86:VAL:HG12	2.03	0.41
56:I:219:HIS:NE2	54:v:87:LYS:HA	2.36	0.41
78:d:110:GLU:O	78:d:114:LYS:HG2	2.21	0.41
79:e:164:LYS:HD3	79:e:167:ASP:HA	2.03	0.41
91:q:44:ASP:O	91:q:47:THR:HG22	2.21	0.41
91:q:147:GLN:O	91:q:150:LYS:HG3	2.20	0.41
93:s:117:GLY:O	93:s:394:TRP:HB3	2.21	0.41
54:t:73:SER:HA	54:w:73:SER:CA	2.50	0.41
11:A:2530:A:H5''	51:D:212:THR:HG21	2.03	0.41
12:A0:82:ARG:HD3	12:A0:85:TRP:CE2	2.56	0.41
20:AB:162:CYS:HB3	20:AB:254:GLN:HG3	2.02	0.41
31:AM:93:LEU:HD13	36:AR:156:TYR:HE2	1.85	0.41
43:AY:315:ILE:HD13	43:AY:315:ILE:HA	1.89	0.41
47:Ay:40:C:H2'	47:Ay:41:A:C8	2.56	0.41
63:OX:335:ILE:HG22	63:OX:337:ALA:H	1.86	0.41
63:OX:385:MET:HE3	63:OX:385:MET:HB3	1.87	0.41
78:d:201:SER:O	78:d:208:VAL:HG12	2.21	0.41
54:t:61:PRO:O	54:t:64:ILE:HG22	2.21	0.41
94:z:87:TYR:CD2	94:z:92:TYR:HB2	2.56	0.41
8:7:269:ILE:HD12	8:7:274:ILE:HB	2.03	0.40
11:A:1829:A:H2'	11:A:1830:G:C8	2.56	0.40
11:A:2275:U:H2'	11:A:2276:C:C6	2.56	0.40
11:A:2286:A:H2'	11:A:2287:U:C6	2.56	0.40
11:A:2553:G:H2'	11:A:2554:A:C8	2.57	0.40
16:A4:159:GLU:HG2	16:A4:163:LEU:HD12	2.03	0.40
19:AA:727:U:H2'	19:AA:728:C:O4'	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:738:A:H3'	19:AA:739:C:C6	2.56	0.40
27:AI:182:PRO:HD2	35:AQ:42:ARG:HD3	2.02	0.40
63:OX:397:LEU:HD13	63:OX:399:GLN:HB3	2.02	0.40
79:e:198:ASN:HB3	79:e:243:PHE:CE1	2.56	0.40
93:s:316:CYS:HB3	93:s:319:GLN:HB2	2.03	0.40
16:A4:62:LYS:HB2	26:AH:66:SER:OG	2.20	0.40
16:A4:196:CYS:HB3	16:A4:265:GLY:HA3	2.03	0.40
16:A4:307:GLU:HG2	16:A4:312:LYS:HE3	2.02	0.40
16:A4:361:LYS:HE2	43:AY:251:PHE:CG	2.56	0.40
19:AA:1056:A:H4'	19:AA:1588:G:N2	2.36	0.40
30:AL:143:LEU:HD11	30:AL:153:LYS:HA	2.02	0.40
33:AO:213:LEU:HB3	33:AO:217:ARG:HH12	1.87	0.40
36:AR:288:GLN:HE22	36:AR:300:LEU:HD22	1.85	0.40
40:AV:96:ARG:HD2	40:AV:101:CYS:SG	2.62	0.40
40:AV:331:LEU:O	40:AV:335:LYS:HG2	2.21	0.40
45:Aw:3:G:H2'	45:Aw:4:U:H6	1.86	0.40
45:Aw:64:U:H2'	45:Aw:65:A:C8	2.56	0.40
46:Ax:52:A:N7	46:Ax:53:U:H1'	2.36	0.40
83:i:38:LEU:HD23	83:i:38:LEU:HA	1.92	0.40
54:u:85:LEU:HA	54:u:88:LYS:HG2	2.03	0.40
16:A4:581:ILE:HG13	16:A4:610:LEU:HD13	2.02	0.40
19:AA:994:A:H2'	19:AA:995:A:O4'	2.20	0.40
22:AD:351:ARG:HD2	22:AD:355:ARG:CZ	2.51	0.40
26:AH:76:LEU:HB2	26:AH:145:LEU:HB2	2.02	0.40
36:AR:254:ASP:HB2	36:AR:275:PHE:CZ	2.55	0.40
54:G:180:GLU:O	54:G:183:LYS:HG3	2.22	0.40
67:S:101:PHE:HE1	84:j:49:TRP:HB3	1.87	0.40
78:d:168:CYS:HB2	78:d:262:HIS:O	2.21	0.40
80:f:80:ILE:HG23	80:f:90:VAL:HG12	2.03	0.40
91:q:117:ARG:O	91:q:121:ILE:HG12	2.21	0.40
54:v:64:ILE:O	54:v:68:VAL:HG23	2.22	0.40
54:x:84:GLU:O	54:x:88:LYS:HG2	2.21	0.40
11:A:2691:U:H2'	11:A:2692:G:C8	2.57	0.40
16:A4:71:LEU:HD11	26:AH:162:ARG:HH12	1.85	0.40
17:A5:394:CYS:HB3	17:A5:406:PRO:HB2	2.02	0.40
17:A5:444:PRO:HB3	18:A6:56:THR:O	2.21	0.40
17:A5:485:PHE:HB2	17:A5:491:ALA:HB2	2.03	0.40
19:AA:946:U:H2'	19:AA:947:U:C6	2.57	0.40
21:AC:42:VAL:HG11	21:AC:51:VAL:HG11	2.03	0.40
42:AX:125:LEU:HD11	42:AX:310:LEU:HG	2.03	0.40
45:Aw:14:A:C6	45:Aw:22:A:C5	3.10	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C:267:GLN:HE21	50:C:297:GLU:HG2	1.86	0.40
54:G:184:ILE:HG13	54:G:185:LYS:N	2.37	0.40
60:M:13:LEU:HD23	60:M:13:LEU:HA	1.86	0.40
72:X:10:LEU:HD23	72:X:10:LEU:HA	1.87	0.40
78:d:40:ARG:HD3	78:d:40:ARG:HA	1.87	0.40
78:d:88:TYR:OH	78:d:91:PRO:HD3	2.21	0.40
7:6:224:HIS:CE1	7:6:227:GLU:H	2.40	0.40
9:8:192:TYR:HB3	80:f:132:ILE:HD11	2.03	0.40
11:A:1722:A:H2'	11:A:1723:A:O4'	2.21	0.40
19:AA:659:U:H2'	19:AA:660:C:H6	1.86	0.40
19:AA:740:G:H2'	19:AA:741:A:H8	1.86	0.40
19:AA:1263:G:N2	26:AH:124:VAL:HG21	2.37	0.40
20:AB:131:PHE:HE2	20:AB:192:LEU:HD13	1.86	0.40
36:AR:128:MET:H	36:AR:128:MET:HG2	1.66	0.40
45:Aw:26:U:H2'	45:Aw:27:A:C8	2.57	0.40
52:E:80:LEU:HD12	52:E:323:GLY:HA3	2.03	0.40
67:S:175:ARG:HB2	67:S:180:PHE:HB3	2.02	0.40
76:b:89:ILE:HA	76:b:92:LYS:HD2	2.03	0.40
54:u:91:LYS:HA	54:w:76:LEU:HD11	2.02	0.40
94:z:293:ALA:O	94:z:304:LEU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	108/188 (57%)	108 (100%)	0	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	389 (99%)	3 (1%)	0	100	100
7	6	352/380 (93%)	346 (98%)	6 (2%)	0	100	100
8	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
9	8	155/206 (75%)	151 (97%)	4 (3%)	0	100	100
10	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
12	A0	213/217 (98%)	209 (98%)	4 (2%)	0	100	100
13	A1	277/323 (86%)	270 (98%)	7 (2%)	0	100	100
14	A2	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
15	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
16	A4	584/689 (85%)	569 (97%)	15 (3%)	0	100	100
17	A5	579/1394 (42%)	550 (95%)	27 (5%)	2 (0%)	36	45
18	A6	72/109 (66%)	65 (90%)	7 (10%)	0	100	100
20	AB	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
21	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
22	AD	341/430 (79%)	335 (98%)	6 (2%)	0	100	100
23	AE	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
24	AF	206/242 (85%)	206 (100%)	0	0	100	100
25	AG	323/396 (82%)	317 (98%)	6 (2%)	0	100	100
26	AH	138/201 (69%)	132 (96%)	5 (4%)	1 (1%)	18	24
27	AI	135/194 (70%)	133 (98%)	1 (1%)	1 (1%)	18	24
28	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
29	AK	99/128 (77%)	99 (100%)	0	0	100	100
30	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
31	AM	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
32	AN	108/130 (83%)	108 (100%)	0	0	100	100
33	AO	191/258 (74%)	186 (97%)	5 (3%)	0	100	100
34	AP	95/142 (67%)	95 (100%)	0	0	100	100
35	AQ	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
36	AR	293/360 (81%)	286 (98%)	7 (2%)	0	100	100
37	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	AT	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
39	AU	174/205 (85%)	174 (100%)	0	0	100	100
40	AV	358/414 (86%)	348 (97%)	10 (3%)	0	100	100
41	AW	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
42	AX	350/398 (88%)	342 (98%)	8 (2%)	0	100	100
43	AY	219/395 (55%)	198 (90%)	19 (9%)	2 (1%)	14	17
44	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
50	C	221/297 (74%)	215 (97%)	6 (3%)	0	100	100
51	D	236/305 (77%)	232 (98%)	4 (2%)	0	100	100
52	E	303/348 (87%)	297 (98%)	6 (2%)	0	100	100
53	F	250/311 (80%)	247 (99%)	3 (1%)	0	100	100
54	G	70/198 (35%)	66 (94%)	4 (6%)	0	100	100
54	t	44/198 (22%)	43 (98%)	1 (2%)	0	100	100
54	u	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
54	v	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
54	w	29/198 (15%)	27 (93%)	2 (7%)	0	100	100
54	x	29/198 (15%)	26 (90%)	3 (10%)	0	100	100
54	y	29/198 (15%)	26 (90%)	3 (10%)	0	100	100
55	H	200/267 (75%)	193 (96%)	7 (4%)	0	100	100
56	I	210/261 (80%)	207 (99%)	3 (1%)	0	100	100
57	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
58	K	176/178 (99%)	174 (99%)	2 (1%)	0	100	100
59	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
60	M	289/296 (98%)	283 (98%)	6 (2%)	0	100	100
61	N	220/251 (88%)	220 (100%)	0	0	100	100
62	O	152/175 (87%)	148 (97%)	4 (3%)	0	100	100
63	OX	293/435 (67%)	279 (95%)	14 (5%)	0	100	100
64	P	142/180 (79%)	139 (98%)	3 (2%)	0	100	100
65	Q	237/292 (81%)	235 (99%)	2 (1%)	0	100	100
66	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
67	S	159/205 (78%)	158 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
69	U	150/153 (98%)	146 (97%)	4 (3%)	0	100	100
70	V	203/216 (94%)	201 (99%)	2 (1%)	0	100	100
71	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
72	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
73	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
74	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
75	a	99/142 (70%)	97 (98%)	2 (2%)	0	100	100
76	b	148/215 (69%)	142 (96%)	6 (4%)	0	100	100
77	c	282/332 (85%)	280 (99%)	2 (1%)	0	100	100
78	d	257/306 (84%)	242 (94%)	15 (6%)	0	100	100
79	e	236/279 (85%)	230 (98%)	6 (2%)	0	100	100
80	f	153/212 (72%)	148 (97%)	5 (3%)	0	100	100
81	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
82	h	108/158 (68%)	106 (98%)	2 (2%)	0	100	100
83	i	95/128 (74%)	95 (100%)	0	0	100	100
84	j	92/123 (75%)	92 (100%)	0	0	100	100
85	k	100/112 (89%)	100 (100%)	0	0	100	100
86	l	80/138 (58%)	78 (98%)	2 (2%)	0	100	100
87	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
89	o	92/102 (90%)	92 (100%)	0	0	100	100
90	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
91	q	175/222 (79%)	175 (100%)	0	0	100	100
92	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
93	s	381/439 (87%)	376 (99%)	5 (1%)	0	100	100
94	z	250/325 (77%)	235 (94%)	15 (6%)	0	100	100
All	All	16051/21917 (73%)	15711 (98%)	334 (2%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	A5	283	ILE
26	AH	126	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	AY	204	ILE
17	A5	257	VAL
27	AI	184	ASN
43	AY	205	ILE

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	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (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%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	270/303 (89%)	270 (100%)	0	100	100
9	8	146/190 (77%)	146 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
12	A0	188/189 (100%)	188 (100%)	0	100	100
13	A1	257/291 (88%)	256 (100%)	1 (0%)	84	89
14	A2	100/100 (100%)	100 (100%)	0	100	100
15	A3	65/166 (39%)	65 (100%)	0	100	100
16	A4	526/609 (86%)	526 (100%)	0	100	100
17	A5	515/1219 (42%)	515 (100%)	0	100	100
18	A6	63/90 (70%)	63 (100%)	0	100	100
20	AB	198/249 (80%)	198 (100%)	0	100	100
21	AC	115/143 (80%)	115 (100%)	0	100	100
22	AD	286/357 (80%)	286 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AE	104/107 (97%)	104 (100%)	0	100	100
24	AF	185/209 (88%)	185 (100%)	0	100	100
25	AG	285/342 (83%)	285 (100%)	0	100	100
26	AH	130/180 (72%)	130 (100%)	0	100	100
27	AI	105/147 (71%)	105 (100%)	0	100	100
28	AJ	93/118 (79%)	93 (100%)	0	100	100
29	AK	91/113 (80%)	91 (100%)	0	100	100
30	AL	158/226 (70%)	158 (100%)	0	100	100
31	AM	97/113 (86%)	97 (100%)	0	100	100
32	AN	96/115 (84%)	96 (100%)	0	100	100
33	AO	174/230 (76%)	174 (100%)	0	100	100
34	AP	88/123 (72%)	88 (100%)	0	100	100
35	AQ	78/78 (100%)	78 (100%)	0	100	100
36	AR	264/318 (83%)	264 (100%)	0	100	100
37	AS	116/164 (71%)	116 (100%)	0	100	100
38	AT	153/157 (98%)	153 (100%)	0	100	100
39	AU	152/174 (87%)	152 (100%)	0	100	100
40	AV	325/364 (89%)	325 (100%)	0	100	100
41	AW	87/158 (55%)	87 (100%)	0	100	100
42	AX	311/351 (89%)	311 (100%)	0	100	100
43	AY	202/357 (57%)	202 (100%)	0	100	100
44	AZ	90/95 (95%)	90 (100%)	0	100	100
50	C	193/245 (79%)	193 (100%)	0	100	100
51	D	192/245 (78%)	192 (100%)	0	100	100
52	E	260/290 (90%)	260 (100%)	0	100	100
53	F	219/262 (84%)	219 (100%)	0	100	100
54	G	60/158 (38%)	60 (100%)	0	100	100
54	t	40/158 (25%)	40 (100%)	0	100	100
54	u	31/158 (20%)	31 (100%)	0	100	100
54	v	31/158 (20%)	31 (100%)	0	100	100
54	w	30/158 (19%)	30 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	x	30/158 (19%)	30 (100%)	0	100	100
54	y	30/158 (19%)	30 (100%)	0	100	100
55	H	182/228 (80%)	182 (100%)	0	100	100
56	I	194/232 (84%)	194 (100%)	0	100	100
57	J	138/150 (92%)	138 (100%)	0	100	100
58	K	155/155 (100%)	155 (100%)	0	100	100
59	L	98/124 (79%)	98 (100%)	0	100	100
60	M	246/249 (99%)	246 (100%)	0	100	100
61	N	189/211 (90%)	189 (100%)	0	100	100
62	O	134/150 (89%)	134 (100%)	0	100	100
63	OX	261/372 (70%)	261 (100%)	0	100	100
64	P	126/155 (81%)	126 (100%)	0	100	100
65	Q	221/256 (86%)	221 (100%)	0	100	100
66	R	118/126 (94%)	118 (100%)	0	100	100
67	S	146/180 (81%)	146 (100%)	0	100	100
68	T	146/176 (83%)	146 (100%)	0	100	100
69	U	134/135 (99%)	134 (100%)	0	100	100
70	V	183/191 (96%)	183 (100%)	0	100	100
71	W	94/119 (79%)	94 (100%)	0	100	100
72	X	220/229 (96%)	220 (100%)	0	100	100
73	Y	163/223 (73%)	163 (100%)	0	100	100
74	Z	113/147 (77%)	113 (100%)	0	100	100
75	a	99/133 (74%)	99 (100%)	0	100	100
76	b	132/186 (71%)	132 (100%)	0	100	100
77	c	251/288 (87%)	251 (100%)	0	100	100
78	d	237/274 (86%)	237 (100%)	0	100	100
79	e	207/236 (88%)	207 (100%)	0	100	100
80	f	139/188 (74%)	139 (100%)	0	100	100
81	g	124/148 (84%)	124 (100%)	0	100	100
82	h	104/148 (70%)	104 (100%)	0	100	100
83	i	86/110 (78%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	j	74/97 (76%)	74 (100%)	0	100	100
85	k	83/89 (93%)	83 (100%)	0	100	100
86	l	76/116 (66%)	76 (100%)	0	100	100
87	m	85/113 (75%)	85 (100%)	0	100	100
89	o	80/87 (92%)	80 (100%)	0	100	100
90	p	135/181 (75%)	135 (100%)	0	100	100
91	q	153/178 (86%)	153 (100%)	0	100	100
92	r	147/169 (87%)	147 (100%)	0	100	100
93	s	339/381 (89%)	339 (100%)	0	100	100
94	z	226/287 (79%)	226 (100%)	0	100	100
All	All	14354/18873 (76%)	14353 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
13	A1	268	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	178	GLN
5	4	95	HIS
6	5	150	GLN
6	5	165	GLN
6	5	191	GLN
6	5	251	HIS
7	6	295	GLN
8	7	287	GLN
9	8	186	GLN
12	A0	24	GLN
13	A1	64	GLN
13	A1	146	HIS
15	A3	158	GLN
15	A3	190	GLN
16	A4	233	GLN
16	A4	453	HIS
16	A4	626	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	A4	656	ASN
17	A5	242	HIS
17	A5	250	ASN
17	A5	474	GLN
17	A5	489	ASN
17	A5	498	ASN
17	A5	509	GLN
17	A5	531	ASN
20	AB	126	GLN
20	AB	148	ASN
20	AB	201	ASN
22	AD	155	GLN
22	AD	369	HIS
22	AD	415	GLN
23	AE	56	GLN
23	AE	92	ASN
24	AF	122	GLN
25	AG	288	HIS
29	AK	124	GLN
30	AL	77	GLN
30	AL	162	GLN
32	AN	52	HIS
33	AO	146	GLN
33	AO	169	GLN
33	AO	181	HIS
36	AR	76	GLN
36	AR	108	GLN
36	AR	290	GLN
36	AR	326	ASN
38	AT	33	ASN
42	AX	81	HIS
42	AX	190	ASN
42	AX	195	ASN
44	AZ	82	GLN
50	C	275	GLN
50	C	281	GLN
50	C	291	HIS
51	D	168	HIS
52	E	52	HIS
52	E	88	HIS
56	I	119	HIS
56	I	228	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	J	84	GLN
57	J	186	GLN
58	K	94	GLN
60	M	30	ASN
61	N	181	HIS
63	OX	206	GLN
64	P	142	ASN
65	Q	107	HIS
66	R	89	ASN
66	R	149	HIS
68	T	145	GLN
69	U	27	GLN
69	U	77	ASN
71	W	65	ASN
72	X	93	ASN
74	Z	148	GLN
74	Z	150	HIS
78	d	193	HIS
78	d	205	GLN
81	g	141	ASN
81	g	155	GLN
83	i	120	HIS
85	k	72	HIS
89	o	91	GLN
90	p	117	GLN
90	p	184	ASN
90	p	194	HIS
91	q	60	GLN
92	r	79	HIS
93	s	152	GLN
93	s	164	HIS
93	s	420	GLN
54	w	69	GLN
94	z	104	HIS
94	z	241	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1558 (99%)	252 (16%)	2 (0%)
19	AA	953/954 (99%)	139 (14%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	Aw	64/76 (84%)	22 (34%)	0
46	Ax	70/71 (98%)	17 (24%)	0
47	Ay	67/76 (88%)	12 (17%)	0
48	Az	33/34 (97%)	13 (39%)	0
49	B	70/72 (97%)	14 (20%)	0
All	All	2813/2841 (99%)	469 (16%)	2 (0%)

All (469) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1681	G
11	A	1689	C
11	A	1692	A
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1708	A
11	A	1709	G
11	A	1711	C
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1736	A
11	A	1748	G
11	A	1750	G
11	A	1765	C
11	A	1777	A
11	A	1805	A
11	A	1806	U
11	A	1807	U
11	A	1808	A
11	A	1812	C
11	A	1817	C
11	A	1821	A
11	A	1827	C
11	A	1828	A
11	A	1829	A
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1854	U
11	A	1856	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	1869	A
11	A	1871	A
11	A	1873	A
11	A	1878	U
11	A	1882	A
11	A	1886	G
11	A	1887	A
11	A	1888	G
11	A	1893	A
11	A	1901	C
11	A	1902	C
11	A	1903	C
11	A	1909	A
11	A	1918	G
11	A	1937	A
11	A	1940	A
11	A	1958	G
11	A	1985	G
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	2001	C
11	A	2003	A
11	A	2015	G
11	A	2022	G
11	A	2030	U
11	A	2036	C
11	A	2037	U
11	A	2039	A
11	A	2044	A
11	A	2054	U
11	A	2060	A
11	A	2071	U
11	A	2079	C
11	A	2099	U
11	A	2113	G
11	A	2125	C
11	A	2126	U
11	A	2147	G
11	A	2159	U
11	A	2160	A
11	A	2163	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2168	U
11	A	2181	A
11	A	2182	G
11	A	2191	A
11	A	2192	A
11	A	2195	A
11	A	2196	A
11	A	2198	A
11	A	2200	A
11	A	2214	A
11	A	2219	C
11	A	2220	A
11	A	2221	C
11	A	2223	A
11	A	2224	C
11	A	2225	C
11	A	2226	U
11	A	2230	A
11	A	2233	U
11	A	2237	A
11	A	2241	A
11	A	2243	A
11	A	2245	A
11	A	2246	A
11	A	2262	C
11	A	2263	C
11	A	2284	C
11	A	2297	A
11	A	2300	G
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2345	G
11	A	2349	G
11	A	2350	A
11	A	2353	A
11	A	2354	A
11	A	2357	C
11	A	2363	A
11	A	2372	U
11	A	2374	A
11	A	2381	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2390	A
11	A	2399	A
11	A	2401	A
11	A	2404	U
11	A	2407	U
11	A	2415	C
11	A	2446	A
11	A	2451	A
11	A	2452	A
11	A	2478	G
11	A	2485	U
11	A	2493	C
11	A	2502	C
11	A	2506	A
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2540	C
11	A	2570	C
11	A	2571	G
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2599	U
11	A	2600	A
11	A	2601	A
11	A	2603	C
11	A	2618	U
11	A	2625	C
11	A	2627	G
11	A	2630	U
11	A	2633	A
11	A	2635	G
11	A	2654	U
11	A	2655	G
11	A	2656	U
11	A	2683	C
11	A	2686	G
11	A	2694	A
11	A	2696	A
11	A	2706	A
11	A	2709	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2718	C
11	A	2719	G
11	A	2723	A
11	A	2724	G
11	A	2725	A
11	A	2732	G
11	A	2733	G
11	A	2745	A
11	A	2762	C
11	A	2763	U
11	A	2765	A
11	A	2767	A
11	A	2768	A
11	A	2782	A
11	A	2783	A
11	A	2786	U
11	A	2790	A
11	A	2810	G
11	A	2832	A
11	A	2833	A
11	A	2844	G
11	A	2847	C
11	A	2864	U
11	A	2865	C
11	A	2882	U
11	A	2885	U
11	A	2888	A
11	A	2889	C
11	A	2893	A
11	A	2907	U
11	A	2913	A
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2927	C
11	A	2928	C
11	A	2935	A
11	A	2956	A
11	A	2962	C
11	A	2971	A
11	A	2985	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2993	U
11	A	3000	A
11	A	3005	A
11	A	3016	G
11	A	3022	G
11	A	3041	U
11	A	3049	U
11	A	3053	A
11	A	3054	G
11	A	3060	C
11	A	3072	U
11	A	3086	U
11	A	3089	A
11	A	3090	G
11	A	3096	U
11	A	3100	U
11	A	3102	U
11	A	3108	U
11	A	3109	U
11	A	3110	C
11	A	3111	A
11	A	3112	A
11	A	3113	A
11	A	3131	G
11	A	3150	U
11	A	3157	C
11	A	3158	A
11	A	3161	G
11	A	3162	C
11	A	3169	C
11	A	3172	C
11	A	3177	A
11	A	3180	A
11	A	3183	U
11	A	3189	C
11	A	3190	A
11	A	3199	U
11	A	3200	U
11	A	3207	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	3209	A
11	A	3210	C
11	A	3212	C
11	A	3217	A
11	A	3218	A
11	A	3220	A
11	A	3228	U
11	A	3229	U
11	A	3230	G
11	A	3231	U
19	AA	651	A
19	AA	680	U
19	AA	688	A
19	AA	704	U
19	AA	706	C
19	AA	721	U
19	AA	722	C
19	AA	735	A
19	AA	737	C
19	AA	738	A
19	AA	753	A
19	AA	761	A
19	AA	766	G
19	AA	773	U
19	AA	791	G
19	AA	794	U
19	AA	796	G
19	AA	808	C
19	AA	829	C
19	AA	830	U
19	AA	832	U
19	AA	835	C
19	AA	836	A
19	AA	860	A
19	AA	861	U
19	AA	868	C
19	AA	871	A
19	AA	881	A
19	AA	890	C
19	AA	893	G
19	AA	903	U
19	AA	904	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	AA	907	A
19	AA	910	A
19	AA	919	A
19	AA	929	A
19	AA	933	G
19	AA	938	A
19	AA	939	A
19	AA	942	A
19	AA	954	C
19	AA	959	C
19	AA	960	C
19	AA	961	U
19	AA	962	C
19	AA	967	A
19	AA	975	A
19	AA	978	A
19	AA	993	A
19	AA	1001	C
19	AA	1002	C
19	AA	1015	A
19	AA	1042	U
19	AA	1046	A
19	AA	1076	5MU
19	AA	1081	U
19	AA	1082	A
19	AA	1096	A
19	AA	1103	A
19	AA	1105	C
19	AA	1106	C
19	AA	1107	U
19	AA	1109	A
19	AA	1116	A
19	AA	1118	A
19	AA	1119	U
19	AA	1121	A
19	AA	1126	A
19	AA	1137	A
19	AA	1138	G
19	AA	1151	C
19	AA	1153	C
19	AA	1155	G
19	AA	1160	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	AA	1167	A
19	AA	1187	U
19	AA	1188	A
19	AA	1189	U
19	AA	1190	C
19	AA	1197	G
19	AA	1215	U
19	AA	1220	A
19	AA	1223	C
19	AA	1225	C
19	AA	1230	C
19	AA	1232	A
19	AA	1235	U
19	AA	1247	G
19	AA	1248	C
19	AA	1250	C
19	AA	1251	A
19	AA	1261	C
19	AA	1271	C
19	AA	1273	G
19	AA	1284	U
19	AA	1285	G
19	AA	1290	C
19	AA	1291	U
19	AA	1292	A
19	AA	1326	A
19	AA	1327	G
19	AA	1343	A
19	AA	1344	U
19	AA	1353	A
19	AA	1354	A
19	AA	1355	G
19	AA	1356	A
19	AA	1376	C
19	AA	1378	C
19	AA	1387	A
19	AA	1390	A
19	AA	1405	C
19	AA	1422	G
19	AA	1430	A
19	AA	1466	C
19	AA	1481	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	AA	1482	A
19	AA	1512	A
19	AA	1519	A
19	AA	1521	U
19	AA	1522	U
19	AA	1525	C
19	AA	1526	U
19	AA	1527	A
19	AA	1533	C
19	AA	1537	C
19	AA	1538	G
19	AA	1539	C
19	AA	1540	A
19	AA	1551	G
19	AA	1557	A
19	AA	1560	U
19	AA	1568	U
19	AA	1571	U
19	AA	1582	G
19	AA	1584	MA6
19	AA	1594	G
19	AA	1595	G
19	AA	1599	A
45	Aw	9	A
45	Aw	13	U
45	Aw	14	A
45	Aw	15	A
45	Aw	16	A
45	Aw	21	A
45	Aw	46	A
45	Aw	49	U
45	Aw	50	A
45	Aw	51	U
45	Aw	52	G
45	Aw	53	A
45	Aw	55	A
45	Aw	56	A
45	Aw	63	A
45	Aw	65	A
45	Aw	68	U
45	Aw	69	A
45	Aw	71	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	Aw	72	A
45	Aw	74	C
45	Aw	75	C
46	Ax	7	G
46	Ax	13	U
46	Ax	16	A
46	Ax	17	U
46	Ax	18	A
46	Ax	22	U
46	Ax	43	A
46	Ax	44	U
46	Ax	47	U
46	Ax	50	U
46	Ax	51	U
46	Ax	52	A
46	Ax	56	C
46	Ax	61	C
46	Ax	63	G
46	Ax	65	A
46	Ax	71	A
47	Ay	9	A
47	Ay	13	U
47	Ay	28	C
47	Ay	29	U
47	Ay	33	U
47	Ay	44	A
47	Ay	45	G
47	Ay	46	A
47	Ay	49	G
47	Ay	58	A
47	Ay	59	U
47	Ay	73	A
48	Az	0	U
48	Az	4	A
48	Az	11	U
48	Az	12	U
48	Az	13	U
48	Az	18	A
48	Az	21	A
48	Az	22	A
48	Az	24	U
48	Az	25	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	Az	26	A
48	Az	27	C
48	Az	31	A
49	B	8	U
49	B	10	2MG
49	B	16	C
49	B	21	A
49	B	45	G
49	B	46	A
49	B	54	C
49	B	55	U
49	B	56	U
49	B	58	A
49	B	59	A
49	B	64	A
49	B	69	U
49	B	76	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2245	A
11	A	2484	C

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

13 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$
49	2MG	B	10	49	23,26,27	0.36	0	33,38,41	0.42	0
49	PSU	B	39	49	18,21,22	1.04	1 (5%)	21,30,33	0.71	0
11	OMU	A	3039	99,11	19,22,23	0.31	0	25,31,34	0.71	1 (4%)
19	B8T	AA	1486	19,97	19,22,23	0.41	0	25,31,34	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	1MA	A	2617	11	21,25,26	0.40	0	30,37,40	0.61	0
11	OMG	A	3040	11,45	23,26,27	0.35	0	32,38,41	0.39	0
19	5MC	AA	1488	19	19,22,23	0.86	1 (5%)	26,32,35	0.51	0
19	MA6	AA	1584	19	23,26,27	0.32	0	33,38,41	0.75	1 (3%)
19	MA6	AA	1583	19	23,26,27	0.35	0	33,38,41	0.76	1 (3%)
19	5MU	AA	1076	19	19,22,23	0.37	0	27,32,35	0.55	0
11	PSU	A	3067	11	18,21,22	1.11	2 (11%)	21,30,33	0.86	1 (4%)
11	OMG	A	2815	99,11,46	23,26,27	0.36	0	32,38,41	0.41	0
49	1MA	B	9	49	21,25,26	0.39	0	30,37,40	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	2MG	B	10	49	-	0/9/27/28	0/3/3/3
49	PSU	B	39	49	-	0/7/25/26	0/2/2/2
11	OMU	A	3039	99,11	-	0/9/27/28	0/2/2/2
19	B8T	AA	1486	19,97	-	1/7/27/28	0/2/2/2
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
11	OMG	A	3040	11,45	-	2/9/27/28	0/3/3/3
19	5MC	AA	1488	19	-	0/7/25/26	0/2/2/2
19	MA6	AA	1584	19	-	1/11/29/30	0/3/3/3
19	MA6	AA	1583	19	-	0/11/29/30	0/3/3/3
19	5MU	AA	1076	19	-	5/7/25/26	0/2/2/2
11	PSU	A	3067	11	-	0/7/25/26	0/2/2/2
11	OMG	A	2815	99,11,46	-	1/9/27/28	0/3/3/3
49	1MA	B	9	49	-	0/7/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B	39	PSU	C6-C5	3.61	1.39	1.35
11	A	3067	PSU	C6-C5	3.45	1.39	1.35
19	AA	1488	5MC	C5-C4	-3.39	1.41	1.44
11	A	3067	PSU	O4'-C1'	-2.45	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	1583	MA6	C2-N1-C6	2.95	119.04	111.83
19	AA	1584	MA6	C2-N1-C6	2.95	119.03	111.83
11	A	3039	OMU	C2'-C1'-N1	-2.78	108.97	114.24
11	A	3067	PSU	O4'-C1'-C2'	2.60	108.75	105.15

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2815	OMG	C1'-C2'-O2'-CM2
19	AA	1076	5MU	O4'-C4'-C5'-O5'
19	AA	1076	5MU	C3'-C4'-C5'-O5'
11	A	3040	OMG	C3'-C4'-C5'-O5'
11	A	3040	OMG	O4'-C4'-C5'-O5'
19	AA	1584	MA6	C4'-C5'-O5'-P
19	AA	1076	5MU	C4'-C5'-O5'-P
19	AA	1486	B8T	O4'-C4'-C5'-O5'
19	AA	1076	5MU	C2'-C1'-N1-C6
19	AA	1076	5MU	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	AA	1486	B8T	1	0
19	AA	1488	5MC	1	0
19	AA	1583	MA6	1	0
11	A	2815	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 279 ligands modelled in this entry, 262 are monoatomic - leaving 17 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
96	SPD	A	3301	-	9,9,9	0.18	0	8,8,8	0.22	0
100	SPM	AA	1780	-	13,13,13	0.18	0	12,12,12	0.21	0
101	NAD	AA	1781	97	46,48,48	1.17	3 (6%)	64,73,73	0.84	2 (3%)
96	SPD	A	3302	-	9,9,9	0.14	0	8,8,8	0.21	0
96	SPD	A	3470	-	9,9,9	0.14	0	8,8,8	0.26	0
102	FES	AP	201	34,23	0,4,4	-	-	-	-	-
96	SPD	A	3471	-	9,9,9	0.18	0	8,8,8	0.29	0
100	SPM	AA	1706	-	13,13,13	0.15	0	12,12,12	0.22	0
104	ATP	AX	403	97	32,33,33	0.55	0	48,52,52	0.34	0
105	VAL	B	101	49	4,6,7	0.80	0	6,7,9	1.03	1 (16%)
98	PUT	A	3309	-	5,5,5	0.13	0	4,4,4	0.23	0
102	FES	AT	201	31,38	0,4,4	-	-	-	-	-
96	SPD	AA	1712	-	9,9,9	0.15	0	8,8,8	0.21	0
96	SPD	O	301	-	9,9,9	0.16	0	8,8,8	0.24	0
102	FES	r	201	92,56	0,4,4	-	-	-	-	-
96	SPD	AA	1779	-	9,9,9	0.16	0	8,8,8	0.25	0
103	GDP	AX	401	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	7 (15%)

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
96	SPD	A	3301	-	-	0/7/7/7	-
100	SPM	AA	1780	-	-	0/11/11/11	-
101	NAD	AA	1781	97	-	2/30/62/62	0/5/5/5
96	SPD	A	3302	-	-	1/7/7/7	-
96	SPD	A	3470	-	-	1/7/7/7	-
102	FES	AP	201	34,23	-	-	0/1/1/1
96	SPD	A	3471	-	-	0/7/7/7	-
100	SPM	AA	1706	-	-	0/11/11/11	-
104	ATP	AX	403	97	-	0/22/38/38	0/3/3/3
105	VAL	B	101	49	-	0/5/6/8	-
98	PUT	A	3309	-	-	0/3/3/3	-
102	FES	AT	201	31,38	-	-	0/1/1/1
96	SPD	AA	1712	-	-	0/7/7/7	-
96	SPD	O	301	-	-	1/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
102	FES	r	201	92,56	-	-	0/1/1/1
96	SPD	AA	1779	-	-	0/7/7/7	-
103	GDP	AX	401	-	-	0/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
101	AA	1781	NAD	PA-O3	4.55	1.64	1.59
103	AX	401	GDP	C5-C4	3.11	1.47	1.38
101	AA	1781	NAD	O4D-C1D	-2.81	1.37	1.40
101	AA	1781	NAD	PN-O3	2.70	1.62	1.59
103	AX	401	GDP	C6-N1	-2.57	1.34	1.38
103	AX	401	GDP	C5-N7	-2.15	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
103	AX	401	GDP	C5-C4-N3	-6.01	118.82	128.39
103	AX	401	GDP	C2-N3-C4	4.88	120.70	112.30
103	AX	401	GDP	N9-C4-N3	4.57	135.08	125.95
103	AX	401	GDP	C6-C5-N7	3.07	135.87	130.29
103	AX	401	GDP	C4-C5-N7	-2.42	106.84	110.67
101	AA	1781	NAD	O3-PA-O1A	-2.39	103.52	110.70
105	B	101	VAL	O-C-CA	-2.37	118.68	124.77
101	AA	1781	NAD	O2A-PA-O1A	2.24	122.89	112.44
103	AX	401	GDP	C3'-C2'-C1'	2.20	105.63	101.46
103	AX	401	GDP	O6-C6-C5	-2.11	120.97	126.53

There are no chirality outliers.

All (5) torsion outliers are listed below:

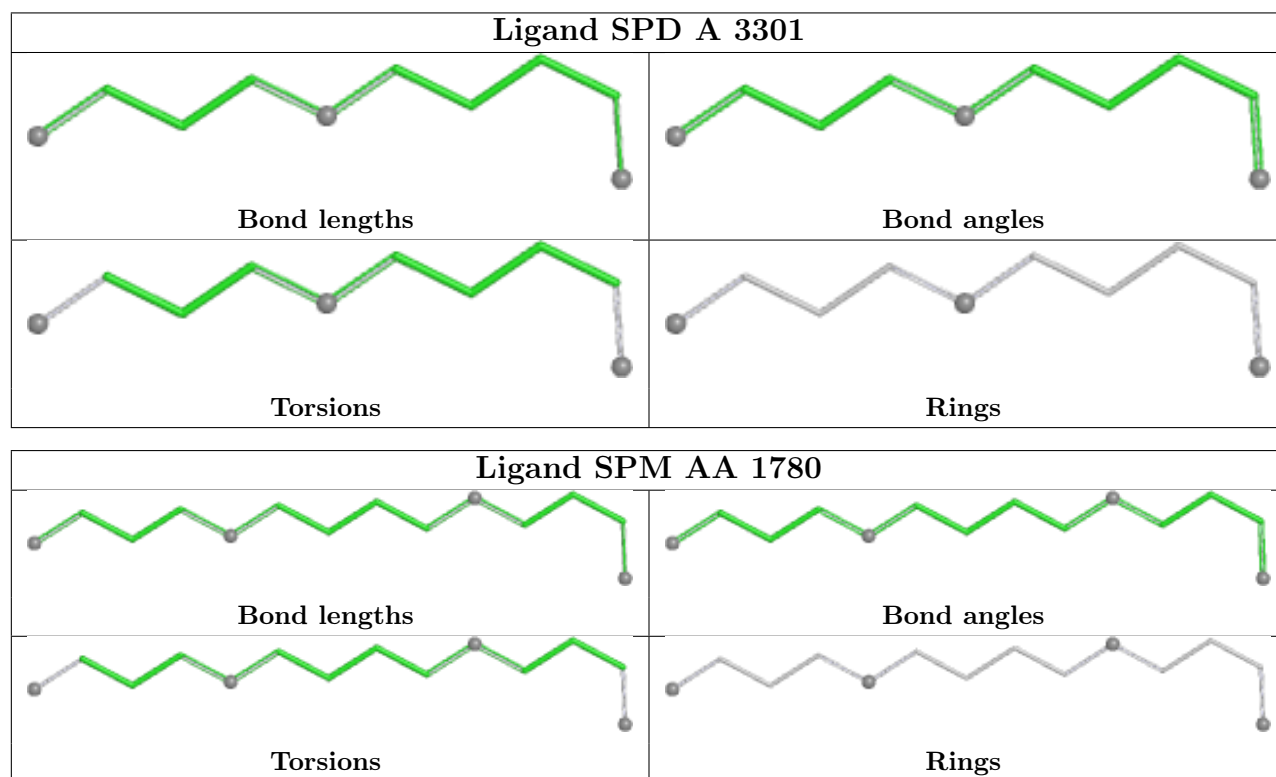
Mol	Chain	Res	Type	Atoms
101	AA	1781	NAD	C5D-O5D-PN-O1N
96	A	3302	SPD	N1-C2-C3-C4
96	A	3470	SPD	C2-C3-C4-C5
96	O	301	SPD	N6-C7-C8-C9
101	AA	1781	NAD	PA-O3-PN-O2N

There are no ring outliers.

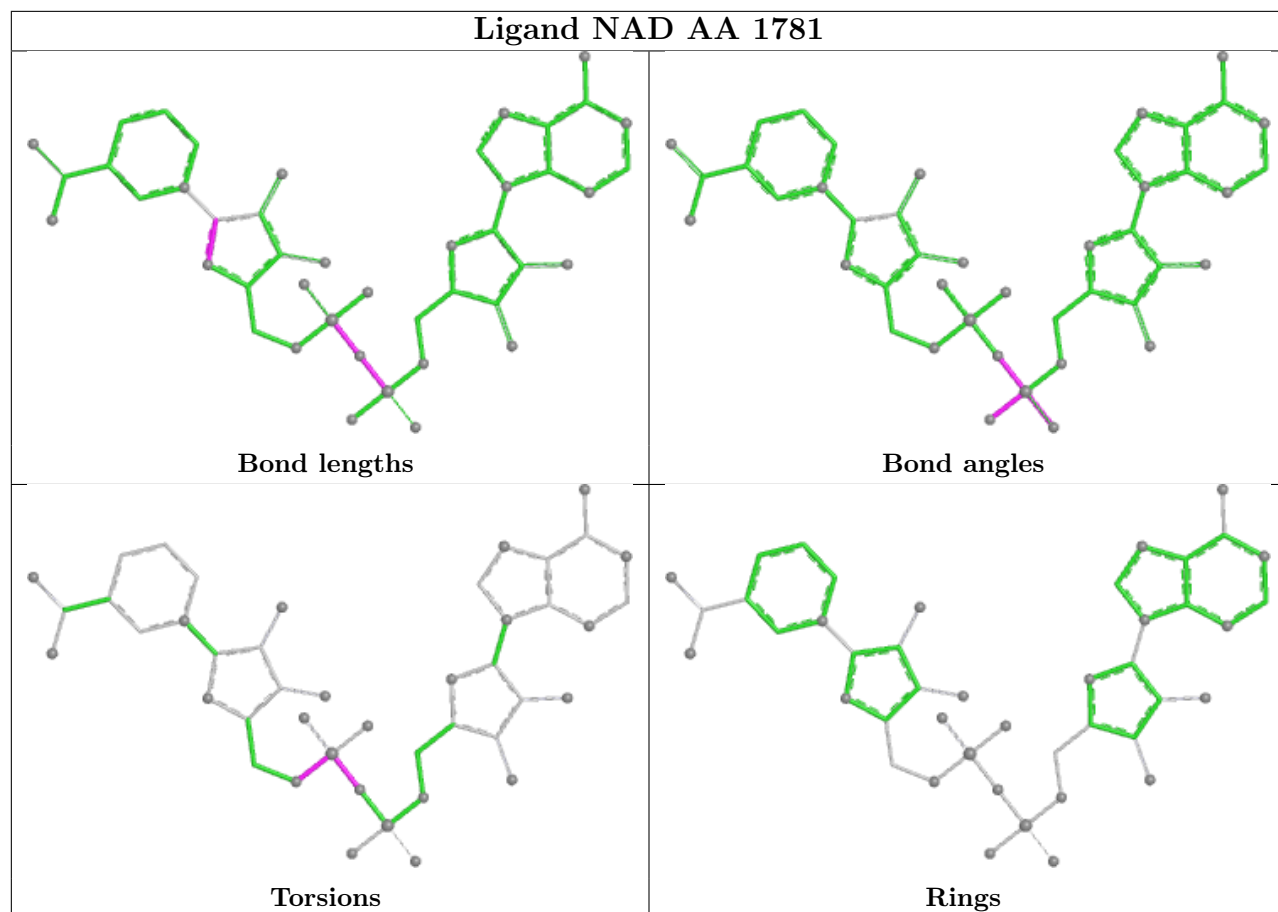
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
101	AA	1781	NAD	1	0
105	B	101	VAL	2	0
102	r	201	FES	1	0
96	AA	1779	SPD	1	0

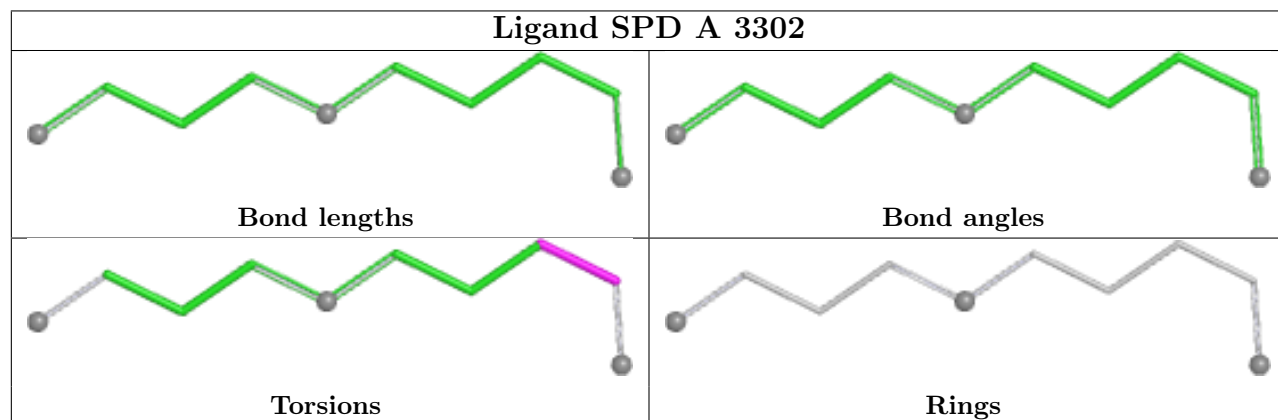
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



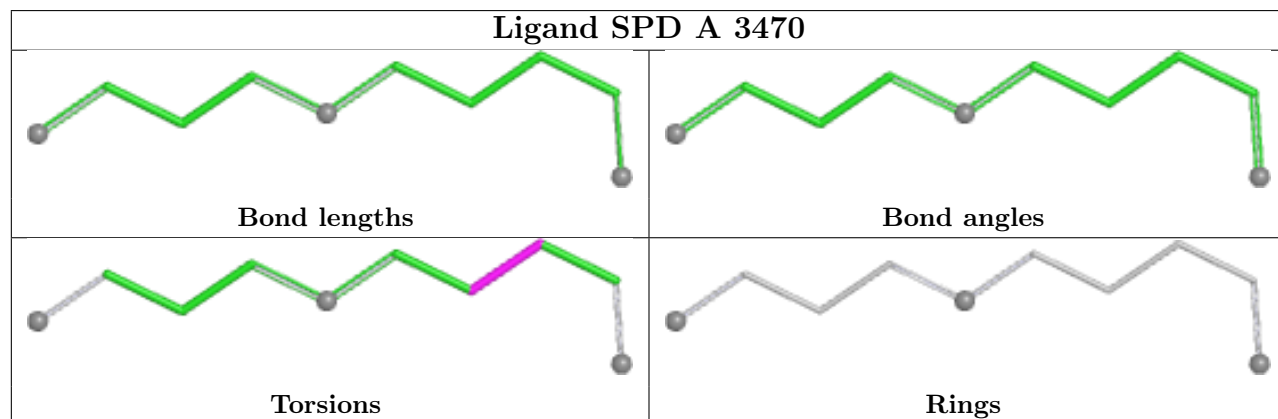
Ligand NAD AA 1781

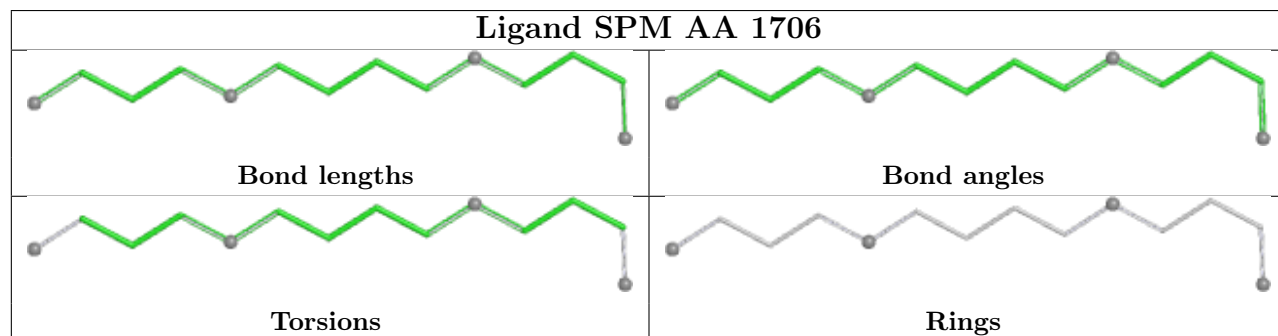
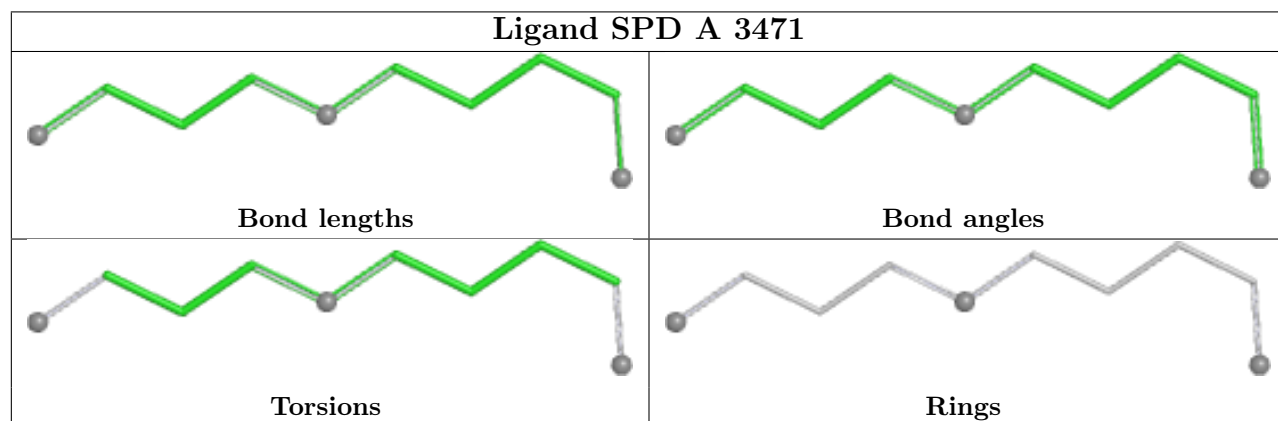
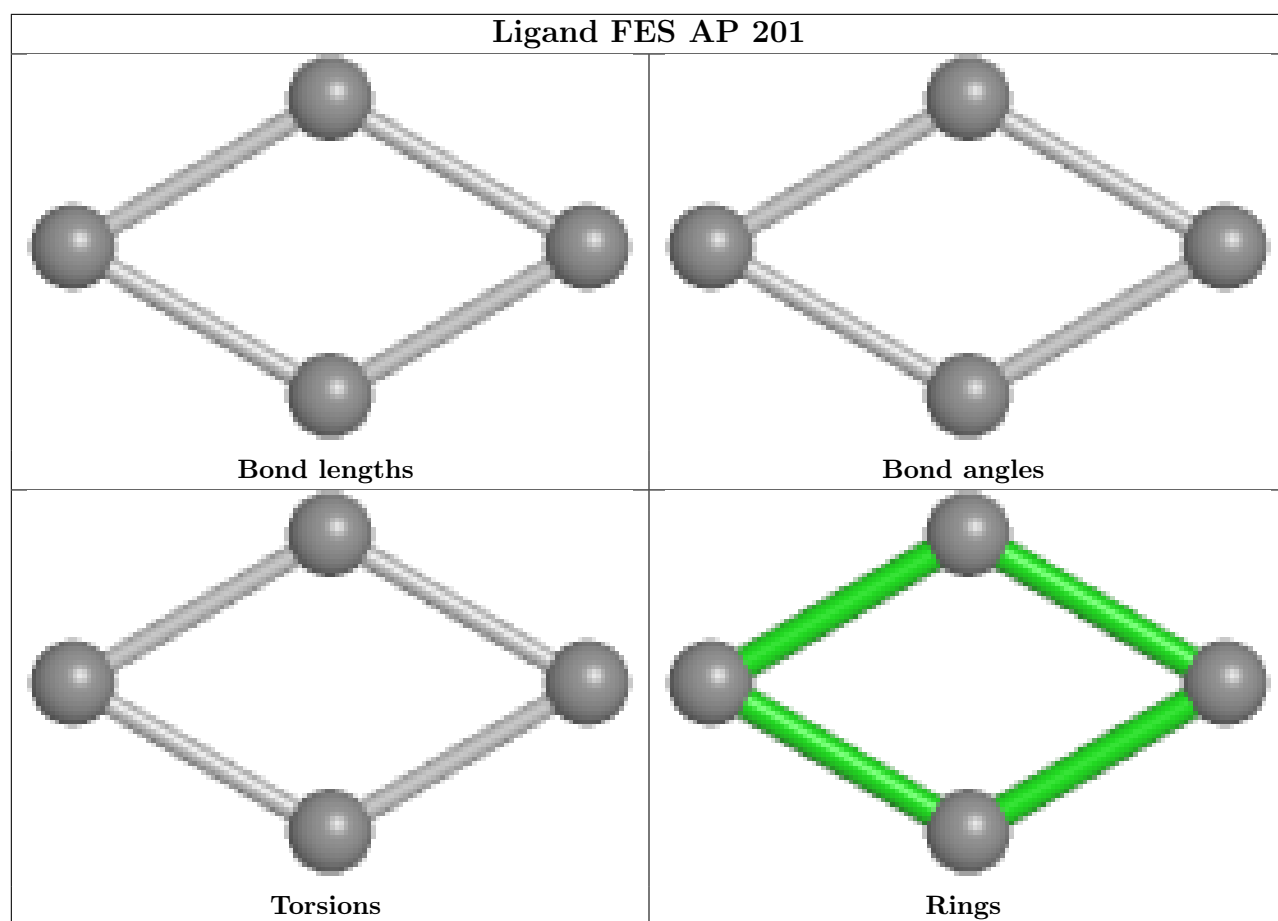


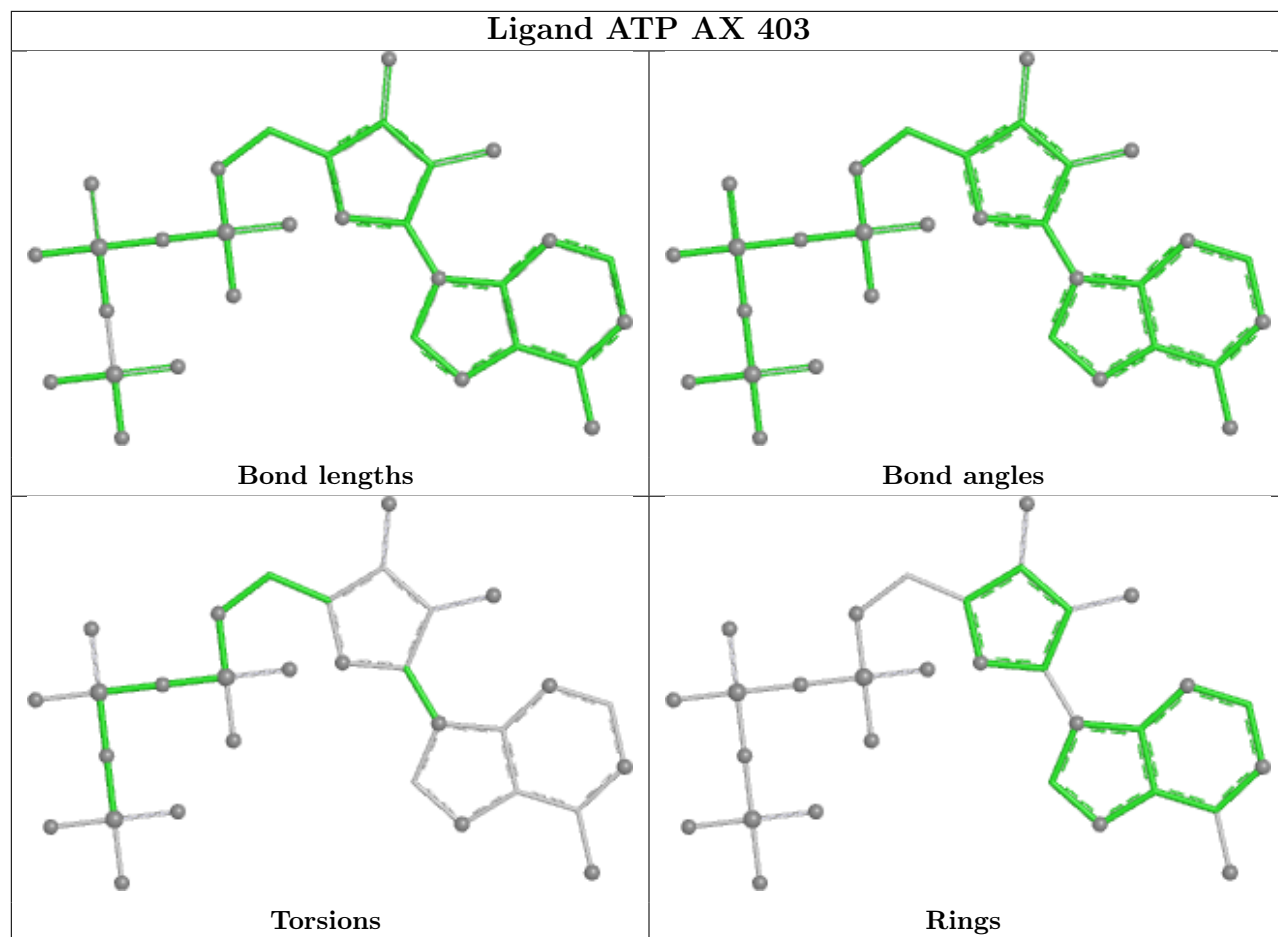
Ligand SPD A 3302

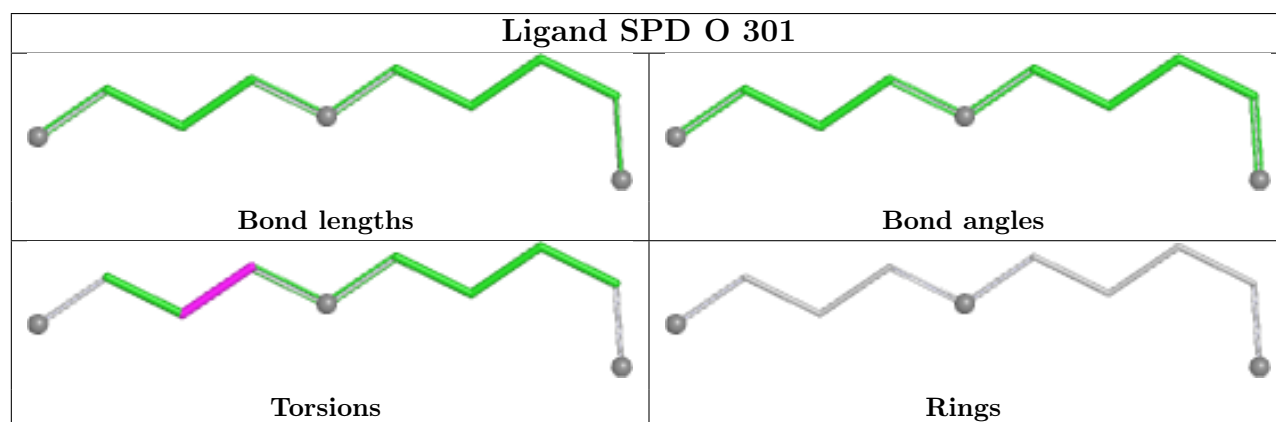
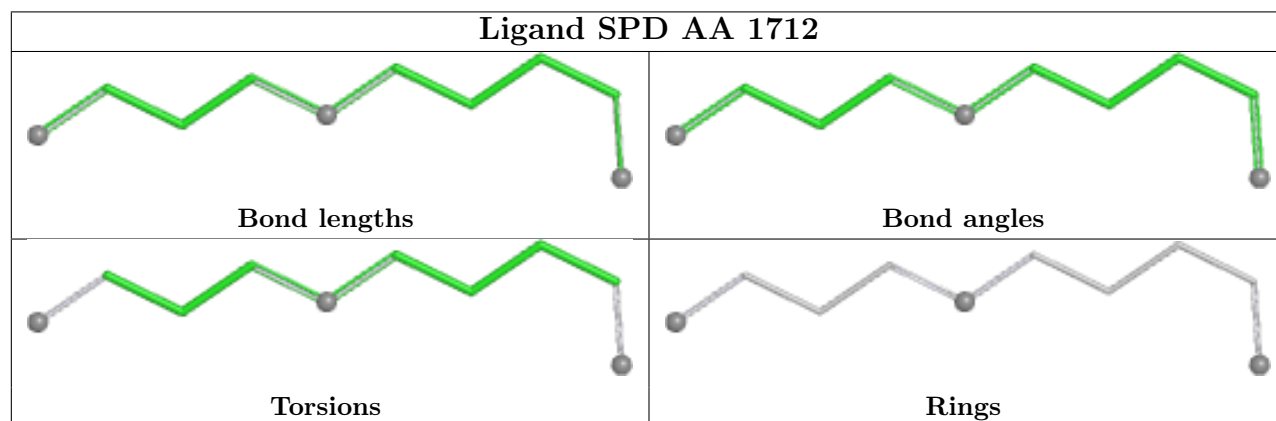
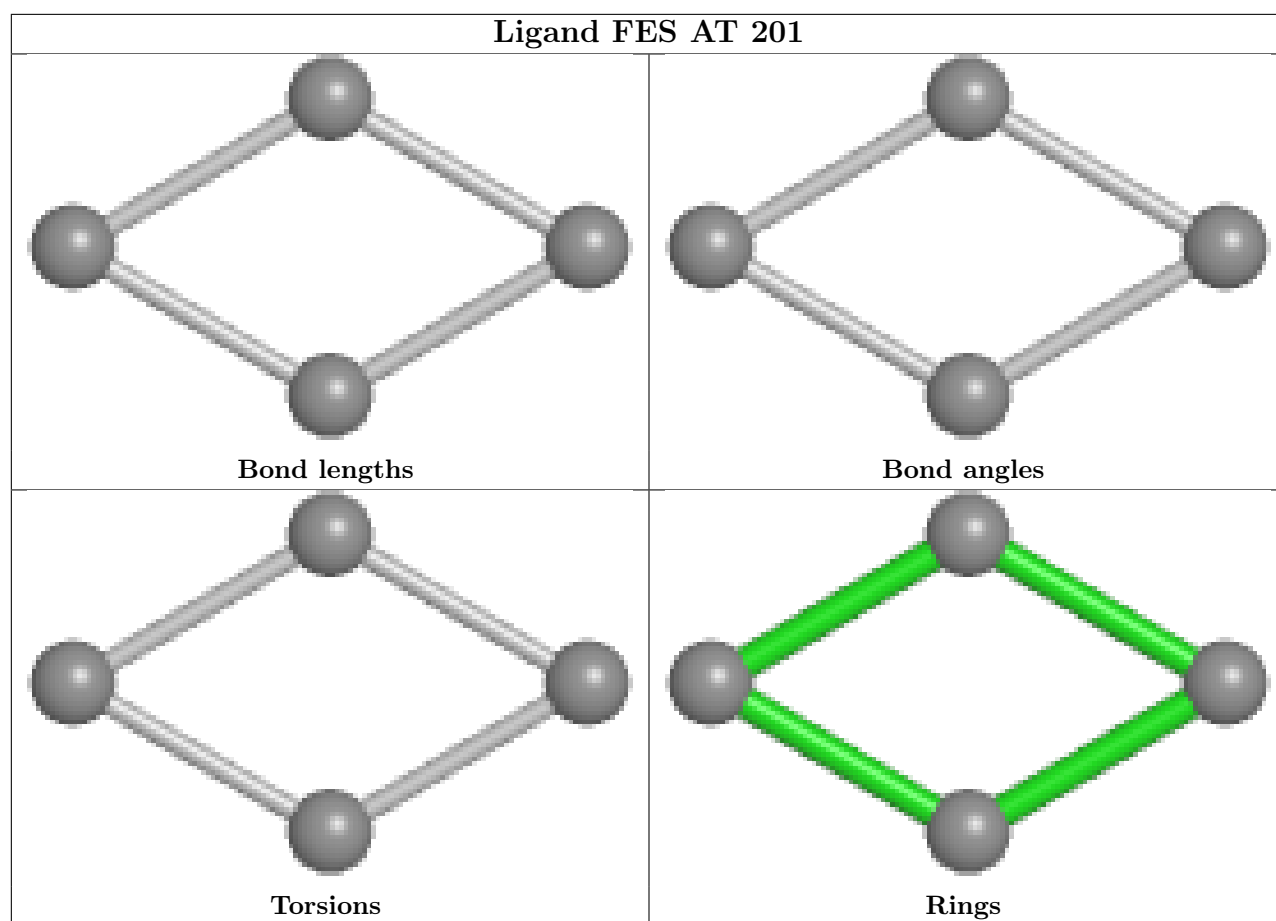


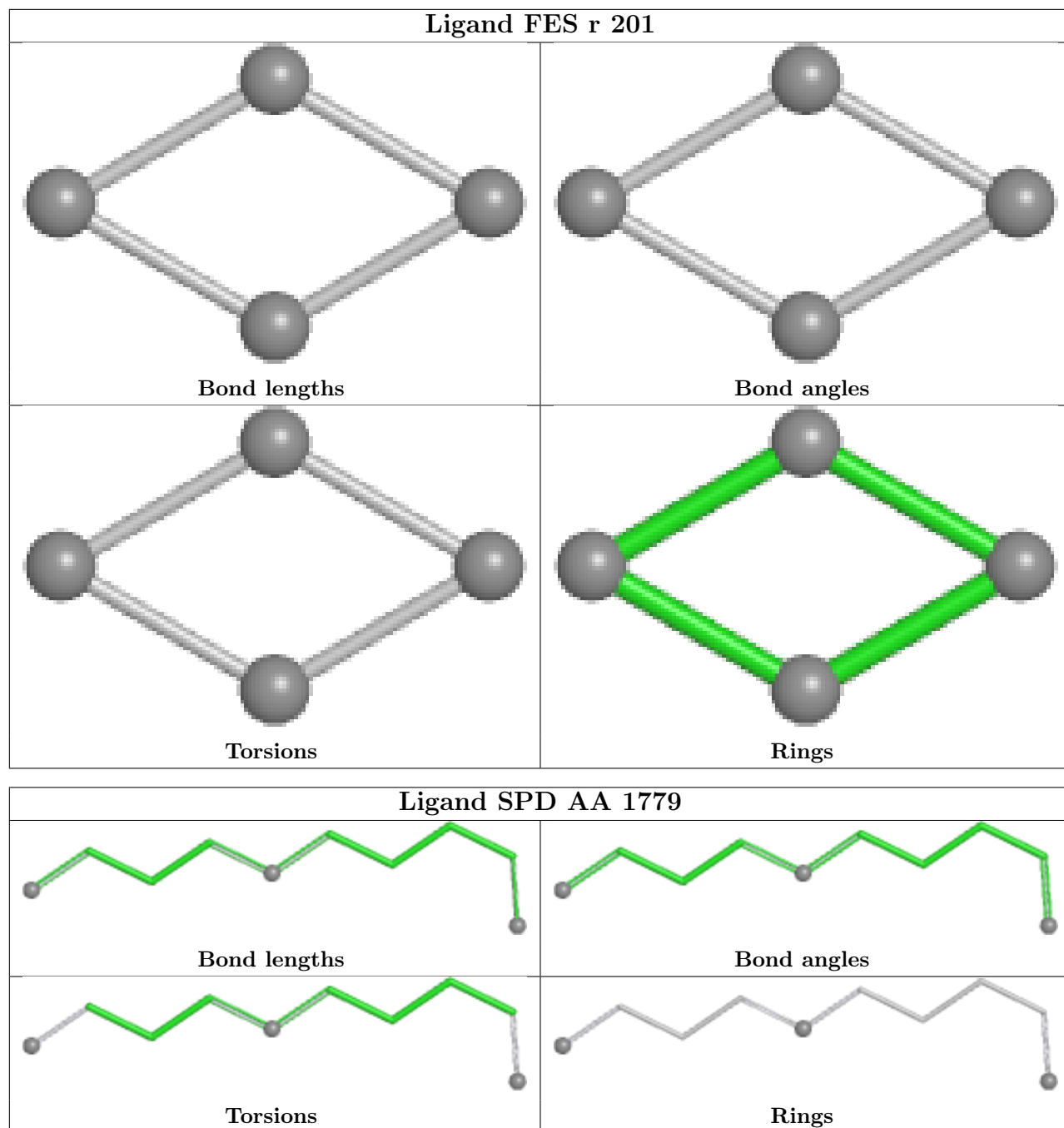
Ligand SPD A 3470

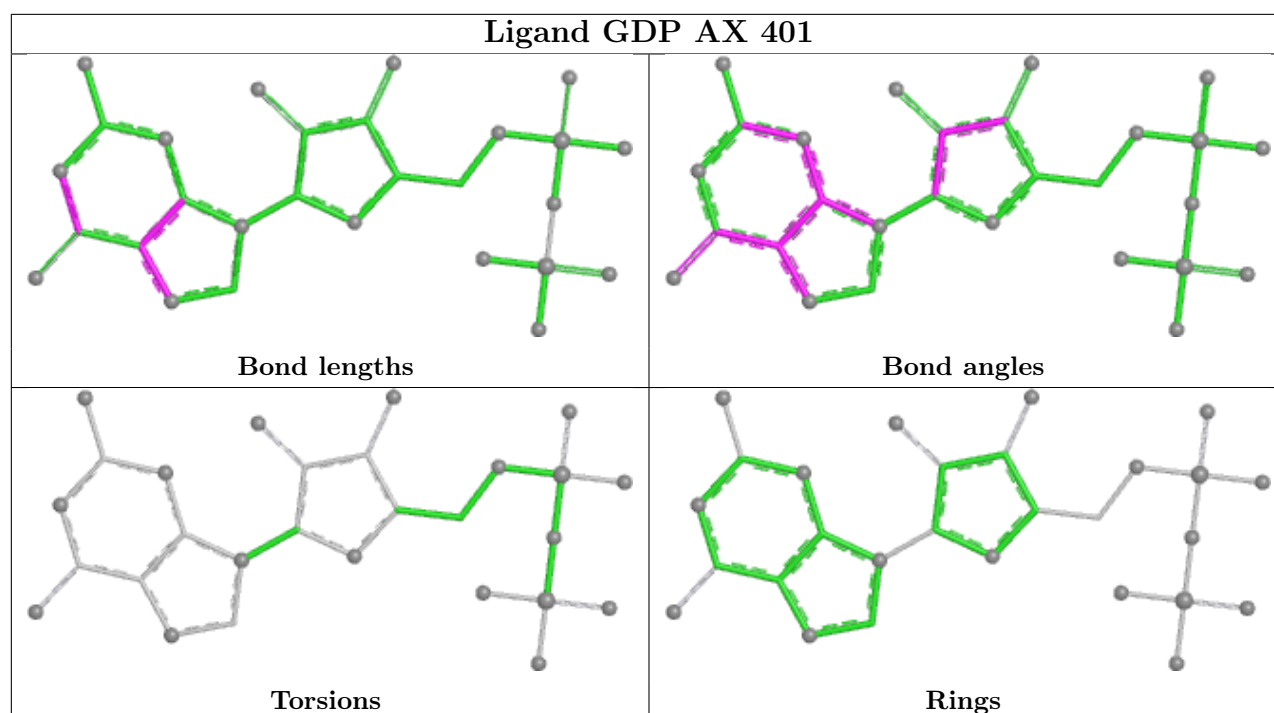












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	A	1
49	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2357:C	O3'	2361:G	P	9.25
1	B	46:A	O3'	48:U	P	4.54

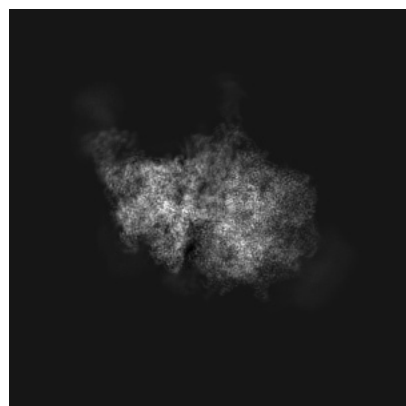
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70592. These allow visual inspection of the internal detail of the map and identification of artifacts.

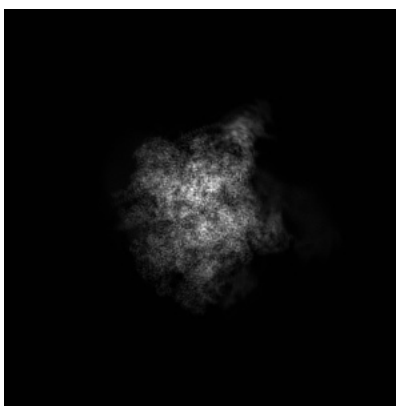
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

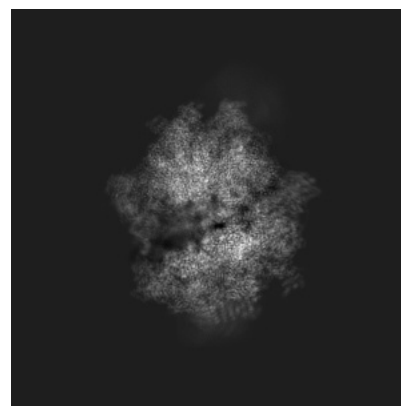
6.1.1 Primary map



X

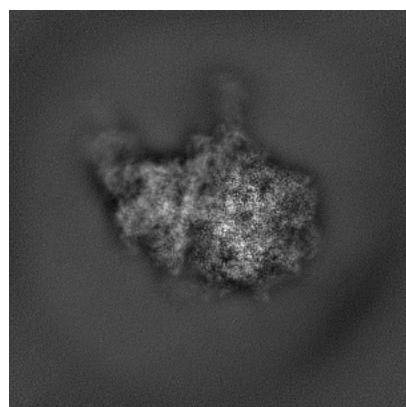


Y

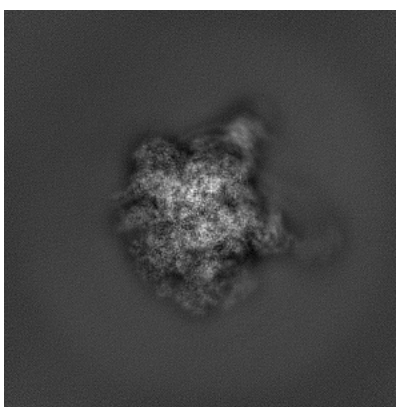


Z

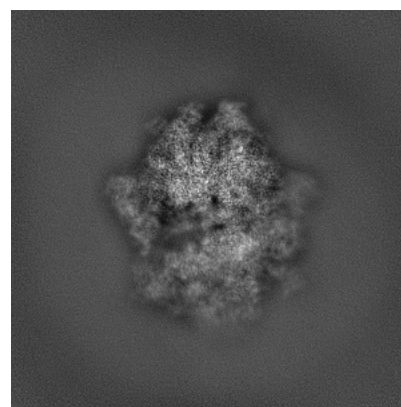
6.1.2 Raw map



X



Y

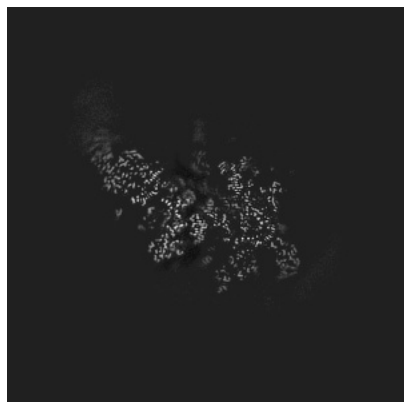


Z

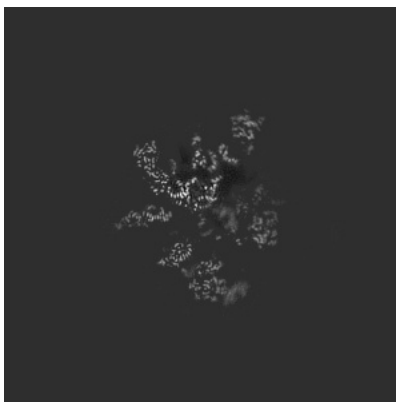
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

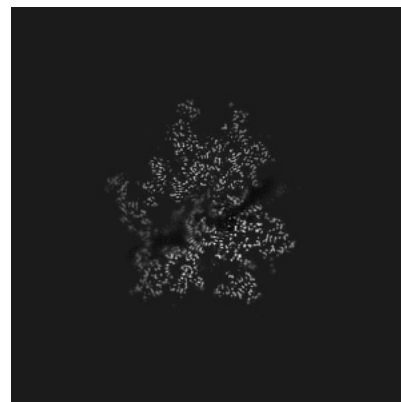
6.2.1 Primary map



X Index: 240

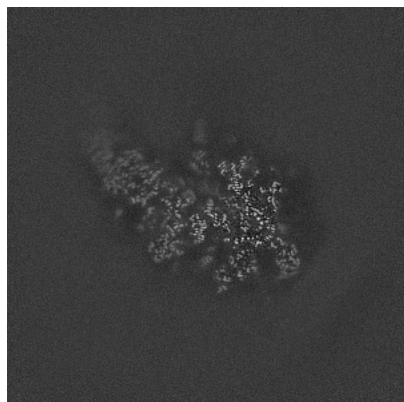


Y Index: 240

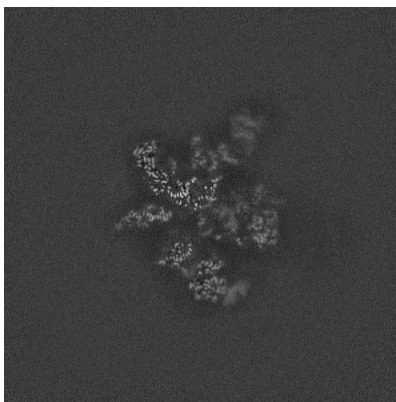


Z Index: 240

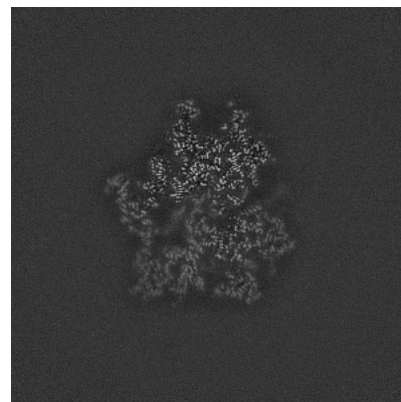
6.2.2 Raw map



X Index: 240



Y Index: 240

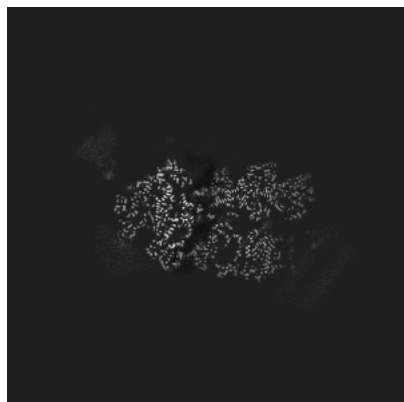


Z Index: 240

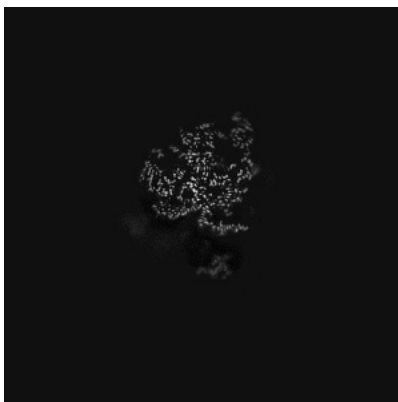
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

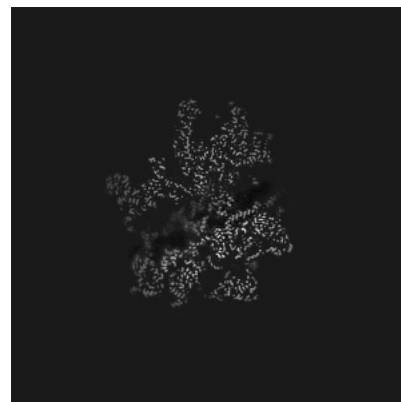
6.3.1 Primary map



X Index: 275

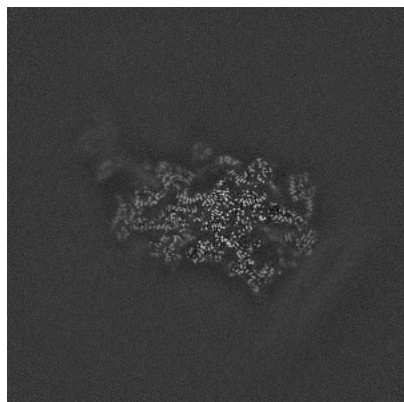


Y Index: 194

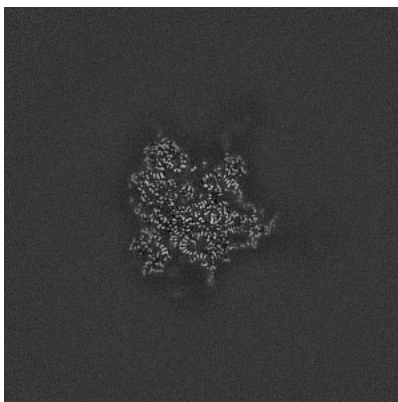


Z Index: 236

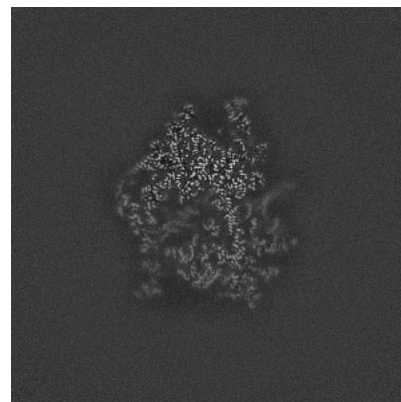
6.3.2 Raw map



X Index: 262



Y Index: 287

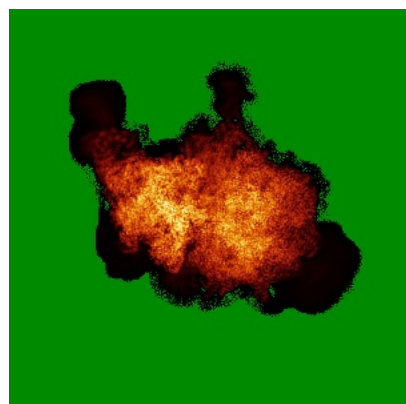


Z Index: 249

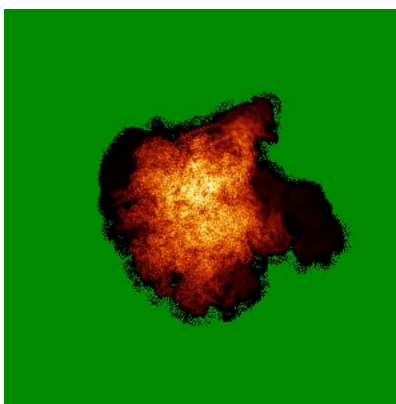
The images above show the largest variance slices of the map in three orthogonal directions.

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

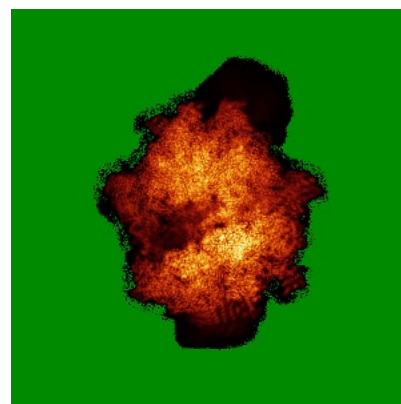
6.4.1 Primary map



X

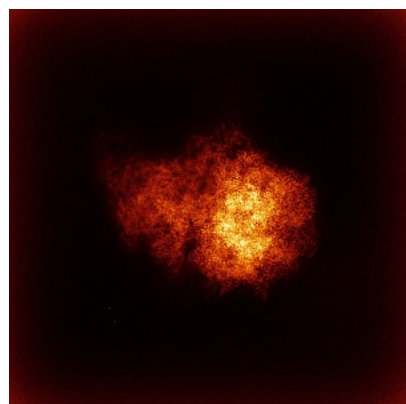


Y

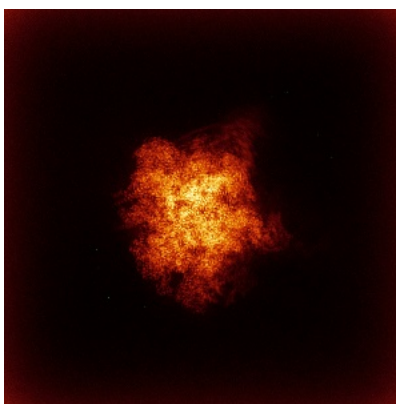


Z

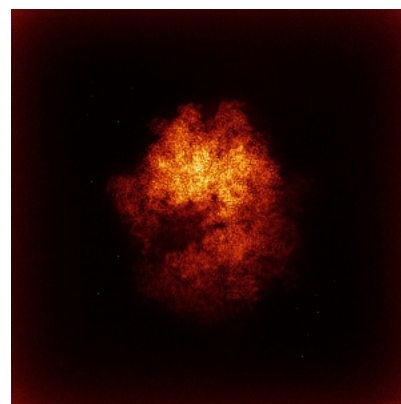
6.4.2 Raw map



X



Y

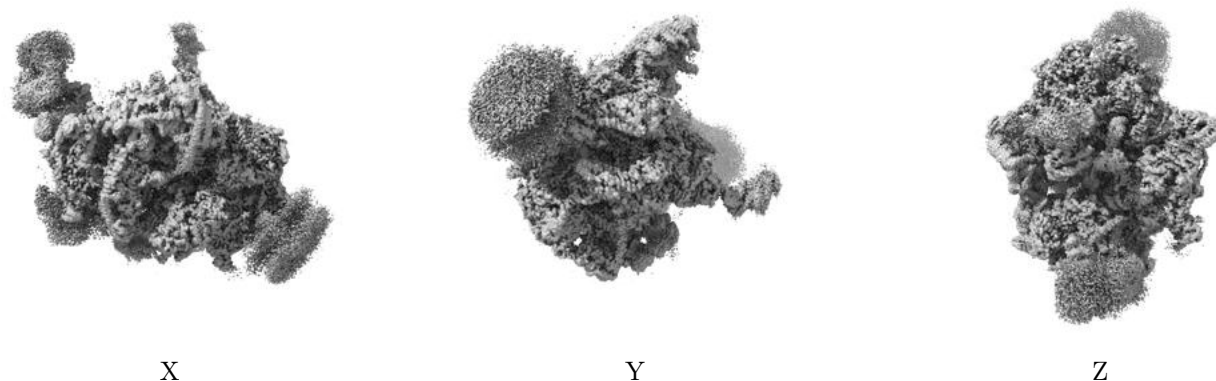


Z

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

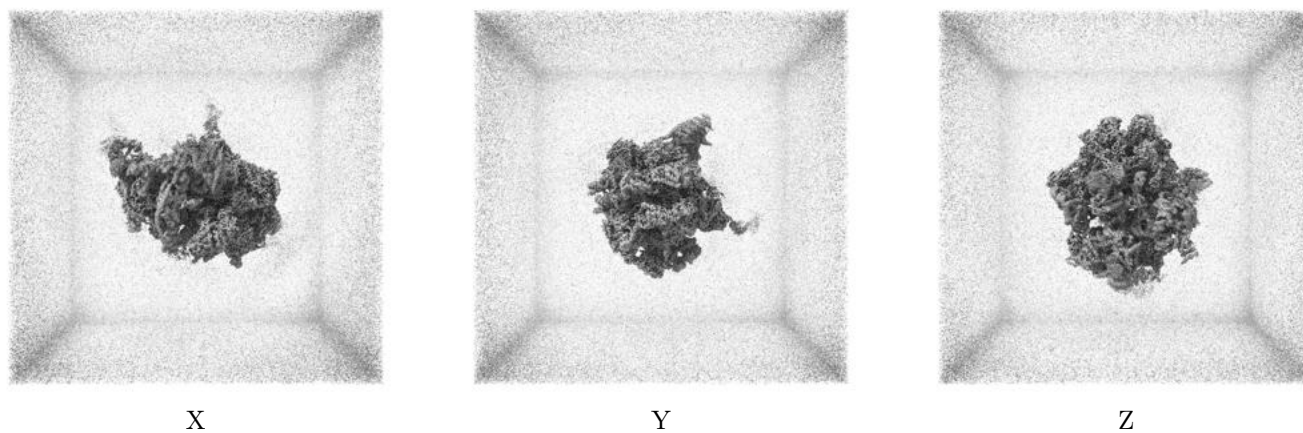
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

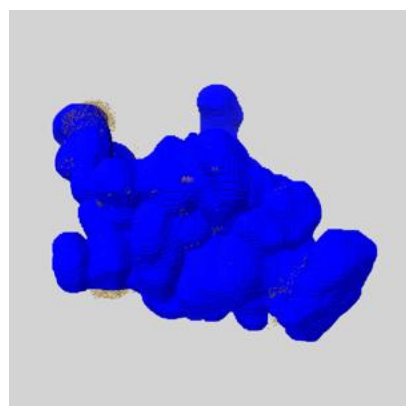
6.6 Mask visualisation [i](#)

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

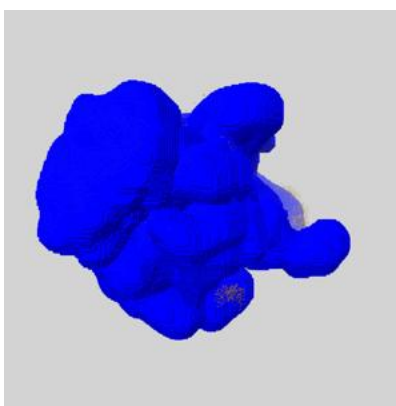
A mask typically either:

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

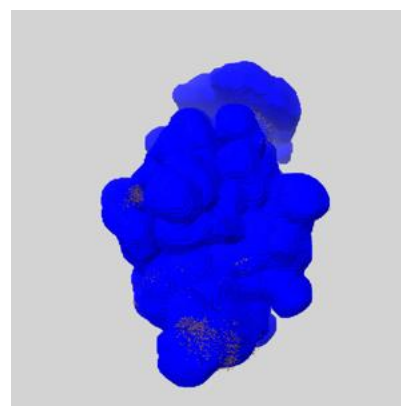
6.6.1 emd_70592_msk_1.map [i](#)



X



Y

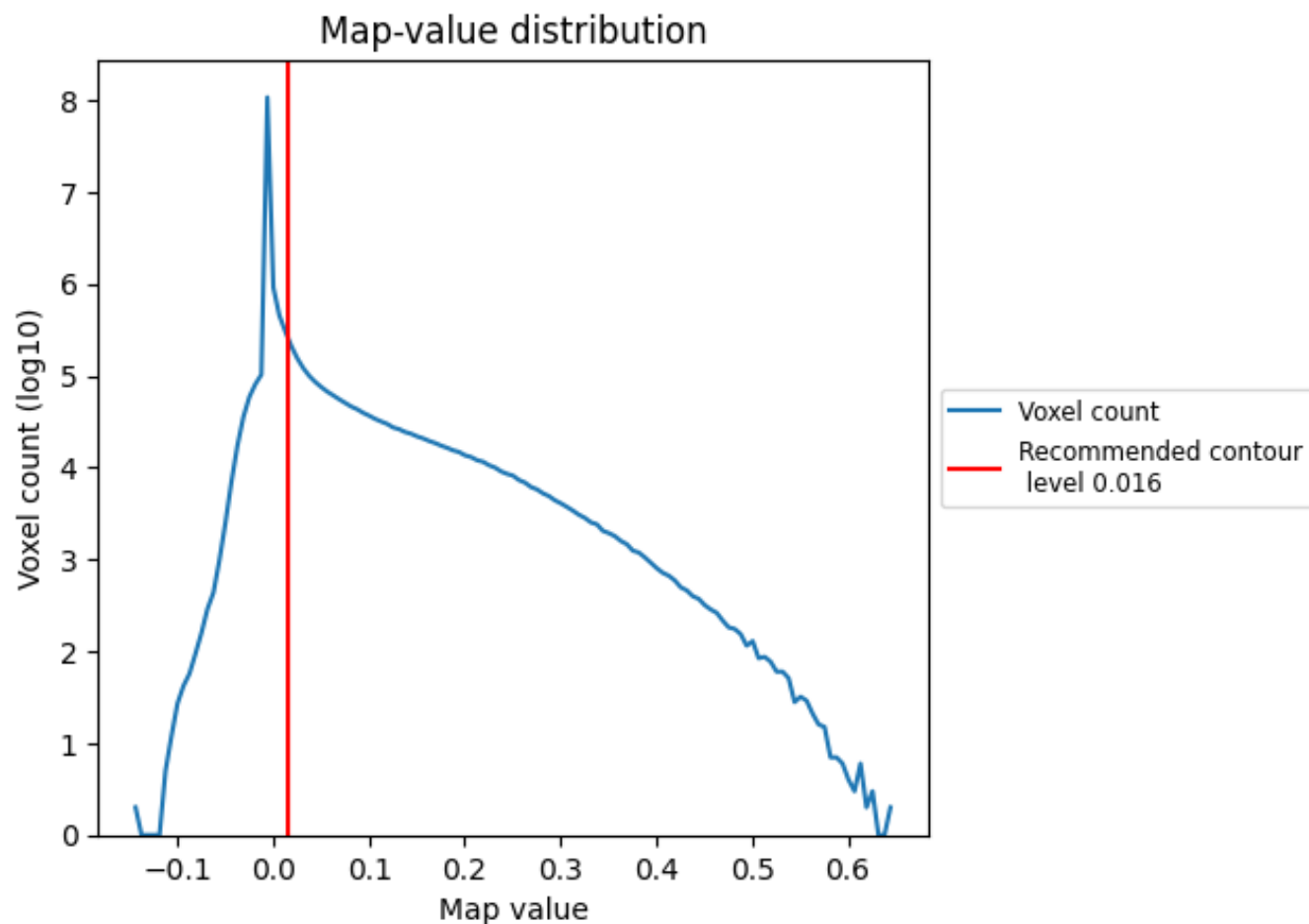


Z

7 Map analysis [i](#)

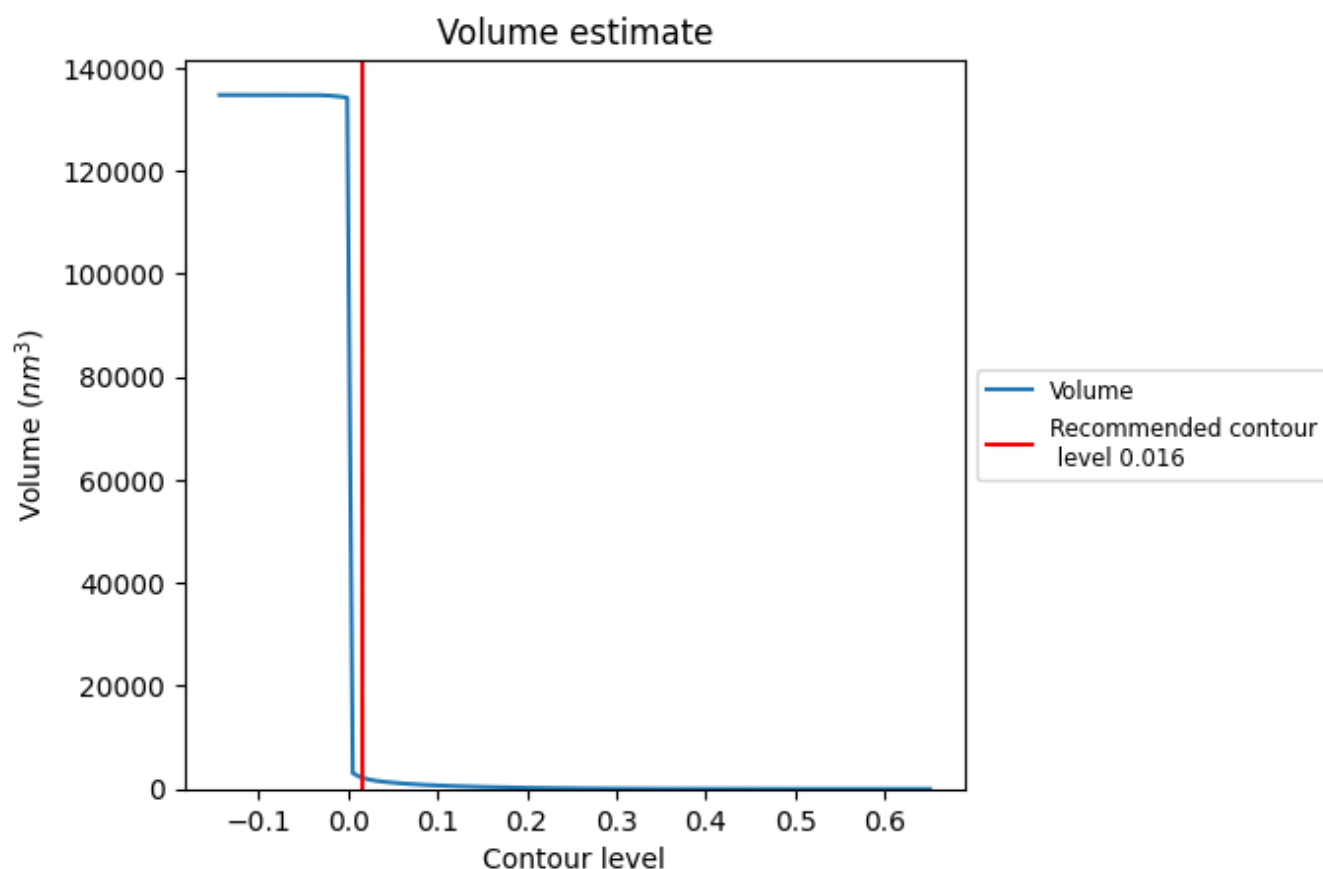
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

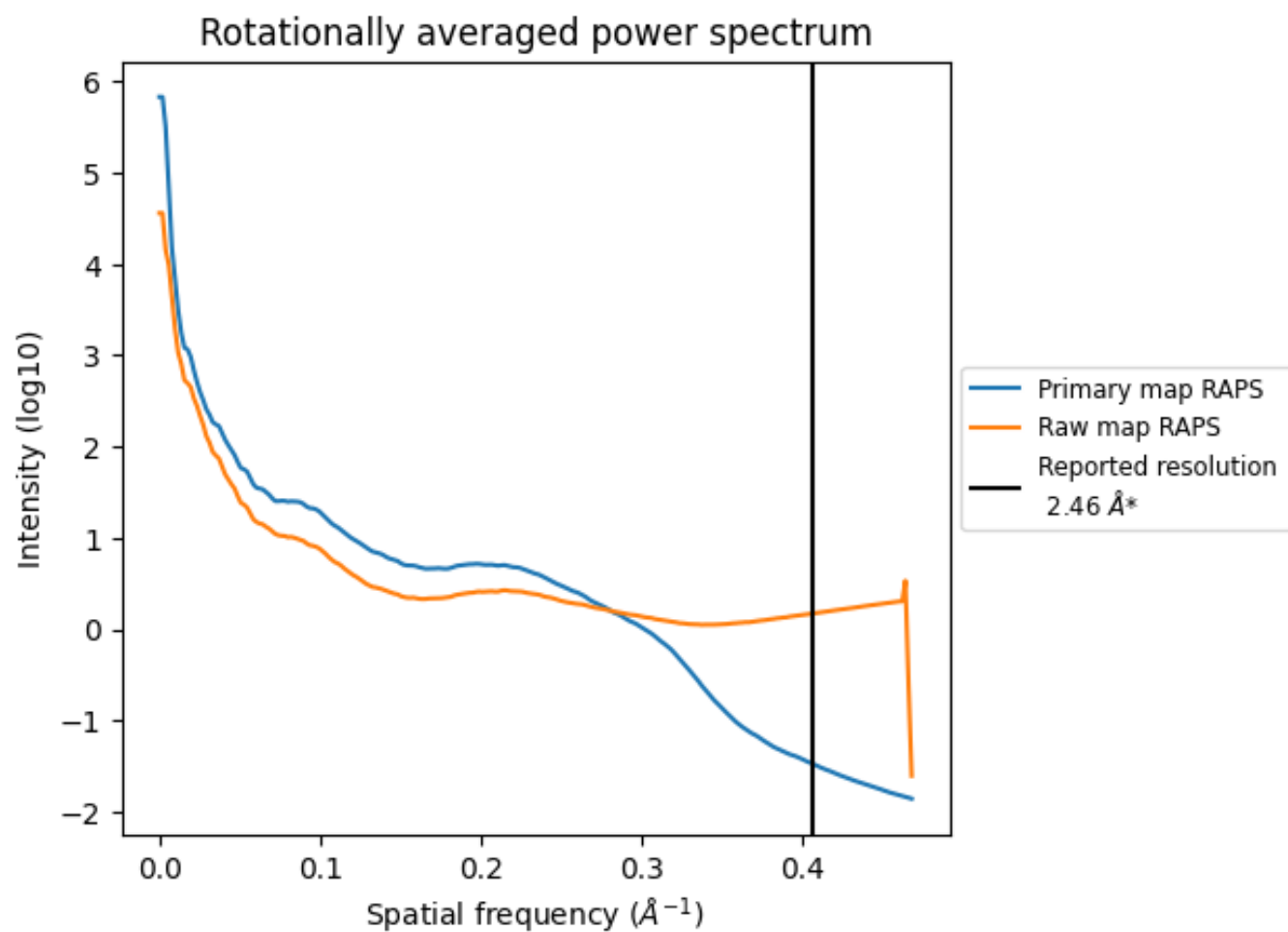
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2209 nm^3 ; this corresponds to an approximate mass of 1995 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

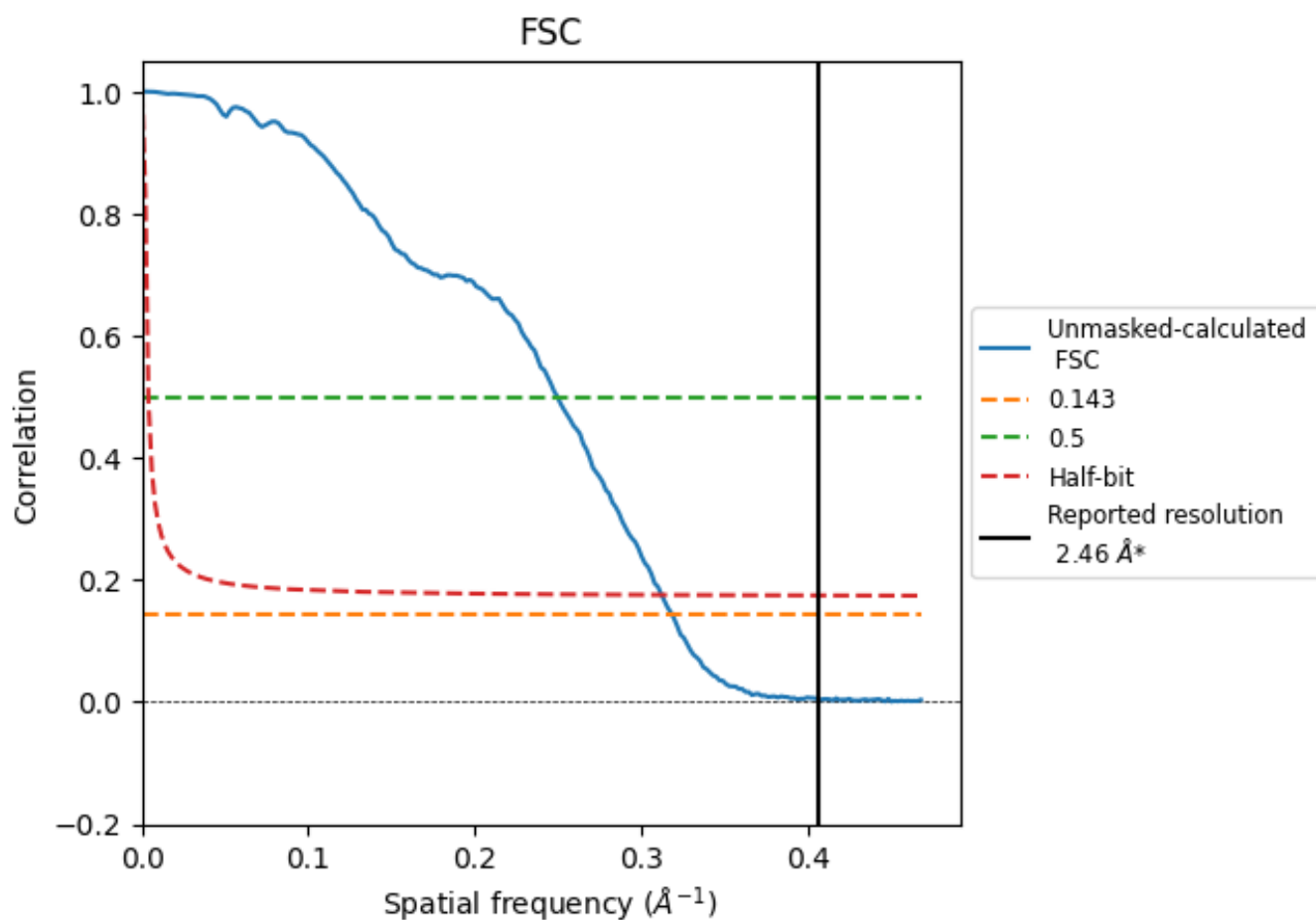


*Reported resolution corresponds to spatial frequency of 0.407 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.407 \AA^{-1}

8.2 Resolution estimates [i](#)

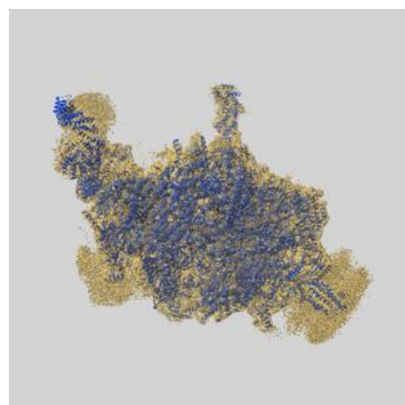
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	4.00	3.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.46 by more than 10 %

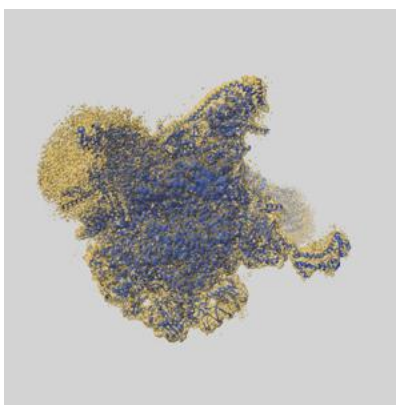
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70592 and PDB model 9OLF. Per-residue inclusion information can be found in [section 3](#) on [page 28](#).

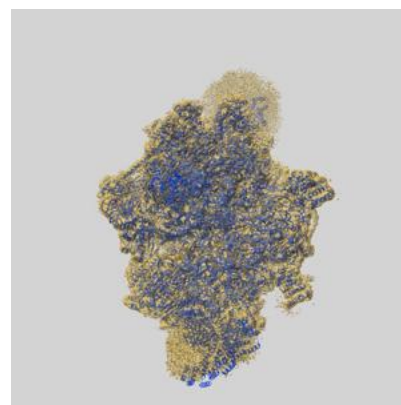
9.1 Map-model overlay [i](#)



X



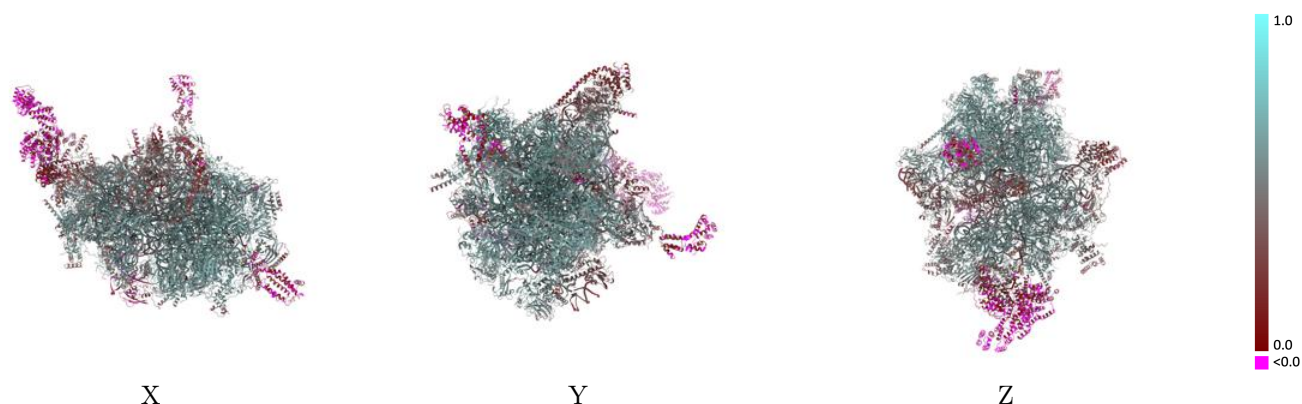
Y



Z

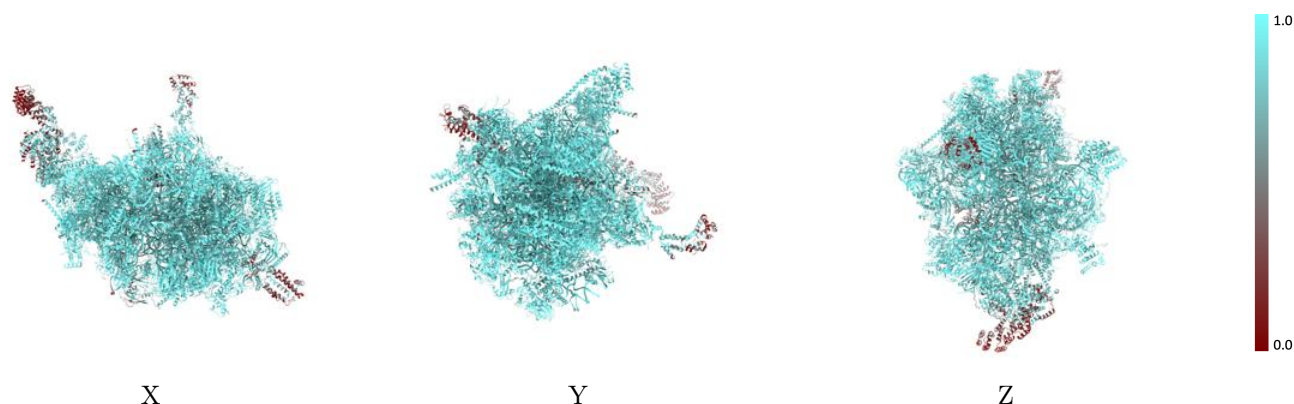
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



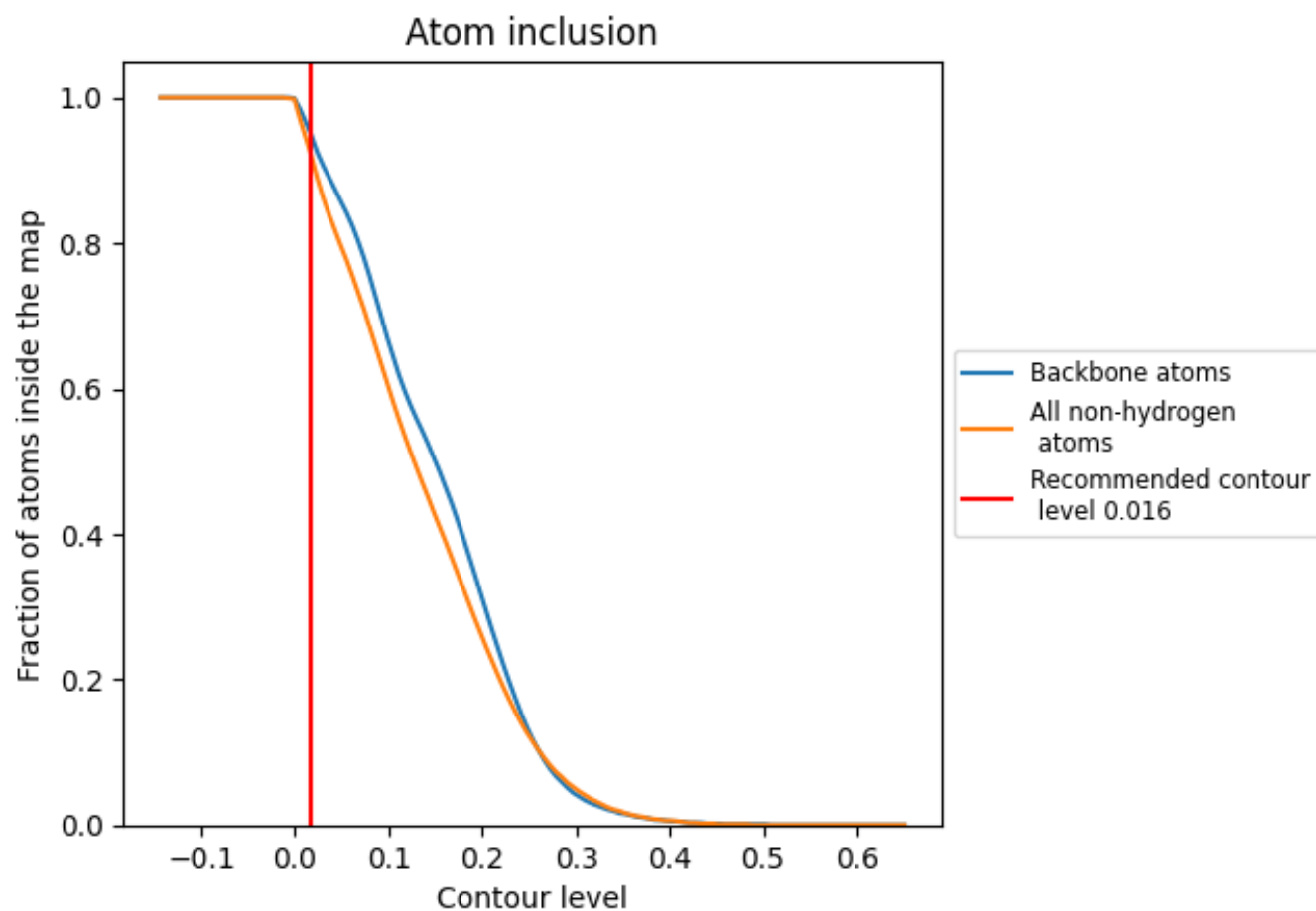
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.4950
0	 0.9690	 0.5980
1	 0.9360	 0.5600
2	 0.9970	 0.6500
3	 0.9930	 0.6430
4	 0.9850	 0.6260
5	 0.9720	 0.5850
6	 0.9580	 0.5330
7	 0.9610	 0.5280
8	 0.8900	 0.3750
9	 0.9610	 0.5640
A	 0.9900	 0.5960
A0	 0.9420	 0.3940
A1	 0.9470	 0.4500
A2	 0.9340	 0.5120
A3	 0.9700	 0.5660
A4	 0.8700	 0.2200
A5	 0.4750	 0.0260
A6	 0.5020	 0.0080
AA	 0.9970	 0.5700
AB	 0.9700	 0.5530
AC	 0.9730	 0.5240
AD	 0.9530	 0.5160
AE	 0.9660	 0.5640
AF	 0.9690	 0.5310
AG	 0.9440	 0.5020
AH	 0.9400	 0.4930
AI	 0.9820	 0.5630
AJ	 0.9660	 0.5630
AK	 0.9820	 0.5850
AL	 0.9530	 0.5330
AM	 0.9450	 0.4670
AN	 0.9560	 0.5640
AO	 0.9630	 0.4830
AP	 0.9790	 0.5710



















































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AQ	 0.9840	 0.5890
AR	 0.9440	 0.4250
AS	 0.9600	 0.4920
AT	 0.9500	 0.5300
AU	 0.9430	 0.4500
AV	 0.9250	 0.2610
AW	 0.9720	 0.5520
AX	 0.9760	 0.4870
AY	 0.6740	 0.2550
AZ	 0.9640	 0.5200
Aw	 0.9690	 0.3340
Ax	 0.9740	 0.4360
Ay	 0.5060	 0.1230
Az	 0.9680	 0.3060
B	 0.9700	 0.3840
C	 0.7170	 0.3440
D	 0.9880	 0.6020
E	 0.9720	 0.6090
F	 0.9890	 0.6210
G	 0.7180	 0.2300
H	 0.8230	 0.3300
I	 0.8830	 0.3920
J	 0.8960	 0.3720
K	 0.9860	 0.6240
L	 0.9840	 0.5950
M	 0.9790	 0.6150
N	 0.9740	 0.6070
O	 0.9820	 0.6110
OX	 0.4950	 0.1340
P	 0.9760	 0.5800
Q	 0.9480	 0.5580
R	 0.9790	 0.6230
S	 0.9760	 0.6100
T	 0.9840	 0.6250
U	 0.9040	 0.5410
V	 0.9560	 0.5430
W	 0.9820	 0.6260
X	 0.9610	 0.5820
Y	 0.9690	 0.5990
Z	 0.9710	 0.6110
a	 0.8880	 0.5060
b	 0.9740	 0.6140

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.9610	 0.5720
d	 0.9140	 0.4860
e	 0.8980	 0.3270
f	 0.9000	 0.4280
g	 0.9730	 0.6000
h	 0.9660	 0.5360
i	 0.9930	 0.6380
j	 0.9540	 0.5590
k	 0.9300	 0.4750
l	 0.9120	 0.4190
m	 0.9280	 0.3680
n	 0.8840	 0.3450
o	 0.9860	 0.6330
p	 0.9150	 0.4960
q	 0.8410	 0.4090
r	 0.9790	 0.5940
s	 0.9730	 0.5950
t	 0.8190	 0.2170
u	 0.7230	 0.1420
v	 0.4650	 0.0500
w	 0.4610	 -0.0330
x	 0.2780	 0.0510
y	 0.1880	 0.0330
z	 0.4730	 0.0930