



## Full wwPDB EM Validation Report ⓘ

Apr 10, 2026 – 01:23 PM UTC

PDB ID : 9PGI / pdb\_00009pgi  
EMDB ID : EMD-71633  
Title : In situ structure of the human mitoribosome in the A-P-E state with TACO1  
Authors : Wang, S.; Xiong, Y.; Zhang, Y.  
Deposited on : 2025-07-07  
Resolution : 3.02 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](mailto: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>.

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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

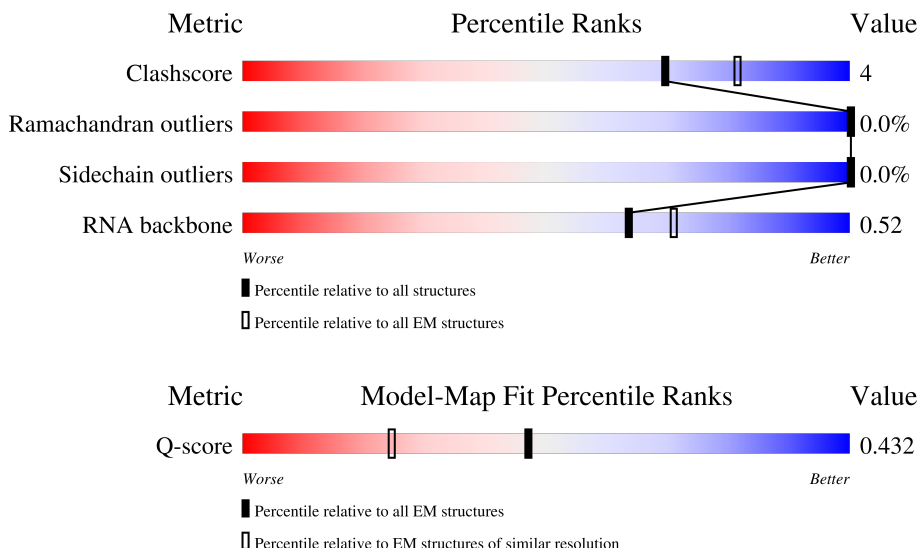
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




The reported resolution of this entry is 3.02 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.














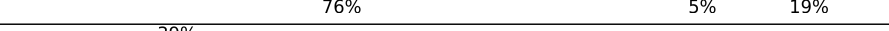



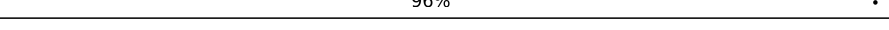

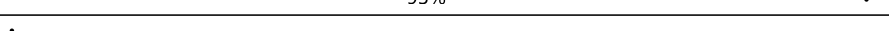

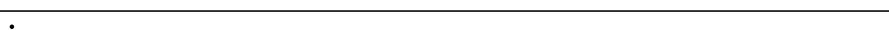

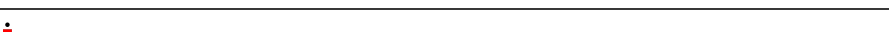
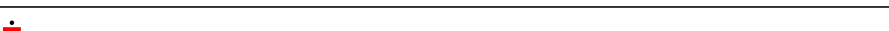


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13913 ( 2.52 - 3.52 )

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  $\geq 3$ , 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	

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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	1561	
12	C	297	
13	D	305	
14	E	348	
15	F	311	
16	H	267	
17	I	261	
18	J	192	
19	K	178	
20	L	145	
21	M	296	
22	N	251	
23	O	175	
24	P	180	
25	Q	292	
26	R	149	
27	S	205	
28	T	206	

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Mol	Chain	Length	Quality of chain
29	U	153	
30	W	148	
31	X	256	
32	Y	250	
33	Z	161	
34	z	325	
35	G	198	
35	t	198	
35	u	198	
36	V	216	
37	b	215	
38	d	306	
39	e	279	
40	g	166	
41	h	158	
42	i	128	
43	j	123	
44	k	112	
45	l	138	
46	m	128	
47	n	43	
48	o	102	
49	q	222	
50	r	196	
51	c	332	

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Mol	Chain	Length	Quality of chain
52	f	212	
53	p	206	
54	s	439	
55	AB	296	
56	AC	167	
57	AD	430	
58	AE	125	
59	AF	242	
60	AG	396	
61	AH	201	
62	AJ	138	
63	AK	128	
64	AL	257	
65	AM	137	
66	AN	130	
67	AO	258	
68	AP	142	
69	AR	360	
70	AS	190	
71	AT	173	
72	AU	205	
73	AV	414	
74	AW	187	
75	AZ	106	
76	A0	217	

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Mol	Chain	Length	Quality of chain
77	A1	323	
78	A3	199	
79	Az	34	
80	AY	395	
81	AA	954	
82	AI	194	
83	OX	435	
84	a	142	
85	Ax	71	
86	Ay	76	
87	Aw	76	
88	A4	689	
89	AX	398	
90	A2	118	
91	AQ	87	
92	B	72	

## 2 Entry composition

There are 103 unique types of molecules in this entry. The entry contains 183684 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		

- Molecule 12 is a protein called Translational activator of cytochrome c oxidase 1.

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

- Molecule 13 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L3, mitochondrial.



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

- Molecule 15 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	181	Total	C	N	O	S	0	0
			1446	932	260	244	10		

- Molecule 18 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 19 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	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 20 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 29 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL1m.

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

- Molecule 35 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	G	72	Total	C	N	O		0	0
			558	358	97	103			
35	t	46	Total	C	N	O		0	0
			354	228	56	70			
35	u	32	Total	C	N	O		0	0
			257	168	40	49			

- Molecule 36 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 44 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	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 45 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 46 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 47 is a protein called Nascent polypeptide.

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

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 49 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 50 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 52 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 53 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 54 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 55 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 56 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 58 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 60 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 61 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 62 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 63 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 64 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 65 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 66 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 67 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 68 is a protein called 28S ribosomal protein S18c, mitochondrial.



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

- Molecule 69 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 71 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 72 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 73 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 74 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 75 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 76 is a protein called Small ribosomal subunit protein mS34.

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

- Molecule 77 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 78 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 79 is a RNA chain called mRNA.

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

- Molecule 80 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AY	119	Total	C	N	O	S	0	0
			1010	654	166	188	2		

- Molecule 81 is a RNA chain called 12S mitochondrial rRNA.

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

- Molecule 82 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 83 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	OX	55	Total	C	N	O	S	0	0
			468	292	93	81	2		

- Molecule 84 is a protein called 39S ribosomal protein L42, mitochondrial.

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

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

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

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

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

- Molecule 87 is a RNA chain called A/A-tRNA.

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

- Molecule 88 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 89 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 90 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	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 91 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	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 92 is a RNA chain called mitochondrial tRNA<sup>Val</sup>.

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

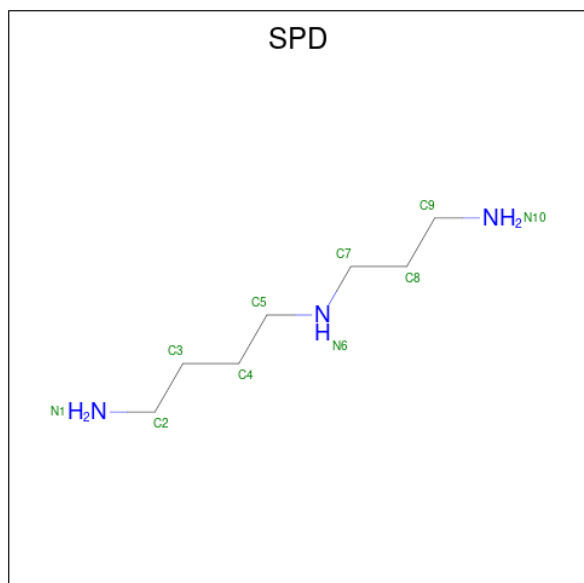
- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
93	0	1	Total	Zn	0
			1	1	
93	4	1	Total	Zn	0
			1	1	
93	AO	1	Total	Zn	0
			1	1	

- Molecule 94 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
94	6	1	Total K 1 1	0
94	A	29	Total K 29 29	0
94	D	1	Total K 1 1	0
94	M	2	Total K 2 2	0
94	N	1	Total K 1 1	0
94	W	1	Total K 1 1	0
94	o	1	Total K 1 1	0
94	AA	18	Total K 18 18	0

- Molecule 95 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



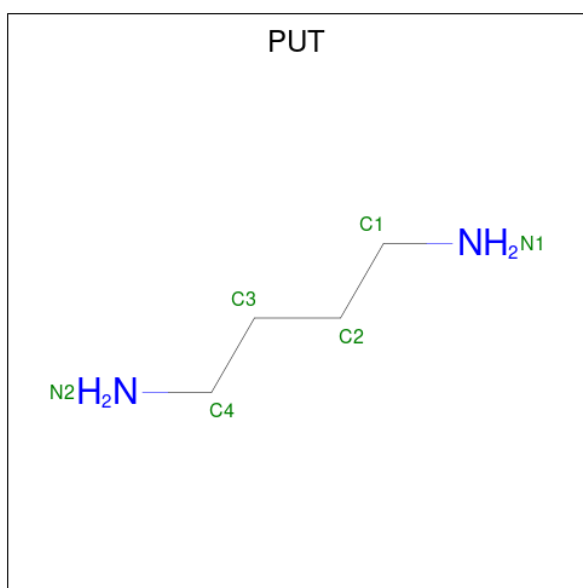
Mol	Chain	Residues	Atoms	AltConf
95	A	1	Total C N 10 7 3	0
95	A	1	Total C N 10 7 3	0

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

- Molecule 96 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ).



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

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

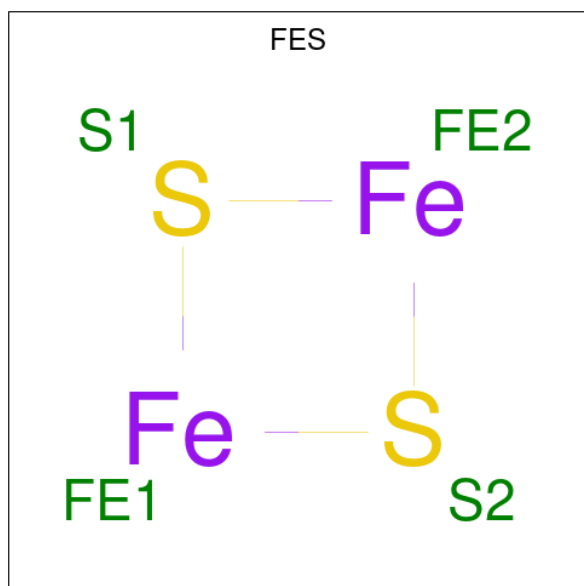
Mol	Chain	Residues	Atoms		AltConf
97	A	137	Total	Mg	0
			137	137	
97	D	2	Total	Mg	0
			2	2	
97	E	1	Total	Mg	0
			1	1	

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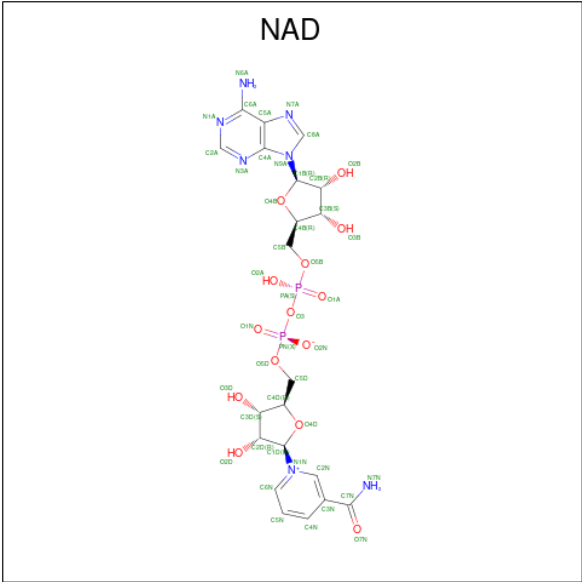
Mol	Chain	Residues	Atoms		AltConf
97	g	1	Total	Mg	0
			1	1	
97	AB	1	Total	Mg	0
			1	1	
97	A3	1	Total	Mg	0
			1	1	
97	AA	60	Total	Mg	0
			60	60	
97	AX	1	Total	Mg	0
			1	1	

- Molecule 98 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



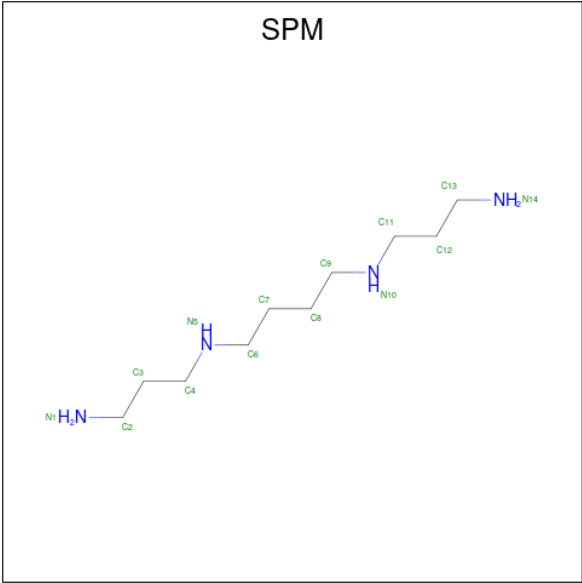
Mol	Chain	Residues	Atoms			AltConf
98	r	1	Total	Fe	S	0
			4	2	2	
98	AP	1	Total	Fe	S	0
			4	2	2	
98	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 99 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:  $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



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

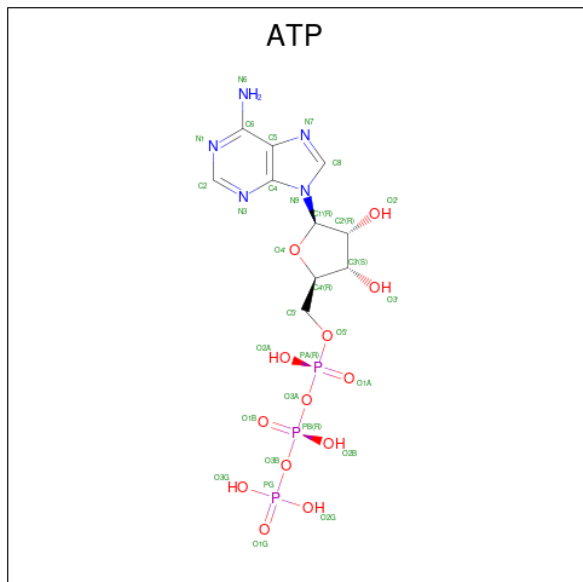
- Molecule 100 is SPERMINE (CCD ID: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



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	

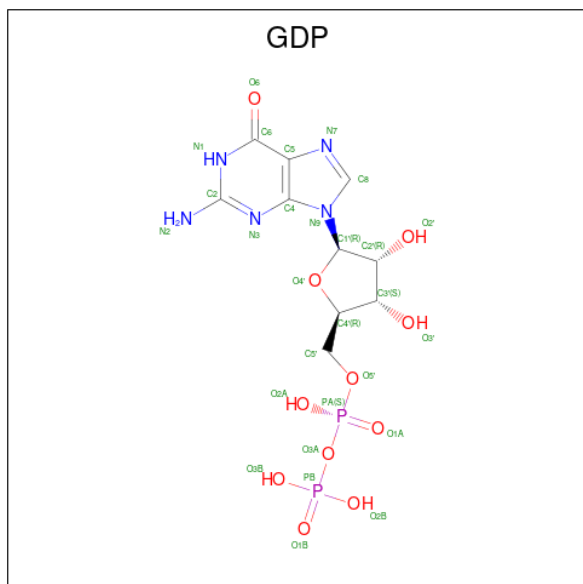


- Molecule 101 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



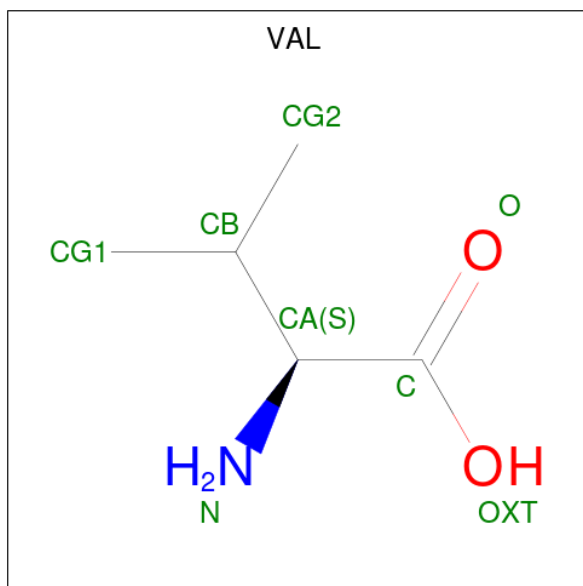
Mol	Chain	Residues	Atoms					AltConf
101	AX	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 102 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).



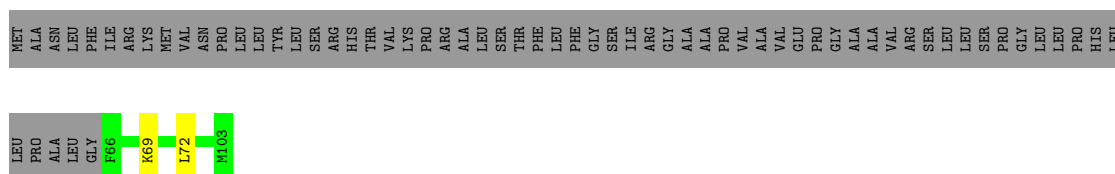
Mol	Chain	Residues	Atoms					AltConf
102	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 103 is VALINE (CCD ID: VAL) (formula:  $C_5H_{11}NO_2$ ).



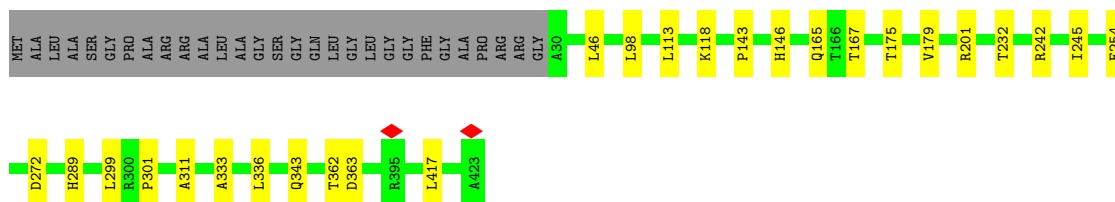
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
103	B	1	7	5	1	1	0





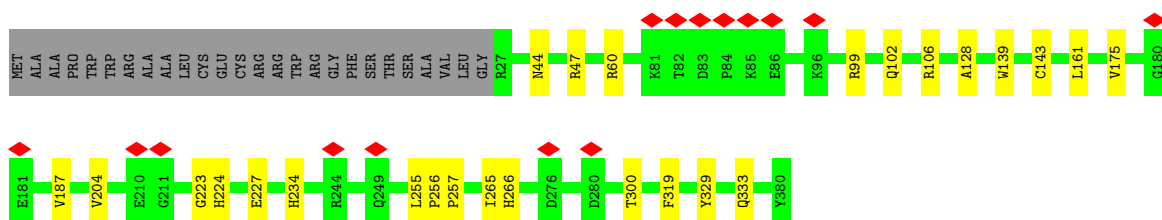
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5: 87% 6% 7%



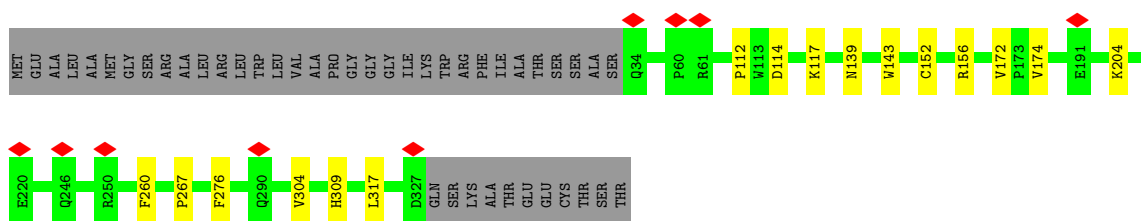
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6: 86% 7% 7%



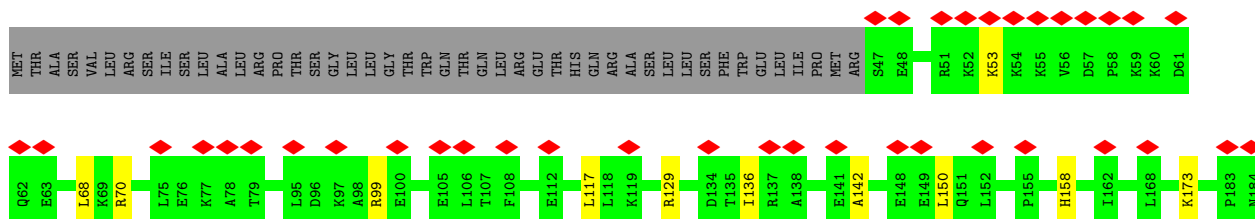
- Molecule 8: 39S ribosomal protein L39, mitochondrial

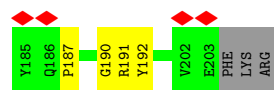
Chain 7: 82% 5% 13%



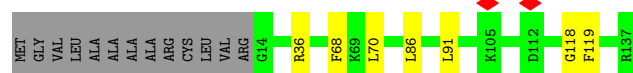
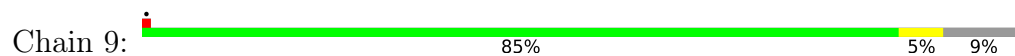
- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8: 20% 69% 7% 24%

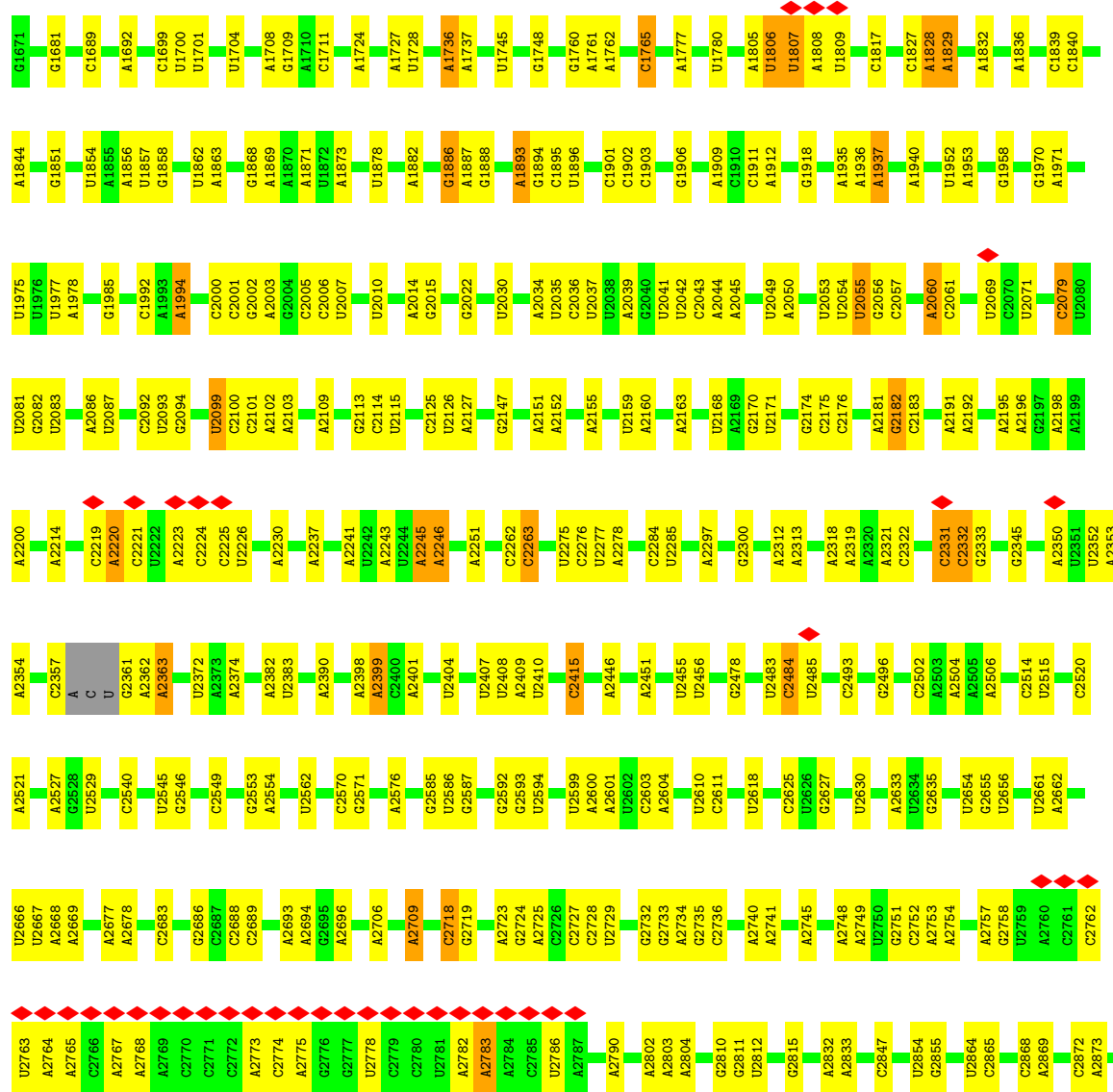


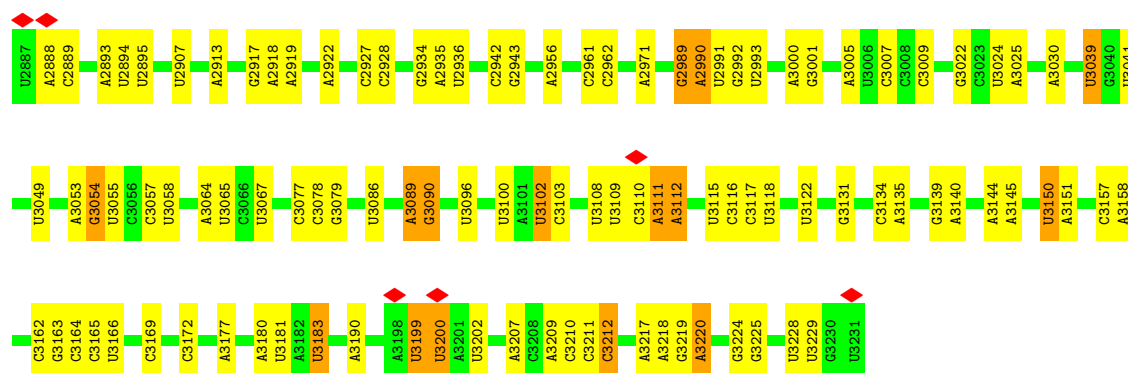


- Molecule 10: 39S ribosomal protein L41, mitochondrial

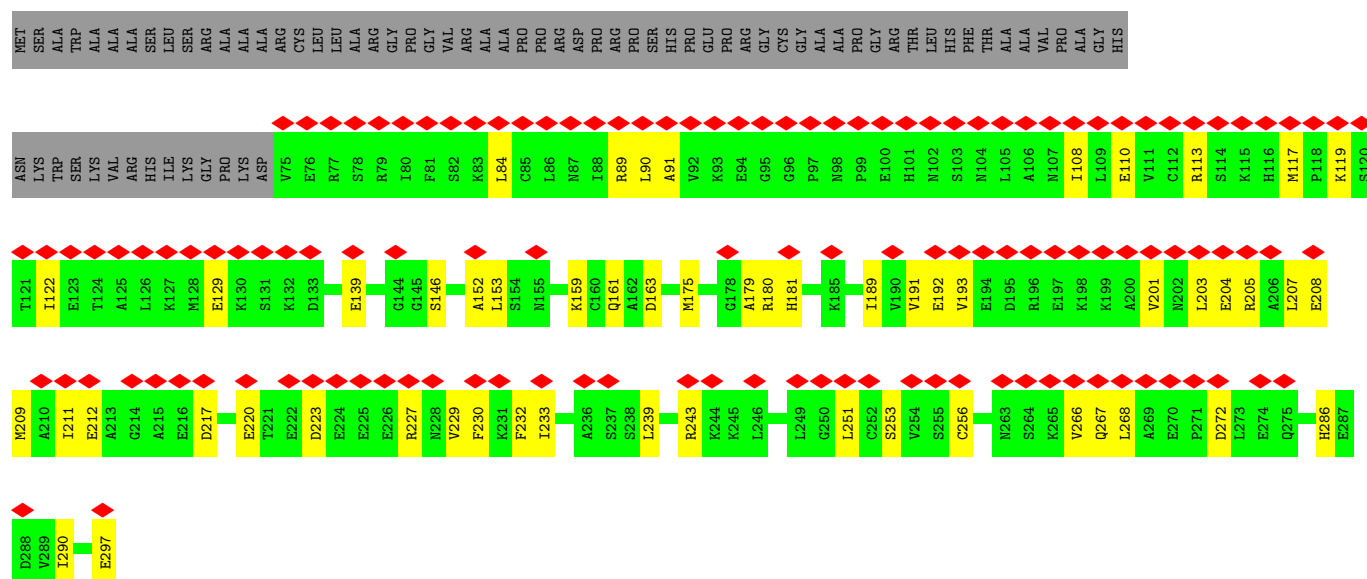
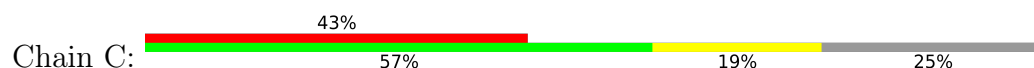


- Molecule 11: 16S mitochondrial rRNA

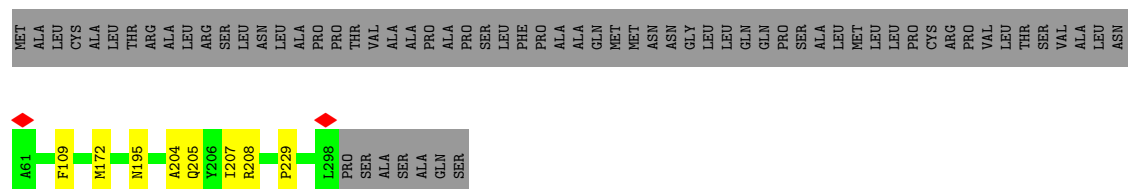
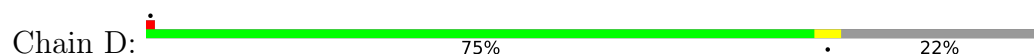




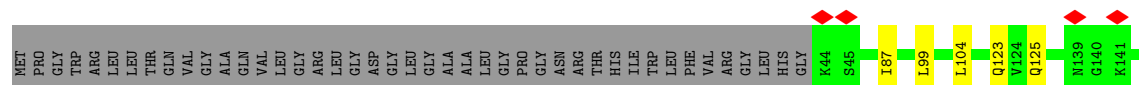
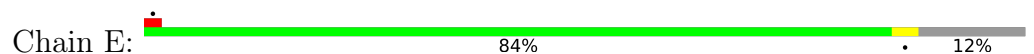
- Molecule 12: Translational activator of cytochrome c oxidase 1



- Molecule 13: 39S ribosomal protein L2, mitochondrial



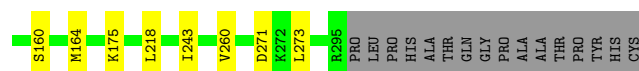
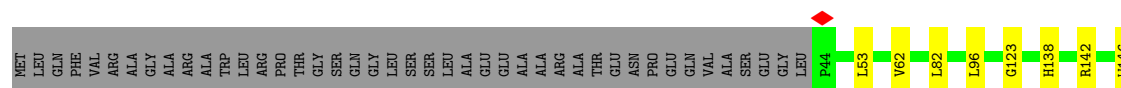
- Molecule 14: 39S ribosomal protein L3, mitochondrial





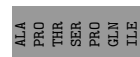
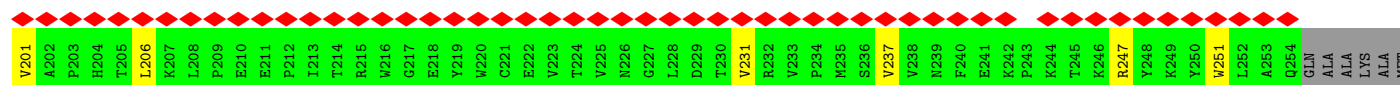
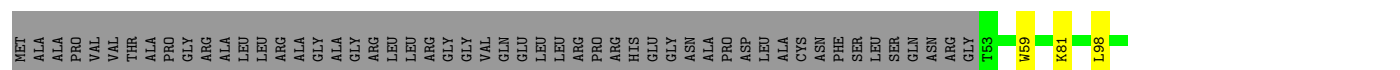
- Molecule 15: 39S ribosomal protein L4, mitochondrial

Chain F: 76% 5% 19%



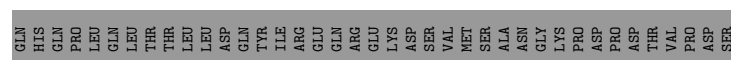
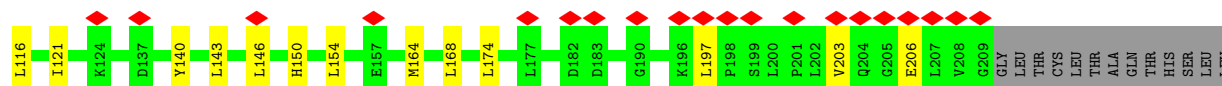
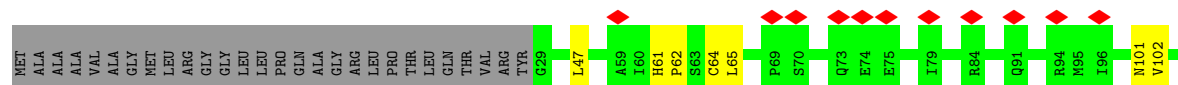
- Molecule 16: 39S ribosomal protein L9, mitochondrial

Chain H: 39% 70% 6% 24%



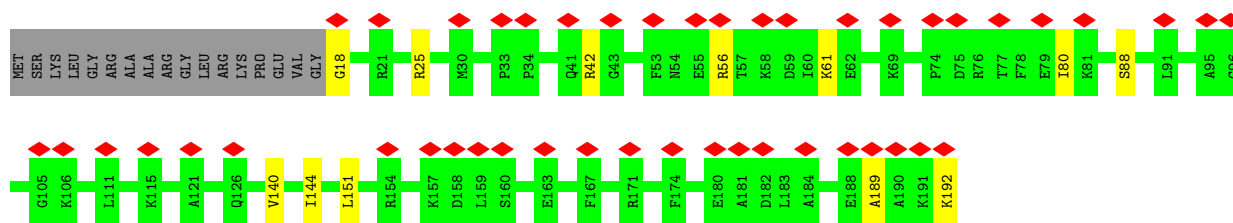
- Molecule 17: 39S ribosomal protein L10, mitochondrial

Chain I: 12% 62% 8% 31%



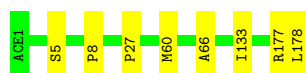
- Molecule 18: 39S ribosomal protein L11, mitochondrial

Chain J: 24% 85% 6% 9%



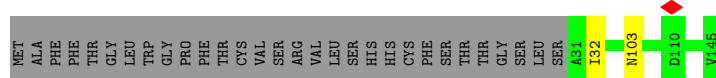
- Molecule 19: Large ribosomal subunit protein uL13m

Chain K: 96%



- Molecule 20: 39S ribosomal protein L14, mitochondrial

Chain L: 78% 21%



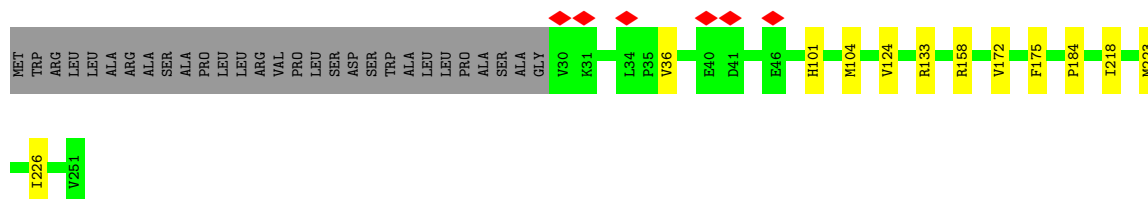
- Molecule 21: 39S ribosomal protein L15, mitochondrial

Chain M: 95%



- Molecule 22: 39S ribosomal protein L16, mitochondrial

Chain N: 84% 5% 12%




- Molecule 23: 39S ribosomal protein L17, mitochondrial

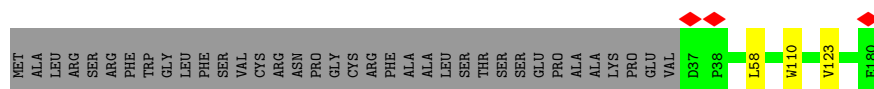
Chain O: 83% 5% 12%




- Molecule 24: 39S ribosomal protein L18, mitochondrial

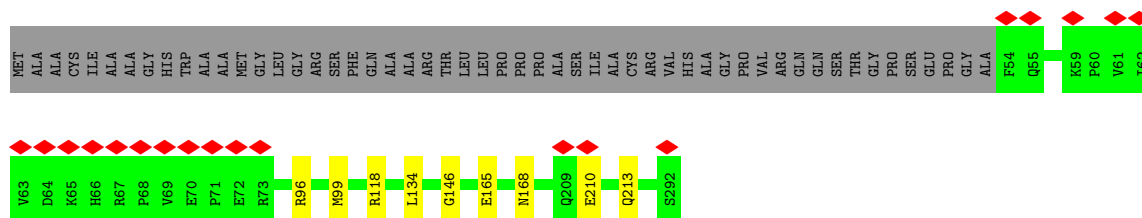


Chain P:  78% 20%



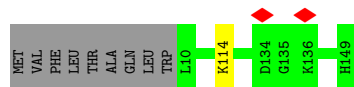
- Molecule 25: 39S ribosomal protein L19, mitochondrial

Chain Q:  7% 79% 18%



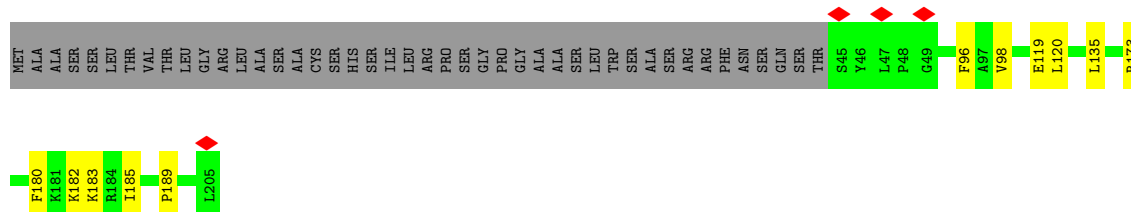
- Molecule 26: 39S ribosomal protein L20, mitochondrial

Chain R:  93% 6%




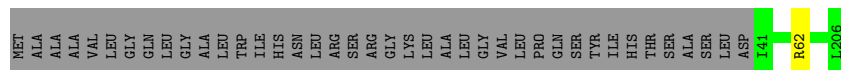
- Molecule 27: 39S ribosomal protein L21, mitochondrial

Chain S:  73% 5% 21%



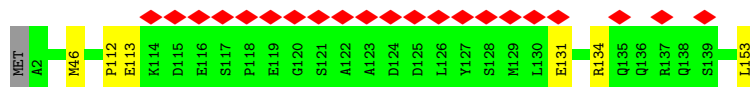
- Molecule 28: 39S ribosomal protein L22, mitochondrial

Chain T:  80% 19%




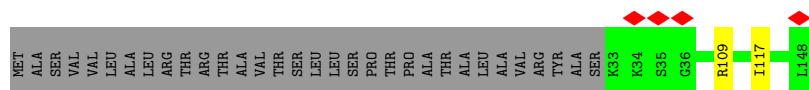
- Molecule 29: 39S ribosomal protein L23, mitochondrial

Chain U:  14% 95%

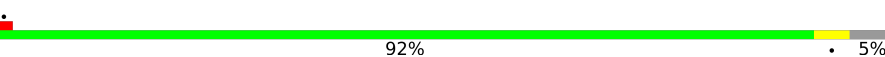


- Molecule 30: 39S ribosomal protein L27, mitochondrial

Chain W:  77% 22%



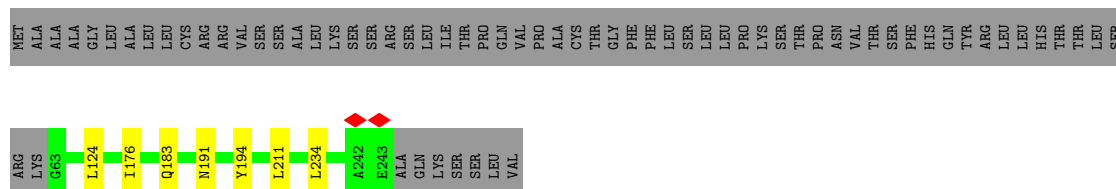
- Molecule 31: 39S ribosomal protein L28, mitochondrial

Chain X:  92% 5%



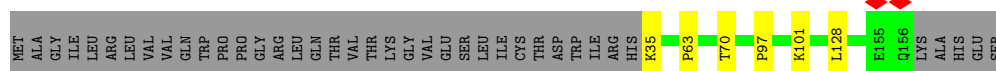
- Molecule 32: 39S ribosomal protein L47, mitochondrial

Chain Y:  70% 28%




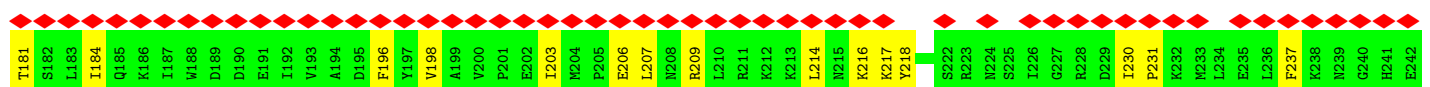
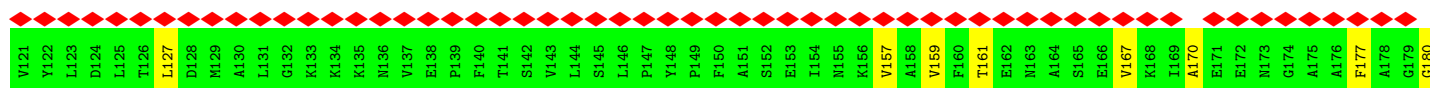
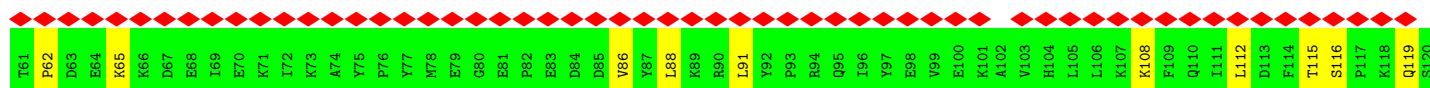
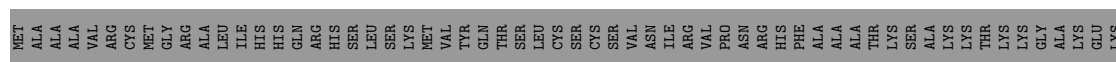
- Molecule 33: 39S ribosomal protein L30, mitochondrial

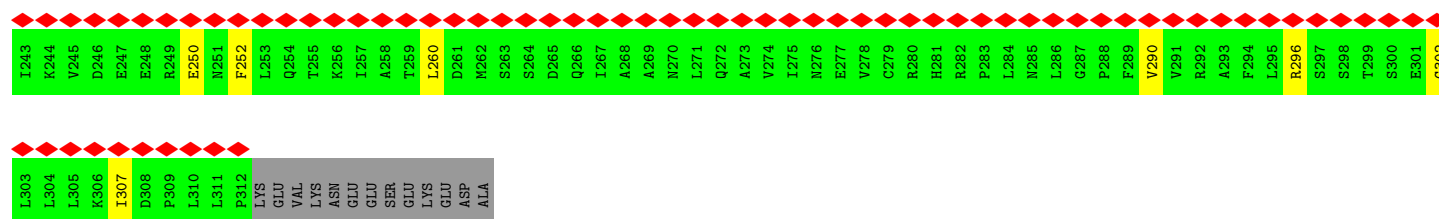
Chain Z:  72% 24%



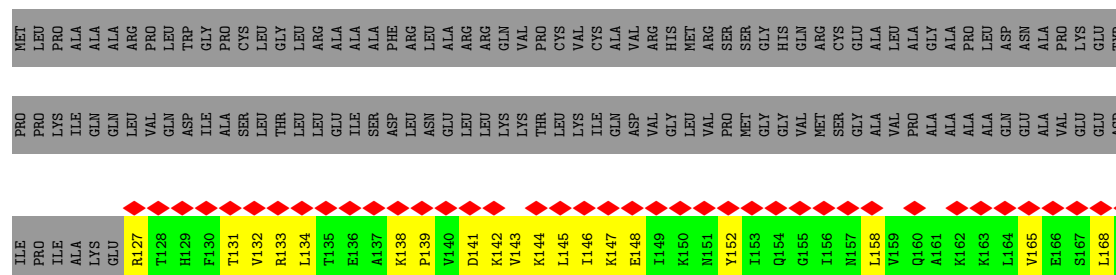
- Molecule 34: Large ribosomal subunit protein uL1m

Chain z:  74% 65% 12% 22%

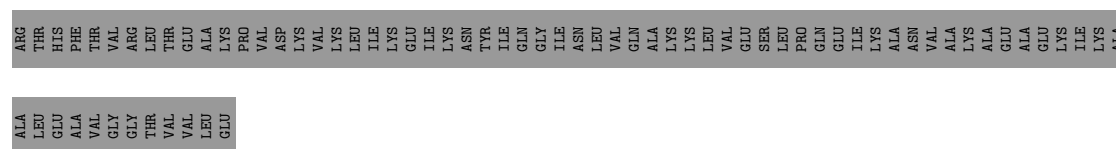
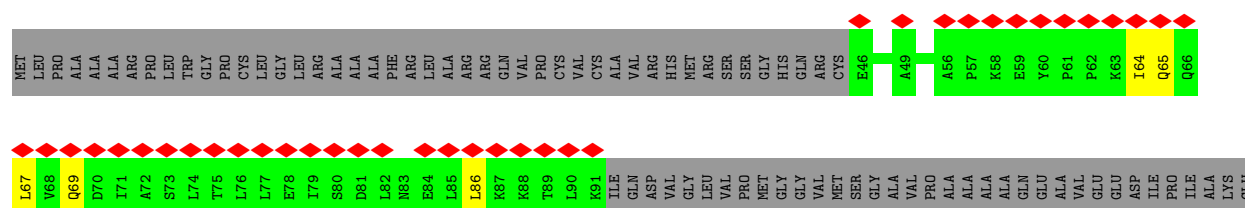




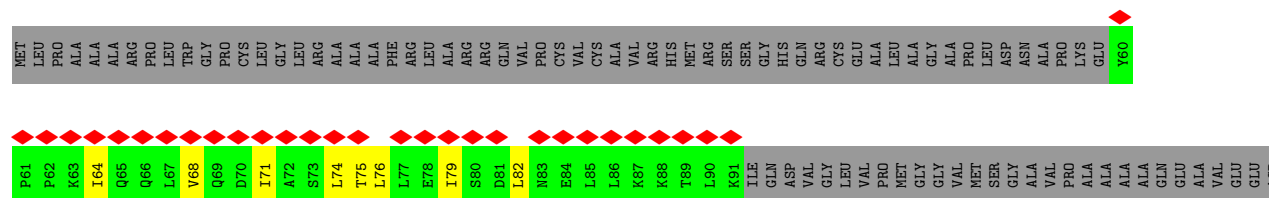
• Molecule 35: 39S ribosomal protein L12, mitochondrial

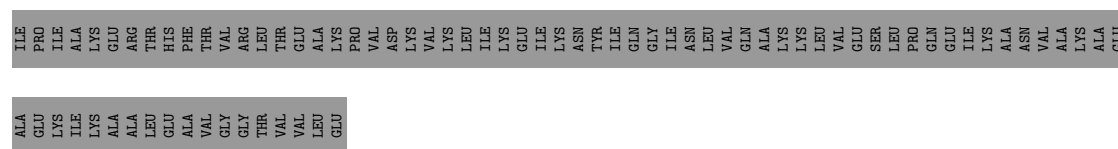


• Molecule 35: 39S ribosomal protein L12, mitochondrial



• Molecule 35: 39S ribosomal protein L12, mitochondrial

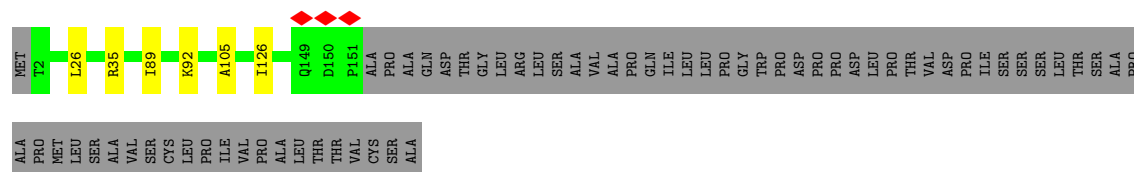




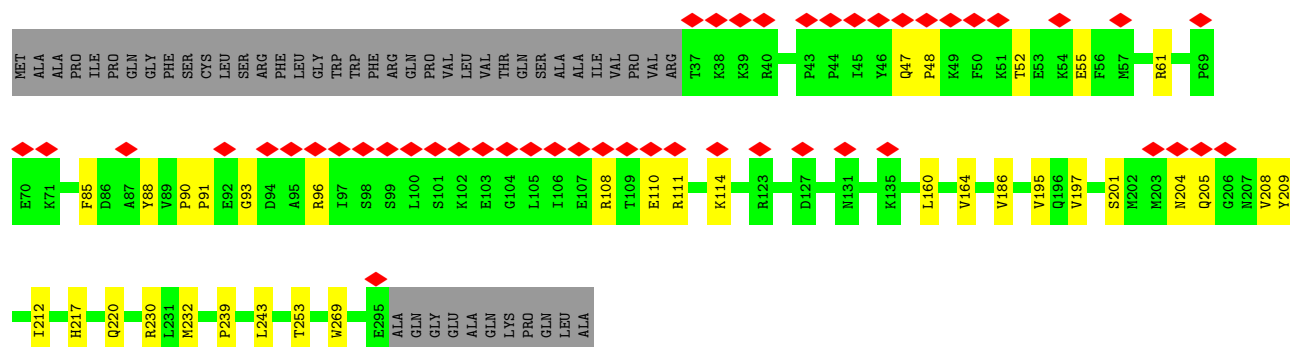
• Molecule 36: 39S ribosomal protein L24, mitochondrial



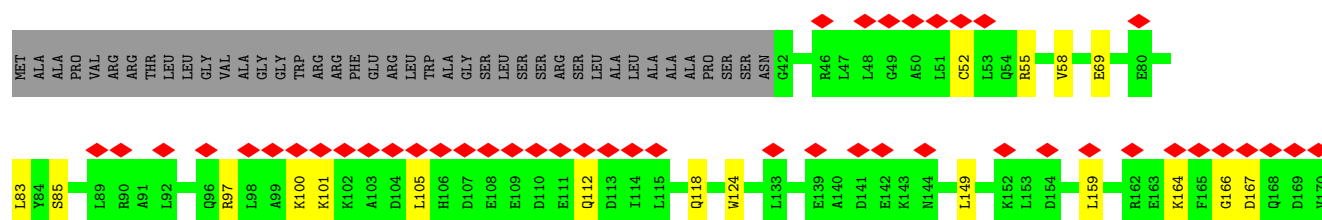
• Molecule 37: 39S ribosomal protein L43, mitochondrial

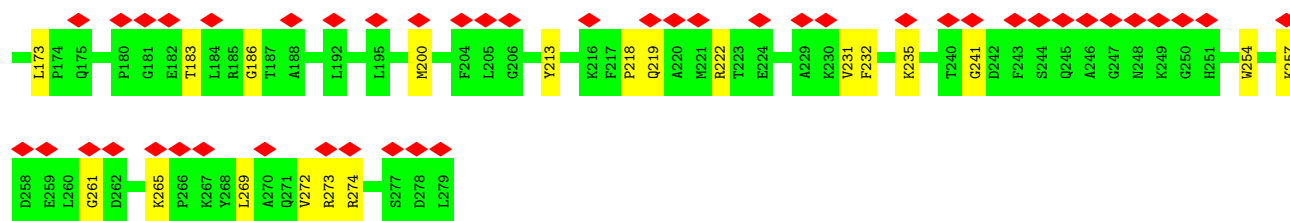


• Molecule 38: 39S ribosomal protein L45, mitochondrial



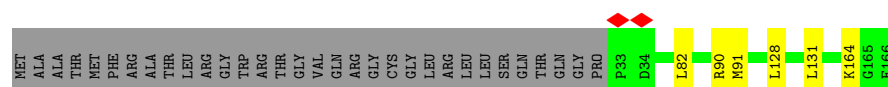
• Molecule 39: 39S ribosomal protein L46, mitochondrial





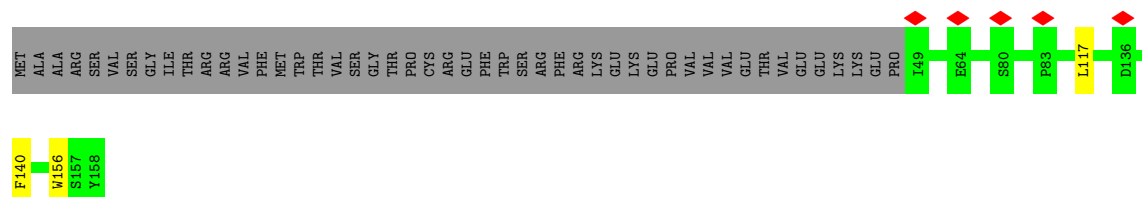
- Molecule 40: 39S ribosomal protein L49, mitochondrial

Chain g: 77% 19%



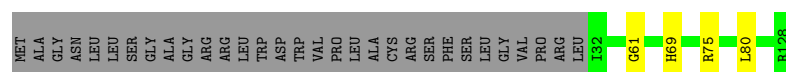
- Molecule 41: 39S ribosomal protein L50, mitochondrial

Chain h: 68% 30%



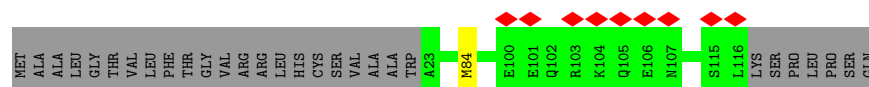
- Molecule 42: 39S ribosomal protein L51, mitochondrial

Chain i: 73% 24%



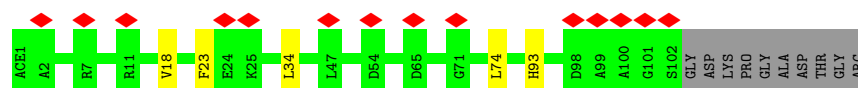
- Molecule 43: 39S ribosomal protein L52, mitochondrial

Chain j: 76% 24%

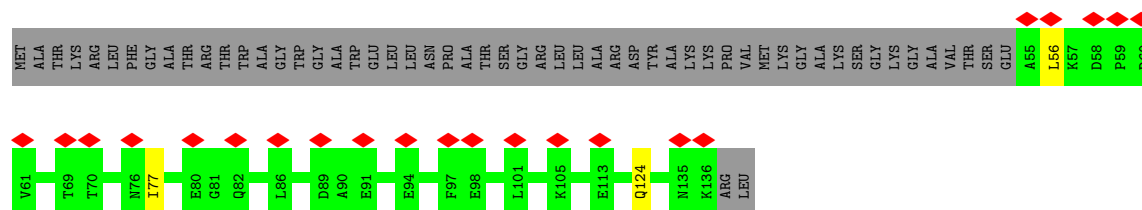


- Molecule 44: Large ribosomal subunit protein mL53

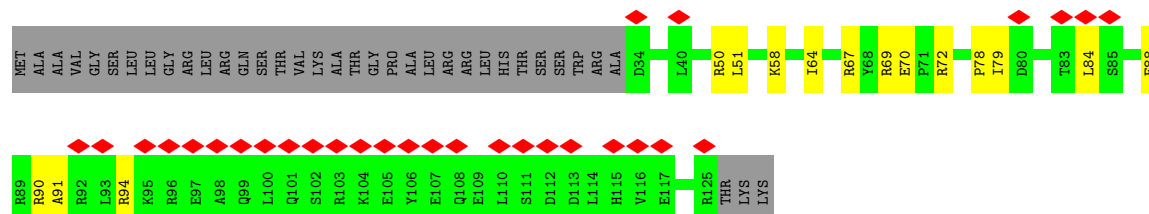
Chain k: 87% 9%



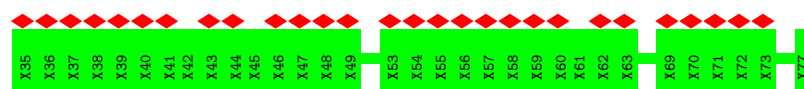
- Molecule 45: 39S ribosomal protein L54, mitochondrial



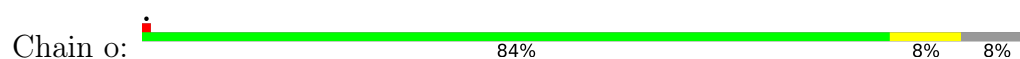
- Molecule 46: 39S ribosomal protein L55, mitochondrial



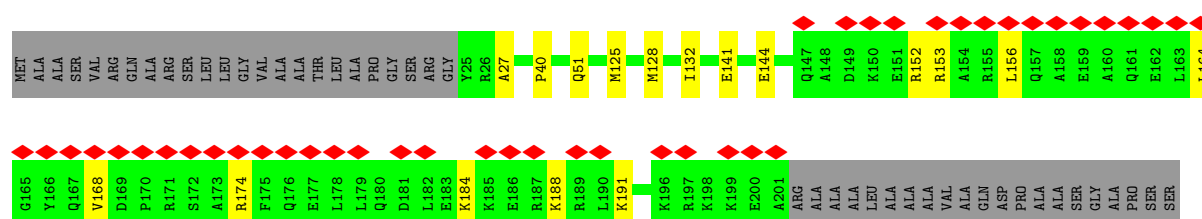
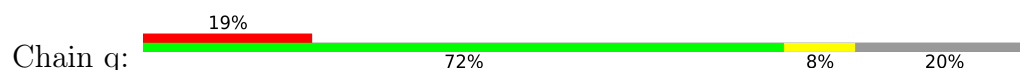
- Molecule 47: Nascent polypeptide



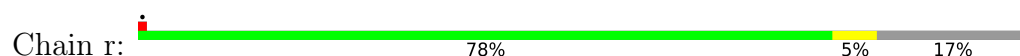
- Molecule 48: Ribosomal protein 63, mitochondrial

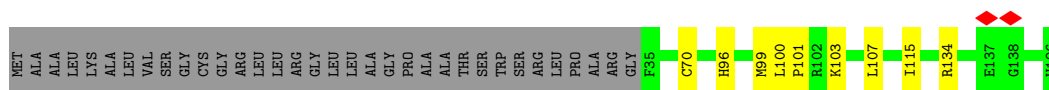


- Molecule 49: Growth arrest and DNA damage-inducible proteins-interacting protein 1



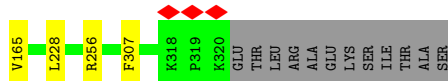
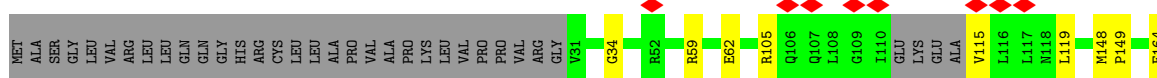
- Molecule 50: 39S ribosomal protein S18a, mitochondrial





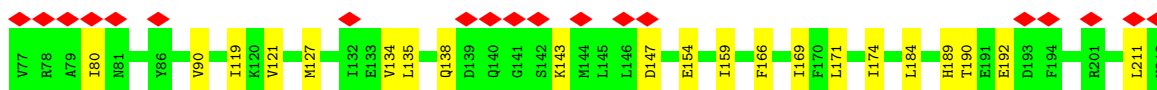
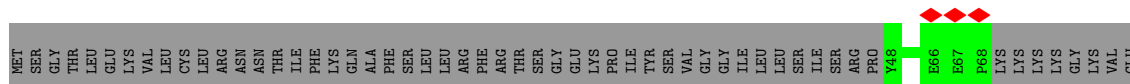
- Molecule 51: 39S ribosomal protein L44, mitochondrial

Chain c: 82% 14%



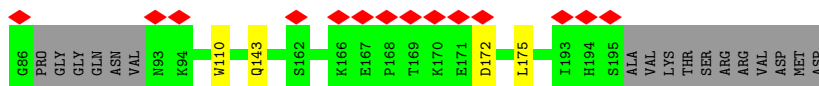
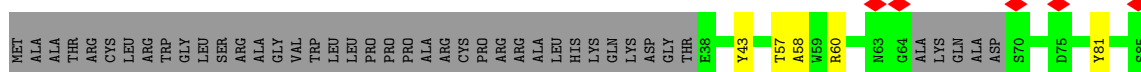
- Molecule 52: 39S ribosomal protein L48, mitochondrial

Chain f: 10% 64% 10% 26%



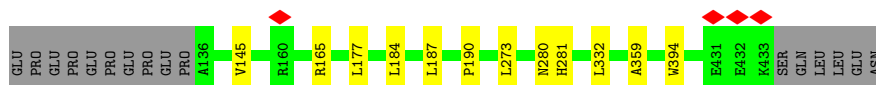
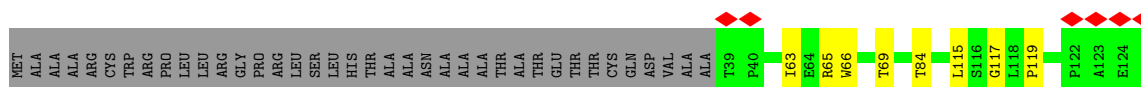
- Molecule 53: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p: 9% 67% 29% 5%




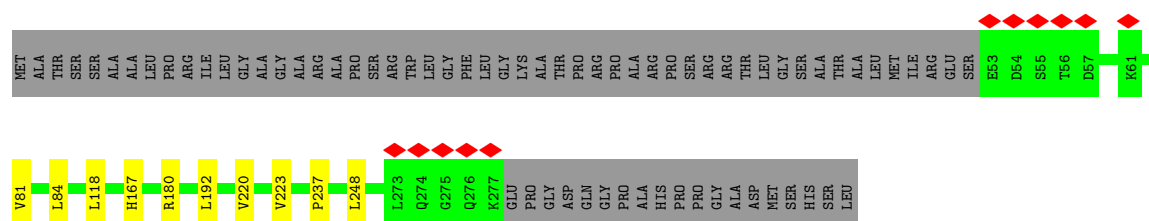
- Molecule 54: 39S ribosomal protein S30, mitochondrial

Chain s: 83% 5% 12%



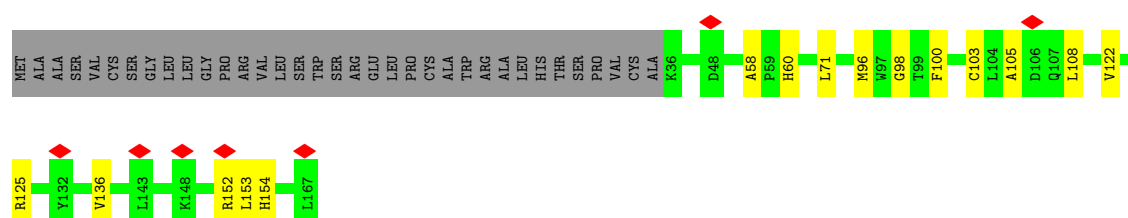
- Molecule 55: 28S ribosomal protein S2, mitochondrial

Chain AB:  73% 24%




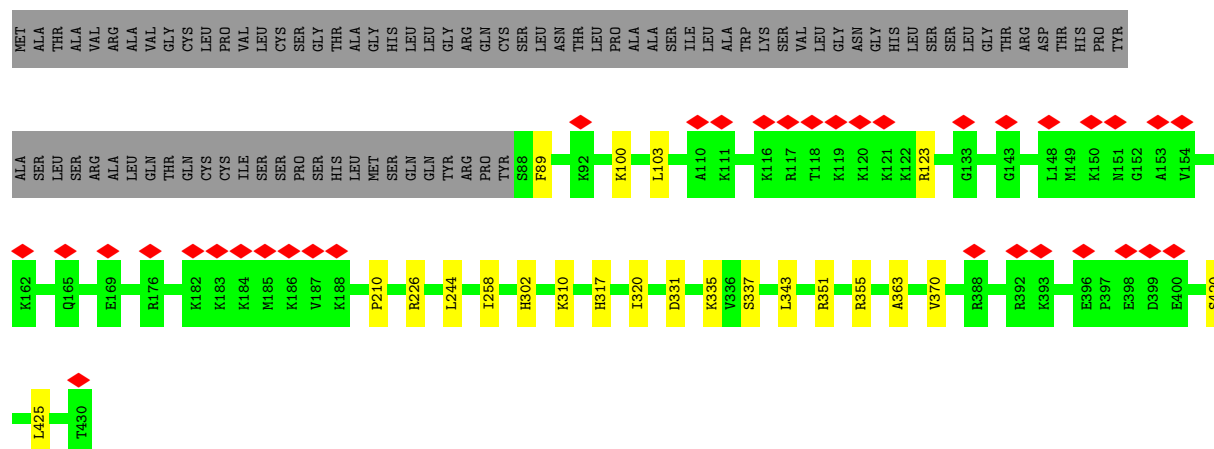
- Molecule 56: 28S ribosomal protein S24, mitochondrial

Chain AC:  70% 9% 21%



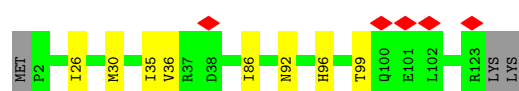
- Molecule 57: 28S ribosomal protein S5, mitochondrial

Chain AD:  8% 75% 5% 20%




- Molecule 58: 28S ribosomal protein S6, mitochondrial

Chain AE:  91% 6%

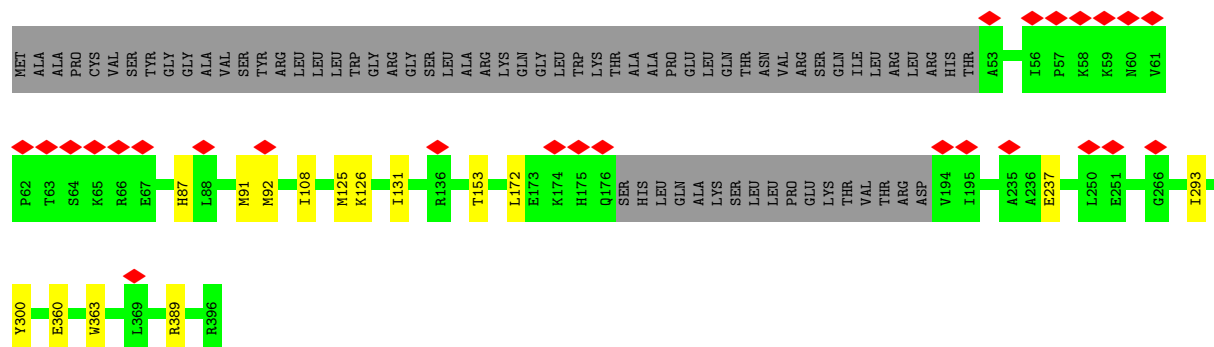
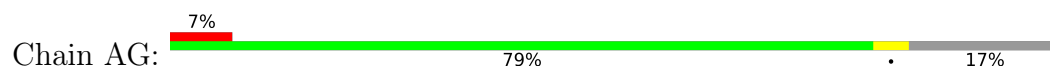


- Molecule 59: 28S ribosomal protein S7, mitochondrial

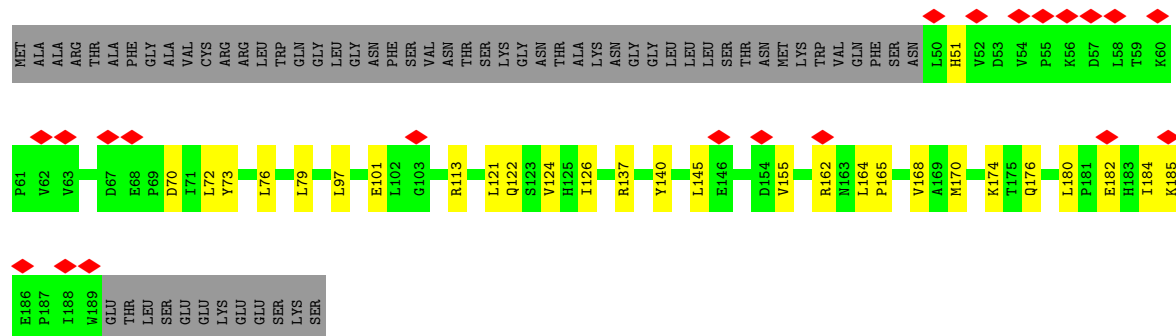
Chain AF:  5% 80% 6% 14%



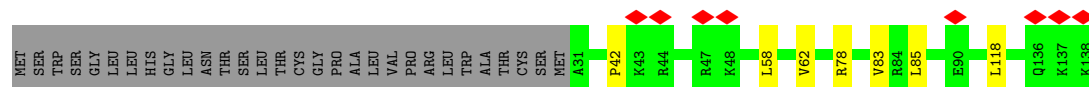
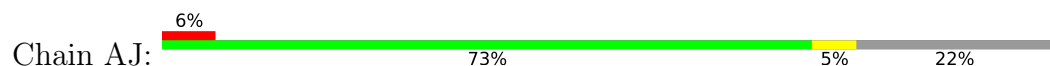
- Molecule 60: 28S ribosomal protein S9, mitochondrial



- Molecule 61: 28S ribosomal protein S10, mitochondrial



- Molecule 62: 28S ribosomal protein S12, mitochondrial

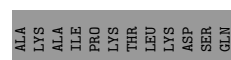
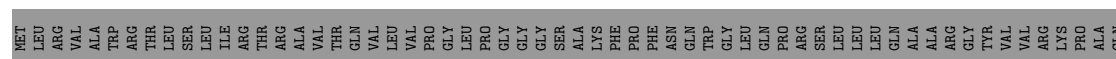


- Molecule 63: 28S ribosomal protein S14, mitochondrial

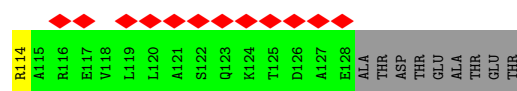
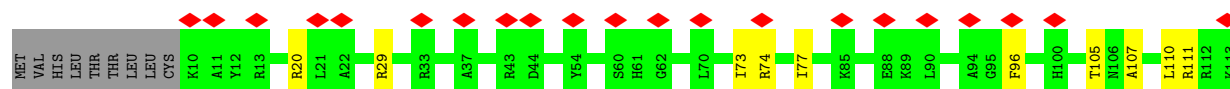
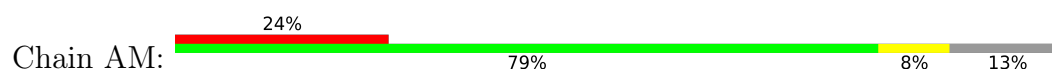




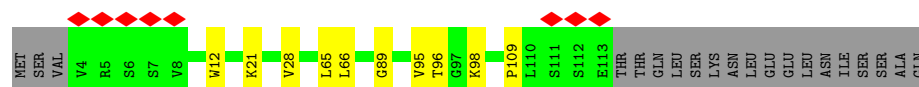
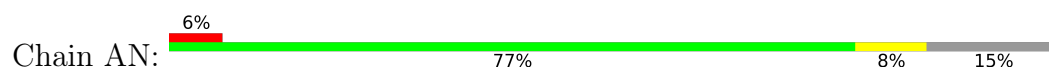
- Molecule 64: 28S ribosomal protein S15, mitochondrial



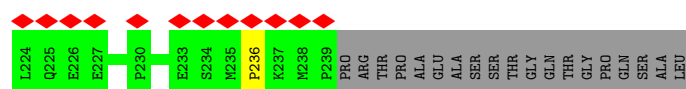
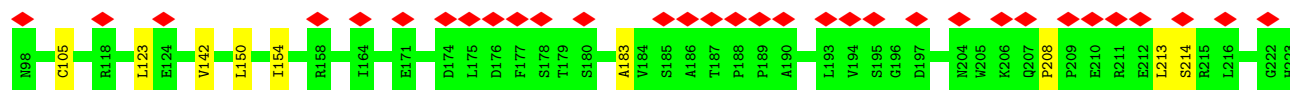
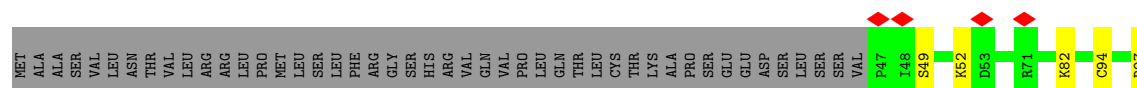
- Molecule 65: 28S ribosomal protein S16, mitochondrial



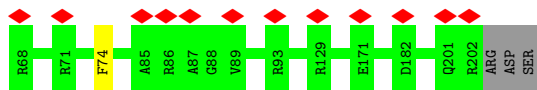
- Molecule 66: 28S ribosomal protein S17, mitochondrial

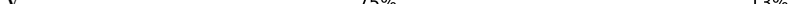


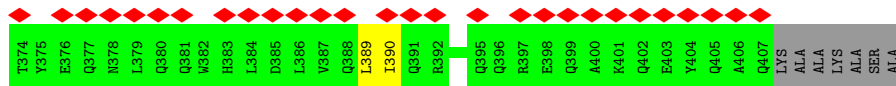
- Molecule 67: 28S ribosomal protein S18b, mitochondrial



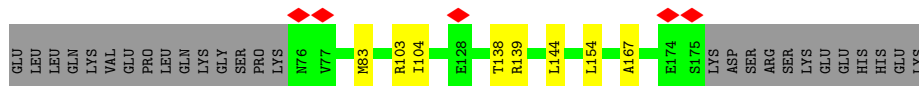


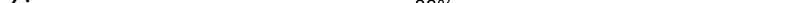


- Chain AV: 



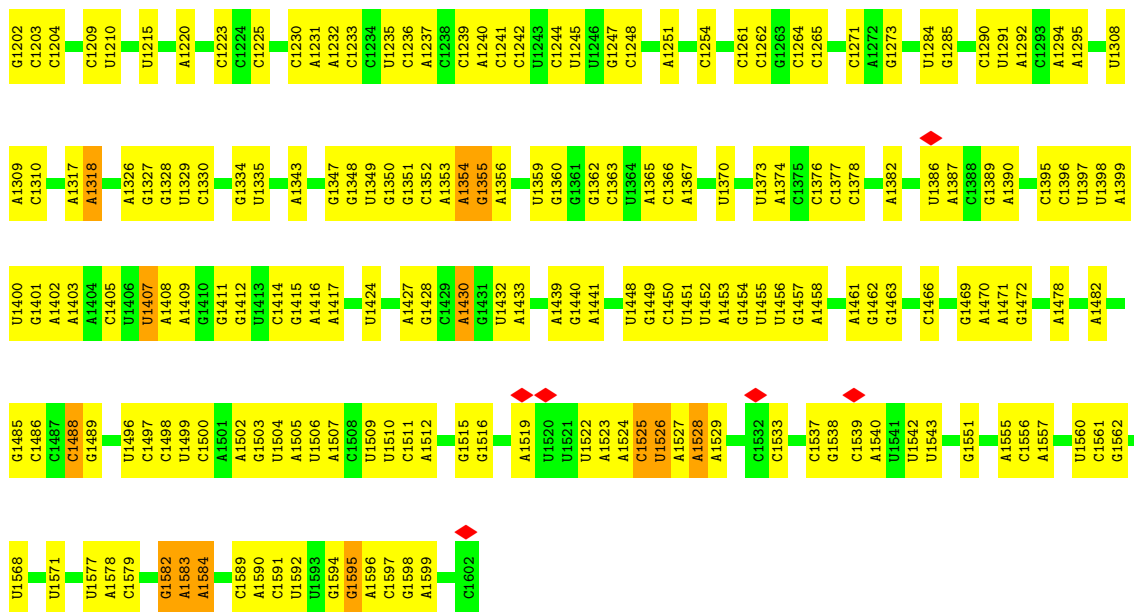
- Chain AW:  49% . 47%



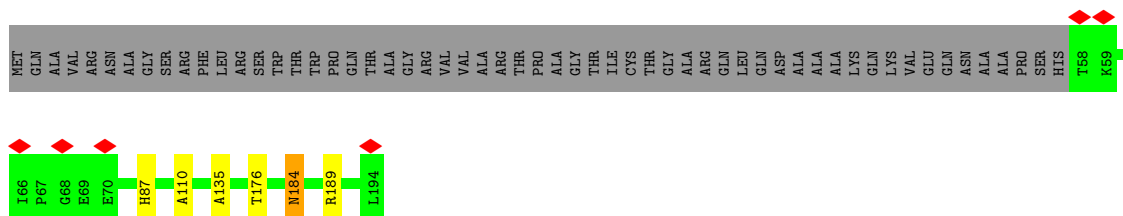
- Chain AZ: 



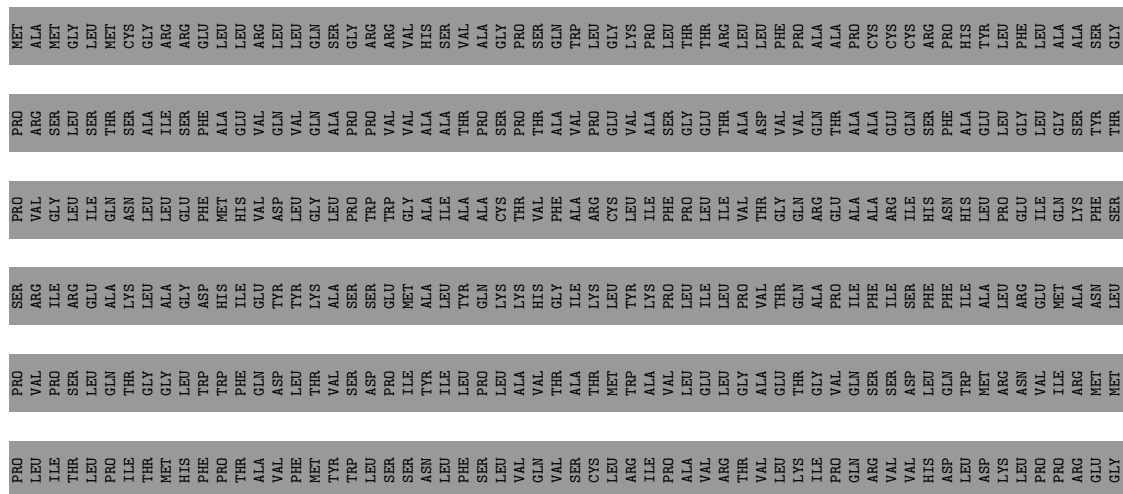


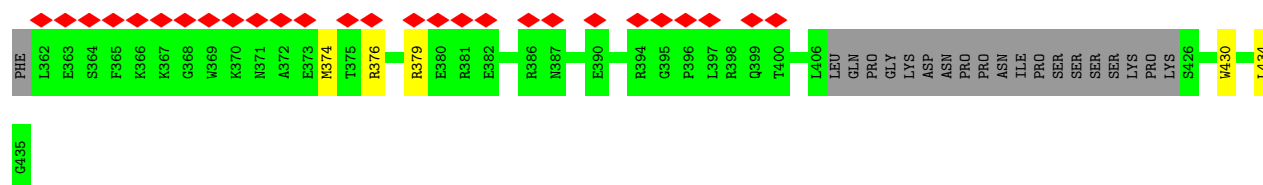


- Molecule 82: 28S ribosomal protein S11, mitochondrial

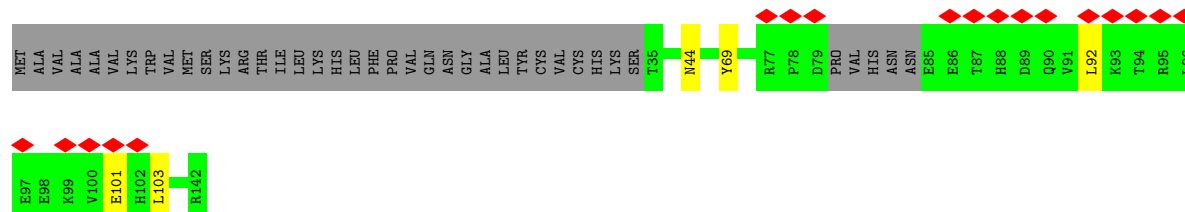


- Molecule 83: Mitochondrial inner membrane protein OXA1L





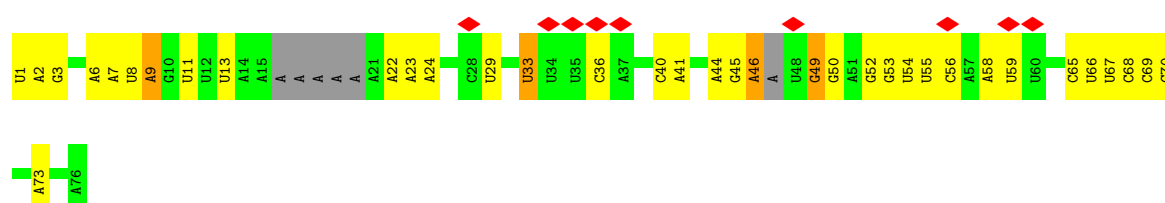
- Molecule 84: 39S ribosomal protein L42, mitochondrial



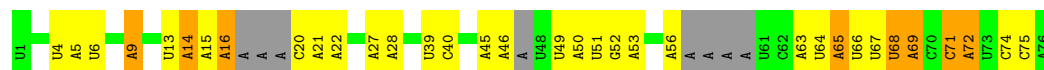
- Molecule 85: P/P-tRNA



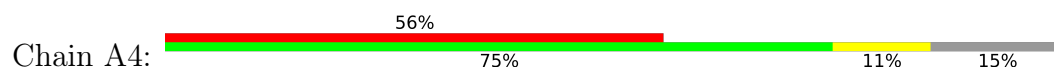
- Molecule 86: E/E-tRNA



- Molecule 87: A/A-tRNA

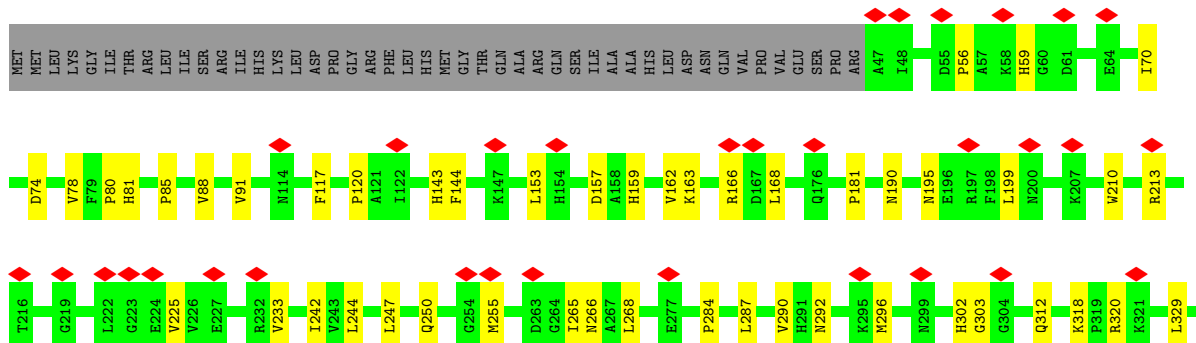
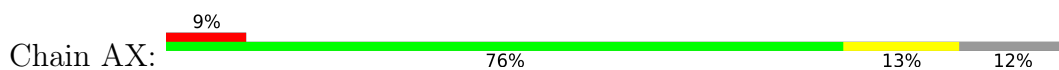


- Molecule 88: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



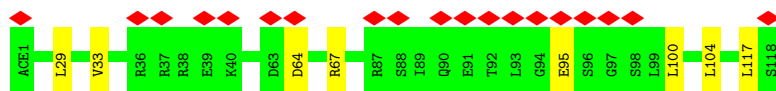


- Molecule 89: 28S ribosomal protein S29, mitochondrial





- Molecule 90: Small ribosomal subunit protein mS37



- Molecule 91: Small ribosomal subunit protein bS21m



- Molecule 92: mitochondrial tRNA<sup>Val</sup>



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104031	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)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.459	Depositor
Minimum map value	-0.219	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.06	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	1.068, 1.068, 1.068	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.44	0/913	0.33	0/1224
2	1	0.40	0/469	0.34	0/621
3	2	0.56	0/383	0.36	0/507
4	3	0.53	0/853	0.36	0/1136
5	4	0.47	0/350	0.30	0/461
6	5	0.41	0/3305	0.35	0/4502
7	6	0.34	0/3043	0.33	0/4140
8	7	0.34	0/2447	0.33	0/3310
9	8	0.22	0/1354	0.36	0/1819
10	9	0.41	0/1025	0.34	0/1379
11	A	0.54	0/36876	0.36	0/57402
12	C	0.20	0/1754	0.34	0/2357
13	D	0.45	0/1896	0.34	0/2549
14	E	0.45	0/2475	0.36	0/3355
15	F	0.49	0/2090	0.36	0/2842
16	H	0.26	0/1698	0.32	0/2292
17	I	0.28	0/1478	0.35	0/1999
18	J	0.21	0/1348	0.32	0/1813
19	K	0.49	0/1497	0.35	0/2031
20	L	0.43	0/905	0.33	0/1218
21	M	0.47	0/2381	0.36	0/3212
22	N	0.43	0/1833	0.34	0/2468
23	O	0.46	0/1283	0.36	0/1727
24	P	0.39	0/1199	0.32	0/1623
25	Q	0.41	0/2039	0.33	0/2750
26	R	0.52	0/1175	0.35	0/1572
27	S	0.49	0/1320	0.39	0/1789
28	T	0.49	0/1403	0.32	0/1886
29	U	0.43	0/1279	0.38	0/1730
30	W	0.48	0/926	0.34	0/1244
31	X	0.41	0/2099	0.30	0/2837

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.46	0/1593	0.32	0/2136
33	Z	0.47	0/1021	0.36	0/1378
34	z	0.16	0/2067	0.38	0/2793
35	G	0.19	0/562	0.53	0/754
35	t	0.16	0/358	0.31	0/486
35	u	0.21	0/259	0.41	0/350
36	V	0.36	0/1721	0.31	0/2333
37	b	0.48	0/1218	0.36	0/1649
38	d	0.29	0/2181	0.37	0/2949
39	e	0.19	0/1970	0.33	0/2658
40	g	0.44	0/1151	0.34	0/1569
41	h	0.32	0/918	0.29	0/1249
42	i	0.52	0/850	0.36	0/1135
43	j	0.41	0/760	0.30	0/1023
44	k	0.24	0/783	0.28	0/1057
45	l	0.21	0/707	0.30	0/960
46	m	0.20	0/805	0.34	0/1081
48	o	0.48	0/819	0.38	0/1097
49	q	0.30	0/1529	0.33	0/2055
50	r	0.42	0/1362	0.35	0/1846
51	c	0.41	0/2347	0.33	0/3171
52	f	0.30	0/1273	0.39	0/1716
53	p	0.32	0/1223	0.33	0/1641
54	s	0.44	0/3231	0.35	0/4389
55	AB	0.31	0/1871	0.30	0/2531
56	AC	0.29	0/1113	0.33	0/1505
57	AD	0.30	0/2783	0.30	0/3724
58	AE	0.32	0/989	0.30	0/1335
59	AF	0.26	0/1767	0.27	0/2373
60	AG	0.26	0/2746	0.30	0/3681
61	AH	0.28	0/1178	0.33	0/1598
62	AJ	0.30	0/855	0.29	0/1148
63	AK	0.29	0/880	0.30	0/1182
64	AL	0.29	0/1477	0.27	0/1974
65	AM	0.20	0/963	0.33	0/1295
66	AN	0.28	0/886	0.30	0/1199
67	AO	0.22	0/1648	0.33	0/2243
68	AP	0.35	0/798	0.33	0/1070
69	AR	0.18	0/2456	0.29	0/3317
70	AS	0.25	0/1138	0.25	0/1533
71	AT	0.26	0/1402	0.32	0/1883
72	AU	0.21	0/1510	0.28	0/2025
73	AV	0.17	0/3030	0.35	0/4093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
74	AW	0.27	0/801	0.29	0/1079
75	AZ	0.23	0/857	0.36	0/1141
76	A0	0.16	0/1834	0.30	0/2484
77	A1	0.22	0/2313	0.30	0/3129
78	A3	0.36	0/636	0.36	0/839
79	Az	0.25	0/804	0.34	0/1248
80	AY	0.21	0/1040	0.27	0/1402
81	AA	0.38	0/22537	0.31	0/35085
82	AI	0.32	0/1039	0.34	0/1400
83	OX	0.25	0/478	0.41	0/639
84	a	0.40	0/891	0.37	0/1208
85	Ax	0.31	0/1673	0.37	0/2602
86	Ay	0.22	0/1655	0.32	0/2567
87	Aw	0.27	0/1600	0.33	0/2476
88	A4	0.17	0/4877	0.34	0/6598
89	AX	0.23	0/2921	0.34	0/3954
90	A2	0.30	0/947	0.32	0/1266
91	AQ	0.35	0/754	0.29	0/1003
92	B	0.26	0/1626	0.31	0/2523
All	All	0.39	0/192577	0.34	0/273622

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [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	4	0
2	1	464	0	511	6	0
3	2	377	0	406	0	0
4	3	832	0	883	6	0
5	4	342	0	361	1	0
6	5	3210	0	3206	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	6	2948	0	2841	15	0
8	7	2390	0	2397	10	0
9	8	1327	0	1368	16	0
10	9	997	0	987	5	0
11	A	33070	0	16797	166	0
12	C	1732	0	1740	35	0
13	D	1859	0	1920	7	0
14	E	2406	0	2415	7	0
15	F	2031	0	2065	11	0
16	H	1661	0	1734	10	0
17	I	1446	0	1532	13	0
18	J	1330	0	1407	8	0
19	K	1455	0	1452	5	0
20	L	890	0	941	1	0
21	M	2327	0	2393	9	0
22	N	1786	0	1817	9	0
23	O	1259	0	1294	5	0
24	P	1173	0	1165	3	0
25	Q	1990	0	2031	5	0
26	R	1154	0	1214	1	0
27	S	1293	0	1365	8	0
28	T	1369	0	1410	1	0
29	U	1248	0	1228	4	0
30	W	904	0	934	2	0
31	X	2044	0	2060	6	0
32	Y	1556	0	1597	6	0
33	Z	996	0	1044	5	0
34	z	2027	0	2076	26	0
35	G	558	0	612	25	0
35	t	354	0	377	4	0
35	u	257	0	283	6	0
36	V	1676	0	1687	7	0
37	b	1193	0	1191	4	0
38	d	2124	0	2125	25	0
39	e	1931	0	1916	28	0
40	g	1113	0	1097	4	0
41	h	895	0	881	2	0
42	i	828	0	857	4	0
43	j	745	0	746	1	0
44	k	774	0	784	3	0
45	l	688	0	674	3	0
46	m	791	0	796	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	n	215	0	51	0	0
48	o	798	0	804	7	0
49	q	1495	0	1492	13	0
50	r	1322	0	1348	8	0
51	c	2299	0	2320	10	0
52	f	1252	0	1269	16	0
53	p	1205	0	1223	6	0
54	s	3148	0	3131	16	0
55	AB	1828	0	1815	8	0
56	AC	1083	0	1088	10	0
57	AD	2731	0	2804	17	0
58	AE	972	0	1000	7	0
59	AF	1725	0	1769	10	0
60	AG	2688	0	2687	11	0
61	AH	1152	0	1183	22	0
62	AJ	839	0	887	4	0
63	AK	862	0	885	9	0
64	AL	1453	0	1540	11	0
65	AM	942	0	965	11	0
66	AN	868	0	928	7	0
67	AO	1592	0	1557	13	0
68	AP	781	0	806	4	0
69	AR	2409	0	2428	13	0
70	AS	1111	0	1115	7	0
71	AT	1371	0	1393	9	0
72	AU	1488	0	1499	6	0
73	AV	2969	0	2961	39	0
74	AW	789	0	802	5	0
75	AZ	839	0	858	6	0
76	A0	1787	0	1796	16	0
77	A1	2265	0	2294	19	0
78	A3	625	0	698	5	0
79	Az	719	0	359	2	0
80	AY	1010	0	957	5	0
81	AA	20260	0	10282	315	0
82	AI	1019	0	1059	6	0
83	OX	468	0	464	4	0
84	a	865	0	829	4	0
85	Ax	1498	0	766	12	0
86	Ay	1483	0	754	24	0
87	Aw	1434	0	728	15	0
88	A4	4768	0	4766	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	AX	2849	0	2844	35	0
90	A2	935	0	971	5	0
91	AQ	744	0	758	3	0
92	B	1524	0	779	21	0
93	0	1	0	0	0	0
93	4	1	0	0	0	0
93	AO	1	0	0	0	0
94	6	1	0	0	0	0
94	A	29	0	0	0	0
94	AA	18	0	0	0	0
94	D	1	0	0	0	0
94	M	2	0	0	0	0
94	N	1	0	0	0	0
94	W	1	0	0	0	0
94	o	1	0	0	0	0
95	A	50	0	95	0	0
95	AA	20	0	38	0	0
96	A	6	0	12	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	D	2	0	0	0	0
97	E	1	0	0	0	0
97	g	1	0	0	0	0
98	AP	4	0	0	0	0
98	AT	4	0	0	0	0
98	r	4	0	0	1	0
99	AA	44	0	26	1	0
100	AA	28	0	52	0	0
101	AX	31	0	12	0	0
102	AX	28	0	12	1	0
103	B	7	0	8	2	0
All	All	183684	0	155500	1227	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 4.

All (1227) 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)
11:A:3112:A:N6	11:A:3200:U:O2	2.06	0.87
39:e:183:THR:HG23	39:e:186:GLY:H	1.46	0.80
34:z:181:THR:HA	34:z:184:ILE:HD12	1.68	0.75
12:C:90:LEU:HG	12:C:153:LEU:HD22	1.69	0.73
34:z:184:ILE:HD13	34:z:206:GLU:HB2	1.70	0.73
81:AA:773:U:H2'	81:AA:774:G:H8	1.54	0.71
9:8:187:PRO:HG2	46:m:79:ILE:HD11	1.71	0.71
73:AV:30:LEU:HD23	73:AV:149:ASP:HB2	1.70	0.71
81:AA:1440:G:H2'	81:AA:1441:A:H8	1.57	0.70
35:G:165:VAL:HA	35:G:168:LEU:HG	1.73	0.70
80:AY:338:LEU:HD11	80:AY:351:MET:HB3	1.75	0.69
12:C:211:ILE:HD12	35:G:143:VAL:HG12	1.74	0.69
49:q:164:LEU:HB3	49:q:168:VAL:HG21	1.75	0.69
51:c:228:LEU:HB2	51:c:307:PHE:HD2	1.58	0.69
28:T:62:ARG:HE	38:d:230:ARG:HD2	1.58	0.69
77:A1:126:LEU:HD11	88:A4:70:VAL:HG13	1.74	0.69
81:AA:1201:A:H2'	81:AA:1202:G:H8	1.58	0.68
88:A4:556:LYS:HE3	88:A4:579:ILE:HD13	1.73	0.68
36:V:79:VAL:HG12	36:V:86:VAL:HG12	1.75	0.68
77:A1:268:GLN:HE22	89:AX:120:PRO:HG3	1.58	0.68
81:AA:1528:A:H2'	81:AA:1529:A:H8	1.58	0.68
34:z:161:THR:HB	34:z:167:VAL:HG22	1.74	0.68
81:AA:1440:G:H2'	81:AA:1441:A:C8	2.30	0.67
2:1:19:ARG:HB2	2:1:62:ILE:HD11	1.77	0.67
81:AA:1398:U:H2'	81:AA:1399:A:H8	1.59	0.67
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.77	0.67
57:AD:244:LEU:HD22	57:AD:343:LEU:HD23	1.77	0.67
81:AA:1347:G:H2'	81:AA:1348:G:H8	1.60	0.67
11:A:2778:U:H5''	34:z:115:THR:HG22	1.77	0.66
81:AA:705:C:H3'	81:AA:706:C:H6	1.61	0.66
89:AX:153:LEU:HD21	89:AX:247:LEU:HD13	1.77	0.66
88:A4:397:MET:HG3	88:A4:431:LEU:HD11	1.77	0.66
12:C:119:LYS:HD3	12:C:122:ILE:HD11	1.78	0.66
34:z:127:LEU:HD22	34:z:290:VAL:HG13	1.78	0.66
22:N:124:VAL:HG12	22:N:158:ARG:HE	1.61	0.65
81:AA:1003:A:H2'	81:AA:1004:G:H8	1.61	0.65
89:AX:242:ILE:HD11	102:AX:503:GDP:C5	2.31	0.65
61:AH:162:ARG:HH21	80:AY:313:PHE:HB2	1.61	0.65
89:AX:181:PRO:HB2	89:AX:233:VAL:HG22	1.78	0.65
6:5:201:ARG:HB3	6:5:232:THR:HG22	1.79	0.64
35:G:185:LYS:HD2	35:G:188:LEU:HD11	1.79	0.64
12:C:207:LEU:HD22	35:G:158:LEU:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AM:114:ARG:HH22	67:AO:236:PRO:HD2	1.63	0.64
81:AA:845:A:H2'	81:AA:846:A:H8	1.63	0.64
88:A4:400:LEU:HA	88:A4:403:LYS:HD3	1.81	0.63
81:AA:1201:A:H2'	81:AA:1202:G:C8	2.33	0.63
52:f:90:VAL:HG13	52:f:189:HIS:HB3	1.81	0.62
12:C:239:LEU:HD11	12:C:256:CYS:HB2	1.82	0.62
11:A:3183:U:H3	19:K:177:ARG:HB3	1.64	0.62
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.80	0.62
12:C:89:ARG:HG3	12:C:129:GLU:HG2	1.81	0.61
60:AG:389:ARG:HB2	81:AA:1433:A:H5''	1.81	0.61
11:A:3150:U:H2'	11:A:3151:A:H8	1.65	0.61
81:AA:872:G:H2'	81:AA:873:G:H8	1.66	0.61
11:A:1994:A:H61	11:A:2736:C:H4'	1.64	0.61
87:Aw:68:U:H2'	87:Aw:69:A:C8	2.35	0.61
81:AA:918:A:H4'	81:AA:920:G:H4'	1.83	0.61
35:G:134:LEU:HA	35:G:195:VAL:HA	1.83	0.61
81:AA:1002:C:H2'	81:AA:1003:A:H8	1.66	0.61
66:AN:95:VAL:HG23	66:AN:96:THR:HG23	1.83	0.60
81:AA:773:U:H2'	81:AA:774:G:C8	2.35	0.60
81:AA:1089:U:H2'	81:AA:1090:A:H8	1.66	0.60
11:A:2740:A:H2'	11:A:2741:A:C8	2.36	0.60
55:AB:180:ARG:HH21	57:AD:210:PRO:HB2	1.65	0.60
81:AA:705:C:H3'	81:AA:706:C:C6	2.36	0.60
2:1:38:ARG:HH12	2:1:41:LEU:HD11	1.65	0.60
58:AE:35:ILE:HD11	64:AL:91:ARG:HE	1.66	0.60
39:e:166:GLY:HA3	103:B:101:VAL:HB	1.84	0.60
39:e:97:ARG:HH11	39:e:112:GLN:HE22	1.50	0.60
82:AI:176:THR:HB	91:AQ:11:THR:HG23	1.82	0.60
77:A1:53:LEU:HD12	88:A4:518:GLU:HG2	1.83	0.60
81:AA:1007:G:H2'	81:AA:1008:A:C8	2.37	0.60
88:A4:343:ARG:HA	88:A4:378:LEU:HD13	1.84	0.60
81:AA:663:A:H2'	81:AA:664:G:C8	2.37	0.59
39:e:213:TYR:HB3	39:e:231:VAL:HB	1.83	0.59
81:AA:681:U:H2'	81:AA:682:A:H8	1.67	0.59
17:I:47:LEU:HD22	22:N:226:ILE:HG12	1.85	0.59
56:AC:125:ARG:HH11	88:A4:94:TYR:HB2	1.67	0.59
81:AA:976:A:H5''	91:AQ:1:ACE:H1	1.85	0.59
81:AA:798:C:H2'	81:AA:799:A:H8	1.68	0.59
81:AA:872:G:H2'	81:AA:873:G:C8	2.38	0.59
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.84	0.59
81:AA:798:C:H2'	81:AA:799:A:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:96:ASN:ND2	11:A:2709:A:H1'	2.19	0.58
9:8:99:ARG:HG2	39:e:83:LEU:HB3	1.84	0.58
81:AA:1562:G:H1'	81:AA:1583:MA6:H2	1.85	0.58
46:m:91:ALA:HA	46:m:94:ARG:HE	1.67	0.58
81:AA:1317:A:H3'	81:AA:1318:A:H8	1.69	0.58
6:5:143:PRO:HA	6:5:146:HIS:HD1	1.67	0.58
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.85	0.58
34:z:161:THR:HG23	34:z:230:ILE:HD12	1.86	0.58
88:A4:332:LEU:HD23	88:A4:368:SER:HB3	1.85	0.58
35:G:139:PRO:HA	35:G:142:LYS:HE3	1.84	0.58
11:A:2099:U:H2'	11:A:2100:C:C6	2.39	0.58
8:7:143:TRP:HE1	8:7:172:VAL:HG23	1.69	0.58
12:C:192:GLU:HA	12:C:227:ARG:HH12	1.69	0.58
35:G:132:VAL:HG23	35:G:172:ILE:HB	1.86	0.58
76:A0:71:LEU:HD11	76:A0:141:LEU:HD11	1.85	0.58
81:AA:1131:C:H2'	81:AA:1132:U:C6	2.39	0.58
81:AA:1239:C:H2'	81:AA:1240:A:H8	1.68	0.58
88:A4:562:GLN:HG2	88:A4:564:ILE:HG22	1.86	0.58
8:7:204:LYS:HE2	84:a:92:LEU:HD22	1.86	0.57
67:AO:208:PRO:HG2	67:AO:213:LEU:HD21	1.85	0.57
81:AA:1239:C:H2'	81:AA:1240:A:C8	2.39	0.57
11:A:2352:U:H3	11:A:2361:G:H1	1.53	0.57
12:C:152:ALA:HA	12:C:290:ILE:HG12	1.86	0.57
61:AH:70:ASP:HA	88:A4:62:LYS:HE3	1.87	0.57
68:AP:54:MET:HE2	70:AS:64:TRP:HB3	1.86	0.57
81:AA:922:C:H2'	81:AA:923:A:C8	2.39	0.57
81:AA:1012:A:H2'	81:AA:1013:A:C8	2.39	0.57
9:8:136:ILE:HD11	52:f:169:ILE:HG23	1.85	0.57
81:AA:916:C:H2'	81:AA:917:C:C6	2.39	0.57
89:AX:366:LEU:HD22	89:AX:398:LEU:HD22	1.86	0.57
92:B:30:A:H2'	92:B:31:A:H8	1.69	0.57
73:AV:68:SER:N	81:AA:1523:A:H5''	2.20	0.57
81:AA:839:A:H2'	81:AA:840:A:H8	1.68	0.57
81:AA:1007:G:H2'	81:AA:1008:A:H8	1.69	0.57
81:AA:1452:U:H2'	81:AA:1453:A:H8	1.70	0.57
81:AA:1578:A:H2'	81:AA:1579:C:C6	2.40	0.57
85:Ax:47:U:H3	85:Ax:58:U:H3	1.52	0.57
92:B:23:A:H2'	92:B:24:G:C8	2.40	0.57
11:A:1936:A:H4'	11:A:1937:A:C8	2.40	0.57
55:AB:81:VAL:HG12	74:AW:83:MET:HE1	1.87	0.56
77:A1:134:PRO:HG3	88:A4:60:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AA:1033:U:H2'	81:AA:1034:U:C6	2.40	0.56
81:AA:838:U:H2'	81:AA:839:A:H8	1.70	0.56
11:A:2718:C:H2'	11:A:2991:U:H4'	1.87	0.56
34:z:214:LEU:HB3	34:z:217:LYS:HB3	1.86	0.56
73:AV:229:ALA:HB1	73:AV:286:VAL:HG11	1.88	0.56
81:AA:739:C:H2'	81:AA:740:G:O4'	2.05	0.56
87:Aw:9:A:H1'	87:Aw:45:A:H2'	1.87	0.56
34:z:184:ILE:HG22	34:z:209:ARG:HH21	1.69	0.56
81:AA:730:A:H61	81:AA:744:A:H1'	1.70	0.56
35:G:148:GLU:O	35:G:152:TYR:HB3	2.05	0.56
76:A0:165:PRO:HG3	76:A0:190:MET:HE2	1.87	0.56
81:AA:1589:C:H2'	81:AA:1590:A:C8	2.40	0.56
81:AA:686:A:H2'	81:AA:687:G:H8	1.71	0.56
81:AA:871:A:H4'	81:AA:872:G:H5'	1.86	0.56
81:AA:985:U:H2'	81:AA:986:G:H8	1.70	0.56
81:AA:852:A:H3'	81:AA:853:C:H6	1.70	0.56
81:AA:1400:U:H2'	81:AA:1401:G:C8	2.41	0.56
17:I:164:MET:HE2	17:I:168:LEU:HD11	1.87	0.55
81:AA:1408:A:H2'	81:AA:1409:A:H8	1.70	0.55
11:A:2740:A:H2'	11:A:2741:A:H8	1.70	0.55
36:V:168:GLU:HB3	83:OX:374:MET:HE1	1.88	0.55
34:z:180:GLY:HA2	34:z:203:ILE:HD12	1.88	0.55
34:z:198:VAL:HB	34:z:230:ILE:HG23	1.88	0.55
55:AB:192:LEU:HD11	55:AB:220:VAL:HG23	1.89	0.55
81:AA:1138:G:H2'	81:AA:1139:A:H8	1.71	0.55
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.41	0.55
12:C:201:VAL:HG22	12:C:205:ARG:HH22	1.71	0.55
38:d:52:THR:HG23	38:d:55:GLU:H	1.71	0.55
73:AV:117:LEU:HA	73:AV:122:GLN:OE1	2.06	0.55
81:AA:1002:C:H2'	81:AA:1003:A:C8	2.41	0.55
81:AA:1349:U:H2'	81:AA:1350:G:C8	2.41	0.55
11:A:3150:U:H2'	11:A:3151:A:C8	2.42	0.55
11:A:2727:C:H2'	11:A:2728:C:C6	2.42	0.55
17:I:101:ASN:HB3	17:I:150:HIS:HB3	1.88	0.55
81:AA:1161:A:H2'	81:AA:1162:A:C8	2.42	0.55
81:AA:1025:A:H2'	81:AA:1026:A:C8	2.41	0.55
11:A:1952:U:H2'	11:A:1953:A:C8	2.42	0.55
12:C:209:MET:HE3	12:C:212:GLU:HB2	1.88	0.55
22:N:124:VAL:HA	22:N:158:ARG:HH21	1.72	0.55
1:0:138:ARG:HB3	11:A:2321:A:C8	2.42	0.54
18:J:56:ARG:HD3	18:J:80:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e:118:GLN:HG2	89:AX:213:ARG:HH12	1.70	0.54
73:AV:70:LEU:HD21	73:AV:390:ILE:HD13	1.89	0.54
11:A:2748:A:H2'	11:A:2749:A:H8	1.72	0.54
69:AR:276:VAL:HG21	69:AR:303:LEU:HD22	1.90	0.54
81:AA:1003:A:H2'	81:AA:1004:G:C8	2.41	0.54
81:AA:1132:U:H2'	81:AA:1133:C:C6	2.41	0.54
9:8:192:TYR:HE1	52:f:134:VAL:HG22	1.73	0.54
75:AZ:10:ARG:HH12	77:A1:239:TRP:CD1	2.26	0.54
85:Ax:40:A:H2'	85:Ax:41:A:C8	2.43	0.54
18:J:88:SER:HA	18:J:151:LEU:HD11	1.88	0.54
81:AA:1042:U:H2'	81:AA:1043:C:C6	2.42	0.54
12:C:84:LEU:HD11	12:C:117:MET:HE3	1.89	0.54
57:AD:310:LYS:HA	57:AD:331:ASP:OD2	2.07	0.54
71:AT:29:VAL:HB	71:AT:79:TYR:HB2	1.90	0.54
12:C:204:GLU:O	12:C:208:GLU:HG2	2.08	0.54
11:A:2318:A:H2'	11:A:2319:A:C8	2.42	0.54
73:AV:76:ILE:HD12	73:AV:112:TRP:HD1	1.72	0.54
87:Aw:66:U:H2'	87:Aw:67:U:C6	2.43	0.54
23:O:44:ALA:HB3	23:O:49:VAL:HG23	1.90	0.54
81:AA:1470:A:H2'	81:AA:1471:A:H8	1.72	0.54
11:A:1851:G:H2'	11:A:2693:A:N7	2.23	0.53
13:D:109:PHE:HB3	13:D:204:ALA:HB3	1.90	0.53
80:AY:290:ASN:HA	88:A4:446:LYS:HD3	1.90	0.53
81:AA:833:A:H2'	81:AA:834:G:C8	2.43	0.53
67:AO:150:LEU:O	67:AO:154:ILE:HD12	2.08	0.53
67:AO:183:ALA:HA	69:AR:183:LYS:HE2	1.89	0.53
40:g:128:LEU:HD23	40:g:131:LEU:HD12	1.90	0.53
73:AV:263:MET:HE1	73:AV:334:PHE:HD1	1.73	0.53
11:A:3089:A:H3'	11:A:3090:G:C5'	2.39	0.53
11:A:3199:U:H5''	11:A:3200:U:H4'	1.91	0.53
58:AE:26:ILE:HG23	58:AE:36:VAL:HG21	1.90	0.53
81:AA:1161:A:H2'	81:AA:1162:A:H8	1.73	0.53
17:I:140:TYR:HB3	17:I:143:LEU:HD12	1.91	0.53
20:L:32:ILE:HD11	20:L:103:ASN:HB3	1.89	0.53
81:AA:1006:U:H2'	81:AA:1007:G:H8	1.73	0.53
35:G:132:VAL:HG12	35:G:197:LEU:HB3	1.91	0.53
73:AV:163:VAL:O	73:AV:167:VAL:HG23	2.09	0.53
89:AX:312:GLN:HE21	89:AX:318:LYS:HB2	1.74	0.53
81:AA:1471:A:H2'	81:AA:1472:G:C8	2.43	0.53
92:B:29:C:H2'	92:B:30:A:H8	1.73	0.53
39:e:265:LYS:HZ3	92:B:76:A:H8	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:AL:126:GLU:HB3	64:AL:181:ILE:HD11	1.90	0.53
81:AA:868:C:H2'	81:AA:869:C:H6	1.74	0.53
89:AX:266:ASN:HA	89:AX:329:LEU:HD23	1.91	0.53
7:6:175:VAL:HG22	7:6:204:VAL:HG13	1.90	0.53
11:A:2093:U:H2'	11:A:2094:G:C8	2.44	0.53
21:M:44:ARG:HG3	21:M:45:ARG:HG3	1.90	0.53
34:z:119:GLN:HB2	34:z:260:LEU:HD12	1.91	0.53
52:f:127:MET:HB2	52:f:154:GLU:HB3	1.91	0.53
73:AV:233:LYS:HB2	73:AV:286:VAL:HG21	1.91	0.53
81:AA:854:U:H2'	81:AA:855:A:C8	2.43	0.53
66:AN:28:VAL:HG21	66:AN:66:LEU:HD11	1.91	0.53
81:AA:1359:U:H2'	81:AA:1360:G:H8	1.74	0.53
81:AA:1471:A:H2'	81:AA:1472:G:H8	1.74	0.53
38:d:208:VAL:HG22	38:d:253:THR:HG23	1.91	0.52
89:AX:85:PRO:HA	89:AX:88:VAL:HG12	1.91	0.52
38:d:108:ARG:HA	38:d:111:ARG:HD2	1.90	0.52
74:AW:103:ARG:HE	74:AW:139:ARG:HH21	1.57	0.52
86:Ay:6:A:H2'	86:Ay:7:A:C8	2.45	0.52
77:A1:134:PRO:HB2	77:A1:137:LEU:HD23	1.91	0.52
81:AA:1042:U:H2'	81:AA:1043:C:H6	1.73	0.52
81:AA:1129:U:H2'	81:AA:1130:G:H8	1.74	0.52
92:B:43:G:H2'	92:B:44:A:C8	2.43	0.52
11:A:2103:A:HO2'	33:Z:35:LYS:N	2.08	0.52
17:I:154:LEU:HD12	17:I:164:MET:HE3	1.91	0.52
69:AR:172:ILE:HD12	69:AR:189:ARG:HG2	1.92	0.52
81:AA:1347:G:H2'	81:AA:1348:G:C8	2.43	0.52
11:A:1857:U:H2'	11:A:1858:G:C8	2.45	0.52
11:A:3054:G:H2'	11:A:3055:U:C6	2.44	0.52
18:J:140:VAL:O	18:J:144:ILE:HG12	2.09	0.52
62:AJ:78:ARG:HG3	62:AJ:118:LEU:HD21	1.91	0.52
88:A4:302:VAL:HG21	88:A4:341:CYS:HB3	1.91	0.52
52:f:134:VAL:HG12	52:f:147:ASP:HB3	1.90	0.52
59:AF:224:HIS:HB3	59:AF:228:LYS:HZ1	1.74	0.52
64:AL:175:TYR:HB2	66:AN:89:GLY:HA3	1.90	0.52
81:AA:799:A:H2'	81:AA:800:C:C6	2.44	0.52
11:A:1936:A:H4'	11:A:1937:A:N7	2.25	0.52
19:K:60:MET:HE2	19:K:133:ILE:HD11	1.92	0.52
52:f:171:LEU:HD13	52:f:174:ILE:HD11	1.91	0.52
73:AV:70:LEU:HD22	73:AV:389:LEU:HG	1.91	0.52
81:AA:1432:U:H2'	81:AA:1433:A:H8	1.73	0.52
88:A4:494:ILE:HD11	88:A4:527:LEU:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:V:102:MET:HE3	38:d:48:PRO:HG2	1.91	0.52
39:e:183:THR:HG23	39:e:186:GLY:N	2.21	0.52
73:AV:175:VAL:HG12	73:AV:177:SER:H	1.75	0.52
11:A:2006:C:H2'	11:A:2007:U:C6	2.46	0.52
11:A:2529:U:OP2	13:D:208:ARG:HD2	2.10	0.52
73:AV:103:TYR:HA	81:AA:1525:C:H5	1.75	0.52
81:AA:1427:A:H2'	81:AA:1428:G:C8	2.45	0.52
11:A:2055:U:H2'	11:A:2056:G:H8	1.75	0.51
16:H:163:THR:HG21	34:z:86:VAL:HG23	1.92	0.51
49:q:164:LEU:HD13	49:q:168:VAL:HG11	1.92	0.51
35:t:64:ILE:HD11	35:u:82:LEU:HB2	1.91	0.51
81:AA:1373:U:H2'	81:AA:1374:A:H8	1.75	0.51
12:C:223:ASP:HB3	12:C:229:VAL:HG11	1.92	0.51
54:s:145:VAL:HG21	54:s:187:LEU:HD11	1.92	0.51
11:A:1935:A:H2'	11:A:1936:A:O4'	2.11	0.51
11:A:2174:G:H4'	18:J:151:LEU:HD23	1.90	0.51
13:D:109:PHE:CE1	13:D:208:ARG:HD3	2.45	0.51
62:AJ:58:LEU:HB3	62:AJ:85:LEU:HD12	1.92	0.51
64:AL:209:LEU:HD12	78:A3:189:TRP:CE2	2.45	0.51
81:AA:1398:U:H2'	81:AA:1399:A:C8	2.43	0.51
57:AD:100:LYS:HG2	81:AA:1262:C:H4'	1.92	0.51
72:AU:64:ARG:HA	72:AU:67:VAL:HG12	1.92	0.51
73:AV:226:TYR:CZ	73:AV:282:VAL:HG11	2.46	0.51
81:AA:832:U:H2'	81:AA:833:A:C8	2.46	0.51
81:AA:832:U:H2'	81:AA:833:A:H8	1.76	0.51
81:AA:1132:U:H2'	81:AA:1133:C:H6	1.76	0.51
12:C:268:LEU:HD23	12:C:272:ASP:HB3	1.92	0.51
79:Az:28:U:H1'	88:A4:414:LYS:HG2	1.92	0.51
81:AA:686:A:H2'	81:AA:687:G:C8	2.45	0.51
81:AA:708:C:H2'	81:AA:709:G:C8	2.45	0.51
7:6:161:LEU:HD23	7:6:300:THR:HG21	1.91	0.51
11:A:1868:G:H2'	21:M:40:PRO:HG3	1.91	0.51
12:C:217:ASP:HB2	12:C:233:ILE:HB	1.92	0.51
88:A4:571:TRP:HE3	88:A4:576:LEU:HD21	1.75	0.51
61:AH:122:GLN:HG3	81:AA:1265:C:H4'	1.93	0.51
73:AV:57:MET:HE1	73:AV:91:TYR:HB3	1.93	0.51
76:A0:64:LEU:HD12	76:A0:139:TRP:CD2	2.45	0.51
76:A0:68:LEU:HD21	76:A0:80:VAL:HG21	1.91	0.51
81:AA:1175:G:H2'	81:AA:1176:G:H8	1.75	0.51
81:AA:1200:G:C2	81:AA:1201:A:C8	2.99	0.51
11:A:2727:C:H2'	11:A:2728:C:H6	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:M:244:LEU:HD12	21:M:245:PRO:HD2	1.91	0.51
65:AM:114:ARG:NH2	67:AO:236:PRO:HD2	2.26	0.51
66:AN:21:LYS:HB3	81:AA:777:G:H5''	1.92	0.51
81:AA:865:A:H2'	81:AA:866:A:C8	2.46	0.51
81:AA:1408:A:H2'	81:AA:1409:A:C8	2.46	0.51
85:Ax:15:A:O2'	85:Ax:16:A:H5'	2.11	0.51
15:F:175:LYS:HG2	15:F:273:LEU:HD13	1.93	0.51
79:Az:30:A:H2'	79:Az:31:A:C4	2.46	0.51
11:A:2748:A:H2'	11:A:2749:A:C8	2.46	0.51
11:A:3078:C:H2'	11:A:3079:G:C8	2.46	0.51
12:C:110:GLU:HA	12:C:113:ARG:HD3	1.93	0.51
6:5:165:GLN:NE2	6:5:175:THR:HG22	2.26	0.50
11:A:2545:U:H5''	11:A:2546:G:H5'	1.93	0.50
31:X:20:ILE:HG22	83:OX:434:LEU:HD23	1.93	0.50
73:AV:66:PRO:HD3	81:AA:1529:A:H1'	1.93	0.50
81:AA:845:A:H2'	81:AA:846:A:C8	2.43	0.50
11:A:2415:C:H3'	54:s:165:ARG:NH2	2.26	0.50
13:D:205:GLN:HA	13:D:208:ARG:HH21	1.77	0.50
38:d:217:HIS:CD2	38:d:243:LEU:HB2	2.47	0.50
81:AA:673:U:H2'	81:AA:674:U:C6	2.47	0.50
83:OX:376:ARG:HG2	83:OX:379:ARG:HH22	1.77	0.50
89:AX:210:TRP:HZ2	89:AX:225:VAL:HG23	1.75	0.50
16:H:174:VAL:HG12	16:H:192:HIS:HB3	1.92	0.50
73:AV:250:ILE:HG23	73:AV:252:LYS:H	1.76	0.50
81:AA:1504:U:H2'	81:AA:1505:A:C8	2.47	0.50
57:AD:335:LYS:HE2	81:AA:649:A:H3'	1.91	0.50
81:AA:956:C:H2'	81:AA:957:C:O4'	2.11	0.50
81:AA:1348:G:H2'	81:AA:1349:U:C6	2.46	0.50
92:B:68:C:H2'	92:B:69:U:C6	2.46	0.50
11:A:2109:A:H5'	22:N:133:ARG:HD3	1.94	0.50
34:z:170:ALA:HA	34:z:231:PRO:HG3	1.93	0.50
81:AA:985:U:H2'	81:AA:986:G:C8	2.46	0.50
81:AA:1461:A:H4'	81:AA:1462:G:C8	2.47	0.50
86:Ay:2:A:H2'	86:Ay:3:G:H8	1.77	0.50
92:B:25:C:H2'	92:B:26:A:H8	1.77	0.50
23:O:50:ASP:HB2	23:O:107:MET:HE1	1.93	0.50
73:AV:103:TYR:CZ	81:AA:1524:A:H4'	2.47	0.50
81:AA:853:C:H2'	81:AA:854:U:C6	2.47	0.50
11:A:2082:G:H2'	11:A:2083:U:O4'	2.11	0.50
11:A:2277:U:H2'	11:A:2278:A:H8	1.76	0.50
12:C:191:VAL:HG11	12:C:251:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:z:108:LYS:O	34:z:112:LEU:HB2	2.11	0.50
56:AC:98:GLY:HA3	75:AZ:71:TYR:CE1	2.47	0.50
57:AD:258:ILE:HD11	57:AD:343:LEU:HD22	1.92	0.50
81:AA:1470:A:H2'	81:AA:1471:A:C8	2.46	0.50
2:1:55:LEU:HD13	49:q:132:ILE:HD13	1.94	0.50
7:6:255:LEU:HD12	7:6:256:PRO:HD2	1.94	0.50
37:b:89:ILE:HA	37:b:92:LYS:HD2	1.94	0.50
38:d:204:ASN:O	38:d:205:GLN:HG2	2.12	0.50
59:AF:201:MET:HA	59:AF:204:LYS:HE2	1.94	0.50
70:AS:134:ARG:HG2	70:AS:136:GLY:H	1.77	0.50
81:AA:1577:U:H2'	81:AA:1578:A:C8	2.47	0.50
89:AX:284:PRO:HA	89:AX:287:LEU:HD23	1.93	0.50
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.92	0.49
39:e:164:LYS:HE2	39:e:167:ASP:HA	1.94	0.49
46:m:69:ARG:HG3	46:m:70:GLU:HG2	1.93	0.49
60:AG:87:HIS:O	60:AG:91:MET:HG2	2.12	0.49
76:A0:99:ARG:HD3	81:AA:1526:U:H2'	1.93	0.49
88:A4:156:ALA:O	88:A4:160:ARG:HG2	2.12	0.49
88:A4:263:ILE:HG13	88:A4:278:LEU:HD23	1.94	0.49
88:A4:349:ALA:HB3	88:A4:378:LEU:HD11	1.94	0.49
2:1:41:LEU:HD23	2:1:43:LEU:HD11	1.94	0.49
11:A:1737:A:H61	11:A:1760:G:H1'	1.77	0.49
12:C:189:ILE:HB	12:C:232:PHE:HB2	1.94	0.49
61:AH:137:ARG:HG3	63:AK:124:GLN:NE2	2.27	0.49
63:AK:103:ARG:HD2	63:AK:104:TRP:CZ2	2.47	0.49
75:AZ:56:HIS:O	75:AZ:60:GLU:HG3	2.11	0.49
35:G:138:LYS:HB2	35:G:141:ASP:HB2	1.92	0.49
39:e:218:PRO:HG3	92:B:75:C:H2'	1.93	0.49
52:f:80:ILE:HG23	52:f:90:VAL:HG12	1.93	0.49
52:f:119:ILE:HD11	52:f:166:PHE:HE2	1.76	0.49
73:AV:81:SER:HB3	73:AV:84:GLU:HG3	1.94	0.49
81:AA:708:C:H2'	81:AA:709:G:H8	1.77	0.49
81:AA:1033:U:H2'	81:AA:1034:U:H6	1.77	0.49
81:AA:1365:A:H4'	81:AA:1389:G:H4'	1.95	0.49
81:AA:1382:A:H5''	89:AX:166:ARG:HH21	1.77	0.49
81:AA:1498:C:H2'	81:AA:1499:U:H6	1.78	0.49
9:8:117:LEU:HD11	39:e:69:GLU:HB3	1.94	0.49
11:A:2151:A:H2'	11:A:2152:A:C8	2.47	0.49
13:D:207:ILE:HG12	13:D:229:PRO:HD3	1.93	0.49
17:I:116:LEU:HG	17:I:121:ILE:HB	1.95	0.49
81:AA:1469:G:H2'	81:AA:1470:A:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3078:C:H2'	11:A:3079:G:H8	1.76	0.49
86:Ay:66:U:H2'	86:Ay:67:U:C6	2.48	0.49
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.93	0.49
6:5:299:LEU:HB3	6:5:301:PRO:HD2	1.94	0.49
16:H:98:LEU:HD11	16:H:105:VAL:HG23	1.94	0.49
44:k:18:VAL:HG11	44:k:34:LEU:HB2	1.93	0.49
50:r:99:MET:HE1	50:r:115:ILE:HG22	1.94	0.49
74:AW:144:LEU:HD23	74:AW:167:ALA:HB2	1.95	0.49
7:6:106:ARG:HG2	24:P:110:TRP:CE2	2.48	0.49
13:D:172:MET:HE1	58:AE:86:ILE:HG12	1.95	0.49
51:c:228:LEU:HB2	51:c:307:PHE:CD2	2.45	0.49
64:AL:209:LEU:HD13	78:A3:173:LEU:HD12	1.94	0.49
81:AA:776:A:H4'	81:AA:777:G:H5'	1.93	0.49
81:AA:1577:U:H2'	81:AA:1578:A:H8	1.78	0.49
66:AN:98:LYS:HE2	66:AN:109:PRO:HA	1.93	0.49
81:AA:1175:G:H2'	81:AA:1176:G:C8	2.48	0.49
11:A:1906:G:H2'	11:A:2014:A:H61	1.78	0.49
12:C:203:LEU:HD13	12:C:230:PHE:HE1	1.77	0.49
35:G:133:ARG:HA	35:G:171:GLU:HA	1.94	0.49
69:AR:207:PRO:HB2	69:AR:209:ILE:HG22	1.95	0.49
73:AV:148:MET:HE2	73:AV:185:VAL:HG21	1.93	0.49
81:AA:839:A:H2'	81:AA:840:A:C8	2.47	0.49
81:AA:1138:G:H2'	81:AA:1139:A:C8	2.48	0.49
10:9:68:PHE:CE2	10:9:70:LEU:HB2	2.48	0.49
11:A:2409:A:H2'	11:A:2410:U:C6	2.48	0.49
17:I:197:LEU:HD22	35:u:76:LEU:HD12	1.94	0.49
34:z:290:VAL:HG11	34:z:307:ILE:HD13	1.95	0.49
35:G:131:THR:HA	35:G:174:ALA:HA	1.94	0.49
35:G:188:LEU:HA	35:G:191:VAL:HG12	1.94	0.49
92:B:74:C:H2'	92:B:75:C:O4'	2.13	0.49
27:S:96:PHE:HB3	37:b:126:ILE:HD13	1.94	0.48
27:S:173:ARG:HB2	27:S:182:LYS:HG3	1.94	0.48
34:z:157:VAL:HG22	34:z:196:PHE:HB3	1.95	0.48
61:AH:164:LEU:HD13	61:AH:170:MET:HE3	1.95	0.48
81:AA:1034:U:H2'	81:AA:1035:U:C6	2.48	0.48
22:N:101:HIS:CD2	22:N:184:PRO:HD3	2.49	0.48
59:AF:172:VAL:HG12	59:AF:240:ARG:HD3	1.94	0.48
61:AH:76:LEU:HB2	61:AH:145:LEU:HB2	1.95	0.48
63:AK:55:ASN:HA	63:AK:58:ARG:HD3	1.95	0.48
67:AO:97:ARG:HH12	81:AA:870:C:H3'	1.78	0.48
76:A0:163:SER:HB3	76:A0:190:MET:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AA:861:U:H2'	81:AA:862:A:H8	1.78	0.48
81:AA:867:C:H2'	81:AA:870:C:N4	2.28	0.48
81:AA:1177:C:H2'	81:AA:1178:G:H8	1.79	0.48
81:AA:1349:U:H2'	81:AA:1350:G:H8	1.76	0.48
88:A4:166:VAL:HG12	88:A4:194:LEU:HG	1.95	0.48
11:A:2894:U:H5''	11:A:2895:U:O4'	2.13	0.48
16:H:98:LEU:HD23	16:H:129:ALA:HB2	1.94	0.48
54:s:63:ILE:HA	54:s:66:TRP:CD1	2.48	0.48
81:AA:1119:U:H2'	81:AA:1120:C:O4'	2.13	0.48
81:AA:1373:U:H2'	81:AA:1374:A:C8	2.47	0.48
11:A:3112:A:C6	11:A:3200:U:O2	2.67	0.48
50:r:70:CYS:HB3	98:r:201:FES:S2	2.53	0.48
86:Ay:66:U:H2'	86:Ay:67:U:H6	1.78	0.48
88:A4:196:CYS:HB3	88:A4:265:GLY:HA3	1.95	0.48
6:5:113:LEU:HD12	6:5:311:ALA:HB1	1.95	0.48
11:A:2668:A:H2'	11:A:2669:A:C8	2.48	0.48
38:d:269:TRP:CD1	38:d:269:TRP:H	2.32	0.48
58:AE:96:HIS:HB3	58:AE:99:THR:HG23	1.96	0.48
73:AV:149:ASP:HA	73:AV:152:ILE:HG22	1.95	0.48
81:AA:982:A:H2'	81:AA:983:C:C6	2.49	0.48
88:A4:335:PHE:CG	88:A4:360:MET:HE2	2.48	0.48
88:A4:429:LEU:HA	88:A4:464:LEU:HD21	1.94	0.48
11:A:3024:U:H2'	11:A:3025:A:H8	1.79	0.48
57:AD:302:HIS:HB2	57:AD:337:SER:HB2	1.95	0.48
81:AA:915:C:H2'	81:AA:916:C:C6	2.48	0.48
81:AA:996:A:H2'	81:AA:997:A:C8	2.49	0.48
81:AA:1502:A:H2'	81:AA:1503:G:O4'	2.14	0.48
11:A:2049:U:H2'	11:A:2050:A:H8	1.79	0.48
35:G:132:VAL:HA	35:G:197:LEU:HA	1.96	0.48
81:AA:1595:G:H2'	81:AA:1596:A:C8	2.48	0.48
89:AX:244:LEU:HD12	89:AX:292:ASN:HB3	1.95	0.48
11:A:1893:A:H4'	11:A:1894:G:H5'	1.95	0.48
59:AF:166:ARG:HD2	86:Ay:36:C:H42	1.78	0.48
64:AL:165:LYS:HE3	81:AA:947:U:H5''	1.95	0.48
81:AA:1396:C:H2'	81:AA:1397:U:C6	2.48	0.48
12:C:146:SER:HA	12:C:266:VAL:HG11	1.96	0.48
22:N:36:VAL:HG11	45:l:124:GLN:HB3	1.95	0.48
49:q:125:MET:HA	49:q:128:MET:HB2	1.96	0.48
60:AG:293:ILE:HB	60:AG:300:TYR:HB3	1.96	0.48
81:AA:946:U:H2'	81:AA:947:U:C6	2.49	0.48
81:AA:958:C:H4'	81:AA:959:C:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:143:LEU:HD23	17:I:146:LEU:HD13	1.95	0.47
51:c:59:ARG:HB2	51:c:62:GLU:HG2	1.95	0.47
61:AH:76:LEU:HD23	61:AH:174:LYS:HA	1.96	0.47
81:AA:838:U:H2'	81:AA:839:A:C8	2.47	0.47
81:AA:1032:C:H2'	81:AA:1033:U:H6	1.79	0.47
81:AA:1504:U:H2'	81:AA:1505:A:H8	1.78	0.47
88:A4:89:PHE:HZ	88:A4:103:SER:HB2	1.79	0.47
88:A4:302:VAL:HG11	88:A4:341:CYS:HB3	1.96	0.47
88:A4:598:LEU:HD23	88:A4:601:LYS:HD2	1.95	0.47
15:F:123:GLY:HA3	15:F:142:ARG:HG2	1.95	0.47
46:m:51:LEU:HD12	46:m:67:ARG:HB3	1.95	0.47
81:AA:1231:A:H1'	81:AA:1236:C:N4	2.29	0.47
88:A4:414:LYS:HE3	88:A4:453:HIS:HE1	1.79	0.47
19:K:178:LEU:HD12	50:r:100:LEU:HD21	1.95	0.47
59:AF:88:ASP:HB3	59:AF:91:ILE:HB	1.96	0.47
81:AA:865:A:H2'	81:AA:866:A:H8	1.78	0.47
11:A:2081:U:H2'	11:A:2082:G:C8	2.49	0.47
11:A:2585:G:H2'	11:A:2586:U:C6	2.50	0.47
18:J:25:ARG:HD2	45:l:56:LEU:HB3	1.94	0.47
31:X:166:LEU:HD13	31:X:196:ILE:HD11	1.96	0.47
81:AA:842:C:H2'	81:AA:843:G:C8	2.49	0.47
89:AX:88:VAL:HA	89:AX:91:VAL:HG22	1.96	0.47
4:3:175:ASP:HB3	4:3:178:GLN:HB2	1.96	0.47
15:F:53:LEU:HD11	15:F:271:ASP:HA	1.97	0.47
58:AE:92:ASN:HB2	68:AP:117:MET:HE3	1.96	0.47
77:A1:162:SER:HA	88:A4:134:GLU:HB2	1.96	0.47
81:AA:871:A:H1'	81:AA:872:G:C8	2.49	0.47
81:AA:1528:A:H2'	81:AA:1529:A:C8	2.44	0.47
11:A:1765:C:H5'	42:i:75:ARG:HH22	1.80	0.47
11:A:2245:A:H4'	11:A:2246:A:OP1	2.14	0.47
11:A:2677:A:H2'	11:A:2678:A:C8	2.49	0.47
38:d:88:TYR:OH	38:d:91:PRO:HD3	2.14	0.47
35:t:64:ILE:HA	35:t:67:LEU:HD12	1.96	0.47
70:AS:51:VAL:HG13	90:A2:117:LEU:HD11	1.97	0.47
81:AA:1578:A:H2'	81:AA:1579:C:H6	1.78	0.47
22:N:218:ILE:HG23	22:N:223:MET:HB2	1.95	0.47
49:q:152:ARG:O	49:q:156:LEU:HG	2.13	0.47
56:AC:100:PHE:HB3	56:AC:103:CYS:HB2	1.97	0.47
56:AC:136:VAL:HG22	56:AC:153:LEU:HD22	1.96	0.47
81:AA:951:G:H2'	81:AA:952:A:H8	1.80	0.47
92:B:9:1MA:N3	92:B:45:G:H2'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:333:ALA:HB1	6:5:363:ASP:HA	1.97	0.47
11:A:2728:C:H2'	11:A:2729:U:H6	1.79	0.47
48:o:12:ILE:HG13	48:o:23:ARG:HB2	1.97	0.47
65:AM:29:ARG:HE	71:AT:147:VAL:HB	1.80	0.47
81:AA:681:U:H2'	81:AA:682:A:C8	2.49	0.47
81:AA:913:A:H2'	81:AA:914:A:C8	2.50	0.47
81:AA:965:C:C4	81:AA:1022:A:H4'	2.50	0.47
85:Ax:25:C:H2'	85:Ax:26:G:H8	1.80	0.47
88:A4:646:THR:O	88:A4:650:MET:HG2	2.15	0.47
11:A:2586:U:H2'	11:A:2587:G:H8	1.79	0.47
11:A:3064:A:H5''	11:A:3065:U:H5'	1.97	0.47
65:AM:96:PHE:HD1	76:A0:169:LEU:HD22	1.80	0.47
71:AT:80:LEU:HD12	71:AT:84:GLU:HB3	1.95	0.47
77:A1:45:GLU:HG2	77:A1:47:PRO:HD2	1.97	0.47
81:AA:913:A:H2'	81:AA:914:A:H8	1.80	0.47
81:AA:1377:C:H5''	89:AX:320:ARG:HD3	1.97	0.47
81:AA:1455:U:H2'	81:AA:1456:U:C6	2.50	0.47
88:A4:377:ARG:NH2	88:A4:418:SER:HA	2.30	0.47
88:A4:532:LEU:HD11	88:A4:555:ILE:HG21	1.95	0.47
89:AX:80:PRO:HG2	89:AX:81:HIS:HD2	1.80	0.47
89:AX:159:HIS:HA	89:AX:162:VAL:HG12	1.97	0.47
11:A:2868:C:H2'	11:A:2869:A:O4'	2.15	0.47
33:Z:70:THR:HG22	33:Z:97:PRO:HA	1.96	0.47
57:AD:420:SER:HA	81:AA:929:A:H4'	1.97	0.47
59:AF:167:PHE:HB2	86:Ay:33:U:H4'	1.96	0.47
73:AV:225:LEU:HD13	73:AV:275:LEU:HD21	1.95	0.47
74:AW:104:ILE:HD13	74:AW:138:THR:HB	1.97	0.47
86:Ay:52:G:H2'	86:Ay:53:G:C8	2.49	0.47
11:A:1977:U:H2'	11:A:1978:A:H8	1.81	0.46
16:H:174:VAL:HG23	16:H:237:VAL:HA	1.96	0.46
17:I:61:HIS:CD2	17:I:62:PRO:HD2	2.49	0.46
21:M:226:PRO:HB3	53:p:58:ALA:HB2	1.96	0.46
39:e:52:CYS:HB3	39:e:235:LYS:HA	1.96	0.46
39:e:257:LYS:HE2	39:e:273:ARG:HE	1.79	0.46
51:c:105:ARG:HH12	51:c:115:VAL:HB	1.80	0.46
81:AA:1034:U:H2'	81:AA:1035:U:H6	1.80	0.46
38:d:217:HIS:HD2	38:d:243:LEU:HB2	1.79	0.46
39:e:85:SER:HB3	46:m:50:ARG:HB3	1.96	0.46
71:AT:118:GLU:HA	71:AT:121:LYS:HD3	1.98	0.46
81:AA:847:G:H2'	81:AA:848:U:C6	2.50	0.46
81:AA:875:U:H2'	81:AA:876:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AA:1414:C:H3'	81:AA:1415:G:H21	1.79	0.46
85:Ax:47:U:H2'	85:Ax:48:G:C8	2.50	0.46
11:A:2331:C:H3'	11:A:2332:C:O4'	2.15	0.46
11:A:2803:A:H2'	11:A:2804:A:O4'	2.15	0.46
14:E:87:ILE:HG23	14:E:317:PRO:HD3	1.97	0.46
81:AA:833:A:H2'	81:AA:834:G:H8	1.80	0.46
4:3:115:LEU:HB2	21:M:83:PHE:HB3	1.97	0.46
6:5:289:HIS:O	6:5:343:GLN:HG2	2.15	0.46
8:7:276:PHE:HB2	8:7:304:VAL:HG22	1.98	0.46
11:A:2182:G:H2'	11:A:2183:C:C6	2.50	0.46
11:A:2942:C:H2'	11:A:2943:G:H8	1.81	0.46
38:d:186:VAL:HG21	38:d:239:PRO:HB3	1.98	0.46
41:h:140:PHE:HB2	41:h:156:TRP:CD2	2.50	0.46
81:AA:981:C:H2'	81:AA:982:A:H8	1.80	0.46
81:AA:1076:5MU:H2'	81:AA:1076:5MU:O2	2.16	0.46
81:AA:1156:C:H2'	81:AA:1157:U:H6	1.79	0.46
81:AA:1488:5MC:H2'	81:AA:1489:G:C8	2.51	0.46
86:Ay:65:C:H2'	86:Ay:66:U:C6	2.51	0.46
9:8:142:ALA:HA	39:e:274:ARG:HH21	1.81	0.46
9:8:191:ARG:NE	52:f:135:LEU:HG	2.30	0.46
65:AM:105:THR:OG1	72:AU:56:LEU:HD13	2.15	0.46
81:AA:921:U:H2'	81:AA:922:C:O4'	2.16	0.46
81:AA:1014:A:H4'	82:AI:184:ASN:CG	2.41	0.46
81:AA:1021:U:H4'	81:AA:1022:A:H5'	1.98	0.46
81:AA:1203:C:H2'	81:AA:1204:C:H6	1.78	0.46
81:AA:1244:C:H2'	81:AA:1245:U:C6	2.51	0.46
81:AA:1523:A:H2'	81:AA:1524:A:C8	2.51	0.46
86:Ay:1:U:H2'	86:Ay:2:A:C8	2.51	0.46
86:Ay:68:C:H2'	86:Ay:69:C:H6	1.79	0.46
92:B:56:U:H5''	92:B:58:A:N7	2.30	0.46
12:C:191:VAL:HG11	12:C:251:LEU:HB3	1.97	0.46
63:AK:86:ARG:HG2	81:AA:1233:C:O2	2.16	0.46
81:AA:1006:U:H2'	81:AA:1007:G:C8	2.49	0.46
81:AA:1452:U:H2'	81:AA:1453:A:C8	2.51	0.46
89:AX:120:PRO:HA	89:AX:302:HIS:HB3	1.97	0.46
2:1:20:MET:HE3	2:1:20:MET:HB3	1.76	0.46
26:R:114:LYS:HD3	84:a:44:ASN:HB3	1.97	0.46
52:f:138:GLN:HE22	52:f:143:LYS:HB2	1.81	0.46
62:AJ:42:PRO:HD3	81:AA:931:C:C2	2.51	0.46
81:AA:884:U:H2'	81:AA:885:U:C6	2.50	0.46
11:A:1911:C:H2'	11:A:1912:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:153:LEU:HD21	38:d:220:GLN:HB2	1.97	0.46
35:G:143:VAL:HA	35:G:146:ILE:HG12	1.98	0.46
67:AO:82:LYS:HB3	81:AA:881:A:N6	2.30	0.46
81:AA:1190:C:H2'	81:AA:1191:C:H6	1.81	0.46
11:A:2610:U:H2'	11:A:2611:C:C6	2.51	0.46
14:E:99:LEU:HD22	14:E:193:LEU:HB3	1.96	0.46
69:AR:128:MET:HE3	69:AR:269:GLY:HA3	1.98	0.46
81:AA:1399:A:H2'	81:AA:1400:U:C6	2.51	0.46
1:O:152:PRO:HG3	1:O:173:ARG:CZ	2.45	0.46
12:C:161:GLN:HG3	12:C:175:MET:HE1	1.98	0.46
15:F:243:ILE:HG22	49:q:27:ALA:HB2	1.98	0.46
64:AL:216:GLU:HG3	78:A3:186:PRO:HB3	1.96	0.46
69:AR:175:ARG:CZ	69:AR:181:LEU:HB2	2.46	0.46
77:A1:268:GLN:NE2	89:AX:120:PRO:HG3	2.29	0.46
81:AA:1203:C:H2'	81:AA:1204:C:C6	2.51	0.46
82:AI:110:ALA:HB3	82:AI:135:ALA:HB2	1.97	0.46
86:Ay:23:A:H2'	86:Ay:24:A:C8	2.51	0.46
7:6:44:ASN:HB2	7:6:47:ARG:HD2	1.98	0.45
60:AG:92:MET:HG3	77:A1:116:PRO:HG2	1.97	0.45
81:AA:1430:A:N1	81:AA:1458:A:H5''	2.31	0.45
8:7:156:ARG:HH12	8:7:260:PHE:HB2	1.80	0.45
11:A:2728:C:H2'	11:A:2729:U:C6	2.51	0.45
11:A:2854:U:H5''	11:A:2855:G:H5''	1.98	0.45
34:z:159:VAL:HB	34:z:177:PHE:O	2.16	0.45
81:AA:1354:A:H2'	81:AA:1355:G:C8	2.52	0.45
86:Ay:54:U:H2'	86:Ay:55:U:O4'	2.15	0.45
89:AX:265:ILE:HD12	89:AX:268:LEU:HD23	1.97	0.45
92:B:23:A:H2'	92:B:24:G:H8	1.80	0.45
11:A:2757:A:H2'	11:A:2758:G:O4'	2.16	0.45
17:I:64:CYS:O	17:I:65:LEU:HB2	2.17	0.45
17:I:203:VAL:HA	17:I:206:GLU:HB2	1.99	0.45
38:d:197:VAL:HG13	38:d:212:ILE:HG12	1.99	0.45
61:AH:124:VAL:HG13	81:AA:1264:C:H1'	1.98	0.45
76:A0:39:GLU:HG2	76:A0:40:THR:HG23	1.98	0.45
81:AA:1395:C:H2'	81:AA:1396:C:H6	1.82	0.45
6:5:242:ARG:HA	6:5:245:ILE:HD12	1.99	0.45
11:A:2127:A:H4'	11:A:2251:A:C5	2.51	0.45
11:A:3163:G:H2'	11:A:3164:C:H6	1.80	0.45
76:A0:145:HIS:CE1	76:A0:146:GLU:HG3	2.52	0.45
81:AA:1122:A:H2'	81:AA:1123:C:C6	2.51	0.45
81:AA:1590:A:H2'	81:AA:1591:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:A4:335:PHE:CE2	88:A4:360:MET:HB2	2.50	0.45
88:A4:392:ILE:HG13	88:A4:393:ILE:N	2.30	0.45
35:G:152:TYR:OH	35:G:173:LYS:HG3	2.17	0.45
49:q:40:PRO:HG2	49:q:51:GLN:HB3	1.99	0.45
55:AB:223:VAL:HG23	55:AB:237:PRO:HA	1.99	0.45
70:AS:48:ARG:HH22	81:AA:1119:U:P	2.40	0.45
73:AV:247:MET:HE2	73:AV:247:MET:HB3	1.79	0.45
73:AV:263:MET:HG2	73:AV:341:LEU:HD11	1.99	0.45
11:A:1839:C:H2'	11:A:1840:C:C6	2.52	0.45
11:A:2514:C:H2'	11:A:2515:U:H6	1.82	0.45
52:f:138:GLN:HE22	52:f:143:LYS:H	1.64	0.45
69:AR:194:GLN:HE22	69:AR:199:LYS:H	1.64	0.45
81:AA:911:U:H2'	81:AA:912:U:C6	2.51	0.45
81:AA:1509:U:H2'	81:AA:1510:U:C6	2.51	0.45
86:Ay:65:C:H2'	86:Ay:66:U:H6	1.82	0.45
86:Ay:68:C:H2'	86:Ay:69:C:C6	2.51	0.45
11:A:2042:U:H2'	11:A:2043:C:H6	1.81	0.45
18:J:18:GLY:HA3	18:J:42:ARG:HH12	1.82	0.45
81:AA:771:A:H2'	81:AA:772:A:C8	2.52	0.45
11:A:1886:G:H1	42:i:61:GLY:HA3	1.81	0.45
11:A:1952:U:H2'	11:A:1953:A:H8	1.78	0.45
38:d:197:VAL:HG22	38:d:212:ILE:HG23	1.98	0.45
49:q:152:ARG:HD3	49:q:153:ARG:NH1	2.32	0.45
35:u:64:ILE:O	35:u:68:VAL:HG23	2.17	0.45
55:AB:180:ARG:HE	57:AD:210:PRO:HG2	1.82	0.45
81:AA:1506:U:H2'	81:AA:1507:A:C8	2.52	0.45
85:Ax:3:U:H2'	85:Ax:4:A:C8	2.51	0.45
88:A4:393:ILE:HA	88:A4:396:ILE:HG22	1.99	0.45
9:8:136:ILE:HD11	52:f:169:ILE:CG2	2.47	0.45
12:C:159:LYS:HE3	87:Aw:66:U:H4'	1.99	0.45
19:K:27:PRO:HA	19:K:66:ALA:O	2.17	0.45
61:AH:72:LEU:HD12	77:A1:133:TRP:CZ3	2.52	0.45
63:AK:41:ARG:HA	63:AK:87:ILE:HD11	1.99	0.45
65:AM:73:ILE:O	65:AM:77:ILE:HG12	2.17	0.45
73:AV:322:THR:HG23	73:AV:325:SER:H	1.80	0.45
81:AA:922:C:H2'	81:AA:923:A:H8	1.80	0.45
81:AA:1402:A:H2'	81:AA:1403:A:C8	2.51	0.45
11:A:1862:U:H2'	11:A:1863:A:H8	1.81	0.45
11:A:2220:A:H5''	50:r:103:LYS:NZ	2.32	0.45
12:C:267:GLN:HG3	12:C:297:GLU:HG2	1.99	0.45
32:Y:234:LEU:HD22	36:V:48:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:G:144:LYS:HB3	35:G:191:VAL:HG22	1.99	0.45
61:AH:79:LEU:HD11	61:AH:140:TYR:HB3	1.98	0.45
81:AA:774:G:H2'	81:AA:775:C:C6	2.52	0.45
81:AA:1005:U:H4'	82:AI:87:HIS:ND1	2.32	0.45
81:AA:1348:G:H2'	81:AA:1349:U:H6	1.81	0.45
88:A4:352:PRO:O	88:A4:355:GLN:HG3	2.16	0.45
92:B:49:U:H2'	92:B:50:U:C6	2.52	0.45
6:5:118:LYS:HD3	6:5:254:GLU:HG2	2.00	0.44
12:C:180:ARG:NH1	12:C:181:HIS:HB3	2.32	0.44
62:AJ:62:VAL:HA	62:AJ:83:VAL:HG12	1.99	0.44
66:AN:12:TRP:HE3	66:AN:65:LEU:HD11	1.82	0.44
81:AA:1059:U:H2'	81:AA:1060:A:H8	1.82	0.44
81:AA:1396:C:H2'	81:AA:1397:U:H6	1.80	0.44
81:AA:1555:A:H2'	81:AA:1556:C:O4'	2.17	0.44
92:B:30:A:H2'	92:B:31:A:C8	2.52	0.44
4:3:106:THR:HG23	4:3:162:THR:HA	1.99	0.44
11:A:3024:U:H2'	11:A:3025:A:C8	2.53	0.44
57:AD:355:ARG:NH1	81:AA:1118:A:H4'	2.33	0.44
76:A0:82:ARG:HD3	76:A0:85:TRP:CE2	2.52	0.44
81:AA:676:G:H2'	81:AA:677:C:C6	2.52	0.44
81:AA:746:A:H2'	81:AA:747:A:H8	1.82	0.44
81:AA:969:A:H2'	81:AA:970:A:H8	1.82	0.44
81:AA:1485:G:H2'	81:AA:1486:B8T:O4'	2.18	0.44
11:A:2092:C:H2'	11:A:2093:U:C6	2.53	0.44
11:A:2382:A:H2'	11:A:2383:U:C6	2.53	0.44
54:s:184:LEU:HD23	54:s:184:LEU:HA	1.78	0.44
56:AC:125:ARG:NH1	88:A4:94:TYR:HB2	2.32	0.44
77:A1:152:ASP:CG	77:A1:174:ARG:HH12	2.25	0.44
77:A1:265:THR:HA	77:A1:268:GLN:HE21	1.81	0.44
81:AA:711:U:H5'	81:AA:712:C:C5	2.53	0.44
81:AA:1432:U:H2'	81:AA:1433:A:C8	2.52	0.44
81:AA:1441:A:H2	81:AA:1449:G:H22	1.64	0.44
6:5:336:LEU:HD21	6:5:362:THR:HG23	1.98	0.44
11:A:2086:A:H2'	11:A:2087:U:C6	2.51	0.44
34:z:157:VAL:HG21	34:z:237:PHE:CD2	2.53	0.44
73:AV:188:HIS:HA	73:AV:353:LEU:HD11	1.98	0.44
9:8:68:LEU:HD21	52:f:211:LEU:HB2	1.99	0.44
11:A:3115:U:H2'	11:A:3116:C:C6	2.52	0.44
37:b:26:LEU:HD22	37:b:105:ALA:HA	2.00	0.44
38:d:160:LEU:HD12	38:d:160:LEU:HA	1.74	0.44
50:r:70:CYS:HB2	50:r:107:LEU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AH:155:VAL:HG21	77:A1:129:PHE:HB3	1.98	0.44
73:AV:340:LYS:HB3	73:AV:340:LYS:HE3	1.81	0.44
78:A3:165:LYS:HG2	78:A3:195:TYR:CE2	2.53	0.44
81:AA:891:C:H2'	81:AA:892:A:O4'	2.17	0.44
89:AX:56:PRO:HB2	89:AX:144:PHE:HB2	1.98	0.44
5:4:69:LYS:HB2	5:4:72:LEU:HD23	2.00	0.44
9:8:53:LYS:NZ	87:Aw:40:C:H5''	2.33	0.44
11:A:1761:A:H2'	11:A:1762:A:C8	2.52	0.44
11:A:2553:G:H2'	11:A:2554:A:C8	2.52	0.44
15:F:218:LEU:HD23	15:F:260:VAL:HB	1.99	0.44
34:z:88:LEU:H	34:z:91:LEU:HD12	1.83	0.44
35:G:145:LEU:HD22	35:G:191:VAL:HG13	1.99	0.44
81:AA:914:A:H2'	81:AA:915:C:C6	2.53	0.44
81:AA:1439:A:H2'	81:AA:1440:G:H8	1.83	0.44
81:AA:1455:U:H2'	81:AA:1456:U:H6	1.81	0.44
81:AA:1496:U:H2'	81:AA:1497:C:C6	2.53	0.44
85:Ax:60:C:H2'	85:Ax:61:C:C6	2.52	0.44
11:A:2734:A:H2'	11:A:2735:G:H8	1.81	0.44
11:A:2774:C:H2'	11:A:2775:A:C5	2.53	0.44
36:V:55:TYR:HB2	36:V:133:ILE:HD11	1.99	0.44
92:B:6:U:H3	92:B:67:G:H1	1.66	0.44
9:8:150:LEU:HG	9:8:158:HIS:HB2	1.98	0.44
11:A:3144:A:H2'	11:A:3145:A:H8	1.83	0.44
34:z:250:GLU:HB3	34:z:252:PHE:CE2	2.53	0.44
38:d:85:PHE:HZ	38:d:209:TYR:HB2	1.83	0.44
51:c:164:GLU:HG2	51:c:165:VAL:N	2.33	0.44
56:AC:152:ARG:HE	56:AC:154:HIS:CE1	2.36	0.44
61:AH:155:VAL:HG13	77:A1:126:LEU:HD12	1.99	0.44
63:AK:52:LEU:HD22	75:AZ:41:PRO:HG3	2.00	0.44
68:AP:103:LYS:HA	68:AP:103:LYS:HD3	1.79	0.44
81:AA:746:A:C4	81:AA:747:A:C8	3.06	0.44
89:AX:81:HIS:CD2	89:AX:190:ASN:HB3	2.53	0.44
11:A:1806:U:H4'	11:A:1807:U:H5'	2.00	0.44
11:A:2415:C:H2'	54:s:165:ARG:NH1	2.33	0.44
69:AR:338:LYS:O	69:AR:342:ILE:HG22	2.18	0.44
73:AV:231:LEU:HD12	73:AV:243:VAL:HG13	2.00	0.44
81:AA:684:U:H2'	81:AA:685:A:H8	1.83	0.44
81:AA:982:A:H2'	81:AA:983:C:H6	1.82	0.44
87:Aw:5:A:H2'	87:Aw:6:U:H6	1.83	0.44
87:Aw:64:U:H2'	87:Aw:65:A:C8	2.52	0.44
89:AX:242:ILE:HD13	89:AX:242:ILE:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3115:U:H2'	11:A:3116:C:H6	1.83	0.43
53:p:172:ASP:HB3	53:p:175:LEU:HG	2.00	0.43
54:s:65:ARG:O	54:s:69:THR:HG23	2.18	0.43
57:AD:226:ARG:HD3	81:AA:659:U:OP1	2.17	0.43
63:AK:81:ASP:HA	63:AK:86:ARG:HD3	1.98	0.43
70:AS:107:GLN:HB2	70:AS:117:LEU:HD21	2.00	0.43
80:AY:292:GLN:HG2	88:A4:446:LYS:HG2	1.99	0.43
81:AA:1395:C:H2'	81:AA:1396:C:C6	2.53	0.43
89:AX:159:HIS:O	89:AX:163:LYS:HG2	2.18	0.43
7:6:223:GLY:HA2	7:6:266:HIS:CE1	2.52	0.43
8:7:152:CYS:HB2	8:7:260:PHE:CD2	2.53	0.43
11:A:2455:U:H2'	11:A:2456:U:C6	2.53	0.43
11:A:2483:U:H2'	11:A:2484:C:O4'	2.18	0.43
60:AG:108:ILE:HG13	60:AG:125:MET:HB2	1.99	0.43
81:AA:745:A:H3'	81:AA:746:A:H8	1.83	0.43
81:AA:959:C:H3'	81:AA:960:C:O4'	2.17	0.43
81:AA:1181:G:H2'	81:AA:1182:C:C6	2.53	0.43
81:AA:1362:G:H2'	81:AA:1363:C:C6	2.53	0.43
88:A4:159:GLU:HG2	88:A4:163:LEU:HD12	2.01	0.43
11:A:2455:U:H2'	11:A:2456:U:H6	1.83	0.43
11:A:3111:A:H2'	11:A:3112:A:H5''	1.99	0.43
11:A:3181:U:H5'	50:r:99:MET:O	2.18	0.43
11:A:3224:G:H2'	11:A:3225:G:H8	1.84	0.43
40:g:90:ARG:HG3	40:g:91:MET:SD	2.59	0.43
60:AG:172:LEU:HD11	60:AG:237:GLU:HG2	2.00	0.43
69:AR:254:ASP:HB2	69:AR:275:PHE:CZ	2.54	0.43
76:A0:21:LEU:O	76:A0:25:LEU:HG	2.18	0.43
81:AA:856:A:C2	81:AA:857:G:C8	3.06	0.43
81:AA:949:U:O2	99:AA:1701:NAD:H6N	2.17	0.43
81:AA:970:A:H2'	81:AA:971:A:C8	2.53	0.43
81:AA:1174:U:H2'	81:AA:1175:G:H8	1.84	0.43
81:AA:1177:C:H2'	81:AA:1178:G:C8	2.53	0.43
86:Ay:2:A:H2'	86:Ay:3:G:C8	2.53	0.43
11:A:1911:C:H2'	11:A:1912:A:H8	1.83	0.43
11:A:2275:U:H5''	51:c:34:GLY:HA2	2.00	0.43
11:A:2553:G:H2'	11:A:2554:A:H8	1.83	0.43
16:H:174:VAL:HG12	16:H:192:HIS:CB	2.48	0.43
29:U:131:GLU:O	29:U:134:ARG:HG3	2.19	0.43
39:e:261:GLY:HA2	39:e:269:LEU:HD13	2.00	0.43
65:AM:110:LEU:O	65:AM:114:ARG:HG3	2.18	0.43
69:AR:155:LYS:HB3	69:AR:177:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AA:852:A:H3'	81:AA:853:C:C6	2.50	0.43
81:AA:1597:C:H5''	81:AA:1598:G:H5'	2.00	0.43
92:B:24:G:H2'	92:B:25:C:O4'	2.18	0.43
9:8:70:ARG:NH1	85:Ax:46:U:H5'	2.34	0.43
11:A:1745:U:H5''	31:X:55:LYS:HD3	2.01	0.43
11:A:2056:G:H2'	11:A:2057:C:H6	1.84	0.43
11:A:2275:U:H2'	11:A:2276:C:C6	2.53	0.43
12:C:193:VAL:HA	12:C:201:VAL:HB	2.00	0.43
33:Z:101:LYS:HD2	43:j:84:MET:HG3	2.01	0.43
35:G:134:LEU:HB2	35:G:195:VAL:HG22	2.00	0.43
49:q:188:LYS:O	49:q:191:LYS:HG2	2.19	0.43
54:s:117:GLY:O	54:s:394:TRP:HB3	2.19	0.43
69:AR:288:GLN:HE22	69:AR:300:LEU:HD22	1.84	0.43
71:AT:78:PHE:HB2	71:AT:86:VAL:HB	2.00	0.43
81:AA:1462:G:H2'	81:AA:1463:G:H8	1.83	0.43
86:Ay:40:C:H2'	86:Ay:41:A:C8	2.53	0.43
8:7:317:LEU:HA	8:7:317:LEU:HD23	1.79	0.43
11:A:2751:G:H2'	11:A:2752:C:C6	2.53	0.43
39:e:97:ARG:HA	39:e:100:LYS:HG2	2.00	0.43
71:AT:161:GLY:HA2	71:AT:164:LYS:HE2	2.00	0.43
72:AU:64:ARG:NH2	81:AA:845:A:H5'	2.33	0.43
75:AZ:24:ARG:HD3	80:AY:349:HIS:CD2	2.54	0.43
81:AA:730:A:H3'	81:AA:731:A:H8	1.83	0.43
81:AA:753:A:H2'	81:AA:754:A:H8	1.84	0.43
81:AA:1351:G:H2'	81:AA:1352:C:C6	2.53	0.43
88:A4:396:ILE:HG12	88:A4:400:LEU:HD23	1.99	0.43
90:A2:33:VAL:HG21	90:A2:104:LEU:HD23	2.00	0.43
6:5:98:LEU:HD22	6:5:272:ASP:HB3	2.00	0.43
7:6:139:TRP:CD1	7:6:143:CYS:HG	2.36	0.43
11:A:2661:U:H2'	11:A:2662:A:C8	2.54	0.43
11:A:3077:C:H2'	11:A:3078:C:H6	1.83	0.43
11:A:3151:A:H4'	25:Q:146:GLY:O	2.18	0.43
14:E:123:GLN:HG2	14:E:125:GLN:HG3	1.99	0.43
31:X:163:ARG:HD3	31:X:204:VAL:O	2.18	0.43
38:d:108:ARG:HG3	38:d:111:ARG:NH1	2.34	0.43
60:AG:92:MET:HE2	60:AG:92:MET:HB2	1.85	0.43
64:AL:132:LEU:HD12	64:AL:132:LEU:HA	1.84	0.43
76:A0:162:ALA:HA	76:A0:194:GLN:HG2	1.99	0.43
81:AA:1334:G:H2'	81:AA:1335:U:O4'	2.19	0.43
86:Ay:1:U:H2'	86:Ay:2:A:H8	1.83	0.43
92:B:51:C:H2'	92:B:52:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:329:TYR:CE1	7:6:333:GLN:HG3	2.53	0.43
12:C:211:ILE:HD13	35:G:147:LYS:HB2	2.01	0.43
25:Q:118:ARG:HB2	25:Q:134:LEU:HD12	2.01	0.43
39:e:159:LEU:HD12	39:e:254:TRP:CH2	2.53	0.43
81:AA:1005:U:H4'	82:AI:87:HIS:CE1	2.53	0.43
81:AA:1145:A:H2'	81:AA:1146:C:H6	1.84	0.43
81:AA:1173:C:H2'	81:AA:1174:U:C6	2.53	0.43
81:AA:1439:A:H2'	81:AA:1440:G:C8	2.54	0.43
88:A4:309:PHE:HB2	88:A4:313:TRP:HZ3	1.83	0.43
11:A:2778:U:O2'	34:z:116:SER:HB2	2.19	0.43
11:A:3116:C:H2'	11:A:3117:C:H6	1.84	0.43
16:H:201:VAL:HG11	16:H:206:LEU:HG	2.01	0.43
35:G:127:ARG:HD2	35:G:127:ARG:HA	1.78	0.43
54:s:177:LEU:HD12	54:s:177:LEU:HA	1.81	0.43
61:AH:180:LEU:HD12	61:AH:184:ILE:HG21	2.01	0.43
81:AA:730:A:N6	81:AA:744:A:H1'	2.33	0.43
81:AA:1080:A:H1'	81:AA:1082:A:N7	2.34	0.43
87:Aw:14:A:C6	87:Aw:22:A:C5	3.06	0.43
89:AX:74:ASP:O	89:AX:78:VAL:HG12	2.19	0.43
9:8:173:LYS:HB3	52:f:184:LEU:HD23	2.00	0.43
14:E:104:LEU:HD23	14:E:104:LEU:HA	1.85	0.43
22:N:104:MET:HE3	22:N:104:MET:HB3	1.86	0.43
49:q:141:GLU:HA	49:q:144:GLU:HG3	2.01	0.43
81:AA:1011:C:C4	81:AA:1063:A:H4'	2.53	0.43
81:AA:1065:C:H2'	81:AA:1066:C:O4'	2.19	0.43
81:AA:1308:U:H2'	81:AA:1309:A:H8	1.84	0.43
81:AA:1456:U:H2'	81:AA:1457:G:O4'	2.18	0.43
82:AI:189:ARG:HH12	91:AQ:44:TYR:HE1	1.66	0.43
12:C:191:VAL:HG22	12:C:253:SER:HA	2.00	0.42
35:t:86:LEU:HG	35:u:71:ILE:HD11	2.00	0.42
63:AK:35:TRP:NE1	63:AK:39:LYS:HD2	2.34	0.42
71:AT:102:ILE:HA	71:AT:105:ILE:HG12	2.00	0.42
88:A4:397:MET:HE3	88:A4:397:MET:HB3	1.81	0.42
6:5:46:LEU:HD12	6:5:46:LEU:HA	1.84	0.42
11:A:2666:U:H2'	11:A:2667:U:O4'	2.19	0.42
11:A:3116:C:H2'	11:A:3117:C:C6	2.53	0.42
36:V:138:THR:HG23	36:V:140:ALA:N	2.34	0.42
38:d:93:GLY:HA3	38:d:96:ARG:HB3	2.00	0.42
53:p:57:THR:HA	53:p:60:ARG:HE	1.83	0.42
57:AD:351:ARG:HD2	57:AD:355:ARG:NH1	2.35	0.42
61:AH:97:LEU:O	61:AH:101:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AH:182:GLU:HA	61:AH:185:LYS:NZ	2.34	0.42
78:A3:193:LYS:HB3	78:A3:196:LEU:HD23	1.99	0.42
81:AA:952:A:H2'	81:AA:953:U:C6	2.54	0.42
81:AA:981:C:H2'	81:AA:982:A:C8	2.54	0.42
81:AA:990:U:H2'	81:AA:991:G:O4'	2.20	0.42
81:AA:1145:A:H2'	81:AA:1146:C:C6	2.54	0.42
81:AA:1407:U:H2'	81:AA:1408:A:H8	1.84	0.42
81:AA:1450:C:H2'	81:AA:1451:U:C6	2.53	0.42
81:AA:1561:C:H2'	81:AA:1562:G:C8	2.55	0.42
85:Ax:4:A:H2'	85:Ax:5:A:H8	1.84	0.42
86:Ay:9:A:C6	86:Ay:46:A:C6	3.08	0.42
88:A4:489:HIS:HB3	88:A4:492:THR:HG23	2.00	0.42
11:A:2989:G:H5''	11:A:2990:A:H5''	2.00	0.42
44:k:74:LEU:HD13	44:k:93:HIS:CD2	2.54	0.42
61:AH:164:LEU:HD12	61:AH:165:PRO:HD2	2.00	0.42
71:AT:37:HIS:CE1	81:AA:955:A:H2'	2.54	0.42
73:AV:30:LEU:HD21	73:AV:181:LEU:HD22	2.01	0.42
18:J:61:LYS:HG2	45:l:77:ILE:O	2.18	0.42
39:e:218:PRO:HG2	103:B:101:VAL:HG22	2.01	0.42
49:q:184:LYS:O	49:q:188:LYS:HG2	2.19	0.42
59:AF:175:PRO:O	59:AF:179:ARG:HG3	2.19	0.42
77:A1:67:PRO:HG3	77:A1:118:ALA:HB2	2.01	0.42
81:AA:959:C:OP2	81:AA:960:C:H1'	2.18	0.42
81:AA:1011:C:N4	81:AA:1063:A:H4'	2.35	0.42
81:AA:1237:A:H1'	81:AA:1254:C:O2	2.19	0.42
85:Ax:22:U:C2	85:Ax:23:A:C8	3.07	0.42
87:Aw:16:A:H3'	87:Aw:20:C:H5'	2.02	0.42
89:AX:56:PRO:HA	89:AX:59:HIS:ND1	2.34	0.42
89:AX:244:LEU:HD22	89:AX:296:MET:HG3	2.01	0.42
90:A2:64:ASP:HA	90:A2:67:ARG:HE	1.84	0.42
4:3:127:ALA:HA	21:M:79:PRO:HD3	2.02	0.42
11:A:2060:A:C8	11:A:2079:C:C4	3.08	0.42
11:A:3211:C:H4'	11:A:3212:C:H5	1.85	0.42
34:z:184:ILE:HG12	34:z:207:LEU:HD13	2.00	0.42
34:z:296:ARG:HB3	34:z:302:GLY:HA2	2.02	0.42
35:G:134:LEU:HD13	35:G:195:VAL:HG22	2.01	0.42
48:o:15:ARG:HB3	48:o:18:ILE:HG12	2.01	0.42
49:q:188:LYS:HD3	49:q:191:LYS:HZ3	1.85	0.42
51:c:228:LEU:HD13	51:c:307:PHE:CD2	2.54	0.42
76:A0:68:LEU:HD13	76:A0:71:LEU:HD12	2.01	0.42
77:A1:194:VAL:HG12	77:A1:229:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AA:1309:A:H2'	81:AA:1310:C:C6	2.54	0.42
88:A4:88:VAL:HG11	88:A4:107:LEU:HD11	2.01	0.42
90:A2:95:GLU:HB3	90:A2:100:LEU:HG	2.02	0.42
10:9:36:ARG:HD2	29:U:46:MET:SD	2.60	0.42
11:A:3039:OMU:O5'	11:A:3039:OMU:H6	2.20	0.42
38:d:160:LEU:O	38:d:164:VAL:HG22	2.19	0.42
39:e:101:LYS:O	39:e:105:LEU:HD23	2.20	0.42
81:AA:818:C:C2	81:AA:819:A:C8	3.08	0.42
81:AA:1071:U:H2'	81:AA:1072:G:H8	1.84	0.42
81:AA:1190:C:H2'	81:AA:1191:C:C6	2.55	0.42
11:A:1895:C:H2'	11:A:1896:U:C6	2.54	0.42
11:A:2688:C:H2'	11:A:2689:C:C6	2.54	0.42
11:A:2753:A:H2'	11:A:2754:A:H8	1.85	0.42
27:S:98:VAL:HG23	27:S:135:LEU:HD22	2.01	0.42
55:AB:84:LEU:HD23	55:AB:248:LEU:HD21	2.02	0.42
57:AD:425:LEU:HD23	57:AD:425:LEU:HA	1.84	0.42
58:AE:35:ILE:HD12	64:AL:97:MET:HE2	2.00	0.42
65:AM:20:ARG:HB2	81:AA:839:A:H5''	2.01	0.42
73:AV:263:MET:HE1	73:AV:334:PHE:CD1	2.53	0.42
77:A1:313:LYS:HB2	89:AX:342:PRO:HD2	2.02	0.42
81:AA:1209:C:H2'	81:AA:1210:U:C6	2.54	0.42
81:AA:1499:U:H2'	81:AA:1500:C:H6	1.84	0.42
89:AX:157:ASP:OD2	89:AX:159:HIS:HB2	2.20	0.42
89:AX:287:LEU:HB2	89:AX:290:VAL:HB	2.02	0.42
11:A:2114:C:H2'	11:A:2115:U:H6	1.83	0.42
12:C:163:ASP:CB	12:C:286:HIS:HE2	2.32	0.42
39:e:149:LEU:HD23	39:e:149:LEU:HA	1.87	0.42
39:e:200:MET:HA	39:e:241:GLY:HA3	2.01	0.42
46:m:84:LEU:HD12	46:m:88:GLU:HG3	2.02	0.42
61:AH:121:LEU:HD23	61:AH:121:LEU:HA	1.89	0.42
65:AM:107:ALA:O	65:AM:111:ARG:HG2	2.19	0.42
68:AP:86:PRO:HA	68:AP:125:LYS:HB2	2.01	0.42
73:AV:152:ILE:HD12	73:AV:185:VAL:HG22	2.01	0.42
81:AA:659:U:H2'	81:AA:660:C:C6	2.55	0.42
81:AA:727:U:H2'	81:AA:728:C:O4'	2.19	0.42
81:AA:1025:A:H2'	81:AA:1026:A:H8	1.85	0.42
10:9:119:PHE:HB2	31:X:227:PHE:CE1	2.55	0.42
11:A:2312:A:H2'	11:A:2313:A:O4'	2.20	0.42
22:N:172:VAL:HA	22:N:175:PHE:CE2	2.55	0.42
38:d:90:PRO:HB2	38:d:269:TRP:HZ2	1.85	0.42
54:s:273:LEU:HD12	54:s:273:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AC:71:LEU:HD23	56:AC:71:LEU:HA	1.92	0.42
57:AD:317:HIS:HB3	57:AD:320:ILE:HG13	2.02	0.42
61:AH:113:ARG:HH22	81:AA:1310:C:H5''	1.85	0.42
67:AO:105:CYS:HB2	67:AO:142:VAL:HA	2.00	0.42
72:AU:57:MET:HE3	72:AU:57:MET:HB3	1.94	0.42
81:AA:702:C:H2'	81:AA:703:A:C8	2.54	0.42
81:AA:848:U:H2'	81:AA:849:U:C6	2.55	0.42
85:Ax:4:A:H2'	85:Ax:5:A:C8	2.55	0.42
88:A4:126:LYS:HA	88:A4:129:GLN:HG2	2.02	0.42
88:A4:535:MET:HE1	88:A4:551:CYS:HB3	2.01	0.42
11:A:2005:C:H2'	11:A:2006:C:C6	2.54	0.42
11:A:2034:A:H2'	11:A:2035:U:O4'	2.19	0.42
11:A:2041:U:H2'	11:A:2042:U:C6	2.55	0.42
11:A:2661:U:H2'	11:A:2662:A:H8	1.84	0.42
25:Q:96:ARG:HA	25:Q:99:MET:HE3	2.02	0.42
27:S:183:LYS:HE2	27:S:185:ILE:HD11	2.02	0.42
54:s:119:PRO:HG3	54:s:394:TRP:CE3	2.54	0.42
60:AG:126:LYS:HB2	60:AG:131:ILE:HD11	2.02	0.42
61:AH:162:ARG:HA	61:AH:162:ARG:HD3	1.87	0.42
81:AA:672:A:H2'	81:AA:673:U:C6	2.55	0.42
81:AA:673:U:H2'	81:AA:674:U:H6	1.83	0.42
81:AA:682:A:H2'	81:AA:683:G:H8	1.84	0.42
81:AA:1510:U:H2'	81:AA:1511:C:C6	2.55	0.42
9:8:129:ARG:HG2	92:B:28:C:H5'	2.00	0.41
11:A:2044:A:C6	11:A:2045:A:C5	3.08	0.41
11:A:2549:C:N4	11:A:2562:U:H2'	2.34	0.41
11:A:3057:C:H2'	11:A:3058:U:O4'	2.20	0.41
11:A:3102:U:H2'	11:A:3103:C:H6	1.85	0.41
11:A:3117:C:H2'	11:A:3118:U:H6	1.84	0.41
11:A:3219:G:H2'	11:A:3220:A:H5''	2.02	0.41
13:D:195:ASN:ND2	13:D:208:ARG:HG3	2.35	0.41
40:g:164:LYS:HA	40:g:164:LYS:HD2	1.94	0.41
46:m:58:LYS:HZ2	46:m:64:ILE:HG23	1.85	0.41
50:r:96:HIS:NE2	50:r:134:ARG:HB2	2.35	0.41
51:c:148:MET:HG3	51:c:149:PRO:HD2	2.02	0.41
64:AL:114:LYS:HG2	64:AL:115:ILE:HG13	2.02	0.41
81:AA:862:A:H2'	81:AA:863:C:C6	2.55	0.41
81:AA:1174:U:H2'	81:AA:1175:G:C8	2.55	0.41
81:AA:1365:A:H2'	81:AA:1366:C:C6	2.54	0.41
7:6:265:ILE:HD13	24:P:58:LEU:HB2	2.01	0.41
11:A:2872:C:H2'	11:A:2873:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:z:216:LYS:HD2	34:z:218:TYR:HE1	1.85	0.41
40:g:82:LEU:HA	40:g:82:LEU:HD23	1.83	0.41
41:h:117:LEU:HD23	41:h:117:LEU:HA	1.83	0.41
57:AD:103:LEU:HD11	57:AD:123:ARG:HB2	2.01	0.41
59:AF:149:LEU:HD23	59:AF:149:LEU:HA	1.89	0.41
63:AK:57:LEU:HD23	63:AK:71:ALA:HB2	2.02	0.41
67:AO:94:CYS:SG	67:AO:105:CYS:HB3	2.60	0.41
73:AV:74:ARG:HH21	73:AV:390:ILE:HD13	1.85	0.41
81:AA:659:U:O2'	81:AA:1285:G:H1'	2.19	0.41
81:AA:682:A:H2'	81:AA:683:G:C8	2.55	0.41
81:AA:1209:C:H2'	81:AA:1210:U:H6	1.85	0.41
81:AA:1363:C:H1'	81:AA:1448:U:O2	2.20	0.41
11:A:2170:G:H2'	11:A:2171:U:C5	2.55	0.41
11:A:3000:A:H2'	11:A:3001:G:C8	2.56	0.41
38:d:88:TYR:OH	38:d:195:VAL:HB	2.20	0.41
39:e:124:TRP:CD2	46:m:72:ARG:HG2	2.55	0.41
56:AC:96:MET:HB2	56:AC:108:LEU:HD11	2.02	0.41
60:AG:389:ARG:HD2	81:AA:1427:A:O2'	2.20	0.41
70:AS:50:ARG:HH22	81:AA:1119:U:H5'	1.85	0.41
77:A1:198:TYR:CZ	77:A1:200:LYS:HA	2.55	0.41
81:AA:664:G:H2'	81:AA:665:C:C6	2.54	0.41
81:AA:969:A:H2'	81:AA:970:A:C8	2.55	0.41
81:AA:1162:A:H2'	81:AA:1163:C:C6	2.55	0.41
81:AA:1416:A:H2'	81:AA:1417:A:C8	2.55	0.41
85:Ax:25:C:H2'	85:Ax:26:G:C8	2.56	0.41
87:Aw:27:A:H2'	87:Aw:28:A:H8	1.85	0.41
87:Aw:39:U:H2'	87:Aw:40:C:C6	2.56	0.41
92:B:21:A:H61	92:B:46:A:H2'	1.85	0.41
1:0:96:ASN:OD1	1:0:97:PRO:HD2	2.20	0.41
11:A:2049:U:H2'	11:A:2050:A:C8	2.54	0.41
11:A:2060:A:H2'	11:A:2061:C:H6	1.85	0.41
15:F:62:VAL:HG23	15:F:82:LEU:HB2	2.01	0.41
21:M:205:LEU:HD11	53:p:43:TYR:CZ	2.55	0.41
56:AC:105:ALA:HB3	56:AC:122:VAL:HG12	2.01	0.41
73:AV:114:ARG:HA	73:AV:117:LEU:HD12	2.02	0.41
81:AA:774:G:H2'	81:AA:775:C:H6	1.84	0.41
81:AA:867:C:H2'	81:AA:870:C:H42	1.86	0.41
81:AA:1241:C:H2'	81:AA:1242:C:C6	2.55	0.41
81:AA:1294:A:O2'	81:AA:1295:A:H8	2.03	0.41
86:Ay:49:G:H2'	86:Ay:50:G:H8	1.85	0.41
92:B:34:U:H2'	92:B:35:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:99:ARG:HH11	7:6:102:GLN:NE2	2.18	0.41
8:7:309:HIS:CE1	14:E:155:PHE:HA	2.55	0.41
11:A:2884:C:H4'	30:W:109:ARG:HH12	1.86	0.41
12:C:139:GLU:HB3	12:C:179:ALA:HB3	2.01	0.41
16:H:247:ARG:HG2	16:H:251:TRP:HE1	1.84	0.41
58:AE:30:MET:HE3	58:AE:30:MET:HB2	1.90	0.41
69:AR:149:GLU:HB3	69:AR:178:SER:C	2.45	0.41
72:AU:49:ASP:HB3	72:AU:52:GLU:HB3	2.02	0.41
73:AV:287:LEU:HD21	73:AV:331:LEU:HB2	2.01	0.41
81:AA:747:A:H2'	81:AA:748:G:H8	1.84	0.41
81:AA:818:C:H2'	81:AA:819:A:C8	2.56	0.41
81:AA:1017:A:H2'	81:AA:1018:G:C8	2.56	0.41
81:AA:1407:U:H2'	81:AA:1408:A:C8	2.55	0.41
86:Ay:23:A:H2'	86:Ay:24:A:H8	1.84	0.41
88:A4:170:VAL:HG23	88:A4:247:ILE:HD11	2.01	0.41
88:A4:450:PRO:HD2	88:A4:453:HIS:CG	2.55	0.41
7:6:60:ARG:HA	7:6:60:ARG:HD2	1.84	0.41
15:F:138:HIS:CD2	15:F:146:TRP:HE1	2.38	0.41
32:Y:124:LEU:HD21	38:d:61:ARG:HD2	2.01	0.41
39:e:52:CYS:HA	39:e:173:LEU:HD21	2.03	0.41
39:e:55:ARG:NH1	39:e:58:VAL:HG23	2.35	0.41
52:f:121:VAL:HG22	52:f:159:ILE:HG22	2.01	0.41
55:AB:118:LEU:HD23	55:AB:118:LEU:HA	1.89	0.41
61:AH:165:PRO:HG2	61:AH:168:VAL:HG21	2.03	0.41
73:AV:167:VAL:HG13	73:AV:172:ALA:HB3	2.02	0.41
76:A0:91:GLU:HB2	76:A0:121:LYS:HD2	2.02	0.41
81:AA:715:G:H2'	81:AA:716:U:C6	2.55	0.41
81:AA:743:C:H2'	81:AA:744:A:O4'	2.21	0.41
81:AA:984:C:H2'	81:AA:985:U:C6	2.56	0.41
81:AA:1503:G:H2'	81:AA:1504:U:C6	2.55	0.41
81:AA:1515:G:H2'	81:AA:1516:G:C8	2.55	0.41
84:a:101:GLU:HA	84:a:103:LEU:HD22	2.02	0.41
86:Ay:9:A:H2'	86:Ay:11:U:O4	2.21	0.41
88:A4:236:VAL:HG13	88:A4:270:ARG:HB3	2.02	0.41
6:5:167:THR:HG21	54:s:281:HIS:CE1	2.55	0.41
11:A:2802:A:H2'	11:A:2803:A:O4'	2.20	0.41
11:A:2815:OMG:HM23	11:A:2815:OMG:H1'	1.69	0.41
17:I:102:VAL:HG22	17:I:174:LEU:HD13	2.02	0.41
27:S:173:ARG:HB3	27:S:180:PHE:HE2	1.86	0.41
46:m:90:ARG:HE	46:m:94:ARG:HG3	1.86	0.41
48:o:12:ILE:HD13	48:o:12:ILE:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:s:84:THR:HB	54:s:280:ASN:HB2	2.03	0.41
61:AH:73:TYR:CE1	61:AH:176:GLN:HB3	2.55	0.41
67:AO:214:SER:HB2	73:AV:317:LEU:HB3	2.02	0.41
71:AT:140:ILE:HG13	71:AT:146:GLN:HG3	2.03	0.41
73:AV:82:ARG:O	73:AV:85:ILE:HG22	2.20	0.41
81:AA:728:C:H2'	81:AA:729:U:O4'	2.21	0.41
81:AA:1032:C:H2'	81:AA:1033:U:C6	2.56	0.41
81:AA:1055:U:C2	81:AA:1056:A:C8	3.09	0.41
88:A4:446:LYS:HB3	88:A4:446:LYS:HE3	1.83	0.41
92:B:16:C:H2'	92:B:18:A:O4'	2.21	0.41
6:5:417:LEU:HD23	6:5:417:LEU:HA	1.85	0.41
11:A:2042:U:H2'	11:A:2043:C:C6	2.56	0.41
11:A:2275:U:H2'	11:A:2276:C:H6	1.85	0.41
11:A:2753:A:C4	11:A:2754:A:C8	3.08	0.41
11:A:3181:U:OP1	50:r:101:PRO:HG3	2.20	0.41
23:O:46:TRP:CD1	23:O:121:ALA:HB2	2.56	0.41
27:S:120:LEU:HD23	27:S:120:LEU:HA	1.78	0.41
34:z:62:PRO:HG2	34:z:65:LYS:HB2	2.03	0.41
54:s:332:LEU:HD21	54:s:359:ALA:HB2	2.02	0.41
69:AR:213:GLU:HG2	69:AR:214:ASN:N	2.36	0.41
87:Aw:4:U:H2'	87:Aw:5:A:C8	2.55	0.41
4:3:156:LYS:HE3	4:3:156:LYS:HB2	1.83	0.41
10:9:118:GLY:HA3	36:V:191:LEU:HD12	2.02	0.41
11:A:1970:G:H2'	11:A:1971:A:O4'	2.20	0.41
11:A:2101:C:H2'	11:A:2102:A:H8	1.86	0.41
11:A:2175:C:H2'	11:A:2176:C:H6	1.86	0.41
11:A:2408:U:H2'	11:A:2409:A:C8	2.55	0.41
11:A:2455:U:H5''	23:O:47:ALA:HB3	2.02	0.41
11:A:2811:G:H2'	11:A:2812:U:H6	1.85	0.41
11:A:3139:G:H2'	11:A:3140:A:C8	2.55	0.41
11:A:3144:A:H2'	11:A:3145:A:C8	2.56	0.41
11:A:3163:G:H2'	11:A:3164:C:C6	2.56	0.41
12:C:113:ARG:HG2	12:C:119:LYS:NZ	2.35	0.41
15:F:160:SER:HB2	42:i:80:LEU:HD22	2.02	0.41
15:F:164:MET:HE2	42:i:69:HIS:CE1	2.56	0.41
21:M:12:ALA:HB2	48:o:88:ILE:HD13	2.02	0.41
25:Q:165:GLU:HB2	25:Q:168:ASN:HB2	2.03	0.41
30:W:117:ILE:HD12	30:W:117:ILE:HA	1.96	0.41
32:Y:176:ILE:HG21	83:OX:430:TRP:CG	2.55	0.41
33:Z:63:PRO:HB3	48:o:51:MET:HB3	2.03	0.41
35:G:180:GLU:O	35:G:183:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:110:GLU:O	38:d:114:LYS:HG2	2.20	0.41
35:u:75:THR:O	35:u:79:ILE:HG13	2.20	0.41
51:c:119:LEU:HD12	51:c:119:LEU:HA	1.88	0.41
52:f:190:THR:HG23	52:f:192:GLU:HG3	2.03	0.41
53:p:81:TYR:HB3	53:p:143:GLN:HE22	1.86	0.41
70:AS:124:ALA:O	70:AS:128:GLU:HG2	2.21	0.41
73:AV:175:VAL:HG12	73:AV:177:SER:N	2.35	0.41
81:AA:862:A:H2'	81:AA:863:C:H6	1.86	0.41
81:AA:970:A:H2'	81:AA:971:A:H8	1.85	0.41
81:AA:1231:A:H1'	81:AA:1236:C:H41	1.86	0.41
81:AA:1328:G:H2'	81:AA:1329:U:C6	2.56	0.41
81:AA:1411:G:H2'	81:AA:1412:G:C8	2.56	0.41
81:AA:1454:G:H2'	81:AA:1455:U:H6	1.85	0.41
86:Ay:22:A:H2'	86:Ay:23:A:C8	2.56	0.41
89:AX:168:LEU:HD13	89:AX:168:LEU:HA	1.95	0.41
6:5:165:GLN:HE21	6:5:179:VAL:HG21	1.87	0.41
11:A:1828:A:H4'	11:A:1829:A:C8	2.56	0.41
11:A:2053:U:OP2	48:o:79:THR:HG23	2.21	0.41
11:A:2263:C:H5'	27:S:180:PHE:CE1	2.56	0.41
11:A:2398:A:H2'	11:A:2399:A:O4'	2.21	0.41
11:A:3134:C:C2	11:A:3135:A:C8	3.08	0.41
12:C:91:ALA:HB2	12:C:108:ILE:HD12	2.03	0.41
12:C:193:VAL:HG12	12:C:230:PHE:HE2	1.86	0.41
15:F:53:LEU:HD23	15:F:53:LEU:HA	1.89	0.41
16:H:59:TRP:NE1	16:H:81:LYS:HB3	2.36	0.41
17:I:146:LEU:HD11	44:k:23:PHE:CZ	2.56	0.41
33:Z:128:LEU:HD23	33:Z:128:LEU:HA	1.92	0.41
35:u:74:LEU:HD23	35:u:79:ILE:HG12	2.03	0.41
54:s:115:LEU:HD12	54:s:394:TRP:NE1	2.36	0.41
76:A0:82:ARG:HB2	76:A0:85:TRP:CG	2.55	0.41
81:AA:824:U:H2'	81:AA:825:U:C6	2.56	0.41
81:AA:995:A:H2'	81:AA:996:A:C8	2.56	0.41
81:AA:1047:A:C5	81:AA:1158:U:H4'	2.56	0.41
81:AA:1542:U:H2'	81:AA:1543:U:C6	2.56	0.41
89:AX:195:ASN:O	89:AX:199:LEU:HD13	2.21	0.41
7:6:128:ALA:HB3	24:P:123:VAL:HG11	2.02	0.40
11:A:1862:U:H2'	11:A:1863:A:C8	2.56	0.40
11:A:3009:C:H5	11:A:3030:A:N6	2.20	0.40
11:A:3165:C:H2'	11:A:3166:U:C6	2.55	0.40
21:M:205:LEU:HD23	21:M:205:LEU:HA	1.84	0.40
25:Q:210:GLU:HB2	25:Q:213:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Y:183:GLN:H	32:Y:183:GLN:HG2	1.62	0.40
38:d:201:SER:O	38:d:208:VAL:HG12	2.21	0.40
38:d:232:MET:HE2	38:d:232:MET:HB3	1.94	0.40
39:e:269:LEU:HA	39:e:272:VAL:HG12	2.03	0.40
73:AV:57:MET:HE3	73:AV:61:PHE:HE2	1.86	0.40
73:AV:188:HIS:CD2	73:AV:353:LEU:HG	2.56	0.40
76:A0:85:TRP:HZ2	76:A0:204:PRO:HG3	1.86	0.40
81:AA:726:C:H2'	81:AA:727:U:H6	1.86	0.40
86:Ay:69:C:H2'	86:Ay:70:C:C6	2.56	0.40
87:Aw:27:A:H2'	87:Aw:28:A:C8	2.56	0.40
87:Aw:71:C:O2'	87:Aw:72:A:H8	2.04	0.40
89:AX:250:GLN:HB3	89:AX:255:MET:SD	2.61	0.40
12:C:203:LEU:HD11	12:C:220:GLU:HB2	2.02	0.40
14:E:272:LYS:HE2	14:E:274:TRP:CZ3	2.55	0.40
14:E:328:LEU:HD23	14:E:328:LEU:HA	1.91	0.40
18:J:189:ALA:HA	18:J:192:LYS:HD2	2.03	0.40
23:O:52:MET:HE3	23:O:52:MET:HB3	1.89	0.40
31:X:40:PRO:HB3	31:X:43:TYR:CZ	2.55	0.40
59:AF:55:VAL:HA	59:AF:58:LEU:HG	2.03	0.40
61:AH:51:HIS:CE1	88:A4:476:LYS:HG3	2.57	0.40
65:AM:74:ARG:HG3	72:AU:74:PHE:CD1	2.57	0.40
81:AA:747:A:H2'	81:AA:748:G:C8	2.56	0.40
81:AA:1180:U:H2'	81:AA:1181:G:H8	1.87	0.40
86:Ay:40:C:H2'	86:Ay:41:A:H8	1.85	0.40
88:A4:236:VAL:HG22	88:A4:270:ARG:HG3	2.03	0.40
89:AX:70:ILE:HG12	89:AX:143:HIS:CE1	2.56	0.40
2:1:44:LEU:HD13	2:1:55:LEU:HD12	2.03	0.40
7:6:224:HIS:CE1	7:6:227:GLU:H	2.39	0.40
9:8:190:GLY:HA3	46:m:78:PRO:HB2	2.02	0.40
11:A:1736:A:H2	11:A:1761:A:N7	2.19	0.40
12:C:243:ARG:HD2	12:C:256:CYS:HB3	2.01	0.40
15:F:96:LEU:HD23	15:F:96:LEU:HA	1.89	0.40
27:S:119:GLU:HG2	27:S:189:PRO:HB2	2.02	0.40
35:G:188:LEU:HD22	35:G:195:VAL:HG21	2.03	0.40
49:q:174:ARG:HA	49:q:174:ARG:HD3	1.79	0.40
51:c:256:ARG:HD2	84:a:69:TYR:CE2	2.57	0.40
54:s:187:LEU:O	54:s:190:PRO:HD2	2.21	0.40
55:AB:167:HIS:CE1	60:AG:153:THR:HA	2.57	0.40
56:AC:58:ALA:HB3	56:AC:60:HIS:CE1	2.57	0.40
57:AD:89:PHE:CE1	75:AZ:62:MET:HG3	2.56	0.40
57:AD:363:ALA:HB2	57:AD:370:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:AF:224:HIS:O	59:AF:228:LYS:HG2	2.21	0.40
60:AG:360:GLU:HA	60:AG:363:TRP:CD1	2.57	0.40
64:AL:219:LYS:HB3	64:AL:223:ARG:HH12	1.87	0.40
65:AM:114:ARG:HH12	67:AO:236:PRO:HD2	1.86	0.40
67:AO:49:SER:H	67:AO:52:LYS:NZ	2.19	0.40
67:AO:123:LEU:HD13	67:AO:154:ILE:HG13	2.02	0.40
74:AW:154:LEU:HB3	90:A2:29:LEU:HG	2.02	0.40
81:AA:875:U:H2'	81:AA:876:U:H6	1.85	0.40
81:AA:1591:C:C2	81:AA:1592:U:C5	3.10	0.40
9:8:150:LEU:HB2	39:e:232:PHE:CE2	2.57	0.40
11:A:2043:C:C2	11:A:2044:A:C8	3.10	0.40
11:A:2362:A:O2'	11:A:2363:A:H8	2.04	0.40
11:A:3117:C:H2'	11:A:3118:U:C6	2.57	0.40
16:H:168:LYS:HD3	16:H:231:VAL:HG13	2.03	0.40
19:K:5:SER:HB2	19:K:8:PRO:HD2	2.04	0.40
29:U:112:PRO:N	29:U:113:GLU:HA	2.36	0.40
35:G:168:LEU:HA	35:G:170:GLN:OE1	2.21	0.40
37:b:35:ARG:HG3	48:o:101:TRP:HB2	2.03	0.40
39:e:219:GLN:HA	39:e:222:ARG:HB2	2.02	0.40
54:s:332:LEU:HA	54:s:332:LEU:HD23	1.82	0.40
66:AN:21:LYS:CB	81:AA:777:G:H5''	2.50	0.40
81:AA:726:C:H2'	81:AA:727:U:C6	2.56	0.40
81:AA:1582:G:H2'	81:AA:1583:MA6:O4'	2.22	0.40
81:AA:1589:C:H2'	81:AA:1590:A:H8	1.84	0.40
87:Aw:71:C:HO2'	87:Aw:72:A:H8	1.69	0.40
88:A4:335:PHE:CD2	88:A4:360:MET:HB2	2.56	0.40
11:A:2783:A:H1'	34:z:296:ARG:NH1	2.37	0.40
32:Y:191:ASN:HB3	32:Y:194:TYR:HB3	2.04	0.40
32:Y:211:LEU:HD23	32:Y:211:LEU:HA	1.84	0.40
35:t:65:GLN:O	35:t:69:GLN:HG2	2.22	0.40
53:p:110:TRP:CD1	53:p:110:TRP:H	2.39	0.40
81:AA:881:A:H2'	81:AA:882:A:C4	2.57	0.40
81:AA:996:A:H2'	81:AA:997:A:H8	1.85	0.40
81:AA:1044:U:H2'	81:AA:1045:G:O4'	2.21	0.40
81:AA:1059:U:H2'	81:AA:1060:A:C8	2.56	0.40
81:AA:1071:U:H2'	81:AA:1072:G:C8	2.57	0.40
89:AX:117:PHE:HB3	89:AX:303:GLY:HA2	2.04	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%)	107 (99%)	1 (1%)	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
4	3	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	379 (97%)	13 (3%)	0	100	100
7	6	352/380 (93%)	338 (96%)	14 (4%)	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%)	117 (96%)	5 (4%)	0	100	100
12	C	221/297 (74%)	209 (95%)	12 (5%)	0	100	100
13	D	236/305 (77%)	227 (96%)	9 (4%)	0	100	100
14	E	303/348 (87%)	292 (96%)	11 (4%)	0	100	100
15	F	250/311 (80%)	243 (97%)	7 (3%)	0	100	100
16	H	200/267 (75%)	196 (98%)	4 (2%)	0	100	100
17	I	179/261 (69%)	174 (97%)	5 (3%)	0	100	100
18	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
19	K	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
20	L	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
21	M	289/296 (98%)	281 (97%)	8 (3%)	0	100	100
22	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
23	O	152/175 (87%)	146 (96%)	6 (4%)	0	100	100
24	P	142/180 (79%)	137 (96%)	5 (4%)	0	100	100
25	Q	237/292 (81%)	233 (98%)	4 (2%)	0	100	100
26	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
28	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
29	U	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
30	W	114/148 (77%)	111 (97%)	3 (3%)	0	100	100
31	X	242/256 (94%)	239 (99%)	3 (1%)	0	100	100
32	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
33	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
34	z	250/325 (77%)	239 (96%)	11 (4%)	0	100	100
35	G	70/198 (35%)	66 (94%)	4 (6%)	0	100	100
35	t	44/198 (22%)	44 (100%)	0	0	100	100
35	u	30/198 (15%)	30 (100%)	0	0	100	100
36	V	203/216 (94%)	200 (98%)	3 (2%)	0	100	100
37	b	148/215 (69%)	141 (95%)	7 (5%)	0	100	100
38	d	257/306 (84%)	239 (93%)	17 (7%)	1 (0%)	30	63
39	e	236/279 (85%)	225 (95%)	11 (5%)	0	100	100
40	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
41	h	108/158 (68%)	101 (94%)	7 (6%)	0	100	100
42	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
43	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
44	k	100/112 (89%)	100 (100%)	0	0	100	100
45	l	80/138 (58%)	77 (96%)	3 (4%)	0	100	100
46	m	90/128 (70%)	88 (98%)	2 (2%)	0	100	100
48	o	92/102 (90%)	92 (100%)	0	0	100	100
49	q	175/222 (79%)	175 (100%)	0	0	100	100
50	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
51	c	282/332 (85%)	276 (98%)	6 (2%)	0	100	100
52	f	153/212 (72%)	148 (97%)	5 (3%)	0	100	100
53	p	141/206 (68%)	137 (97%)	4 (3%)	0	100	100
54	s	381/439 (87%)	371 (97%)	10 (3%)	0	100	100
55	AB	223/296 (75%)	219 (98%)	4 (2%)	0	100	100
56	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	AD	341/430 (79%)	331 (97%)	10 (3%)	0	100	100
58	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
59	AF	206/242 (85%)	203 (98%)	3 (2%)	0	100	100
60	AG	323/396 (82%)	316 (98%)	7 (2%)	0	100	100
61	AH	138/201 (69%)	132 (96%)	5 (4%)	1 (1%)	18	51
62	AJ	106/138 (77%)	103 (97%)	3 (3%)	0	100	100
63	AK	99/128 (77%)	99 (100%)	0	0	100	100
64	AL	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
65	AM	117/137 (85%)	113 (97%)	4 (3%)	0	100	100
66	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
67	AO	191/258 (74%)	188 (98%)	3 (2%)	0	100	100
68	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
69	AR	293/360 (81%)	286 (98%)	7 (2%)	0	100	100
70	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
71	AT	166/173 (96%)	162 (98%)	4 (2%)	0	100	100
72	AU	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
73	AV	358/414 (86%)	344 (96%)	14 (4%)	0	100	100
74	AW	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
75	AZ	98/106 (92%)	98 (100%)	0	0	100	100
76	A0	213/217 (98%)	208 (98%)	5 (2%)	0	100	100
77	A1	277/323 (86%)	265 (96%)	12 (4%)	0	100	100
78	A3	68/199 (34%)	66 (97%)	2 (3%)	0	100	100
80	AY	117/395 (30%)	115 (98%)	2 (2%)	0	100	100
82	AI	135/194 (70%)	133 (98%)	1 (1%)	1 (1%)	18	51
83	OX	51/435 (12%)	48 (94%)	3 (6%)	0	100	100
84	a	99/142 (70%)	98 (99%)	1 (1%)	0	100	100
88	A4	584/689 (85%)	565 (97%)	19 (3%)	0	100	100
89	AX	350/398 (88%)	339 (97%)	11 (3%)	0	100	100
90	A2	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
91	AQ	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
All	All	14908/19622 (76%)	14518 (97%)	387 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
61	AH	126	ILE
82	AI	184	ASN
38	d	47	GLN

### 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	C	193/245 (79%)	193 (100%)	0	100	100
13	D	192/245 (78%)	192 (100%)	0	100	100
14	E	260/290 (90%)	260 (100%)	0	100	100
15	F	219/262 (84%)	219 (100%)	0	100	100
16	H	182/228 (80%)	182 (100%)	0	100	100
17	I	165/232 (71%)	165 (100%)	0	100	100
18	J	138/150 (92%)	138 (100%)	0	100	100
19	K	155/155 (100%)	155 (100%)	0	100	100
20	L	98/124 (79%)	98 (100%)	0	100	100
21	M	246/249 (99%)	245 (100%)	1 (0%)	84	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	N	189/211 (90%)	189 (100%)	0	100	100
23	O	134/150 (89%)	134 (100%)	0	100	100
24	P	126/155 (81%)	126 (100%)	0	100	100
25	Q	221/256 (86%)	221 (100%)	0	100	100
26	R	118/126 (94%)	118 (100%)	0	100	100
27	S	146/180 (81%)	146 (100%)	0	100	100
28	T	146/176 (83%)	146 (100%)	0	100	100
29	U	134/135 (99%)	134 (100%)	0	100	100
30	W	94/119 (79%)	94 (100%)	0	100	100
31	X	220/229 (96%)	220 (100%)	0	100	100
32	Y	163/223 (73%)	163 (100%)	0	100	100
33	Z	113/147 (77%)	113 (100%)	0	100	100
34	z	226/287 (79%)	226 (100%)	0	100	100
35	G	60/158 (38%)	60 (100%)	0	100	100
35	t	40/158 (25%)	40 (100%)	0	100	100
35	u	31/158 (20%)	31 (100%)	0	100	100
36	V	183/191 (96%)	183 (100%)	0	100	100
37	b	132/186 (71%)	132 (100%)	0	100	100
38	d	237/274 (86%)	237 (100%)	0	100	100
39	e	207/236 (88%)	207 (100%)	0	100	100
40	g	124/148 (84%)	124 (100%)	0	100	100
41	h	104/148 (70%)	104 (100%)	0	100	100
42	i	86/110 (78%)	86 (100%)	0	100	100
43	j	74/97 (76%)	74 (100%)	0	100	100
44	k	83/89 (93%)	83 (100%)	0	100	100
45	l	76/116 (66%)	76 (100%)	0	100	100
46	m	85/113 (75%)	85 (100%)	0	100	100
48	o	80/87 (92%)	80 (100%)	0	100	100
49	q	153/178 (86%)	153 (100%)	0	100	100
50	r	147/169 (87%)	147 (100%)	0	100	100
51	c	251/288 (87%)	251 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	f	139/188 (74%)	139 (100%)	0	100	100
53	p	135/181 (75%)	135 (100%)	0	100	100
54	s	339/381 (89%)	339 (100%)	0	100	100
55	AB	198/249 (80%)	198 (100%)	0	100	100
56	AC	115/143 (80%)	115 (100%)	0	100	100
57	AD	286/357 (80%)	286 (100%)	0	100	100
58	AE	104/107 (97%)	104 (100%)	0	100	100
59	AF	185/209 (88%)	185 (100%)	0	100	100
60	AG	285/342 (83%)	285 (100%)	0	100	100
61	AH	130/180 (72%)	130 (100%)	0	100	100
62	AJ	93/118 (79%)	93 (100%)	0	100	100
63	AK	91/113 (80%)	91 (100%)	0	100	100
64	AL	158/226 (70%)	158 (100%)	0	100	100
65	AM	97/113 (86%)	97 (100%)	0	100	100
66	AN	96/115 (84%)	96 (100%)	0	100	100
67	AO	174/230 (76%)	174 (100%)	0	100	100
68	AP	88/123 (72%)	88 (100%)	0	100	100
69	AR	264/318 (83%)	264 (100%)	0	100	100
70	AS	116/164 (71%)	116 (100%)	0	100	100
71	AT	153/157 (98%)	153 (100%)	0	100	100
72	AU	152/174 (87%)	152 (100%)	0	100	100
73	AV	325/364 (89%)	325 (100%)	0	100	100
74	AW	87/158 (55%)	87 (100%)	0	100	100
75	AZ	90/95 (95%)	90 (100%)	0	100	100
76	A0	188/189 (100%)	188 (100%)	0	100	100
77	A1	257/291 (88%)	257 (100%)	0	100	100
78	A3	65/166 (39%)	65 (100%)	0	100	100
80	AY	110/357 (31%)	110 (100%)	0	100	100
82	AI	105/147 (71%)	105 (100%)	0	100	100
83	OX	49/372 (13%)	49 (100%)	0	100	100
84	a	99/133 (74%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
88	A4	526/609 (86%)	526 (100%)	0	100	100
89	AX	311/351 (89%)	311 (100%)	0	100	100
90	A2	100/100 (100%)	100 (100%)	0	100	100
91	AQ	78/78 (100%)	78 (100%)	0	100	100
All	All	13322/16932 (79%)	13321 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
21	M	30	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	170	ASN
4	3	185	ASN
6	5	165	GLN
6	5	214	ASN
7	6	292	GLN
7	6	295	GLN
9	8	103	GLN
9	8	186	GLN
12	C	98	ASN
12	C	275	GLN
12	C	281	GLN
13	D	233	GLN
14	E	281	ASN
16	H	178	ASN
16	H	196	ASN
16	H	254	GLN
18	J	186	GLN
19	K	64	HIS
20	L	59	HIS
21	M	6	GLN
21	M	30	ASN
22	N	86	ASN
22	N	101	HIS
22	N	138	HIS
22	N	178	GLN
22	N	210	GLN

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Mol	Chain	Res	Type
23	O	150	GLN
23	O	154	GLN
25	Q	132	GLN
25	Q	172	GLN
25	Q	209	GLN
25	Q	237	ASN
27	S	196	ASN
30	W	41	ASN
31	X	4	HIS
31	X	27	HIS
31	X	93	ASN
31	X	177	HIS
32	Y	225	ASN
34	z	119	GLN
34	z	136	ASN
36	V	35	ASN
37	b	90	HIS
37	b	123	ASN
37	b	129	GLN
38	d	77	HIS
40	g	73	GLN
40	g	155	GLN
42	i	120	HIS
42	i	124	HIS
43	j	30	GLN
48	o	21	HIS
49	q	60	GLN
35	t	65	GLN
51	c	128	GLN
51	c	155	ASN
51	c	168	HIS
51	c	172	ASN
53	p	117	GLN
54	s	107	GLN
54	s	152	GLN
54	s	154	HIS
54	s	238	ASN
54	s	239	ASN
54	s	281	HIS
54	s	314	GLN
54	s	358	GLN
54	s	420	GLN

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Mol	Chain	Res	Type
55	AB	69	HIS
55	AB	201	ASN
57	AD	130	GLN
57	AD	155	GLN
57	AD	273	ASN
57	AD	341	ASN
58	AE	56	GLN
59	AF	113	GLN
59	AF	122	GLN
59	AF	224	HIS
60	AG	130	GLN
60	AG	139	GLN
60	AG	176	GLN
60	AG	242	GLN
60	AG	288	HIS
61	AH	125	HIS
65	AM	75	HIS
67	AO	130	HIS
68	AP	137	ASN
69	AR	247	HIS
69	AR	278	ASN
69	AR	320	GLN
70	AS	66	HIS
71	AT	18	GLN
73	AV	246	ASN
73	AV	358	GLN
74	AW	135	GLN
76	A0	24	GLN
77	A1	268	GLN
78	A3	190	GLN
80	AY	295	GLN
84	a	126	HIS
88	A4	72	GLN
88	A4	90	GLN
88	A4	274	GLN
88	A4	453	HIS
88	A4	656	ASN
89	AX	81	HIS
89	AX	148	GLN
89	AX	190	ASN

### 5.3.3 RNA ⓘ



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1561 (99%)	257 (16%)	2 (0%)
79	Az	33/34 (97%)	13 (39%)	0
81	AA	953/954 (99%)	139 (14%)	1 (0%)
85	Ax	70/71 (98%)	15 (21%)	0
86	Ay	67/76 (88%)	13 (19%)	0
87	Aw	64/76 (84%)	21 (32%)	0
92	B	70/72 (97%)	15 (21%)	0
All	All	2813/2844 (98%)	473 (16%)	3 (0%)

All (473) 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	1701	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	1765	C
11	A	1777	A
11	A	1780	U
11	A	1805	A
11	A	1806	U
11	A	1807	U
11	A	1808	A
11	A	1809	U
11	A	1817	C
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

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Mol	Chain	Res	Type
11	A	1856	A
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	1975	U
11	A	1985	G
11	A	1992	C
11	A	1994	A
11	A	2000	C
11	A	2001	C
11	A	2002	G
11	A	2003	A
11	A	2010	U
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	2054	U
11	A	2055	U
11	A	2060	A
11	A	2069	U
11	A	2071	U
11	A	2079	C
11	A	2099	U
11	A	2113	G
11	A	2125	C

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Mol	Chain	Res	Type
11	A	2126	U
11	A	2147	G
11	A	2155	A
11	A	2159	U
11	A	2160	A
11	A	2163	A
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	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	2285	U
11	A	2297	A
11	A	2300	G
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2333	G
11	A	2345	G
11	A	2350	A
11	A	2353	A

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Mol	Chain	Res	Type
11	A	2354	A
11	A	2357	C
11	A	2363	A
11	A	2372	U
11	A	2374	A
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	2478	G
11	A	2485	U
11	A	2493	C
11	A	2496	G
11	A	2502	C
11	A	2504	A
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	2576	A
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	2604	A
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

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Mol	Chain	Res	Type
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
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	2764	A
11	A	2765	A
11	A	2767	A
11	A	2768	A
11	A	2773	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	2847	C
11	A	2864	U
11	A	2865	C
11	A	2883	A
11	A	2884	C
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

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Mol	Chain	Res	Type
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2927	C
11	A	2928	C
11	A	2934	G
11	A	2935	A
11	A	2936	U
11	A	2956	A
11	A	2961	C
11	A	2962	C
11	A	2971	A
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2993	U
11	A	3005	A
11	A	3007	C
11	A	3022	G
11	A	3041	U
11	A	3049	U
11	A	3053	A
11	A	3054	G
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	3122	U
11	A	3131	G
11	A	3150	U
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3169	C
11	A	3172	C

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Mol	Chain	Res	Type
11	A	3177	A
11	A	3180	A
11	A	3183	U
11	A	3190	A
11	A	3199	U
11	A	3200	U
11	A	3202	U
11	A	3207	A
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
79	Az	0	U
79	Az	4	A
79	Az	11	U
79	Az	12	U
79	Az	13	U
79	Az	16	A
79	Az	18	A
79	Az	21	A
79	Az	22	A
79	Az	25	U
79	Az	26	A
79	Az	27	C
79	Az	30	A
81	AA	651	A
81	AA	680	U
81	AA	688	A
81	AA	704	U
81	AA	706	C
81	AA	712	C
81	AA	721	U
81	AA	722	C
81	AA	737	C
81	AA	738	A
81	AA	753	A
81	AA	761	A
81	AA	766	G

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Mol	Chain	Res	Type
81	AA	773	U
81	AA	791	G
81	AA	794	U
81	AA	796	G
81	AA	828	C
81	AA	830	U
81	AA	832	U
81	AA	835	C
81	AA	860	A
81	AA	861	U
81	AA	868	C
81	AA	870	C
81	AA	871	A
81	AA	881	A
81	AA	890	C
81	AA	893	G
81	AA	903	U
81	AA	904	C
81	AA	907	A
81	AA	919	A
81	AA	929	A
81	AA	931	C
81	AA	938	A
81	AA	939	A
81	AA	942	A
81	AA	954	C
81	AA	958	C
81	AA	959	C
81	AA	960	C
81	AA	961	U
81	AA	962	C
81	AA	963	C
81	AA	967	A
81	AA	978	A
81	AA	993	A
81	AA	1001	C
81	AA	1011	C
81	AA	1012	A
81	AA	1015	A
81	AA	1031	G
81	AA	1046	A
81	AA	1076	5MU

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Mol	Chain	Res	Type
81	AA	1081	U
81	AA	1082	A
81	AA	1096	A
81	AA	1103	A
81	AA	1105	C
81	AA	1106	C
81	AA	1107	U
81	AA	1109	A
81	AA	1116	A
81	AA	1118	A
81	AA	1119	U
81	AA	1121	A
81	AA	1126	A
81	AA	1138	G
81	AA	1151	C
81	AA	1153	C
81	AA	1155	G
81	AA	1160	A
81	AA	1167	A
81	AA	1187	U
81	AA	1189	U
81	AA	1190	C
81	AA	1215	U
81	AA	1220	A
81	AA	1223	C
81	AA	1225	C
81	AA	1230	C
81	AA	1232	A
81	AA	1235	U
81	AA	1247	G
81	AA	1248	C
81	AA	1251	A
81	AA	1261	C
81	AA	1271	C
81	AA	1273	G
81	AA	1284	U
81	AA	1290	C
81	AA	1291	U
81	AA	1292	A
81	AA	1318	A
81	AA	1326	A
81	AA	1327	G

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Mol	Chain	Res	Type
81	AA	1330	C
81	AA	1343	A
81	AA	1353	A
81	AA	1354	A
81	AA	1355	G
81	AA	1356	A
81	AA	1367	A
81	AA	1370	U
81	AA	1376	C
81	AA	1378	C
81	AA	1386	U
81	AA	1387	A
81	AA	1390	A
81	AA	1405	C
81	AA	1407	U
81	AA	1424	U
81	AA	1430	A
81	AA	1466	C
81	AA	1478	A
81	AA	1482	A
81	AA	1512	A
81	AA	1519	A
81	AA	1522	U
81	AA	1525	C
81	AA	1526	U
81	AA	1527	A
81	AA	1528	A
81	AA	1533	C
81	AA	1537	C
81	AA	1538	G
81	AA	1539	C
81	AA	1540	A
81	AA	1551	G
81	AA	1557	A
81	AA	1560	U
81	AA	1568	U
81	AA	1571	U
81	AA	1582	G
81	AA	1584	MA6
81	AA	1594	G
81	AA	1595	G
81	AA	1599	A

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Mol	Chain	Res	Type
85	Ax	13	U
85	Ax	16	A
85	Ax	17	U
85	Ax	18	A
85	Ax	22	U
85	Ax	43	A
85	Ax	44	U
85	Ax	47	U
85	Ax	48	G
85	Ax	51	U
85	Ax	52	A
85	Ax	56	C
85	Ax	63	G
85	Ax	65	A
85	Ax	71	A
86	Ay	8	U
86	Ay	9	A
86	Ay	13	U
86	Ay	29	U
86	Ay	33	U
86	Ay	44	A
86	Ay	45	G
86	Ay	46	A
86	Ay	49	G
86	Ay	56	C
86	Ay	58	A
86	Ay	59	U
86	Ay	73	A
87	Aw	9	A
87	Aw	13	U
87	Aw	14	A
87	Aw	15	A
87	Aw	16	A
87	Aw	21	A
87	Aw	46	A
87	Aw	49	U
87	Aw	50	A
87	Aw	51	U
87	Aw	52	G
87	Aw	53	A
87	Aw	56	A
87	Aw	63	A

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Mol	Chain	Res	Type
87	Aw	65	A
87	Aw	68	U
87	Aw	69	A
87	Aw	71	C
87	Aw	72	A
87	Aw	74	C
87	Aw	75	C
92	B	8	U
92	B	10	2MG
92	B	16	C
92	B	21	A
92	B	45	G
92	B	46	A
92	B	54	C
92	B	55	U
92	B	56	U
92	B	58	A
92	B	59	A
92	B	64	A
92	B	69	U
92	B	72	G
92	B	76	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2245	A
11	A	2484	C
81	AA	1137	A

## 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
11	PSU	A	3067	11	18,21,22	1.18	2 (11%)	21,30,33	0.81	1 (4%)
81	5MC	AA	1488	81	19,22,23	0.95	1 (5%)	26,32,35	0.57	0
81	MA6	AA	1583	81	23,26,27	0.41	0	33,38,41	0.75	1 (3%)
11	OMG	A	3040	11,87	23,26,27	0.39	0	32,38,41	0.41	0
81	MA6	AA	1584	81	23,26,27	0.37	0	33,38,41	0.75	1 (3%)
81	B8T	AA	1486	81,97	19,22,23	0.47	0	25,31,34	0.32	0
92	1MA	B	9	92	21,25,26	0.43	0	30,37,40	0.67	0
92	PSU	B	39	92	18,21,22	1.06	1 (5%)	21,30,33	0.72	0
11	OMU	A	3039	11,94	19,22,23	0.36	0	25,31,34	0.67	1 (4%)
11	OMG	A	2815	85,11,94	23,26,27	0.42	0	32,38,41	0.41	0
11	1MA	A	2617	11	21,25,26	0.48	0	30,37,40	0.62	0
81	5MU	AA	1076	81	19,22,23	0.41	0	27,32,35	0.66	0
92	2MG	B	10	92	23,26,27	0.37	0	33,38,41	0.43	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
11	PSU	A	3067	11	-	1/7/25/26	0/2/2/2
81	5MC	AA	1488	81	-	0/7/25/26	0/2/2/2
81	MA6	AA	1583	81	-	0/11/29/30	0/3/3/3
11	OMG	A	3040	11,87	-	0/9/27/28	0/3/3/3
81	MA6	AA	1584	81	-	1/11/29/30	0/3/3/3
81	B8T	AA	1486	81,97	-	1/7/27/28	0/2/2/2
92	1MA	B	9	92	-	0/7/25/26	0/3/3/3
92	PSU	B	39	92	-	0/7/25/26	0/2/2/2
11	OMU	A	3039	11,94	-	0/9/27/28	0/2/2/2
11	OMG	A	2815	85,11,94	-	1/9/27/28	0/3/3/3
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
81	5MU	AA	1076	81	-	5/7/25/26	0/2/2/2
92	2MG	B	10	92	-	0/9/27/28	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AA	1488	5MC	C5-C4	-3.67	1.41	1.44
92	B	39	PSU	C6-C5	3.44	1.39	1.35
11	A	3067	PSU	C6-C5	3.35	1.39	1.35
11	A	3067	PSU	O4'-C1'	-2.79	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AA	1583	MA6	C2-N1-C6	2.93	119.00	111.83
81	AA	1584	MA6	C2-N1-C6	2.88	118.88	111.83
11	A	3039	OMU	C2'-C1'-N1	-2.58	109.34	114.24
11	A	3067	PSU	O4'-C1'-C2'	2.41	108.49	105.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2815	OMG	C1'-C2'-O2'-CM2
81	AA	1076	5MU	O4'-C4'-C5'-O5'
81	AA	1076	5MU	C3'-C4'-C5'-O5'
81	AA	1076	5MU	C4'-C5'-O5'-P
81	AA	1584	MA6	C4'-C5'-O5'-P
81	AA	1076	5MU	C2'-C1'-N1-C2
81	AA	1486	B8T	O4'-C4'-C5'-O5'
81	AA	1076	5MU	C2'-C1'-N1-C6
11	A	3067	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	AA	1488	5MC	1	0
81	AA	1583	MA6	2	0
81	AA	1486	B8T	1	0
92	B	9	1MA	1	0
11	A	3039	OMU	1	0
11	A	2815	OMG	1	0
81	AA	1076	5MU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 278 ligands modelled in this entry, 261 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	$\# Z  > 2$
95	SPD	A	3472	-	9,9,9	0.18	0	8,8,8	0.30	0
98	FES	r	201	17,50	0,4,4	-	-	-		
100	SPM	AA	1781	-	13,13,13	0.18	0	12,12,12	0.31	0
95	SPD	A	3471	-	9,9,9	0.14	0	8,8,8	0.37	0
95	SPD	A	3301	-	9,9,9	0.19	0	8,8,8	0.23	0
98	FES	AP	201	58,68	0,4,4	-	-	-		
95	SPD	AA	1703	-	9,9,9	0.16	0	8,8,8	0.28	0
96	PUT	A	3303	-	5,5,5	0.11	0	4,4,4	0.28	0
102	GDP	AX	503	-	29,30,30	1.19	3 (10%)	45,47,47	1.77	6 (13%)
95	SPD	AA	1783	-	9,9,9	0.17	0	8,8,8	0.23	0
95	SPD	A	3470	-	9,9,9	0.17	0	8,8,8	0.25	0
99	NAD	AA	1701	97	46,48,48	1.17	3 (6%)	64,73,73	0.89	3 (4%)
100	SPM	AA	1702	-	13,13,13	0.19	0	12,12,12	0.27	0
101	ATP	AX	501	97	32,33,33	0.83	2 (6%)	48,52,52	0.39	0
103	VAL	B	101	92	4,6,7	0.79	0	6,7,9	1.01	1 (16%)
98	FES	AT	201	65,71	0,4,4	-	-	-		
95	SPD	A	3302	-	9,9,9	0.16	0	8,8,8	0.22	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
95	SPD	A	3472	-	-	1/7/7/7	-
98	FES	r	201	17,50	-	-	0/1/1/1
100	SPM	AA	1781	-	-	0/11/11/11	-
95	SPD	A	3471	-	-	1/7/7/7	-
95	SPD	A	3301	-	-	0/7/7/7	-
102	GDP	AX	503	-	-	6/16/32/32	0/3/3/3
95	SPD	AA	1703	-	-	0/7/7/7	-
96	PUT	A	3303	-	-	0/3/3/3	-
98	FES	AP	201	58,68	-	-	0/1/1/1
95	SPD	AA	1783	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
95	SPD	A	3470	-	-	0/7/7/7	-
99	NAD	AA	1701	97	-	4/30/62/62	0/5/5/5
100	SPM	AA	1702	-	-	0/11/11/11	-
101	ATP	AX	501	97	-	2/22/38/38	0/3/3/3
103	VAL	B	101	92	-	1/5/6/8	-
98	FES	AT	201	65,71	-	-	0/1/1/1
95	SPD	A	3302	-	-	2/7/7/7	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
99	AA	1701	NAD	PA-O3	4.12	1.63	1.59
101	AX	501	ATP	PB-O3B	-3.38	1.55	1.59
102	AX	503	GDP	C5-C4	3.07	1.47	1.38
99	AA	1701	NAD	O4D-C1D	-2.88	1.37	1.40
101	AX	501	ATP	PA-O3A	-2.64	1.56	1.59
102	AX	503	GDP	C6-N1	-2.59	1.34	1.38
102	AX	503	GDP	C5-N7	-2.20	1.34	1.39
99	AA	1701	NAD	PN-O3	2.07	1.61	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
102	AX	503	GDP	C5-C4-N3	-6.01	118.83	128.39
102	AX	503	GDP	C2-N3-C4	4.82	120.60	112.30
102	AX	503	GDP	N9-C4-N3	4.49	134.94	125.95
102	AX	503	GDP	C6-C5-N7	3.22	136.16	130.29
99	AA	1701	NAD	O3-PA-O1A	-2.80	102.27	110.70
102	AX	503	GDP	C4-C5-N7	-2.54	106.64	110.67
103	B	101	VAL	O-C-CA	-2.37	118.66	124.77
102	AX	503	GDP	C3'-C2'-C1'	2.36	105.92	101.46
99	AA	1701	NAD	O2A-PA-O1A	2.26	122.96	112.44
99	AA	1701	NAD	O7N-C7N-N7N	2.01	125.53	122.62

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
99	AA	1701	NAD	C5D-O5D-PN-O3
99	AA	1701	NAD	C5D-O5D-PN-O1N

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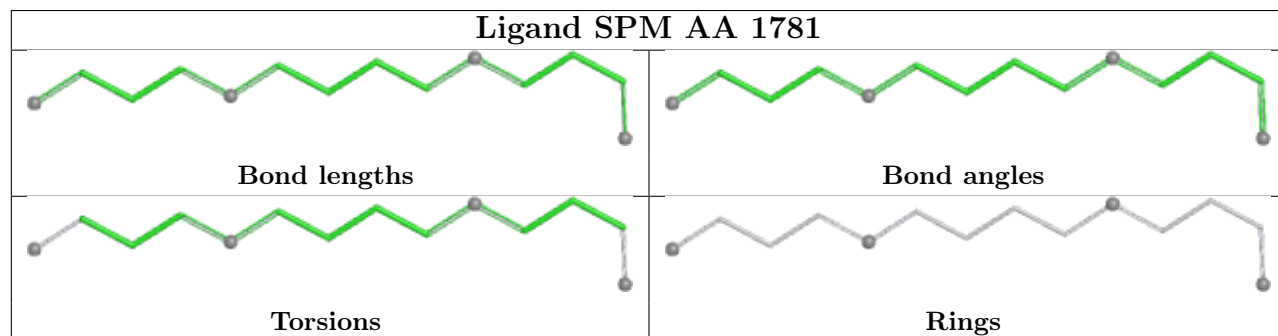
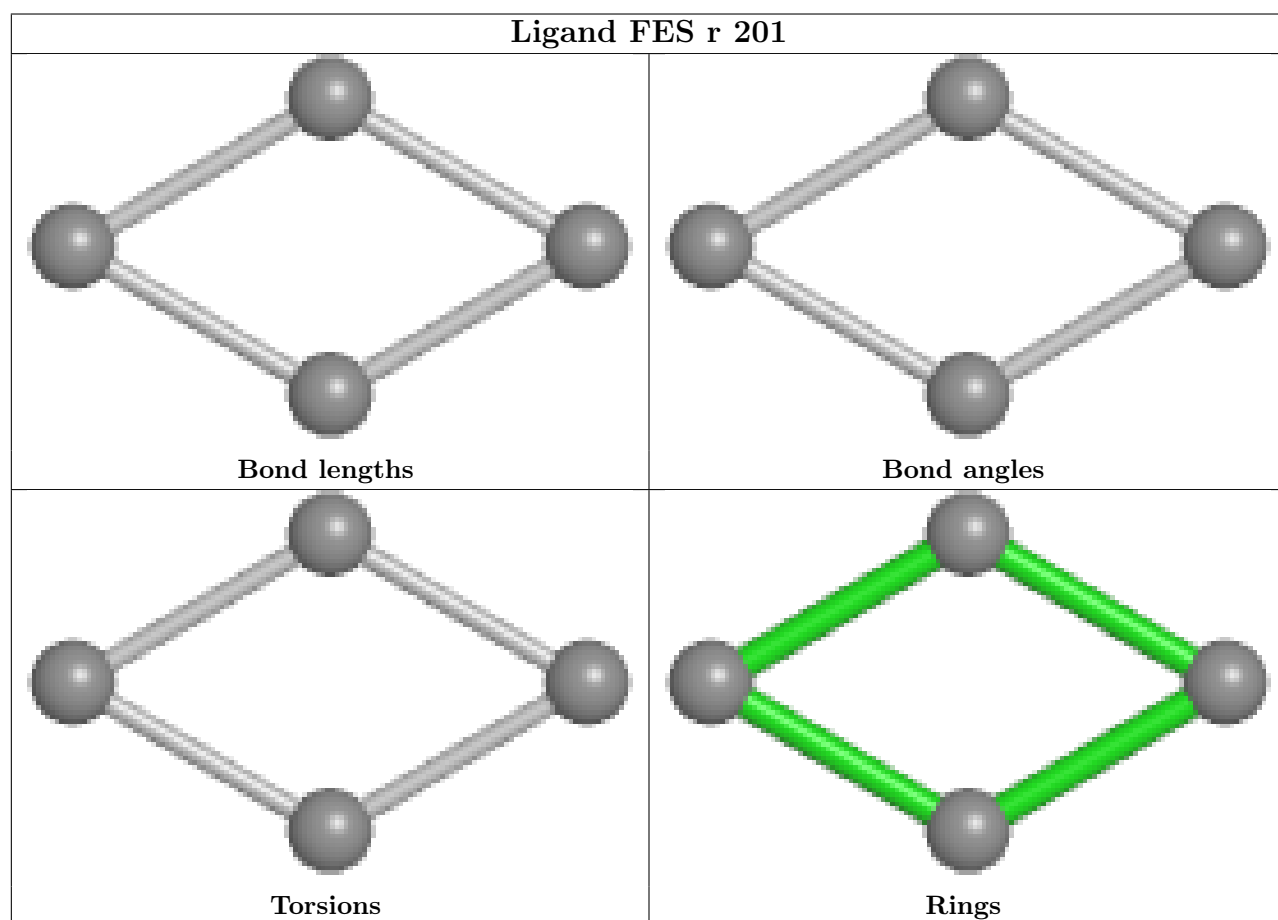
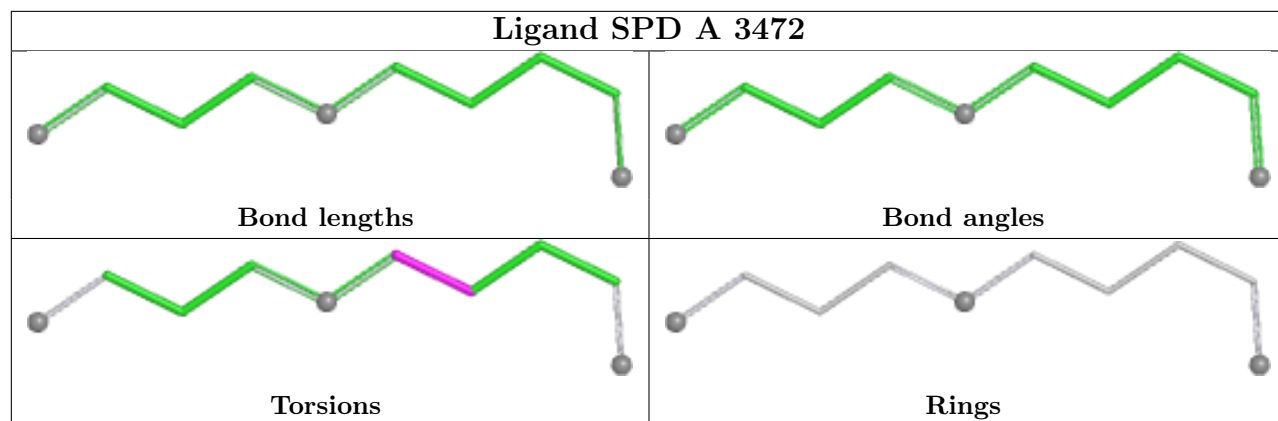
Mol	Chain	Res	Type	Atoms
102	AX	503	GDP	PA-O3A-PB-O3B
102	AX	503	GDP	C5'-O5'-PA-O3A
102	AX	503	GDP	C5'-O5'-PA-O1A
103	B	101	VAL	C-CA-CB-CG2
95	A	3472	SPD	C3-C4-C5-N6
99	AA	1701	NAD	C3D-C4D-C5D-O5D
99	AA	1701	NAD	O4D-C4D-C5D-O5D
95	A	3302	SPD	N1-C2-C3-C4
101	AX	501	ATP	PB-O3B-PG-O3G
102	AX	503	GDP	C5'-O5'-PA-O2A
102	AX	503	GDP	PA-O3A-PB-O2B
95	A	3471	SPD	C2-C3-C4-C5
95	A	3302	SPD	C8-C7-N6-C5
102	AX	503	GDP	PA-O3A-PB-O1B
101	AX	501	ATP	PG-O3B-PB-O2B

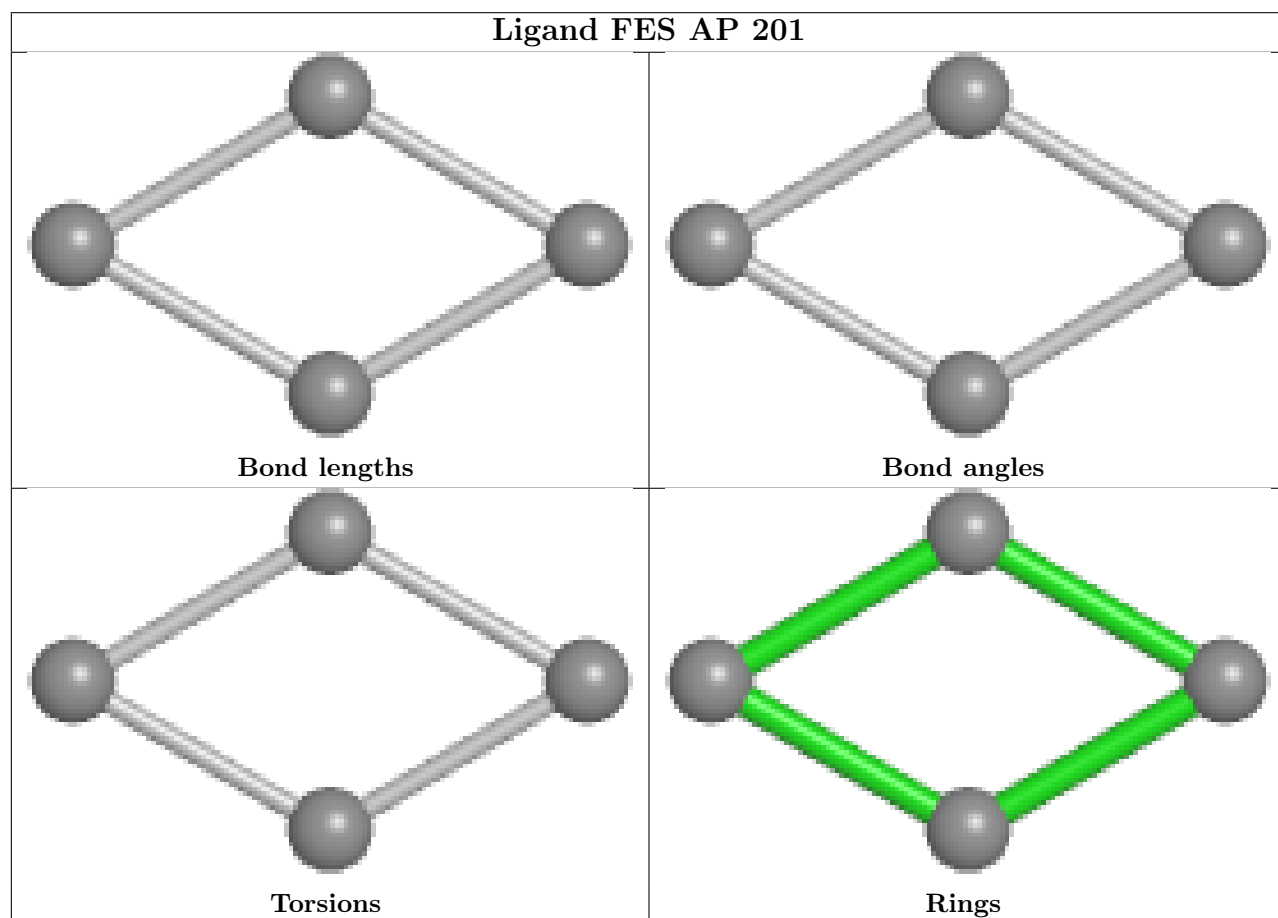
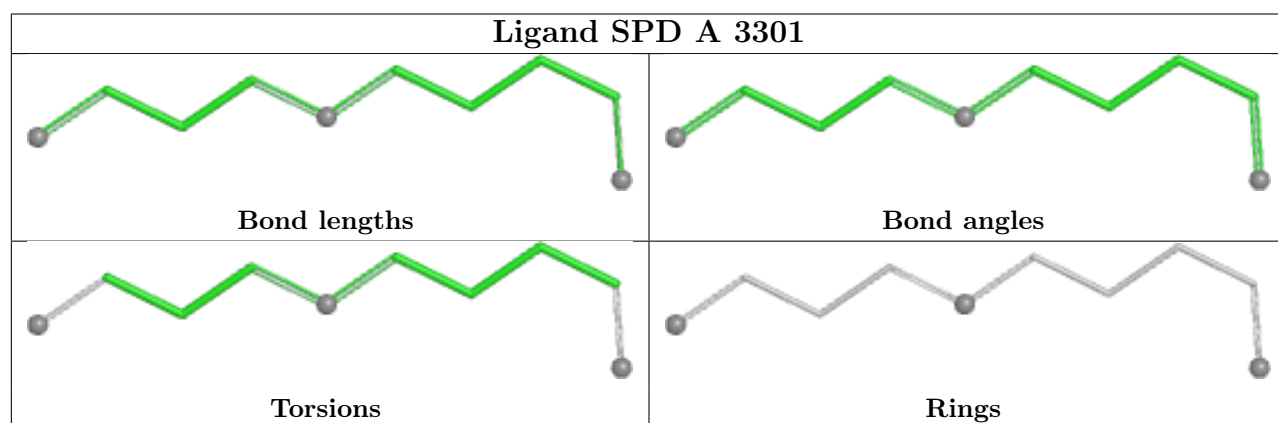
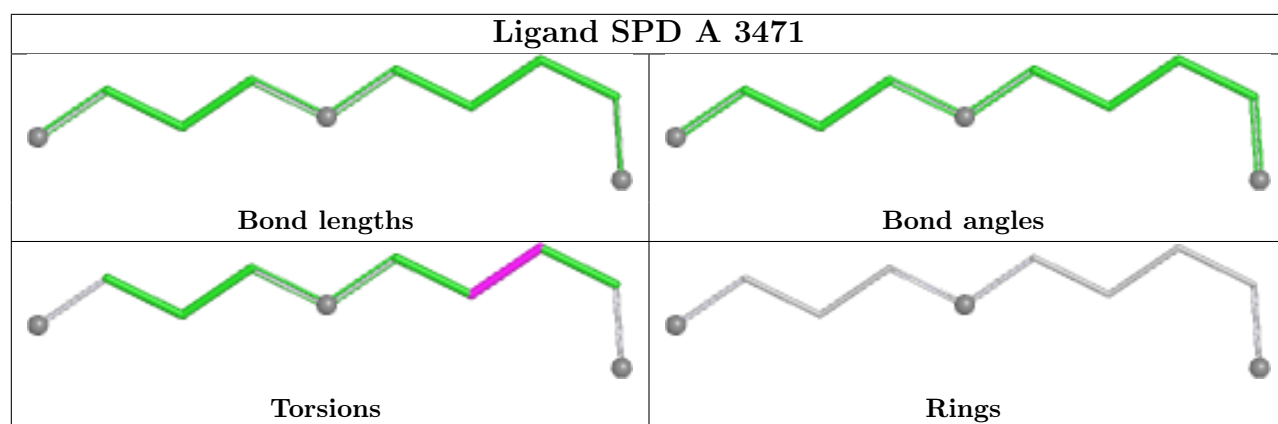
There are no ring outliers.

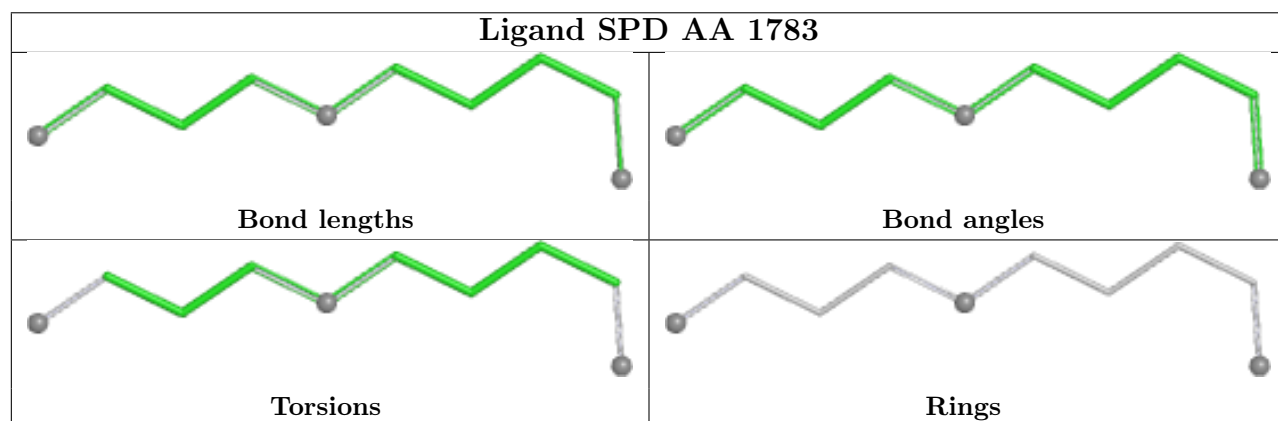
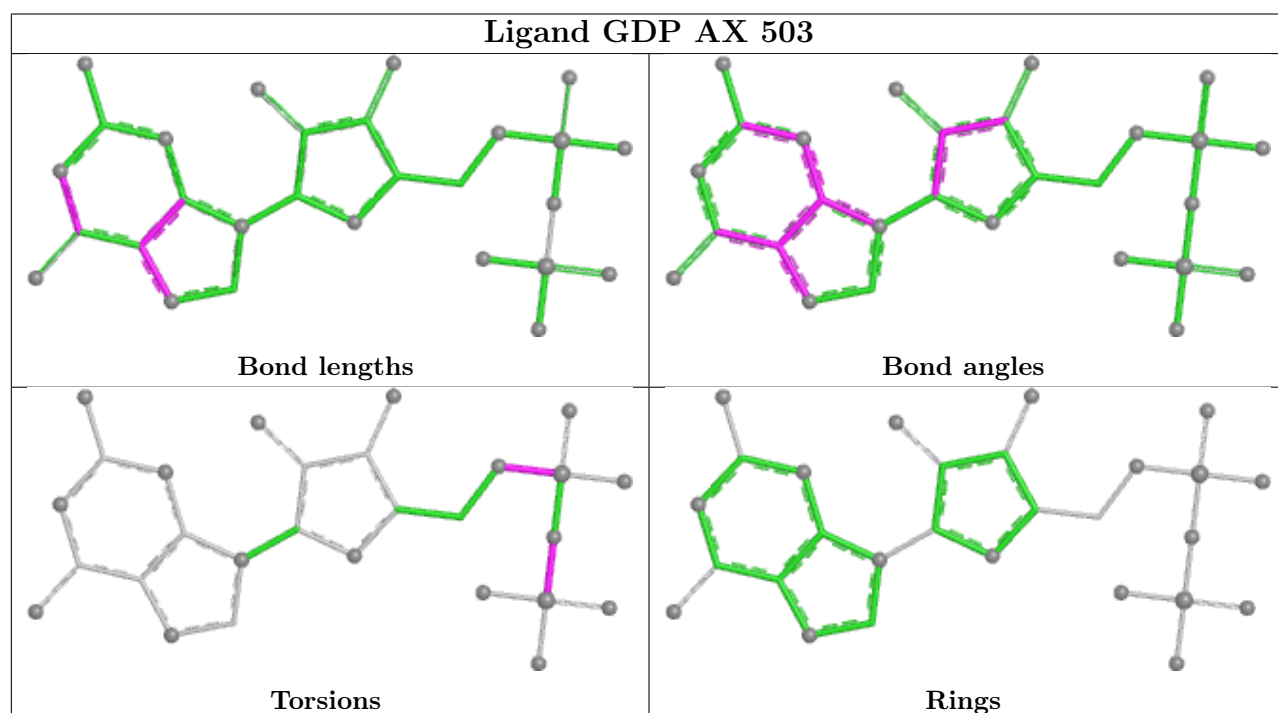
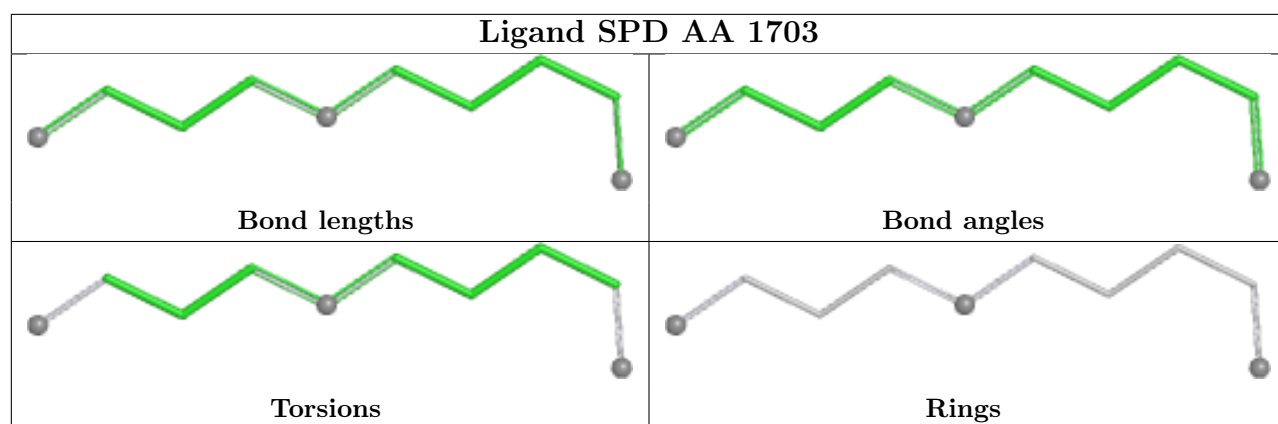
4 monomers are involved in 5 short contacts:

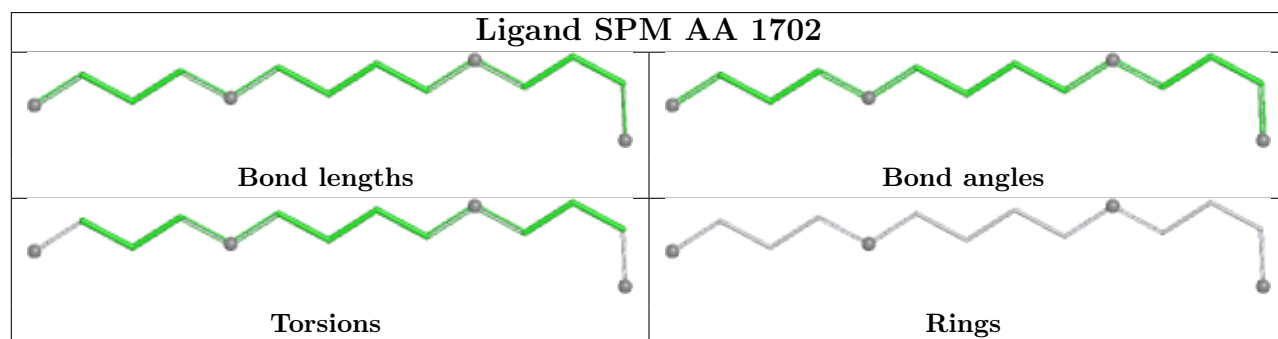
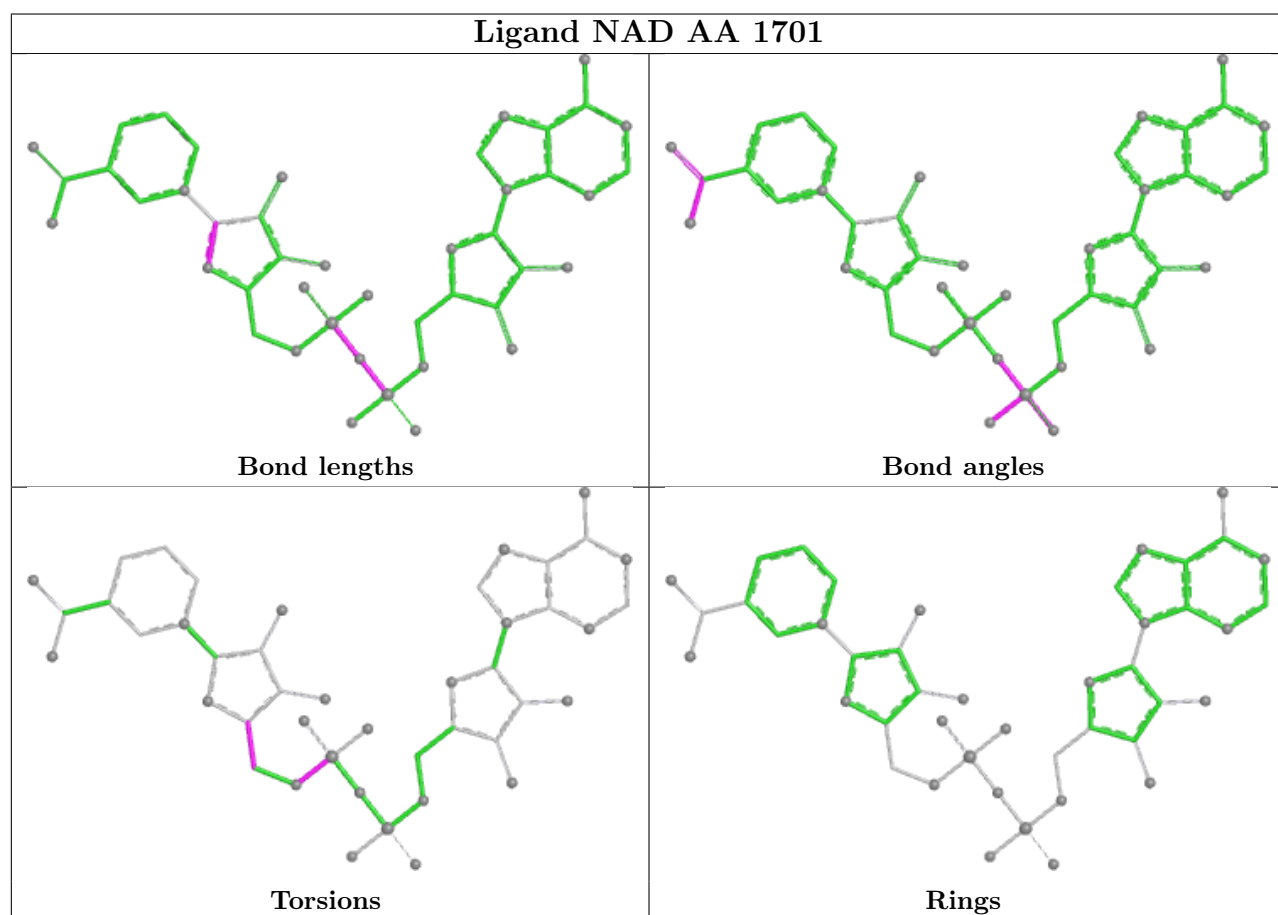
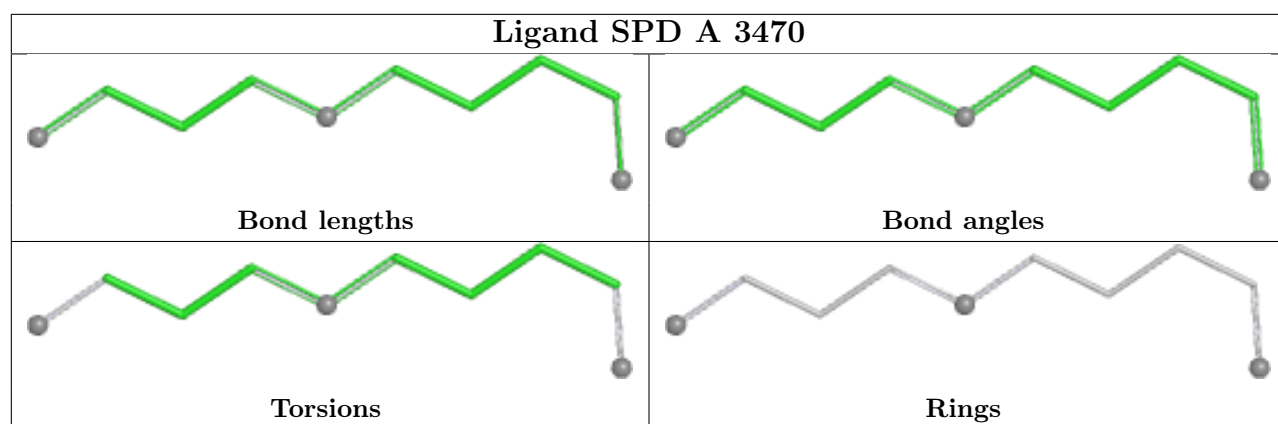
Mol	Chain	Res	Type	Clashes	Symm-Clashes
98	r	201	FES	1	0
102	AX	503	GDP	1	0
99	AA	1701	NAD	1	0
103	B	101	VAL	2	0

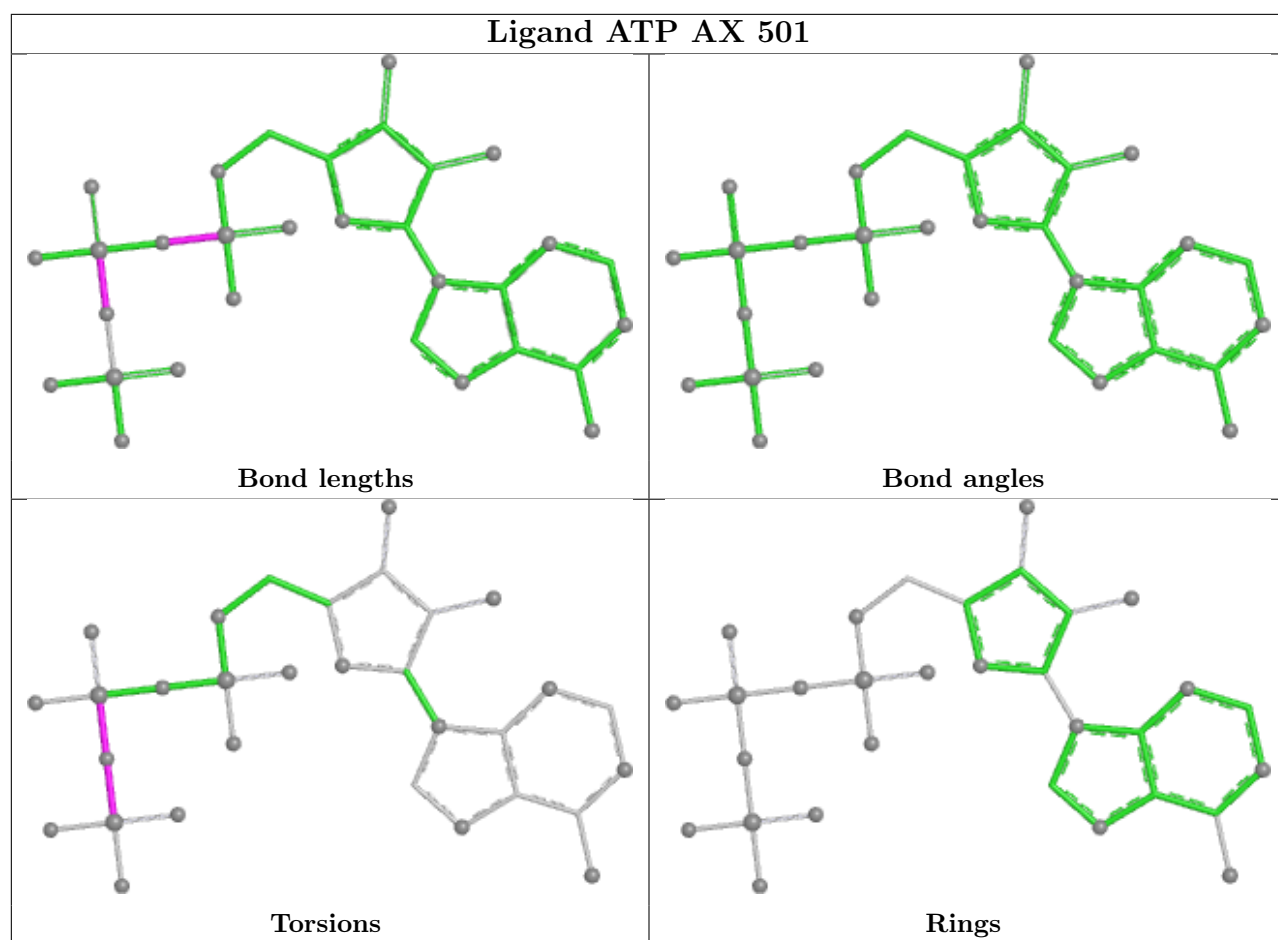
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

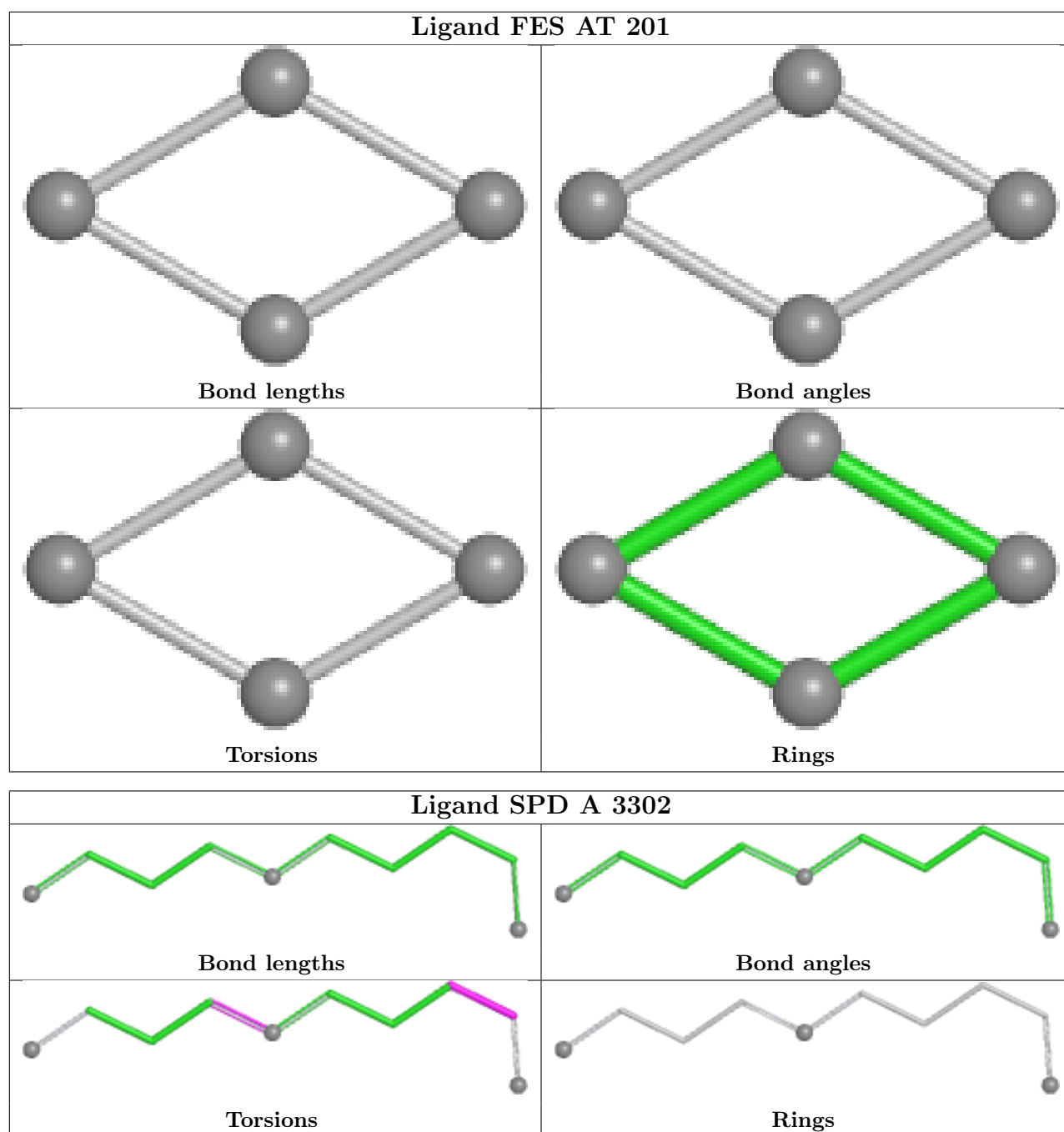












## 5.7 Other polymers [i](#)

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
92	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	46:A	O3'	48:U	P	4.56



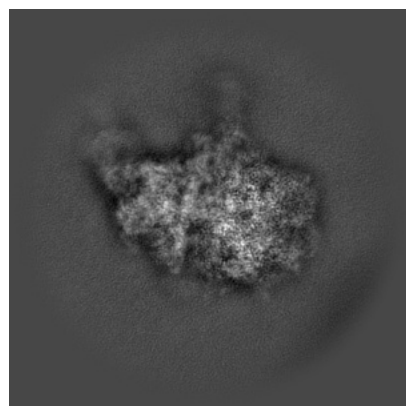
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71633. These allow visual inspection of the internal detail of the map and identification of artifacts.

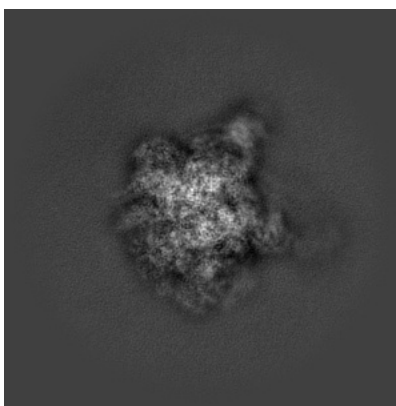
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

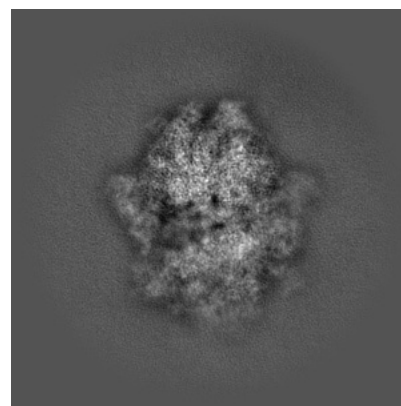
#### 6.1.1 Primary map



X

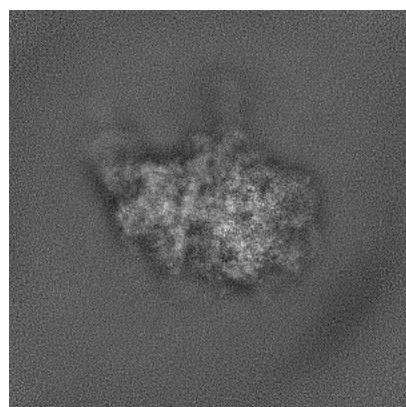


Y

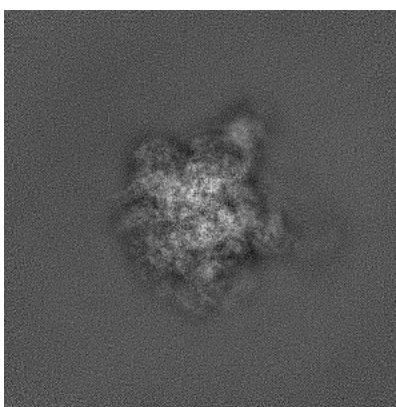


Z

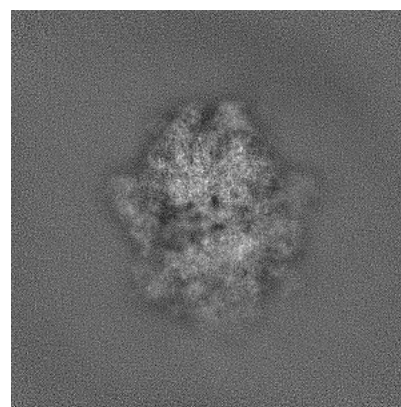
#### 6.1.2 Raw map



X



Y

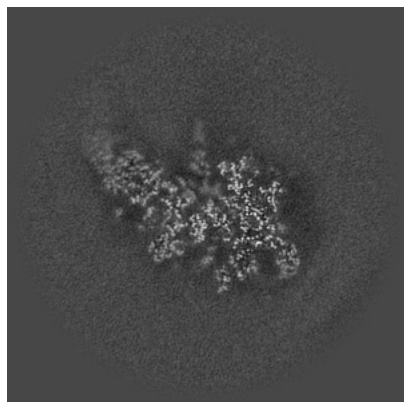


Z

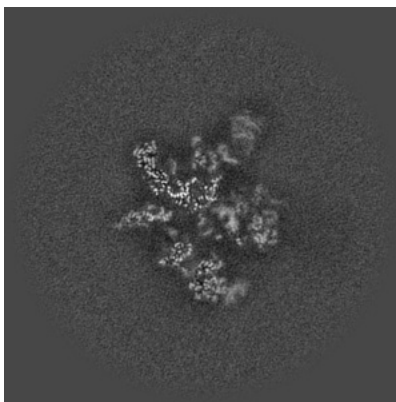
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

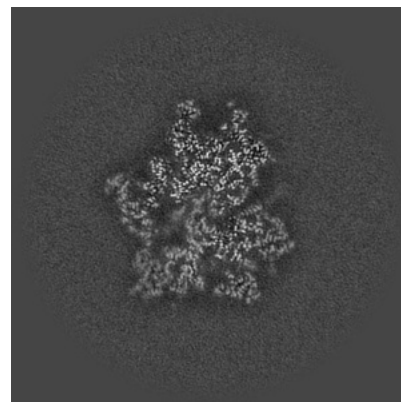
### 6.2.1 Primary map



X Index: 240

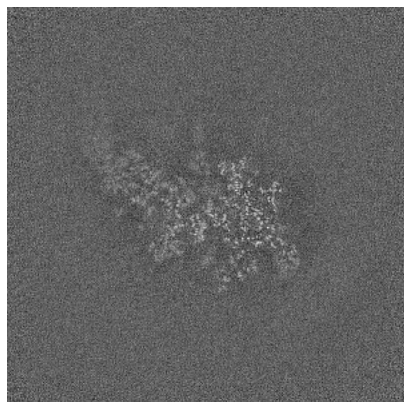


Y Index: 240

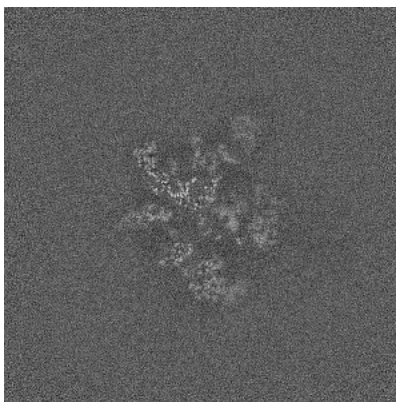


Z Index: 240

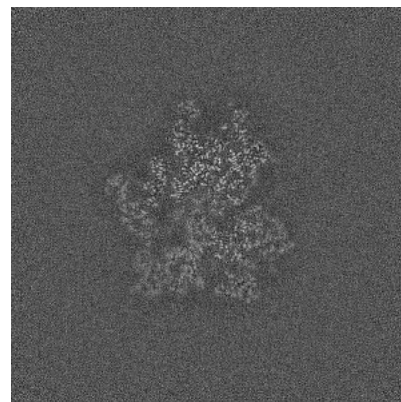
### 6.2.2 Raw map



X Index: 240



Y Index: 240

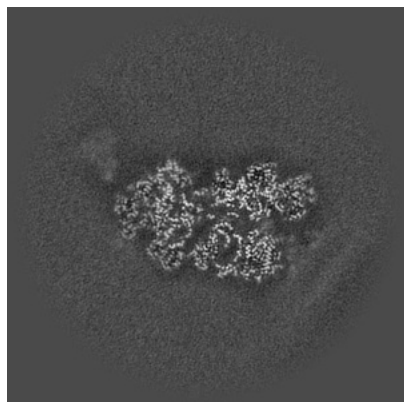


Z Index: 240

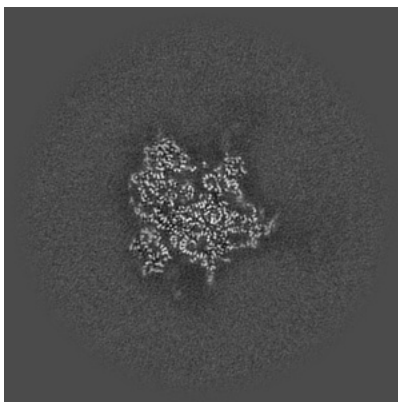
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

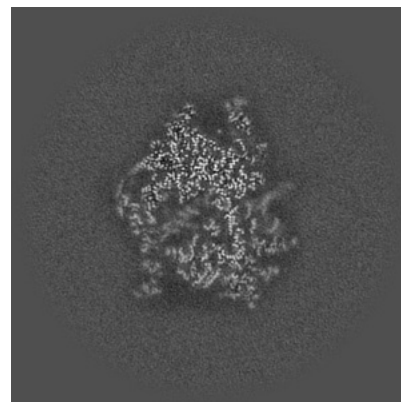
### 6.3.1 Primary map



X Index: 275

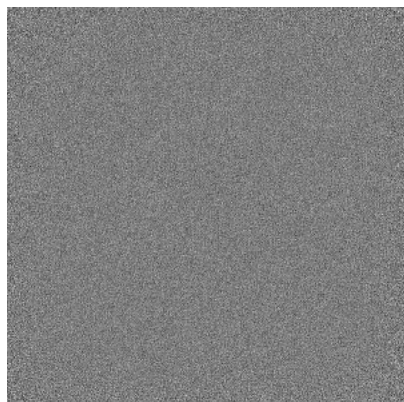


Y Index: 287

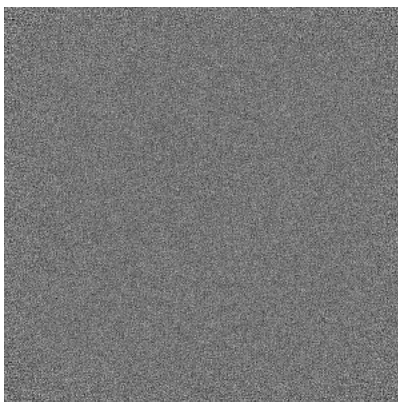


Z Index: 249

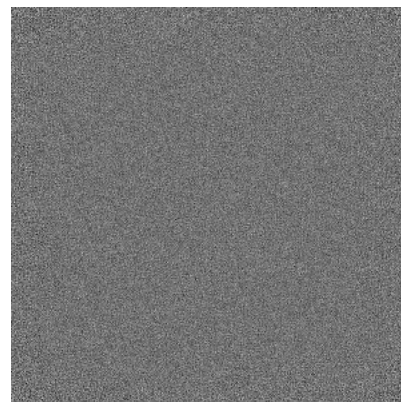
### 6.3.2 Raw map



X Index: 0



Y Index: 0



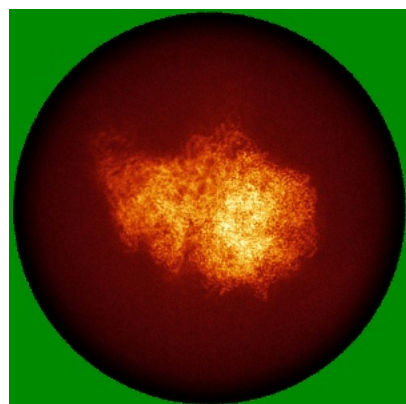
Z Index: 0

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

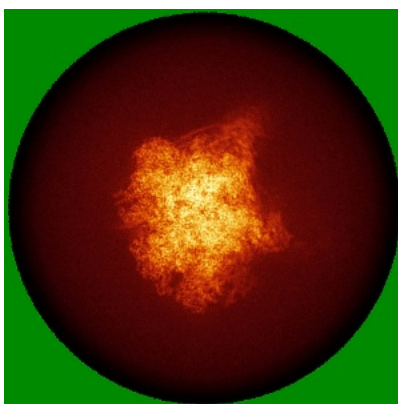


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

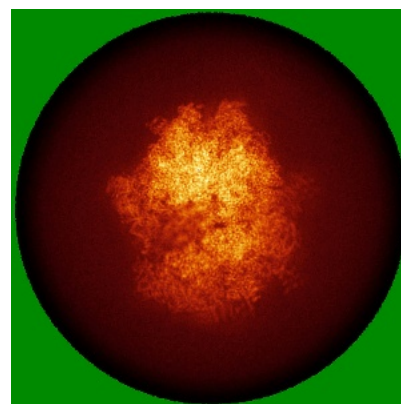
### 6.4.1 Primary map



X

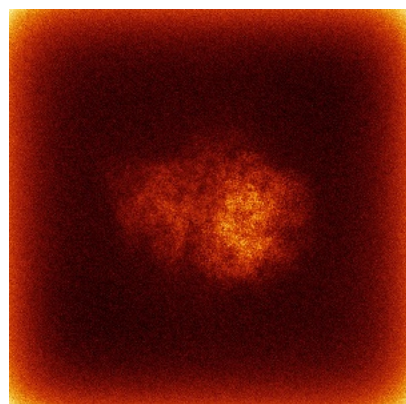


Y

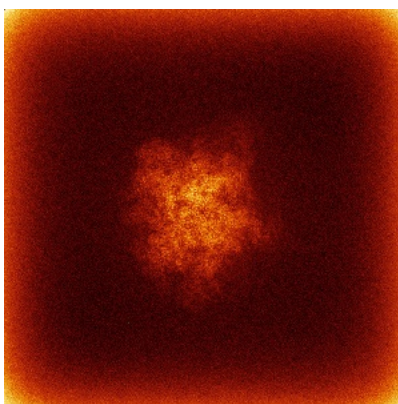


Z

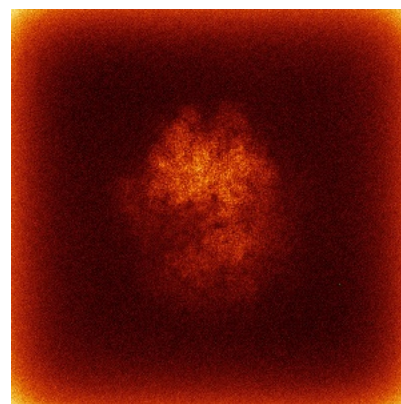
### 6.4.2 Raw map



X



Y

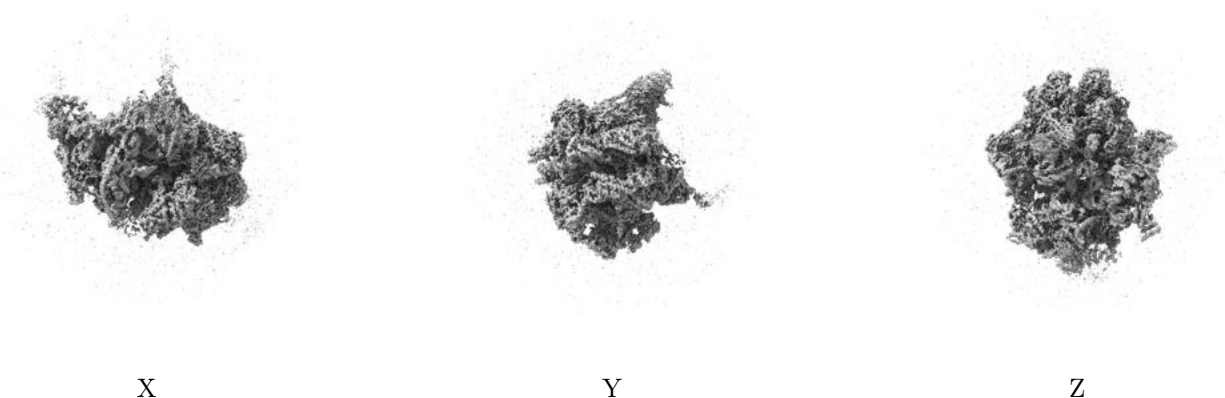


Z

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.

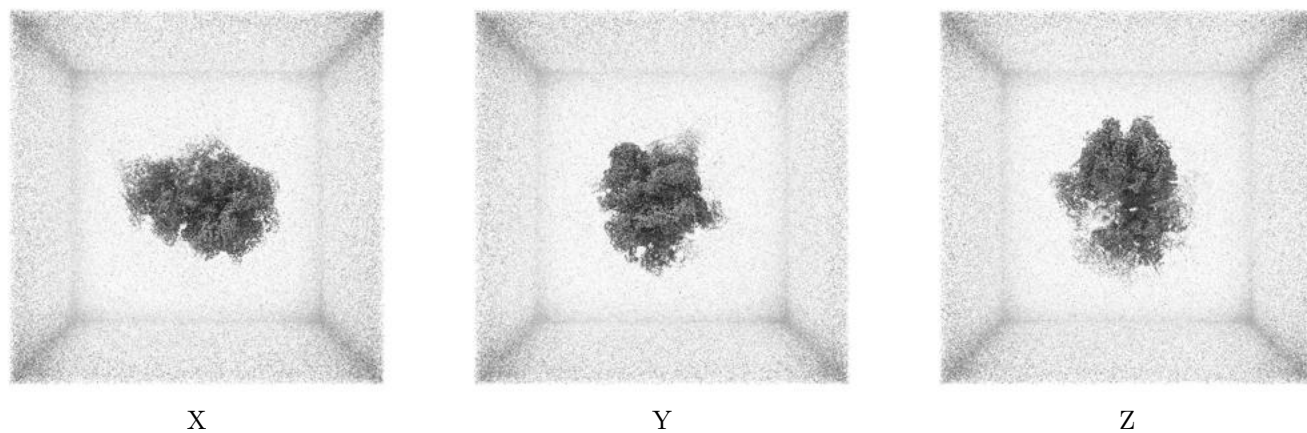
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

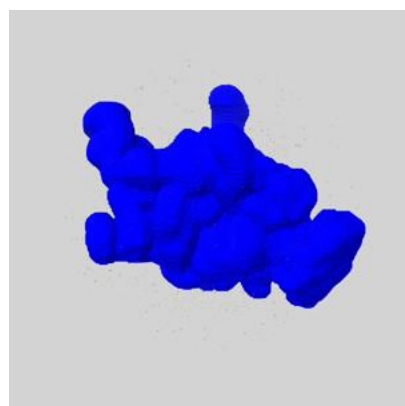
## 6.6 Mask visualisation [i](#)

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

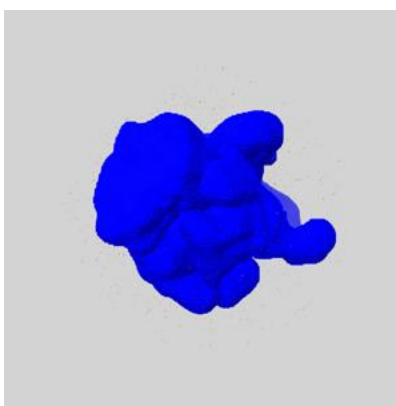
A mask typically either:

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

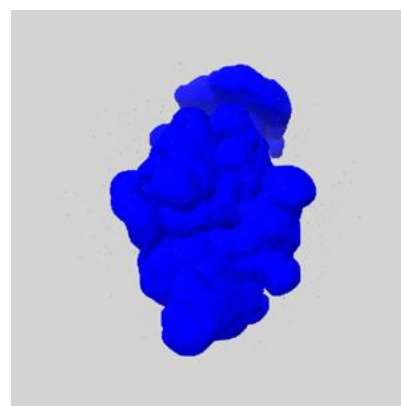
### 6.6.1 emd\_71633\_msk\_1.map [i](#)



X



Y

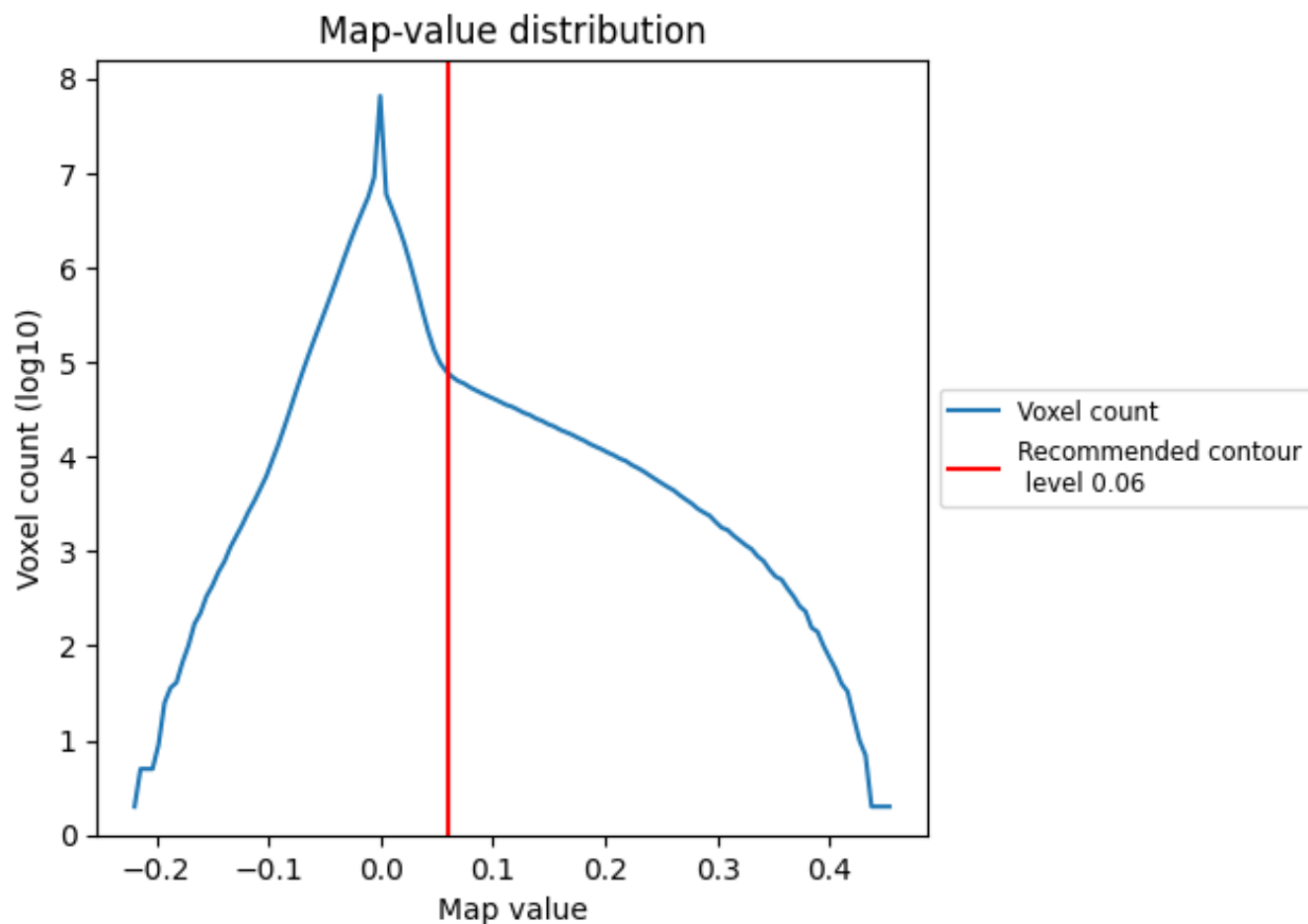


Z

## 7 Map analysis [i](#)

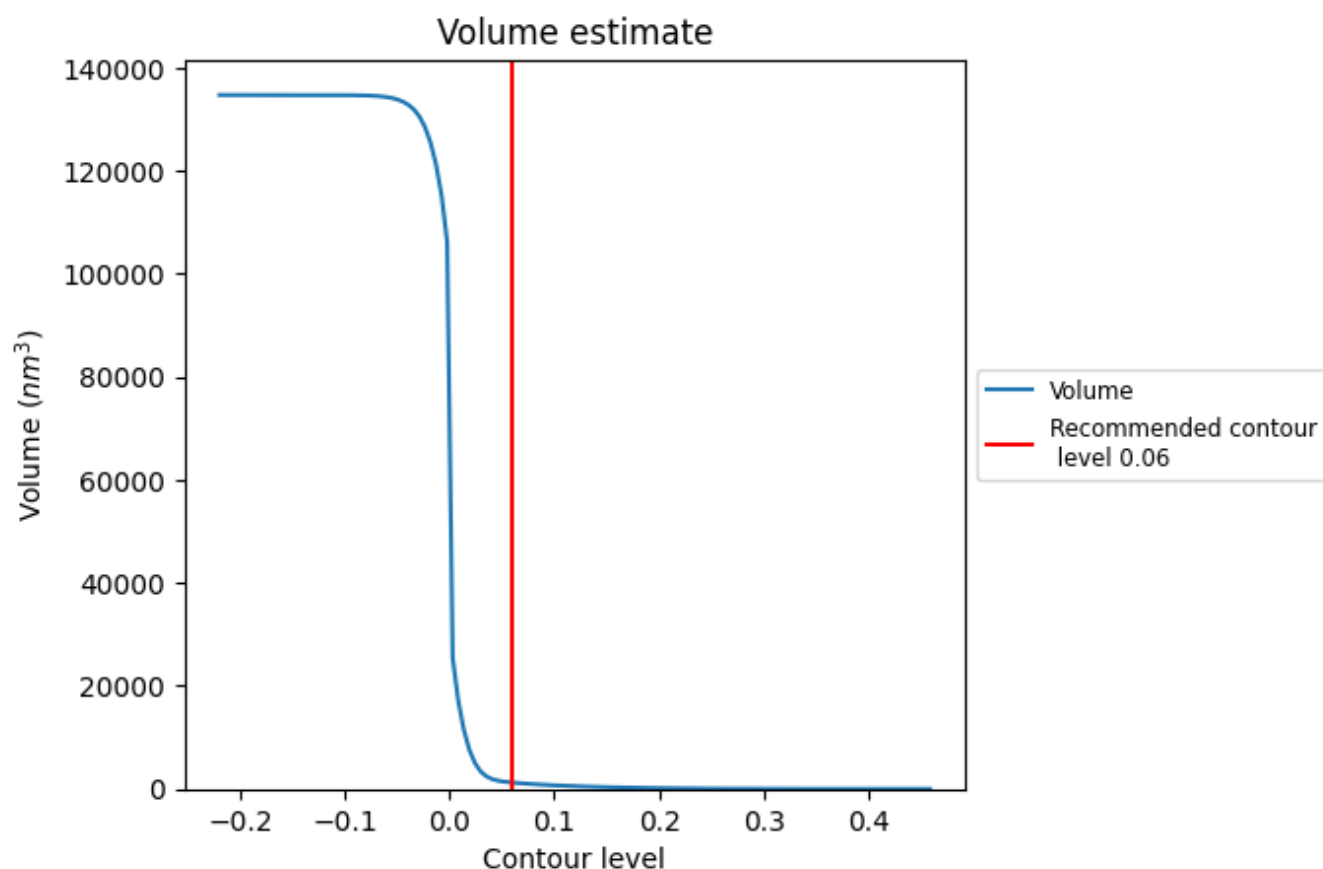
This section contains the results of statistical analysis of the map.

### 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](#)

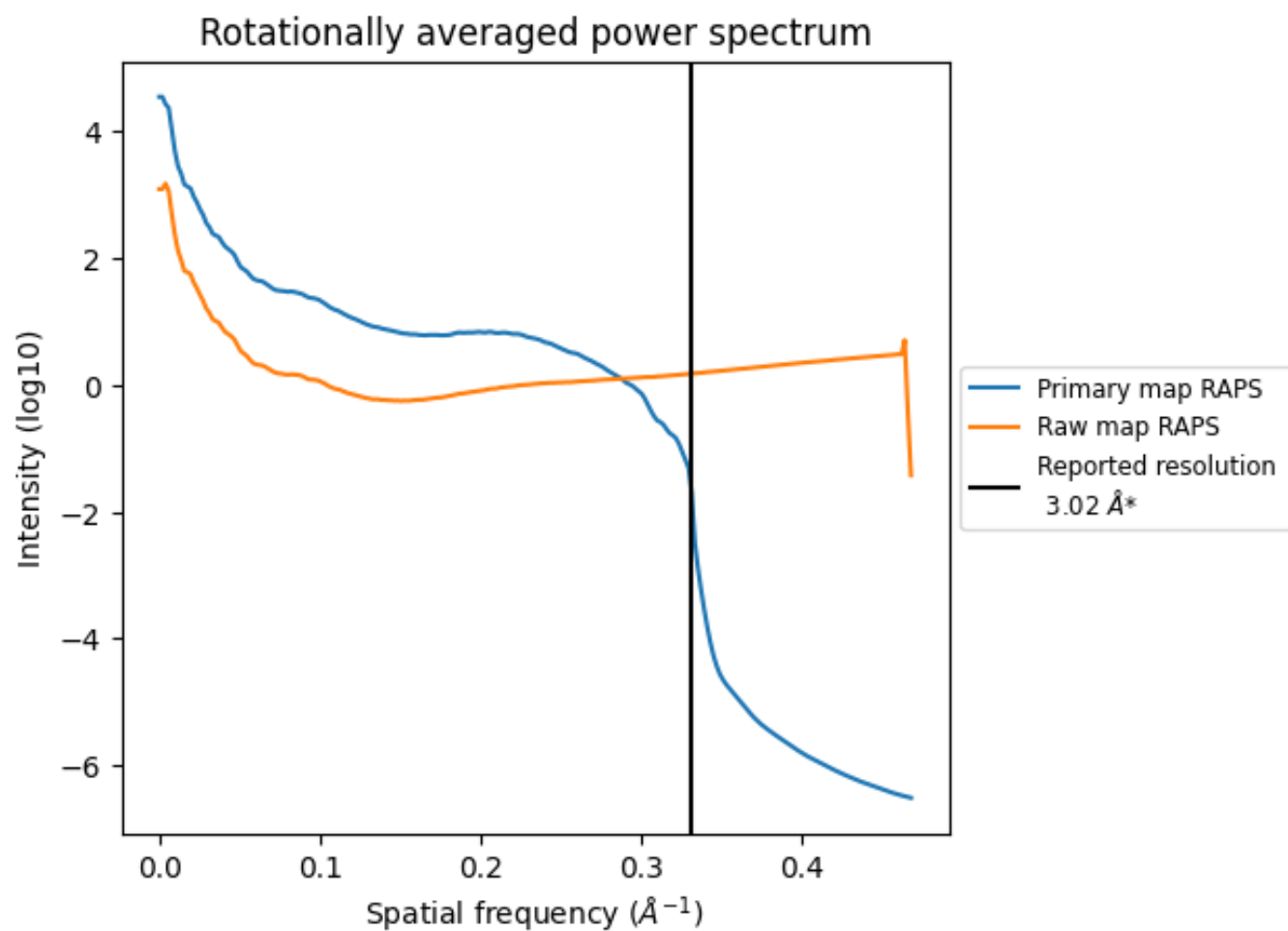


The volume at the recommended contour level is 1240  $\text{nm}^3$ ; this corresponds to an approximate mass of 1120 kDa.

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 ⓘ

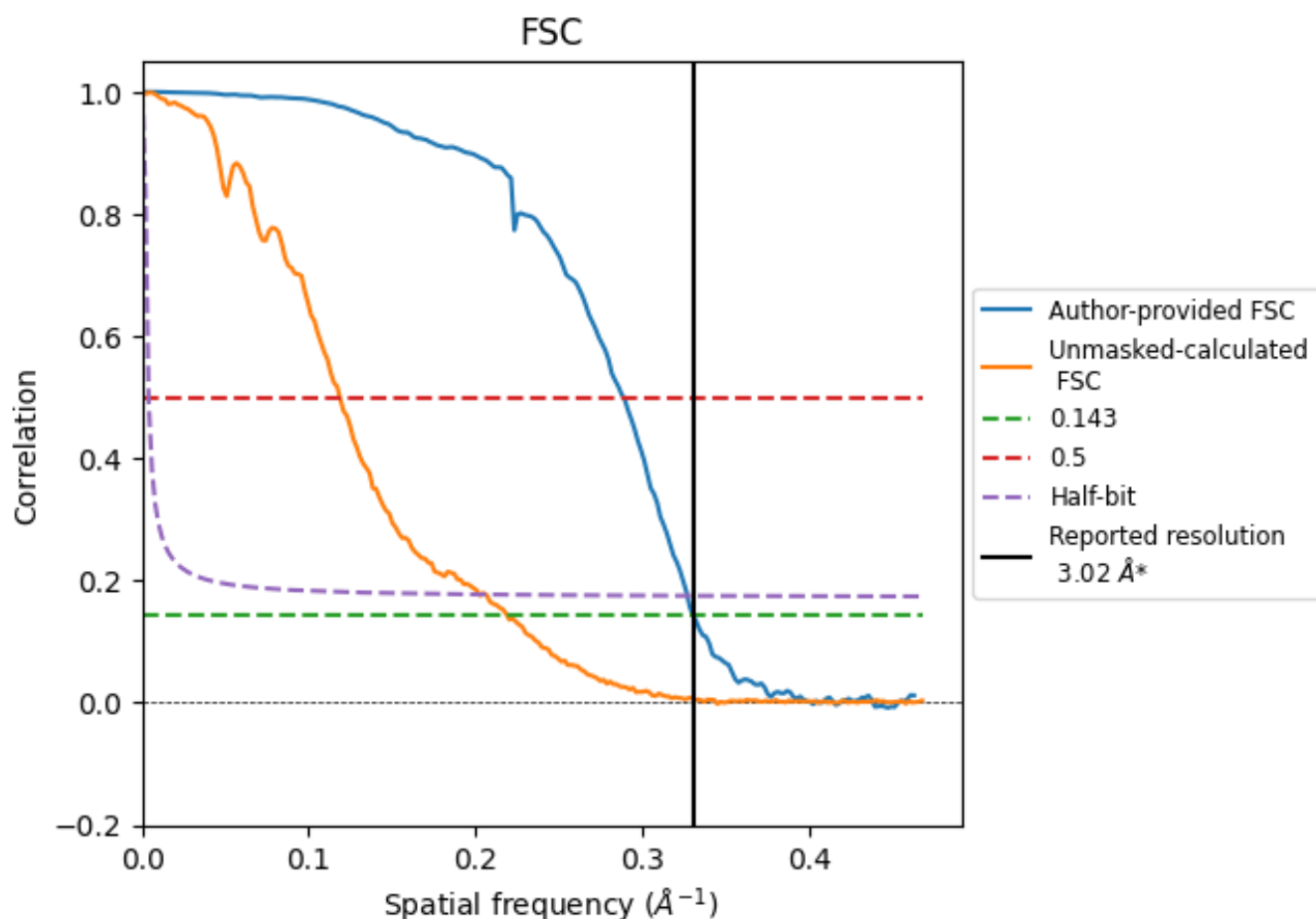


\*Reported resolution corresponds to spatial frequency of 0.331  $\text{\AA}^{-1}$

## 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 0.331  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

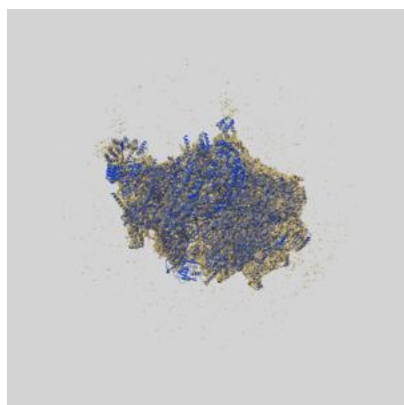
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.46	3.06
Unmasked-calculated*	4.57	8.43	4.94

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.57 differs from the reported value 3.02 by more than 10 %

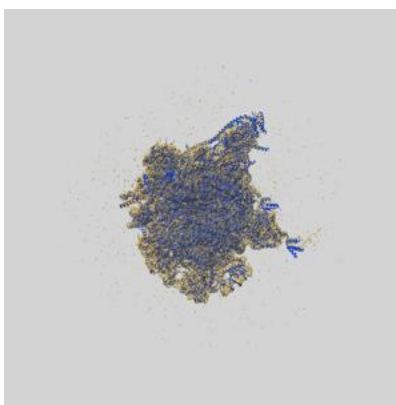
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71633 and PDB model 9PGI. Per-residue inclusion information can be found in section [3](#) on page [27](#).

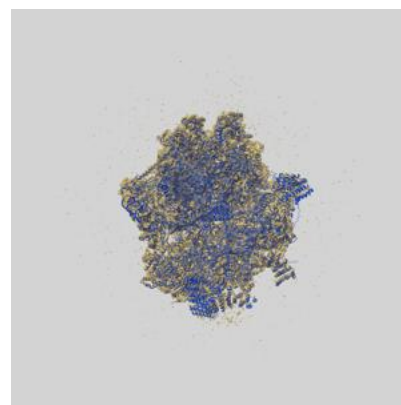
### 9.1 Map-model overlay [i](#)



X



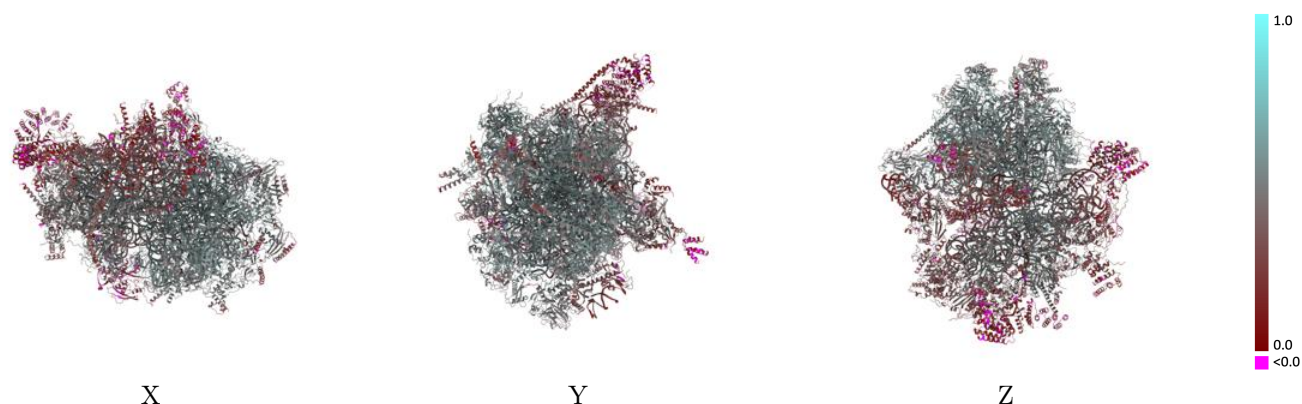
Y



Z

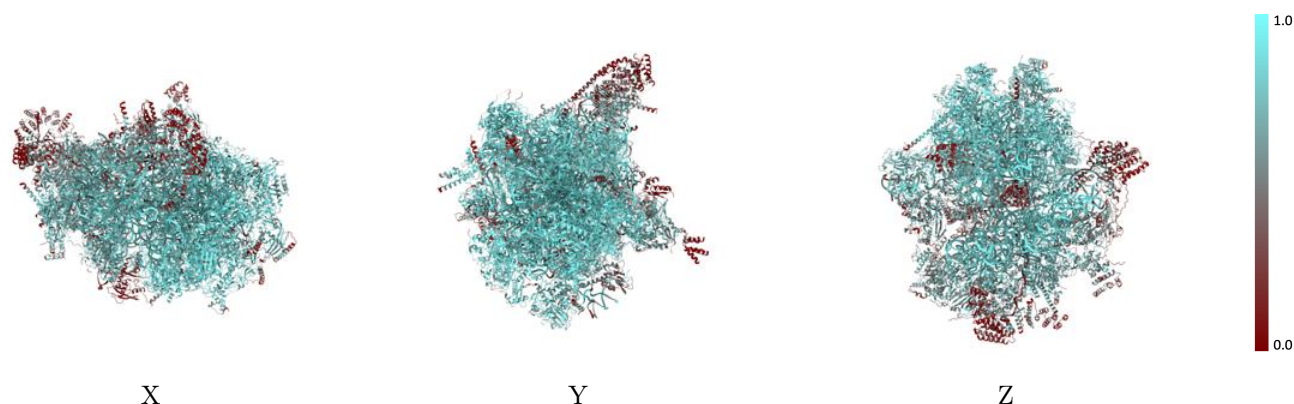
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



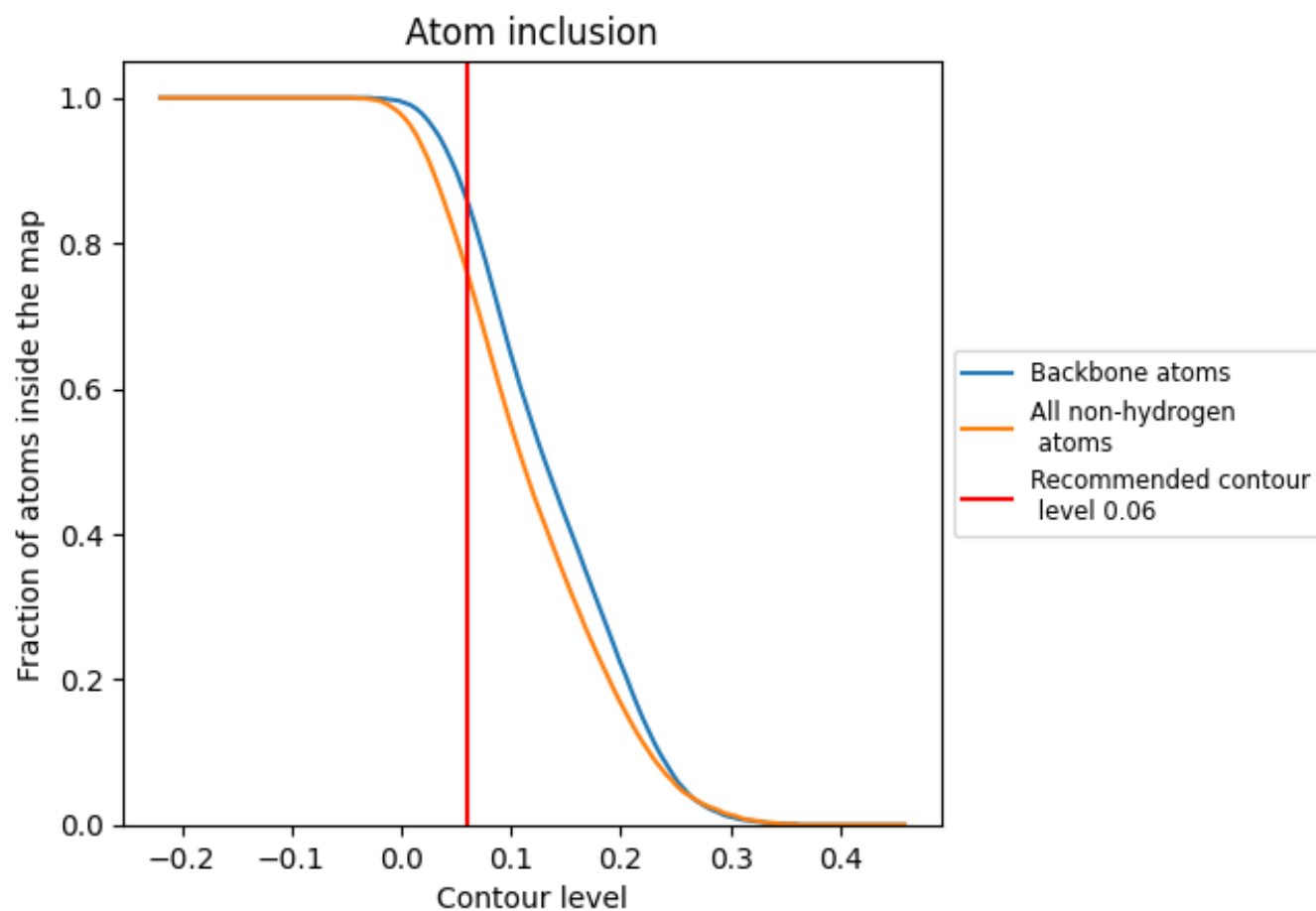
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.4320
0	 0.8580	 0.5230
1	 0.7690	 0.4860
2	 0.9500	 0.5620
3	 0.9210	 0.5600
4	 0.9110	 0.5510
5	 0.8510	 0.5120
6	 0.7820	 0.4540
7	 0.7710	 0.4650
8	 0.5410	 0.3170
9	 0.8230	 0.4980
A	 0.9400	 0.5080
A0	 0.3900	 0.2130
A1	 0.5810	 0.3290
A2	 0.6800	 0.4380
A3	 0.8170	 0.4880
A4	 0.2970	 0.1820
AA	 0.9350	 0.4520
AB	 0.7540	 0.4440
AC	 0.7150	 0.4450
AD	 0.6880	 0.4280
AE	 0.7570	 0.4790
AF	 0.6890	 0.4170
AG	 0.6770	 0.3950
AH	 0.6410	 0.3980
AI	 0.7480	 0.4630
AJ	 0.7560	 0.4750
AK	 0.7740	 0.4350
AL	 0.7050	 0.4310
AM	 0.5510	 0.2990
AN	 0.6880	 0.4400
AO	 0.5810	 0.3250
AP	 0.7480	 0.4670
AQ	 0.8120	 0.4860
AR	 0.4960	 0.2770



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Chain	Atom inclusion	Q-score
AS	 0.6420	 0.3870
AT	 0.6790	 0.3970
AU	 0.5830	 0.3040
AV	 0.2140	 0.1530
AW	 0.7070	 0.4490
AX	 0.6430	 0.3560
AY	 0.5340	 0.3140
AZ	 0.6430	 0.3750
Aw	 0.9000	 0.3070
Ax	 0.8240	 0.3720
Ay	 0.6470	 0.1970
Az	 0.4550	 0.2420
B	 0.7610	 0.3180
C	 0.3260	 0.3160
D	 0.8880	 0.5480
E	 0.8610	 0.5330
F	 0.8910	 0.5440
G	 0.1070	 0.1920
H	 0.4060	 0.3040
I	 0.6220	 0.3640
J	 0.5510	 0.2870
K	 0.9000	 0.5420
L	 0.8410	 0.5340
M	 0.8670	 0.5320
N	 0.8440	 0.5270
O	 0.8820	 0.5360
OX	 0.4610	 0.3150
P	 0.8220	 0.4970
Q	 0.7780	 0.4930
R	 0.8940	 0.5430
S	 0.8500	 0.5370
T	 0.8960	 0.5550
U	 0.7760	 0.4750
V	 0.7970	 0.4880
W	 0.8550	 0.5450
X	 0.8270	 0.5070
Y	 0.8600	 0.5220
Z	 0.8660	 0.5350
a	 0.7260	 0.4620
b	 0.8900	 0.5430
c	 0.8210	 0.4970
d	 0.6530	 0.4330

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Chain	Atom inclusion	Q-score
e	 0.4650	 0.2680
f	 0.6290	 0.3820
g	 0.8560	 0.5250
h	 0.7710	 0.4580
i	 0.9160	 0.5560
j	 0.7940	 0.4830
k	 0.6490	 0.3950
l	 0.5900	 0.3320
m	 0.5170	 0.3250
n	 0.3440	 0.3500
o	 0.9040	 0.5500
p	 0.6890	 0.4260
q	 0.6060	 0.3590
r	 0.8490	 0.5160
s	 0.8540	 0.5190
t	 0.1590	 0.1560
u	 0.0900	 0.1030
z	 0.0620	 0.0970