



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 11:28 PM EDT

PDB ID : 9PSM / pdb_00009psm
EMDB ID : EMD-71829
Title : In situ structure of the human mitoribosome in the A/P-P/E state
Authors : Shuhui, W.; Yong, X.
Deposited on : 2025-07-25
Resolution : 2.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 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) : 2.50

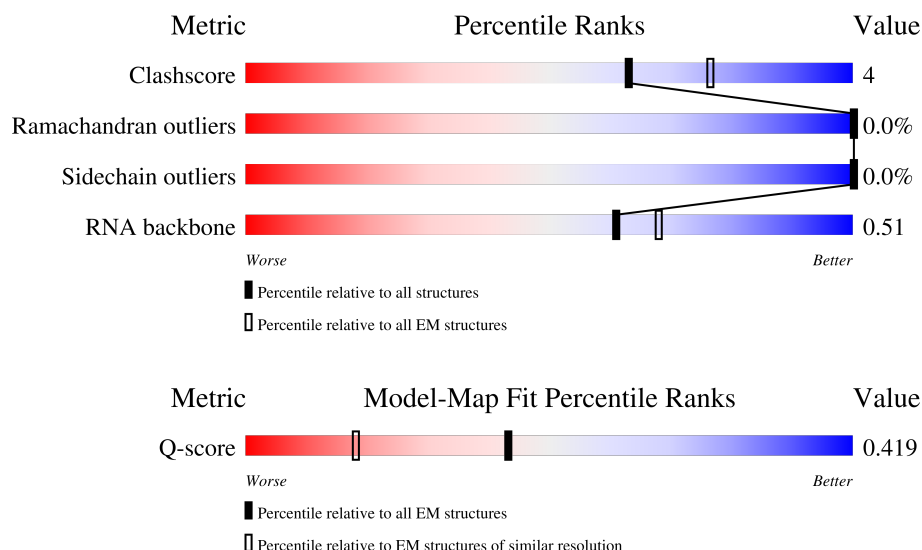
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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.



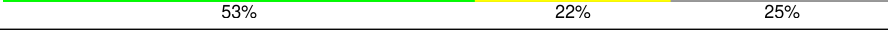
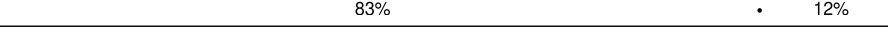
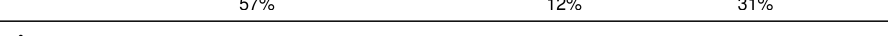
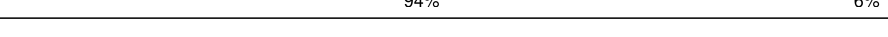
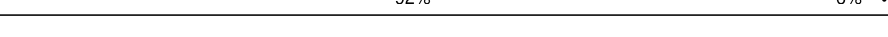
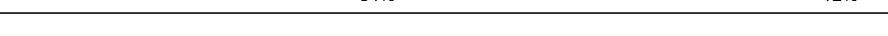
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13236 (2.48 - 3.48)

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

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

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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	1558	
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	

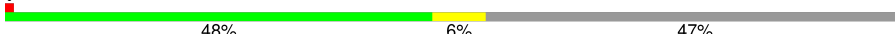
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Mol	Chain	Length	Quality of chain
29	U	153	
30	W	148	
31	X	256	
32	Y	250	
33	Z	161	
34	z	325	
35	G	198	
35	t	198	
35	u	198	
36	V	216	
37	b	215	
38	d	306	
39	e	279	
40	g	166	
41	h	158	
42	i	128	
43	j	123	
44	k	112	
45	l	138	
46	m	128	
47	n	43	
48	o	102	
49	q	222	
50	r	196	
51	AB	296	

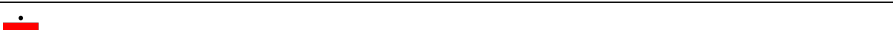
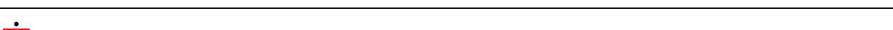
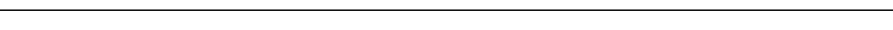
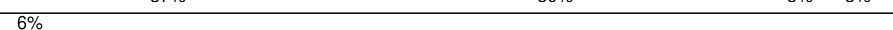
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Mol	Chain	Length	Quality of chain
52	AC	167	
53	AD	430	
54	AE	125	
55	AF	242	
56	AG	396	
57	AH	201	
58	AJ	138	
59	AK	128	
60	AL	257	
61	AM	137	
62	AN	130	
63	AO	258	
64	AP	142	
65	AR	360	
66	AS	190	
67	AT	173	
68	AU	205	
69	AV	414	
70	AW	187	
71	AZ	106	
72	A0	217	
73	A1	323	
74	A3	199	
75	Az	34	
76	AY	395	

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Mol	Chain	Length	Quality of chain
77	AA	954	
78	AI	194	
79	A4	689	
80	AX	398	
81	A2	118	
82	AQ	87	
83	c	332	
84	f	212	
85	p	206	
86	s	439	
87	OX	435	
88	a	142	
89	Aw	76	
90	Ax	76	
91	B	72	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
102	VAL	B	101	-	-	X	-

2 Entry composition

There are 102 unique types of molecules in this entry. The entry contains 181859 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 12 is a protein called 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	226	Total	C	N	O	S	0	0
			1878	1202	332	335	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	68	Total	C	N	O	S	0	0
			567	349	117	99	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 28S ribosomal protein S2, mitochondrial.

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

- Molecule 52 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 53 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 54 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 55 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 56 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 58 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 60 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 61 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 62 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 63 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 64 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 65 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 66 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 67 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 68 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 69 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 71 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 72 is a protein called Small ribosomal subunit protein mS34.

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

- Molecule 73 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 74 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 75 is a RNA chain called mRNA.

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

- Molecule 76 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 77 is a RNA chain called 12S mitochondrial rRNA.

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

- Molecule 78 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 79 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 80 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 81 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	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 82 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	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 83 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 84 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 85 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

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

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

- Molecule 87 is a protein called Mitochondrial inner membrane protein OXA1L.

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

- Molecule 88 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 89 is a RNA chain called A/P-tRNA.

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

- Molecule 90 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	Ax	70	Total	C	N	O	P	0	0
			1482	665	260	487	70		

- Molecule 91 is a RNA chain called mitochondrial tRNAVal.

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

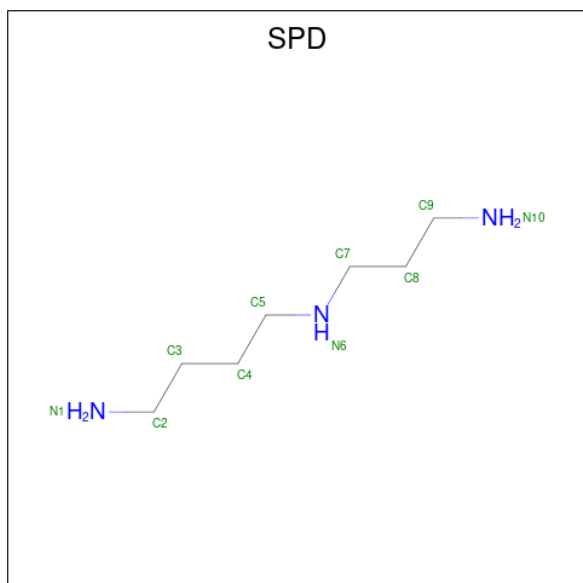
- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
92	0	1	Total	Zn	0
			1	1	
92	4	1	Total	Zn	0
			1	1	
92	AO	1	Total	Zn	0
			1	1	

- Molecule 93 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
93	6	1	Total K 1 1	0
93	A	30	Total K 30 30	0
93	D	1	Total K 1 1	0
93	M	2	Total K 2 2	0
93	N	1	Total K 1 1	0
93	o	1	Total K 1 1	0
93	AJ	1	Total K 1 1	0
93	AA	17	Total K 17 17	0

- Molecule 94 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



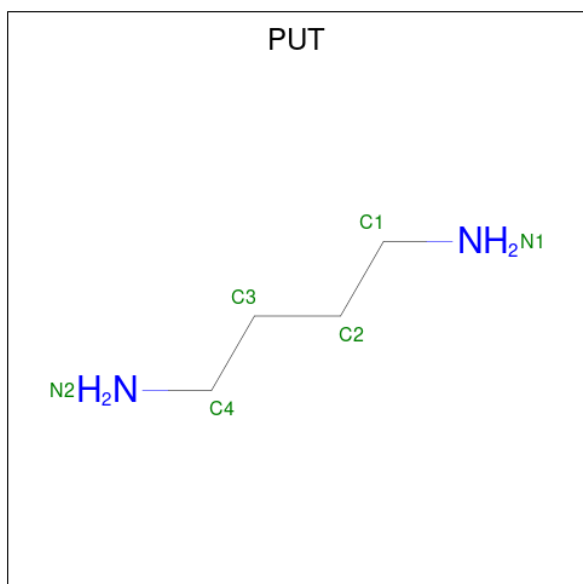
Mol	Chain	Residues	Atoms	AltConf
94	A	1	Total C N 10 7 3	0
94	A	1	Total C N 10 7 3	0

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

- Molecule 95 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



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

- Molecule 96 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

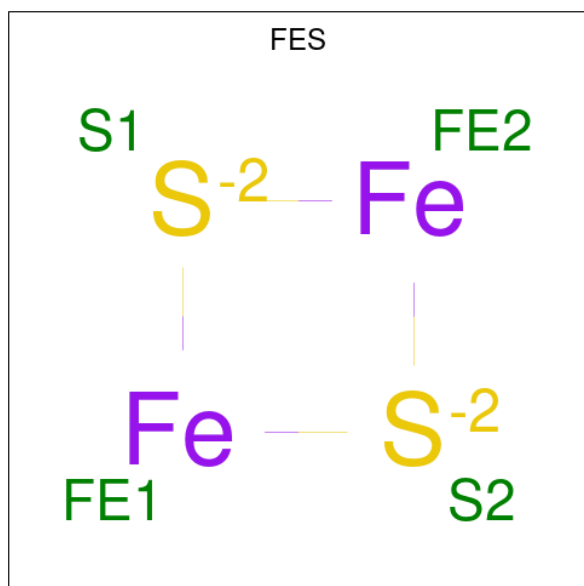
Mol	Chain	Residues	Atoms		AltConf
96	A	137	Total	Mg	0
			137	137	
96	D	2	Total	Mg	0
			2	2	

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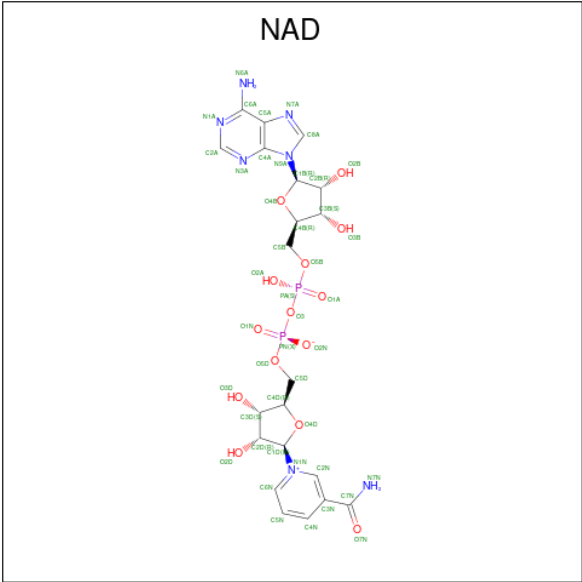
Mol	Chain	Residues	Atoms		AltConf
96	E	1	Total	Mg	0
			1	1	
96	g	1	Total	Mg	0
			1	1	
96	AB	1	Total	Mg	0
			1	1	
96	A3	1	Total	Mg	0
			1	1	
96	AA	60	Total	Mg	0
			60	60	
96	AX	1	Total	Mg	0
			1	1	

- Molecule 97 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



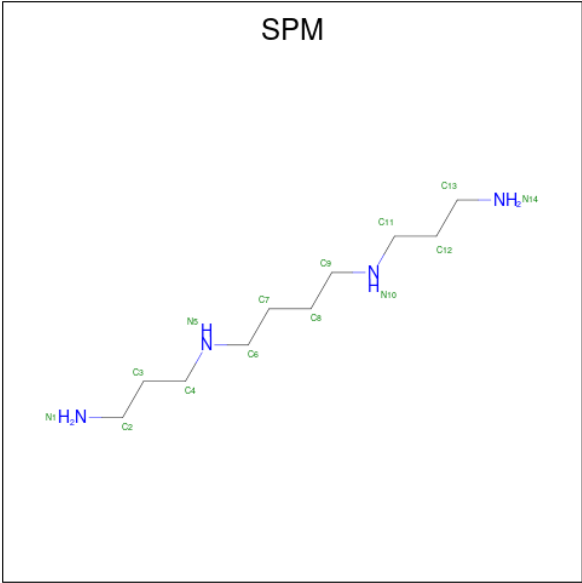
Mol	Chain	Residues	Atoms			AltConf
97	r	1	Total	Fe	S	0
			4	2	2	
97	AP	1	Total	Fe	S	0
			4	2	2	
97	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 98 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).



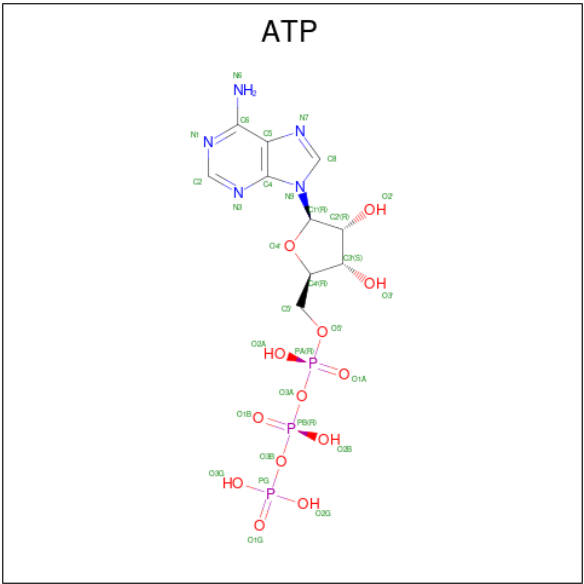
Mol	Chain	Residues	Atoms					AltConf
98	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 99 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



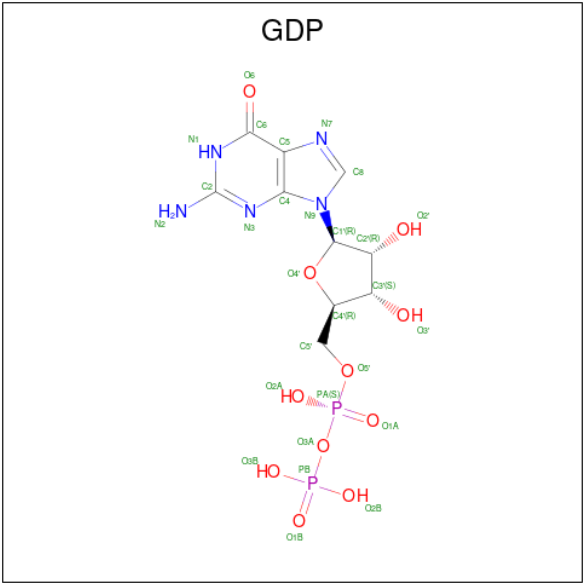
Mol	Chain	Residues	Atoms			AltConf
99	AA	1	Total	C	N	0
			14	10	4	
99	AA	1	Total	C	N	0
			14	10	4	

- Molecule 100 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



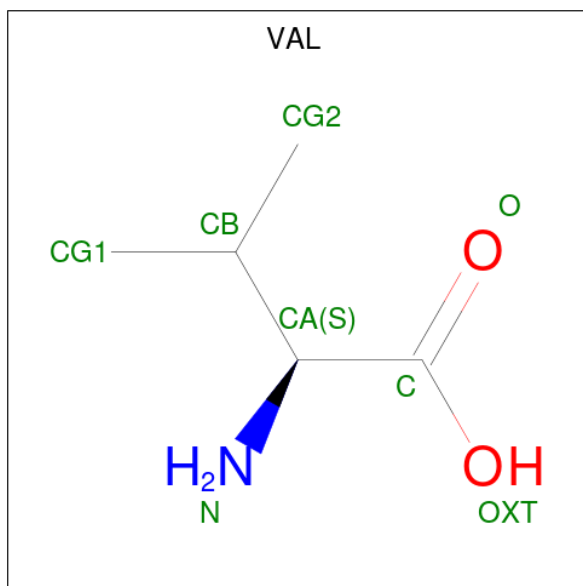
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
100	AX	1	31	10	5	13	3	0

- Molecule 101 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 102 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).

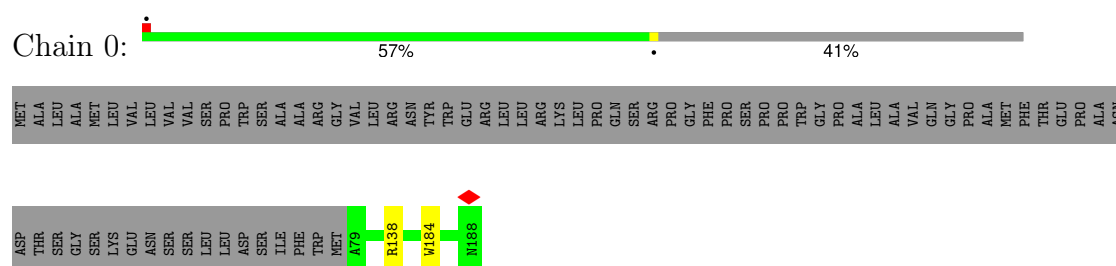


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
102	B	1	7	5	1	1	0

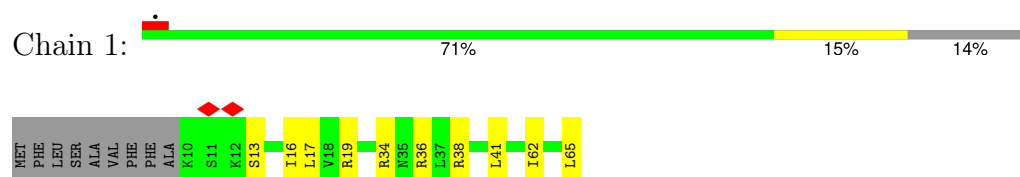
3 Residue-property plots [i](#)

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

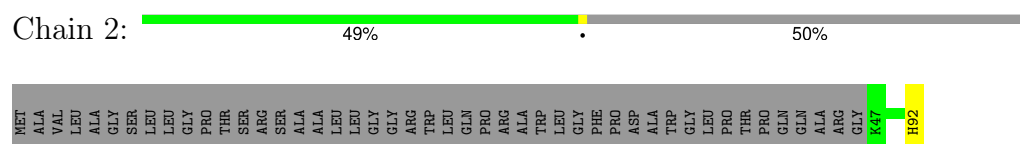
- Molecule 1: 39S ribosomal protein L32, mitochondrial



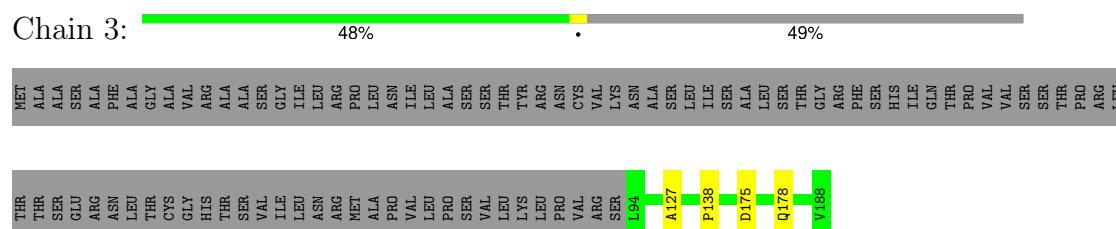
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial

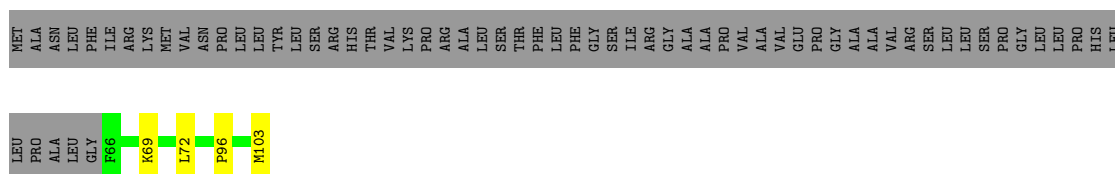


- Molecule 4: 39S ribosomal protein L35, mitochondrial



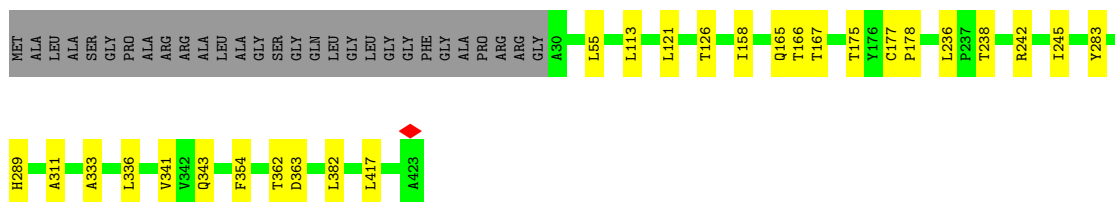
- Molecule 5: 39S ribosomal protein L36, mitochondrial





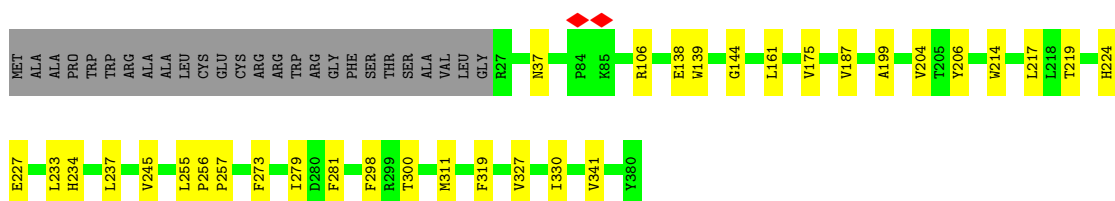
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5: 87% 6% 7%



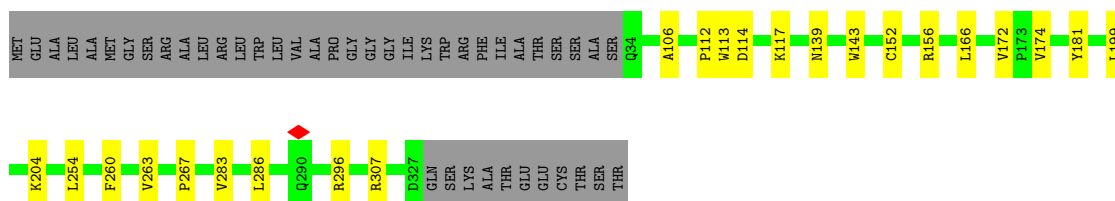
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6: 84% 9% 7%



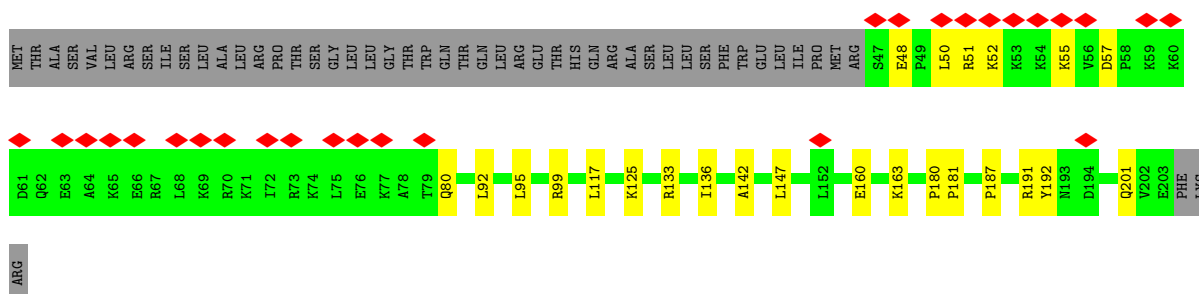
- Molecule 8: 39S ribosomal protein L39, mitochondrial

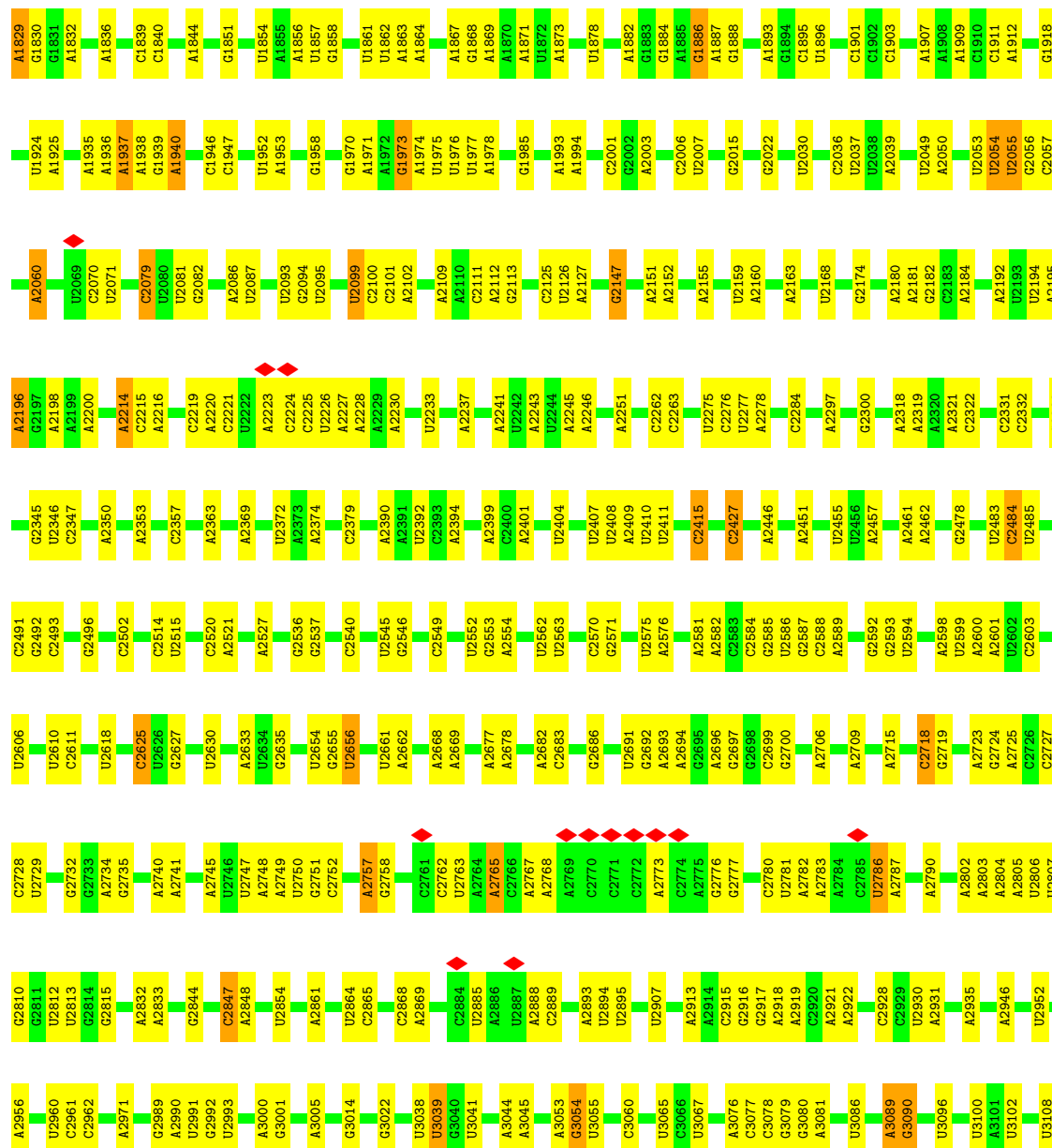
Chain 7: 80% 7% 13%

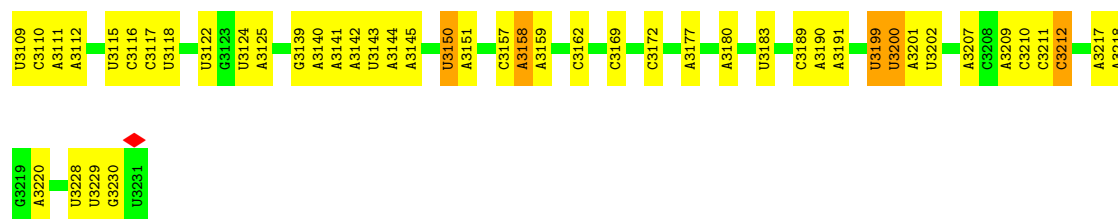


- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8: 13% 65% 12% 24%

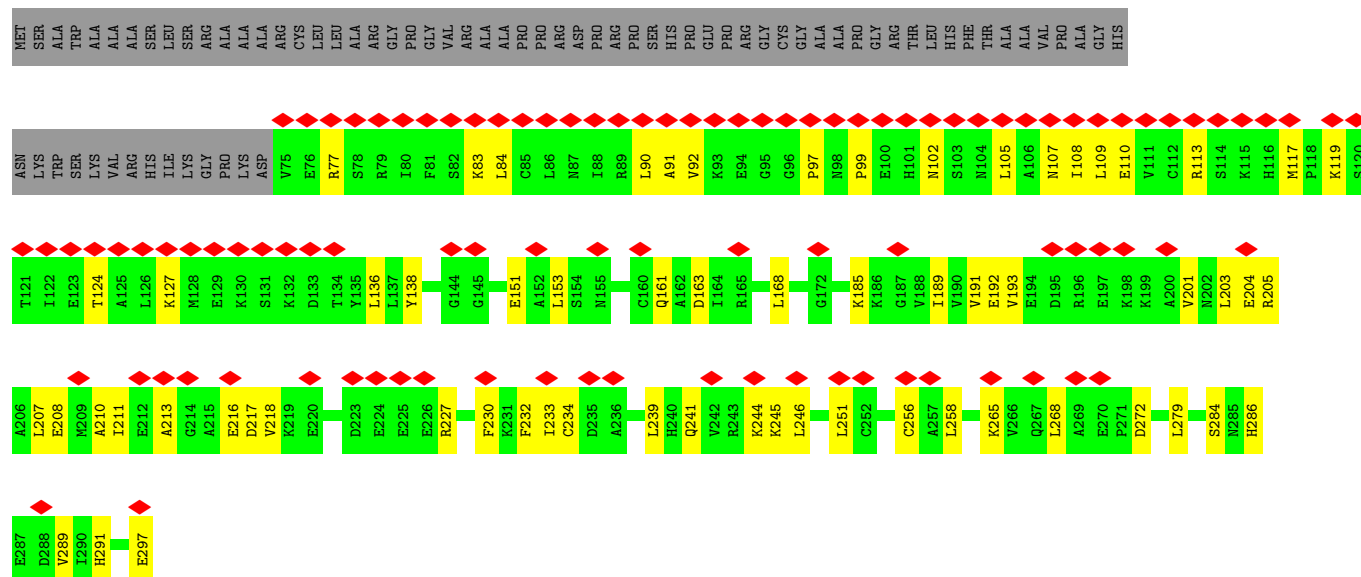






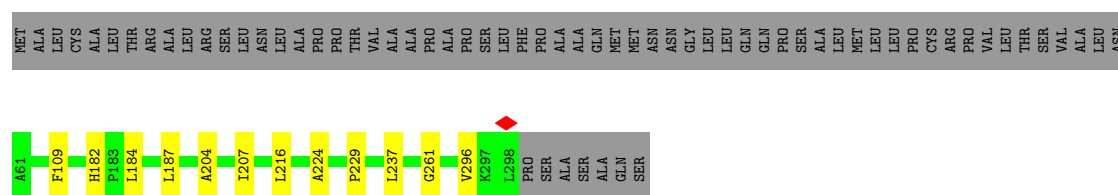
- Molecule 12: Translational activator of cytochrome c oxidase 1

Chain C: 34% 53% 22% 25%



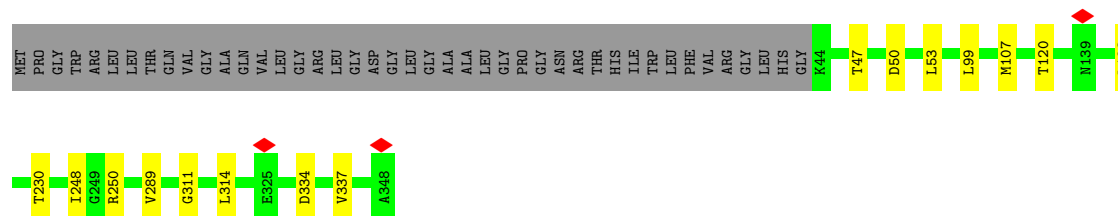
- Molecule 13: 39S ribosomal protein L2, mitochondrial

Chain D: 74% 22%



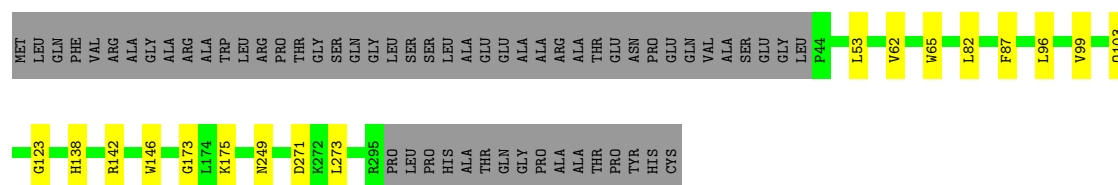
- Molecule 14: 39S ribosomal protein L3, mitochondrial

Chain E: 83% 12%



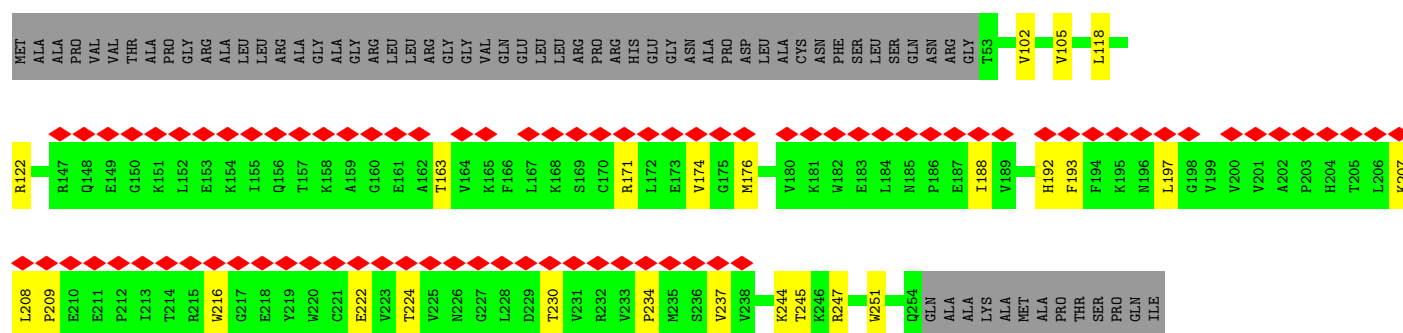
- Molecule 15: 39S ribosomal protein L4, mitochondrial

Chain F: 



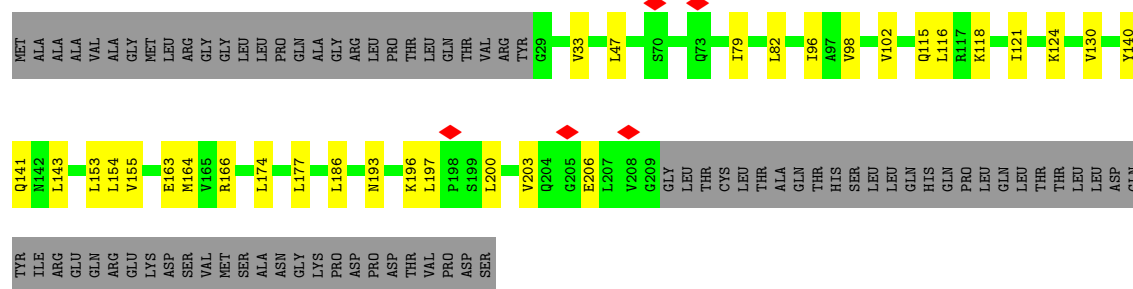
- Molecule 16: 39S ribosomal protein L9, mitochondrial

Chain H: 



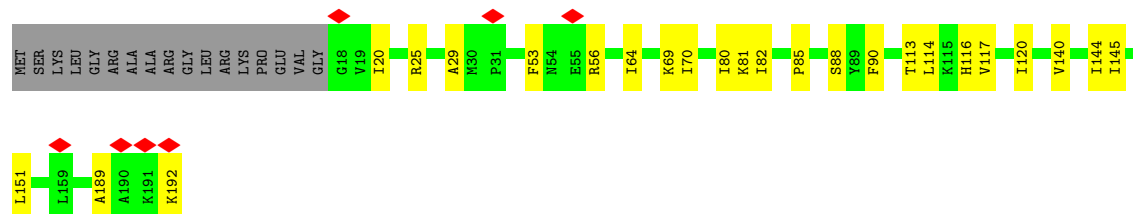
- Molecule 17: 39S ribosomal protein L10, mitochondrial

Chain I: 

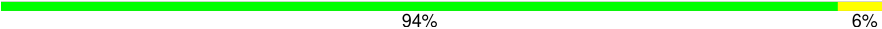


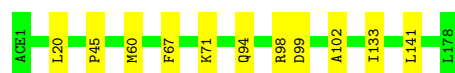
- Molecule 18: 39S ribosomal protein L11, mitochondrial

Chain J: 



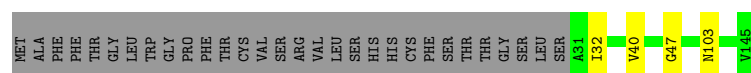
- Molecule 19: Large ribosomal subunit protein uL13m

Chain K:  94% 6%



- Molecule 20: 39S ribosomal protein L14, mitochondrial

Chain L:  77% 21%



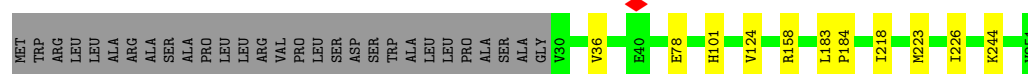
- Molecule 21: 39S ribosomal protein L15, mitochondrial

Chain M:  92% 6%



- Molecule 22: 39S ribosomal protein L16, mitochondrial

Chain N:  84% 12%



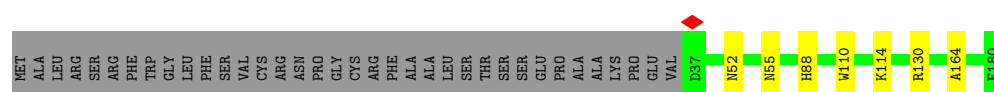
- Molecule 23: 39S ribosomal protein L17, mitochondrial

Chain O:  83% 5% 12%



- Molecule 24: 39S ribosomal protein L18, mitochondrial

Chain P:  76% 20%



- Molecule 25: 39S ribosomal protein L19, mitochondrial

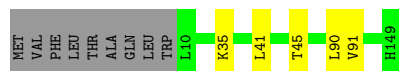
Chain Q:  72% 5% 23%





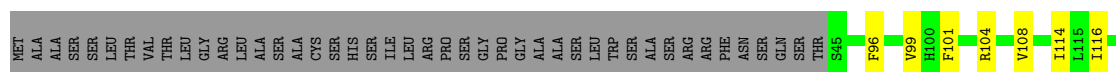
- Molecule 26: 39S ribosomal protein L20, mitochondrial

Chain R: 91% 6%



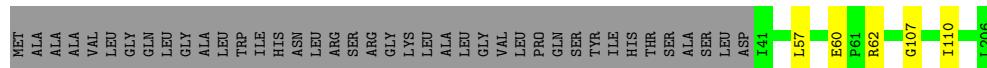
- Molecule 27: 39S ribosomal protein L21, mitochondrial

Chain S: 70% 9% 21%



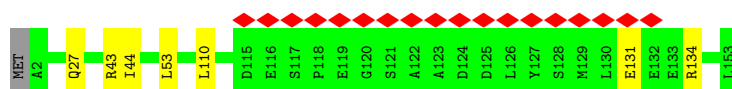
- Molecule 28: 39S ribosomal protein L22, mitochondrial

Chain T: 78% 19%



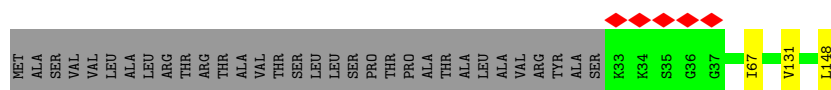
- Molecule 29: 39S ribosomal protein L23, mitochondrial

Chain U: 12% 95% 5%



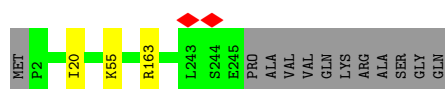
- Molecule 30: 39S ribosomal protein L27, mitochondrial

Chain W: 76% 22%



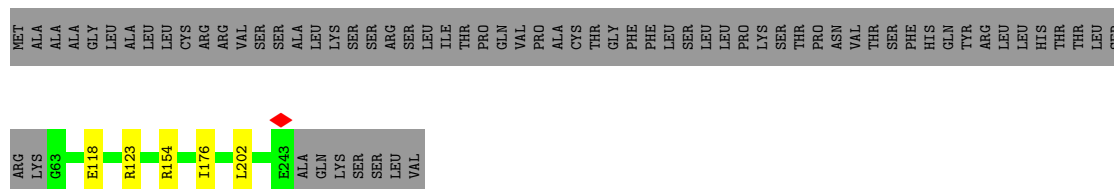
- Molecule 31: 39S ribosomal protein L28, mitochondrial

Chain X: 94% 5%



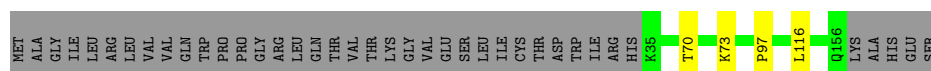
- Molecule 32: 39S ribosomal protein L47, mitochondrial

Chain Y: 



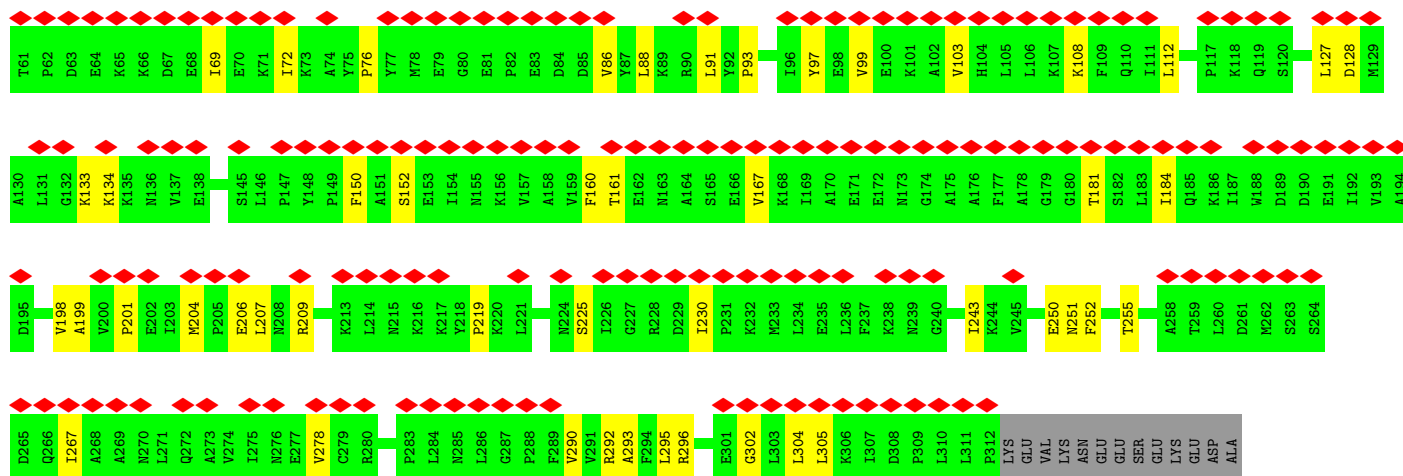
- Molecule 33: 39S ribosomal protein L30, mitochondrial

Chain Z: 



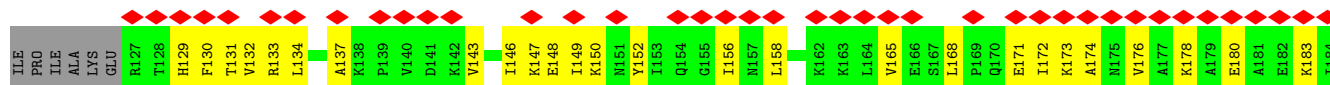
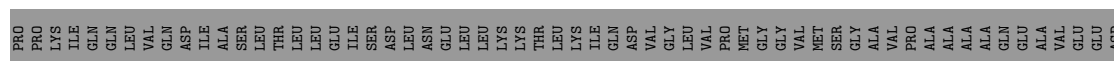
- Molecule 34: Large ribosomal subunit protein uL1m

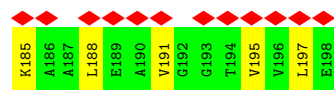
Chain z: 



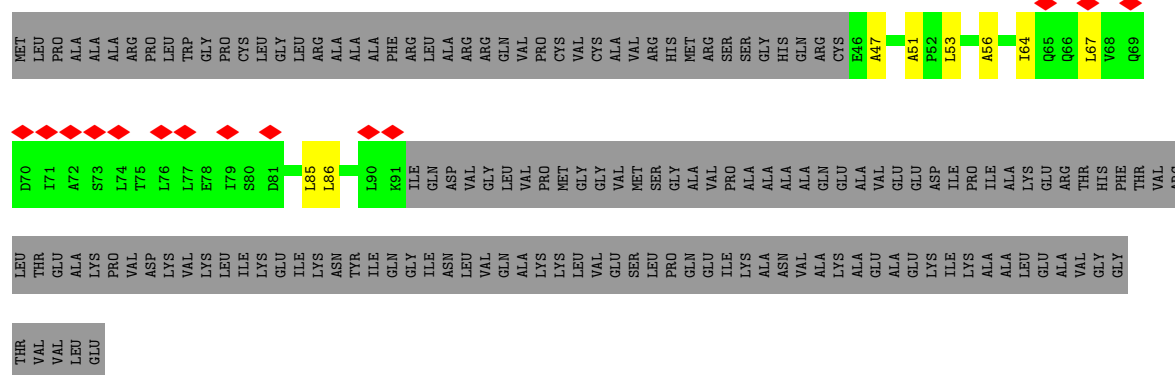
- Molecule 35: 39S ribosomal protein L12, mitochondrial

Chain G: 

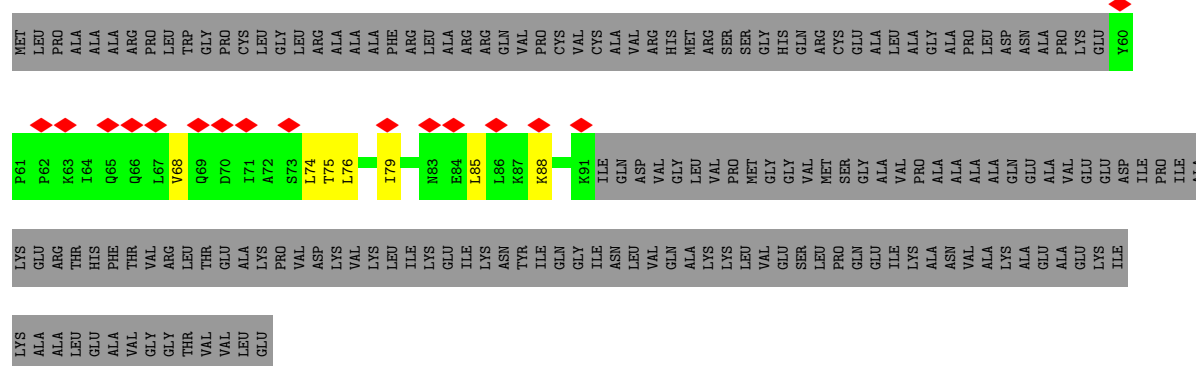




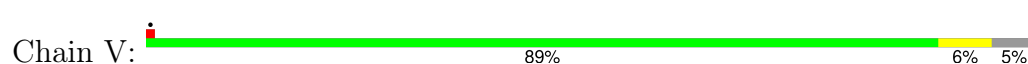
- Molecule 35: 39S ribosomal protein L12, mitochondrial



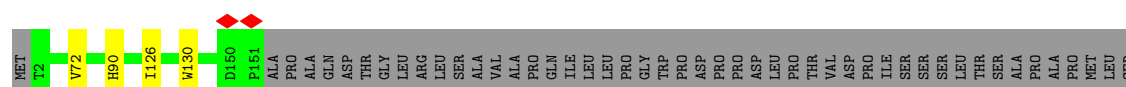
- Molecule 35: 39S ribosomal protein L12, mitochondrial



- Molecule 36: 39S ribosomal protein L24, mitochondrial



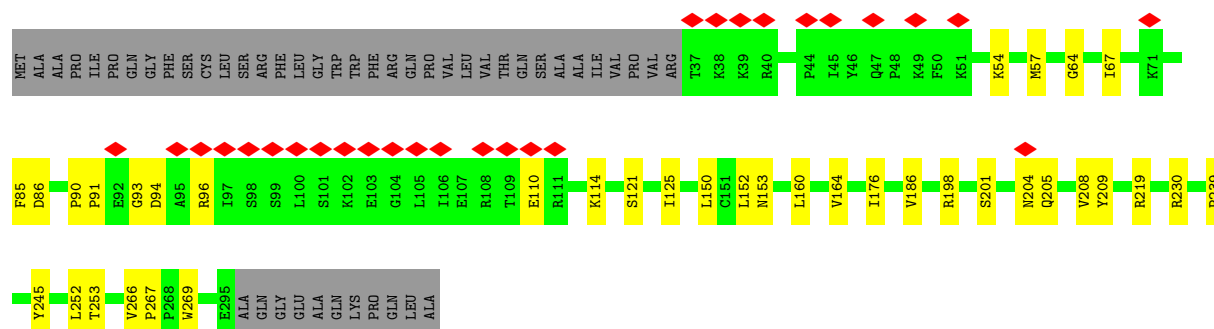
- Molecule 37: 39S ribosomal protein L43, mitochondrial



ALA
VAL
SER
CYS
LEU
PRO
PRO
ILE
VAL
PHE
SER
ALA
LEU
THR
THR
VAL
CYS
SER
ALA

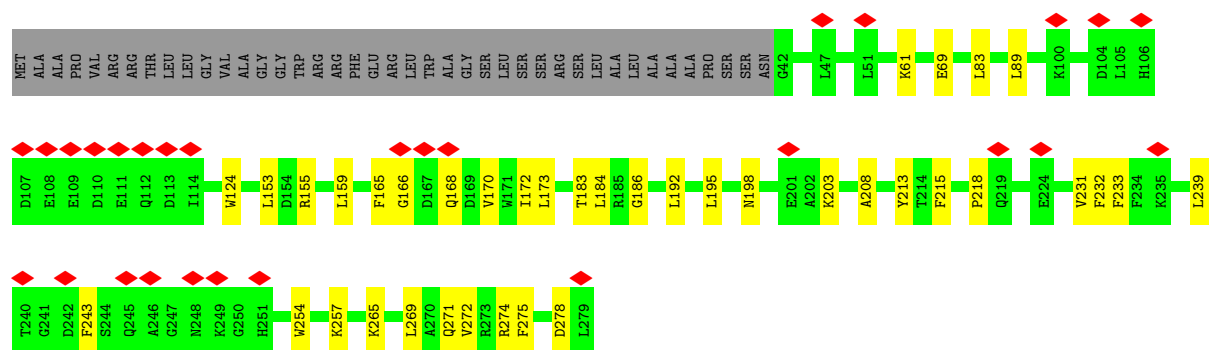
• Molecule 38: 39S ribosomal protein L45, mitochondrial

Chain d:  9% 73% 12% 15%



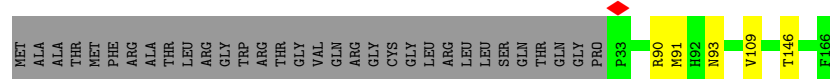
• Molecule 39: 39S ribosomal protein L46, mitochondrial

Chain e:  10% 71% 14% 15%



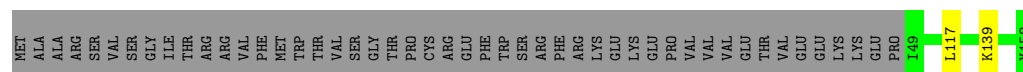
• Molecule 40: 39S ribosomal protein L49, mitochondrial

Chain g:  78% 19%



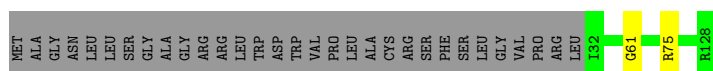
• Molecule 41: 39S ribosomal protein L50, mitochondrial

Chain h:  68% 30%

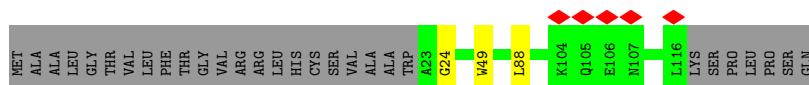


• Molecule 42: 39S ribosomal protein L51, mitochondrial

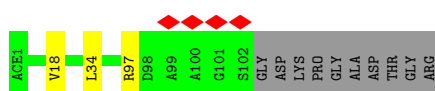
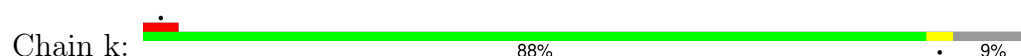
Chain i:  74% 24%



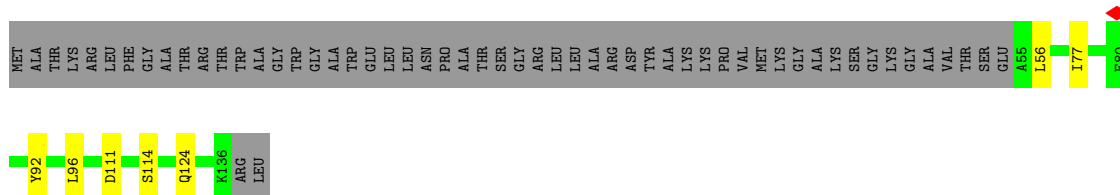
- Molecule 43: 39S ribosomal protein L52, mitochondrial



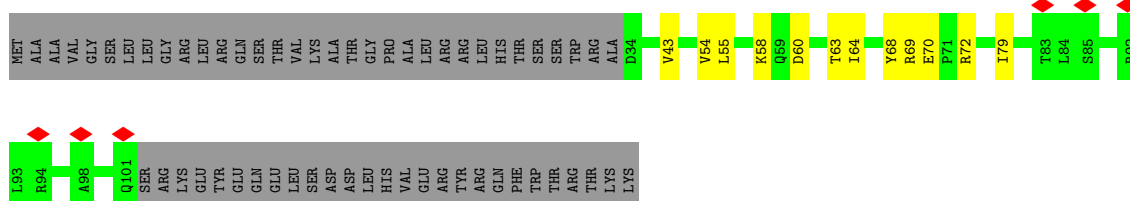
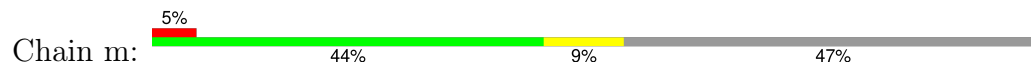
- Molecule 44: Large ribosomal subunit protein mL53



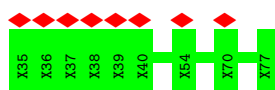
- Molecule 45: 39S ribosomal protein L54, mitochondrial



- Molecule 46: 39S ribosomal protein L55, mitochondrial



- Molecule 47: Nascent polypeptide



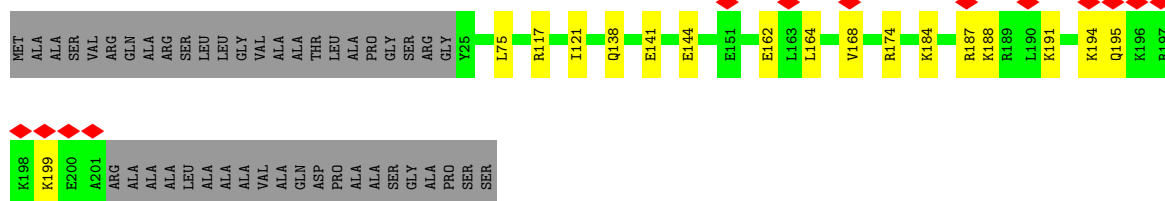
- Molecule 48: Ribosomal protein 63, mitochondrial

Chain o:  86% 6% 8%



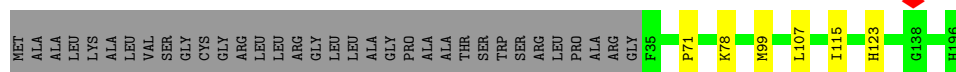
- Molecule 49: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:  6% 72% 8% 20%



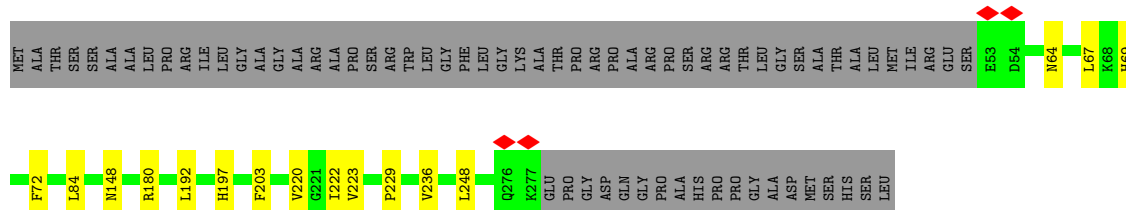
- Molecule 50: 39S ribosomal protein S18a, mitochondrial

Chain r:  80% 17%



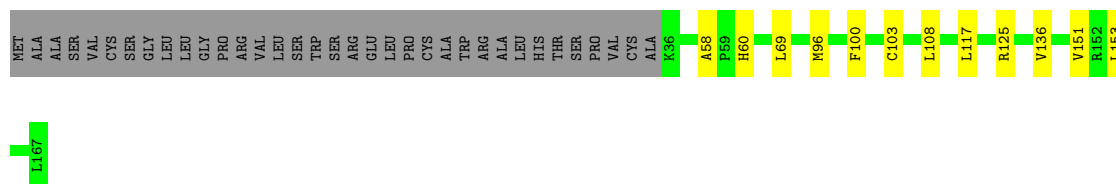
- Molecule 51: 28S ribosomal protein S2, mitochondrial

Chain AB:  71% 5% 24%



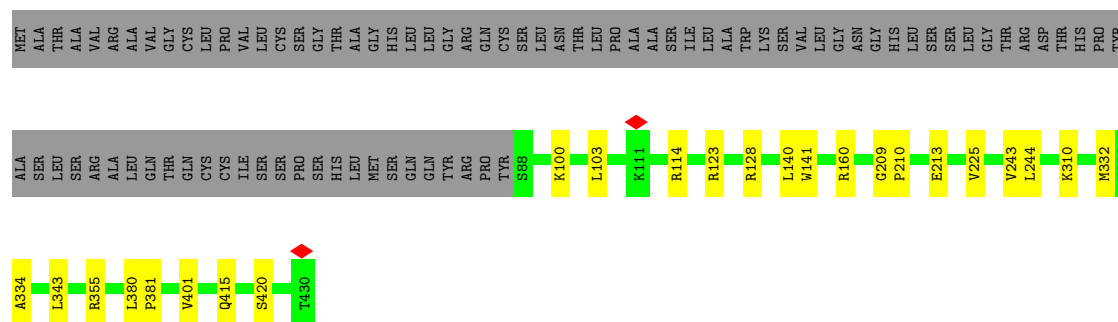
- Molecule 52: 28S ribosomal protein S24, mitochondrial

Chain AC:  72% 7% 21%



- Molecule 53: 28S ribosomal protein S5, mitochondrial

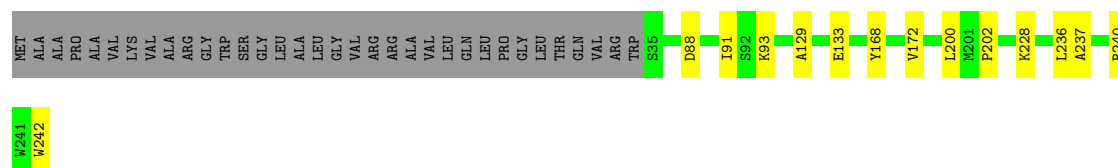
Chain AD:  74% 6% 20%



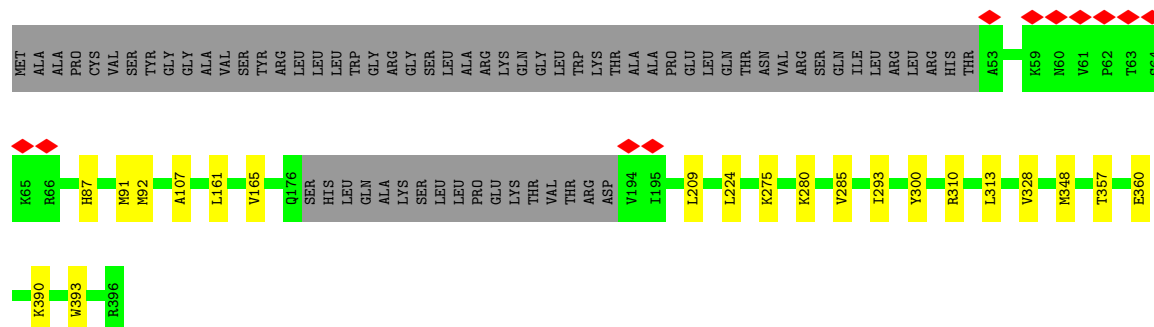
Chain AE: 85% 13%



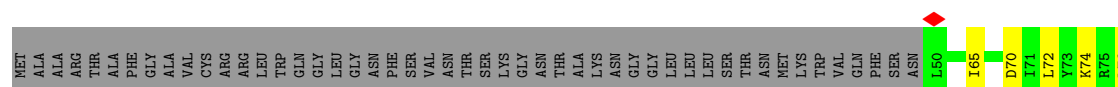
Chain AF: 80% 6% 14%



Chain AG: 77% 5% 17%



Chain AH: 55% 14% 30%

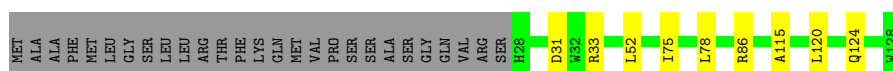




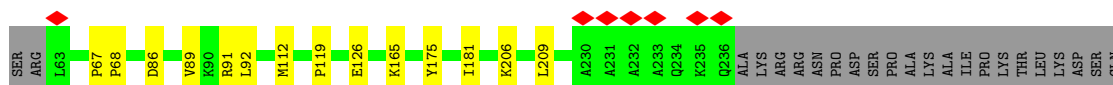
- Molecule 58: 28S ribosomal protein S12, mitochondrial



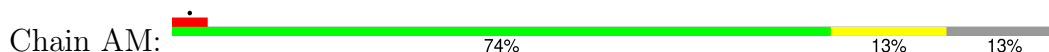
- Molecule 59: 28S ribosomal protein S14, mitochondrial



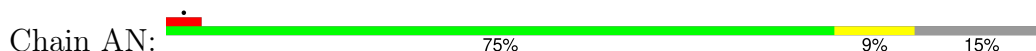
- Molecule 60: 28S ribosomal protein S15, mitochondrial



- Molecule 61: 28S ribosomal protein S16, mitochondrial

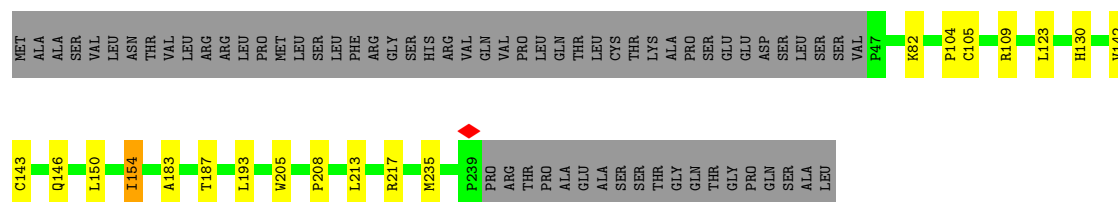


- Molecule 62: 28S ribosomal protein S17, mitochondrial

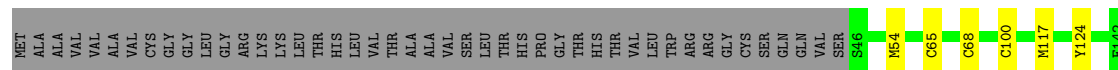


- Molecule 63: 28S ribosomal protein S18b, mitochondrial

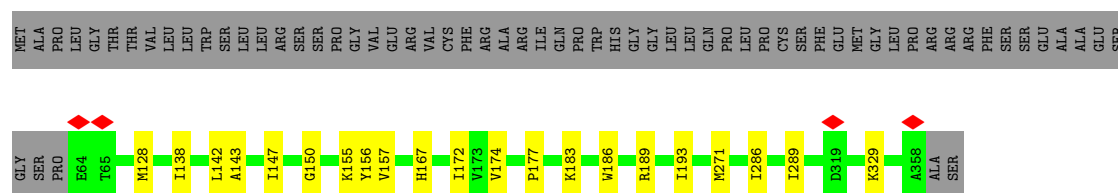
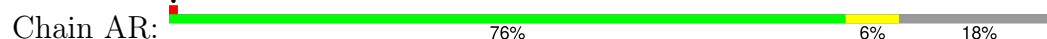




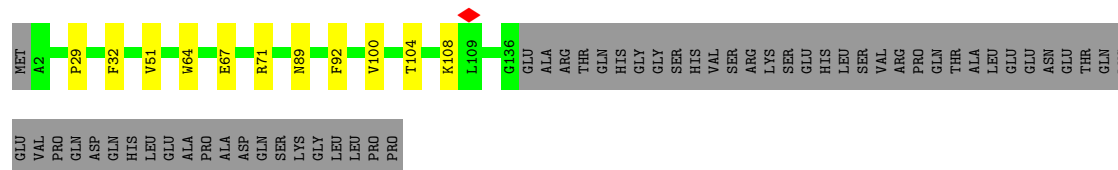
- Molecule 64: 28S ribosomal protein S18c, mitochondrial



- Molecule 65: 28S ribosomal protein S22, mitochondrial



- Molecule 66: 28S ribosomal protein S23, mitochondrial



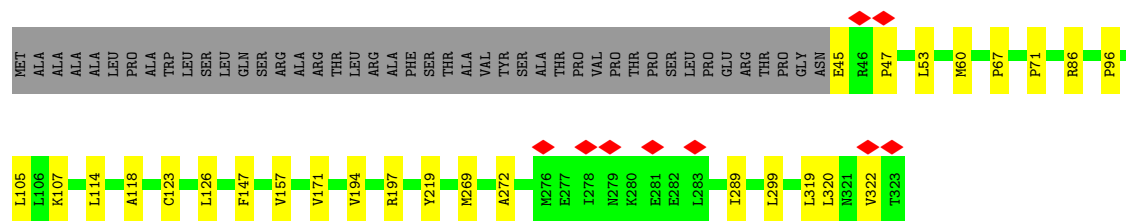
- Molecule 67: 28S ribosomal protein S25, mitochondrial



- Molecule 68: 28S ribosomal protein S26, mitochondrial

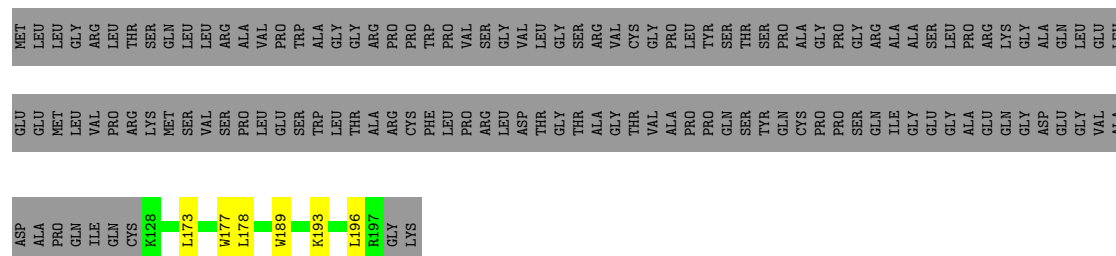


- Molecule 69: 28S ribosomal protein S27, mitochondrial



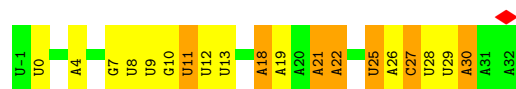
• Molecule 74: Aurora kinase A-interacting protein

Chain A3: 32% 65%



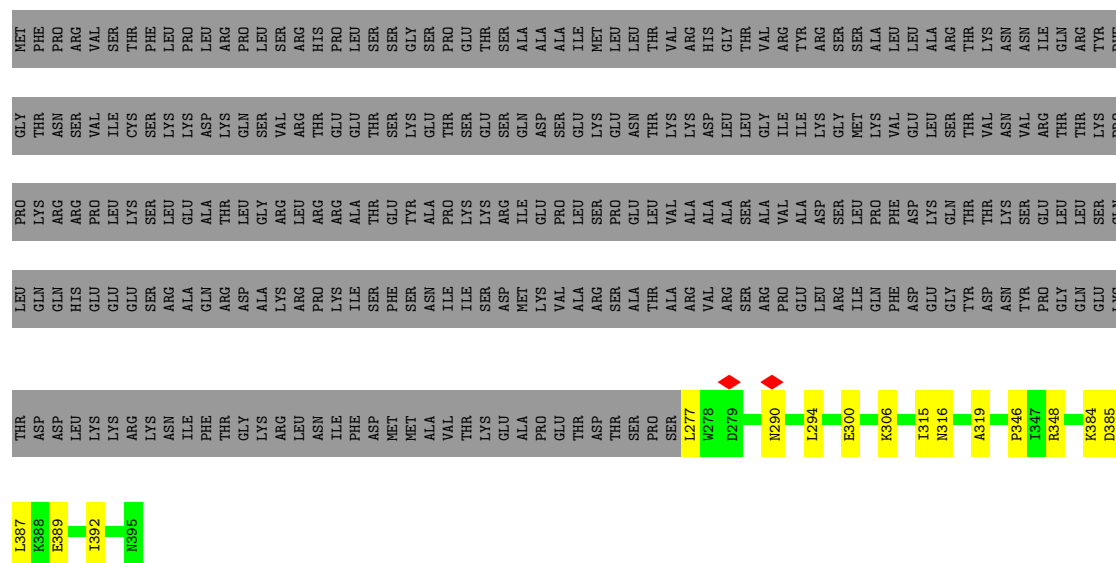
• Molecule 75: mRNA

Chain Az: 44% 35% 21%



• Molecule 76: 28S ribosomal protein S31, mitochondrial

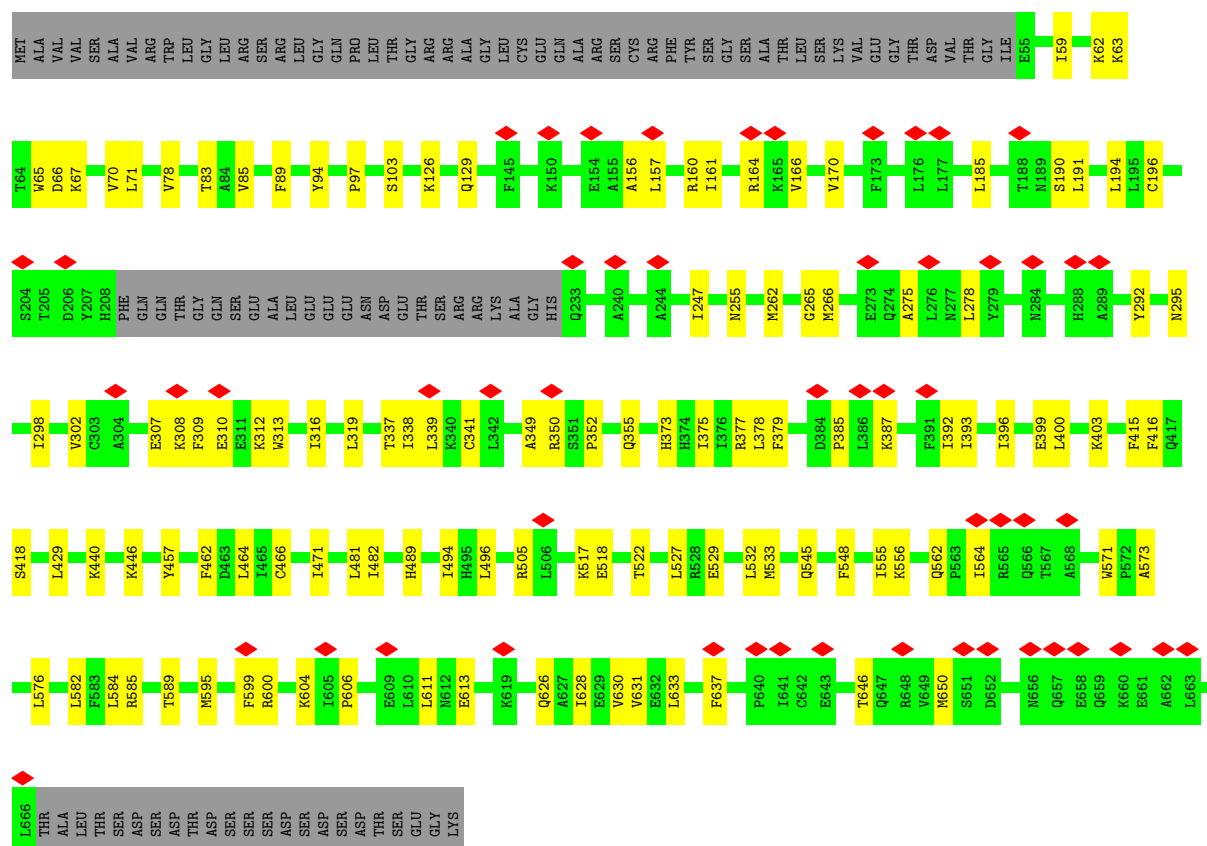
Chain AY: 26% 70%



• Molecule 77: 12S mitochondrial rRNA

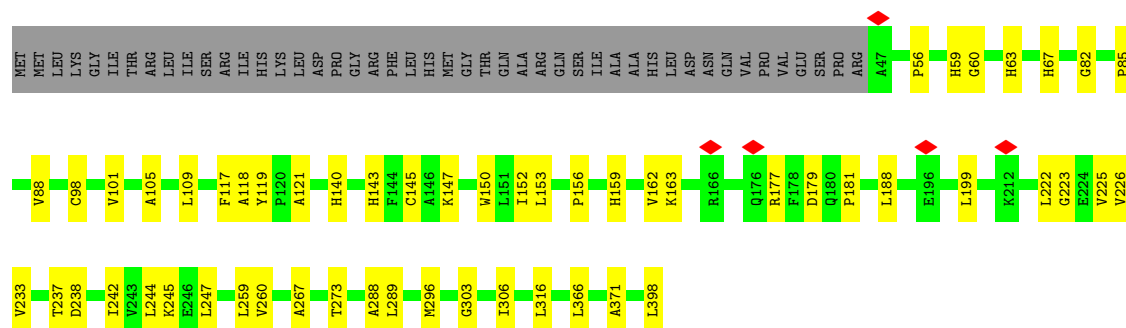
Chain AA: 51% 45%

Chain A4: 

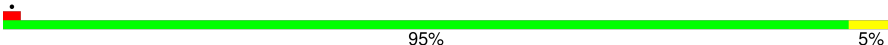


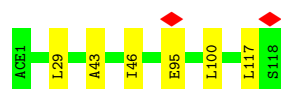
- Molecule 80: 28S ribosomal protein S29, mitochondrial

Chain AX: 



- Molecule 81: Small ribosomal subunit protein mS37

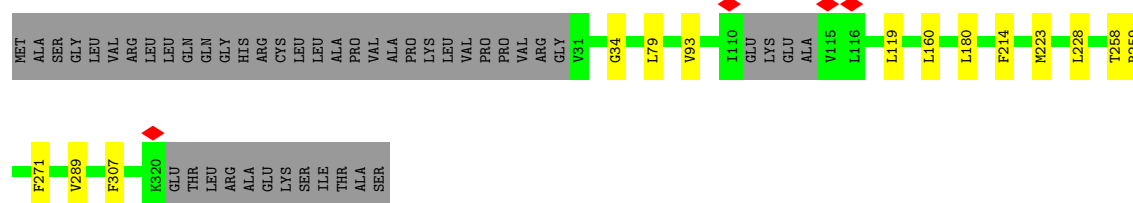
Chain A2: 



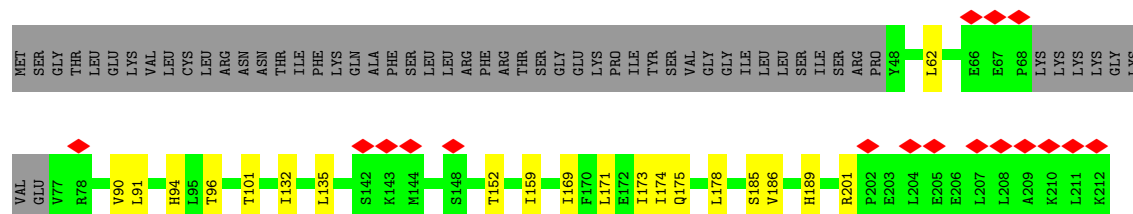
- Molecule 82: Small ribosomal subunit protein bS21m

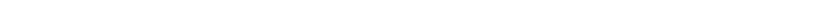
Diagram illustrating the 1000 Genomes Project, showing a sequence of populations: ACE1, H4, T11, M66, E67, M68, and C87. The populations are represented by colored blocks (yellow and green) connected by lines, indicating a genetic lineage.

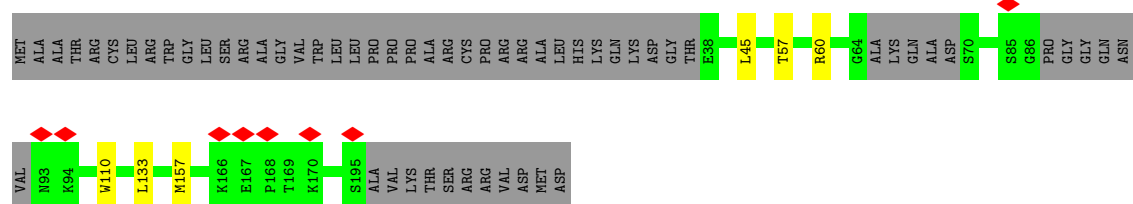
- Chain c: 82% 14%



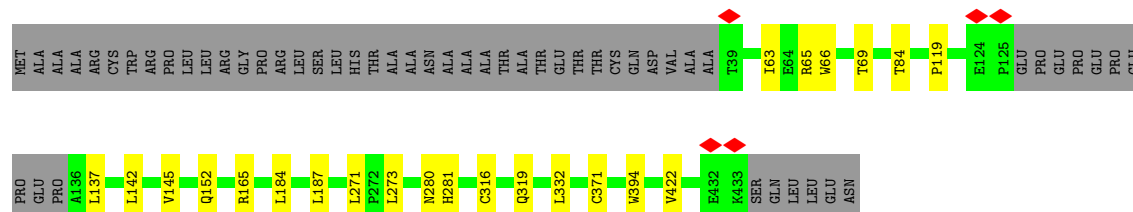
- Chain f:



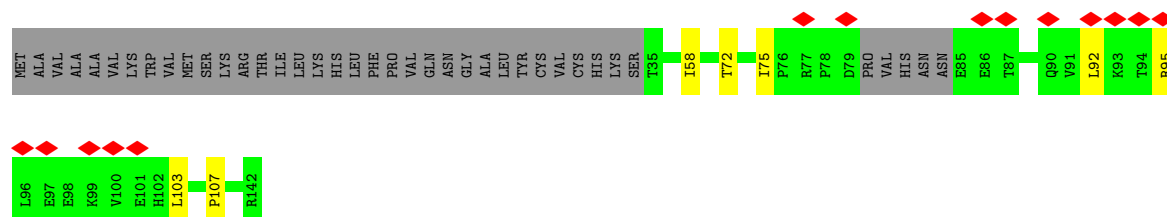
- Chain p:  68% 29%



- Chain s: 82% 5% 12%



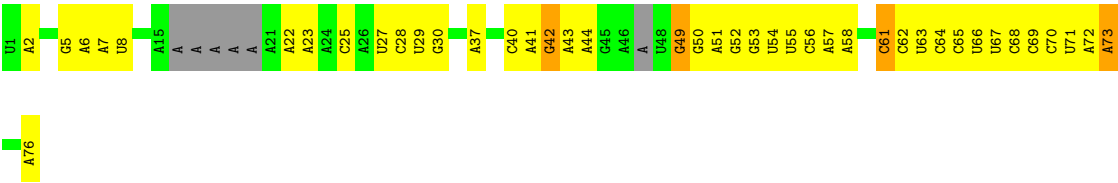
Chain OX: 12% 87%



Chain Aw:



Chain Ax:



• Molecule 91: mitochondrial tRNAVal



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64516	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	0.622	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.24	0/913	0.25	0/1224
2	1	0.22	0/469	0.29	0/621
3	2	0.29	0/383	0.26	0/507
4	3	0.29	0/853	0.28	0/1136
5	4	0.28	0/350	0.26	0/461
6	5	0.22	0/3305	0.29	0/4502
7	6	0.20	0/3043	0.29	0/4140
8	7	0.19	0/2447	0.28	0/3310
9	8	0.14	0/1354	0.34	0/1819
10	9	0.22	0/1025	0.27	0/1379
11	A	0.28	0/36876	0.30	0/57402
12	C	0.14	0/1754	0.33	0/2357
13	D	0.23	0/1896	0.28	0/2549
14	E	0.25	0/2475	0.30	0/3355
15	F	0.27	0/2090	0.29	0/2842
16	H	0.16	0/1698	0.31	0/2292
17	I	0.17	0/1478	0.30	0/1999
18	J	0.15	0/1348	0.30	0/1813
19	K	0.27	0/1497	0.28	0/2031
20	L	0.22	0/905	0.28	0/1218
21	M	0.26	0/2381	0.29	0/3212
22	N	0.24	0/1833	0.28	0/2468
23	O	0.26	0/1283	0.29	0/1727
24	P	0.21	0/1199	0.26	0/1623
25	Q	0.22	0/1921	0.26	0/2588
26	R	0.27	0/1175	0.26	0/1572
27	S	0.26	0/1320	0.29	0/1789
28	T	0.26	0/1403	0.27	0/1886
29	U	0.25	0/1279	0.35	0/1730
30	W	0.26	0/926	0.26	0/1244
31	X	0.23	0/2099	0.24	0/2837

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.25	0/1593	0.25	0/2136
33	Z	0.26	0/1021	0.30	0/1378
34	z	0.15	0/2067	0.36	0/2793
35	G	0.19	0/562	0.50	0/754
35	t	0.13	0/358	0.30	0/486
35	u	0.19	0/259	0.40	0/350
36	V	0.20	0/1721	0.27	0/2333
37	b	0.25	0/1218	0.29	0/1649
38	d	0.19	0/2181	0.35	0/2949
39	e	0.15	0/1970	0.33	0/2658
40	g	0.25	0/1151	0.29	0/1569
41	h	0.18	0/918	0.26	0/1249
42	i	0.28	0/850	0.28	0/1135
43	j	0.22	0/760	0.25	0/1023
44	k	0.16	0/783	0.22	0/1057
45	l	0.14	0/707	0.29	0/960
46	m	0.12	0/575	0.31	0/772
48	o	0.26	0/819	0.30	0/1097
49	q	0.18	0/1529	0.29	0/2055
50	r	0.24	0/1362	0.29	0/1846
51	AB	0.19	0/1871	0.27	0/2531
52	AC	0.20	0/1113	0.30	0/1505
53	AD	0.20	0/2783	0.27	0/3724
54	AE	0.15	0/989	0.27	0/1335
55	AF	0.15	0/1767	0.24	0/2373
56	AG	0.17	0/2746	0.26	0/3681
57	AH	0.20	0/1178	0.29	0/1598
58	AJ	0.19	0/855	0.29	0/1148
59	AK	0.19	0/880	0.29	0/1182
60	AL	0.16	0/1477	0.22	0/1974
61	AM	0.18	0/963	0.32	0/1295
62	AN	0.19	0/886	0.26	0/1199
63	AO	0.18	0/1648	0.30	0/2243
64	AP	0.17	0/798	0.27	0/1070
65	AR	0.16	0/2456	0.28	0/3317
66	AS	0.17	0/1138	0.25	0/1533
67	AT	0.18	0/1402	0.28	0/1883
68	AU	0.15	0/1510	0.25	0/2025
69	AV	0.17	0/3030	0.36	0/4093
70	AW	0.17	0/801	0.25	0/1079
71	AZ	0.16	0/857	0.26	0/1141
72	A0	0.15	0/1834	0.32	0/2484
73	A1	0.15	0/2313	0.28	0/3129

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	A3	0.20	0/636	0.31	0/839
75	Az	0.16	0/804	0.33	0/1248
76	AY	0.17	0/1040	0.27	0/1402
77	AA	0.23	0/22537	0.28	0/35085
78	AI	0.18	0/1039	0.27	0/1400
79	A4	0.16	0/4877	0.33	0/6598
80	AX	0.15	0/2921	0.33	0/3954
81	A2	0.17	0/947	0.28	0/1266
82	AQ	0.18	0/754	0.25	0/1003
83	c	0.22	0/2347	0.26	0/3171
84	f	0.16	0/1273	0.34	0/1716
85	p	0.17	0/1223	0.26	0/1641
86	s	0.25	0/3231	0.30	0/4389
87	OX	0.18	0/478	0.42	0/639
88	a	0.23	0/891	0.33	0/1208
89	Aw	0.16	0/1600	0.36	0/2476
90	Ax	0.16	0/1654	0.32	0/2565
91	B	0.16	0/1626	0.27	0/2523
All	All	0.22	0/190555	0.30	0/270547

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	2	0
2	1	464	0	511	6	0
3	2	377	0	406	1	0
4	3	832	0	883	3	0
5	4	342	0	361	3	0
6	5	3210	0	3204	20	0
7	6	2948	0	2841	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	7	2390	0	2397	14	0
9	8	1327	0	1368	25	0
10	9	997	0	987	2	0
11	A	33070	0	16795	172	0
12	C	1732	0	1740	43	0
13	D	1859	0	1920	8	0
14	E	2406	0	2415	9	0
15	F	2031	0	2065	10	0
16	H	1661	0	1734	14	0
17	I	1446	0	1532	19	0
18	J	1330	0	1407	19	0
19	K	1455	0	1452	6	0
20	L	890	0	941	2	0
21	M	2327	0	2395	13	0
22	N	1786	0	1817	8	0
23	O	1259	0	1294	6	0
24	P	1173	0	1165	5	0
25	Q	1878	0	1909	9	0
26	R	1154	0	1214	4	0
27	S	1293	0	1365	11	0
28	T	1369	0	1410	3	0
29	U	1248	0	1228	4	0
30	W	904	0	935	2	0
31	X	2044	0	2060	4	0
32	Y	1556	0	1597	5	0
33	Z	996	0	1044	2	0
34	z	2027	0	2076	32	0
35	G	558	0	612	24	0
35	t	354	0	377	6	0
35	u	257	0	283	7	0
36	V	1676	0	1687	7	0
37	b	1193	0	1191	3	0
38	d	2124	0	2125	23	0
39	e	1931	0	1916	38	0
40	g	1113	0	1097	3	0
41	h	895	0	881	2	0
42	i	828	0	857	2	0
43	j	745	0	746	3	0
44	k	774	0	784	2	0
45	l	688	0	674	9	0
46	m	567	0	591	8	0
47	n	215	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	o	798	0	804	5	0
49	q	1495	0	1492	13	0
50	r	1322	0	1348	4	0
51	AB	1828	0	1815	9	0
52	AC	1083	0	1088	8	0
53	AD	2731	0	2802	18	0
54	AE	972	0	1000	11	0
55	AF	1725	0	1769	9	0
56	AG	2688	0	2687	13	0
57	AH	1152	0	1183	20	0
58	AJ	839	0	887	17	0
59	AK	862	0	885	8	0
60	AL	1453	0	1540	12	0
61	AM	942	0	965	14	0
62	AN	868	0	928	8	0
63	AO	1592	0	1557	16	0
64	AP	781	0	806	5	0
65	AR	2409	0	2428	15	0
66	AS	1111	0	1115	7	0
67	AT	1371	0	1393	10	0
68	AU	1488	0	1499	11	0
69	AV	2969	0	2961	52	0
70	AW	789	0	802	8	0
71	AZ	839	0	858	5	0
72	A0	1787	0	1796	28	0
73	A1	2265	0	2294	21	0
74	A3	625	0	698	6	0
75	Az	719	0	360	9	0
76	AY	1010	0	957	10	0
77	AA	20260	0	10288	328	0
78	AI	1019	0	1059	6	0
79	A4	4768	0	4766	79	0
80	AX	2849	0	2843	36	0
81	A2	935	0	969	6	0
82	AQ	744	0	758	5	0
83	c	2299	0	2320	10	0
84	f	1252	0	1269	14	0
85	p	1205	0	1223	4	0
86	s	3148	0	3131	16	0
87	OX	468	0	464	4	0
88	a	865	0	829	7	0
89	Aw	1434	0	728	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	Ax	1482	0	753	29	0
91	B	1524	0	779	22	0
92	0	1	0	0	0	0
92	4	1	0	0	0	0
92	AO	1	0	0	0	0
93	6	1	0	0	0	0
93	A	30	0	0	0	0
93	AA	17	0	0	0	0
93	AJ	1	0	0	0	0
93	D	1	0	0	0	0
93	M	2	0	0	0	0
93	N	1	0	0	0	0
93	o	1	0	0	0	0
94	A	50	0	95	1	0
94	AA	30	0	57	4	0
95	A	6	0	12	0	0
96	A	137	0	0	0	0
96	A3	1	0	0	0	0
96	AA	60	0	0	0	0
96	AB	1	0	0	0	0
96	AX	1	0	0	0	0
96	D	2	0	0	0	0
96	E	1	0	0	0	0
96	g	1	0	0	0	0
97	AP	4	0	0	0	0
97	AT	4	0	0	0	0
97	r	4	0	0	1	0
98	AA	44	0	26	1	0
99	AA	28	0	52	0	0
100	AX	31	0	12	0	0
101	AX	28	0	12	3	0
102	B	7	0	8	4	0
All	All	181859	0	154427	1396	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 (1396) 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)
35:G:148:GLU:O	35:G:152:TYR:HB3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e:218:PRO:HG2	102:B:101:VAL:HG22	1.60	0.82
39:e:172:ILE:HD13	91:B:76:A:H2	1.46	0.81
15:F:103:GLN:HE22	15:F:249:ASN:HD22	1.29	0.79
77:AA:1587:U:H2'	77:AA:1588:G:H8	1.52	0.75
35:G:165:VAL:HA	35:G:168:LEU:HG	1.68	0.74
39:e:183:THR:HG23	39:e:186:GLY:H	1.49	0.74
9:8:187:PRO:HG2	46:m:79:ILE:HD11	1.70	0.74
16:H:207:LYS:HB3	16:H:222:GLU:HB3	1.69	0.73
34:z:161:THR:HB	34:z:167:VAL:HG22	1.71	0.73
32:Y:123:ARG:HD3	38:d:64:GLY:HA2	1.71	0.72
22:N:124:VAL:HG12	22:N:158:ARG:HE	1.55	0.72
9:8:147:LEU:HD21	39:e:208:ALA:HB1	1.72	0.71
39:e:172:ILE:HD13	91:B:76:A:C2	2.25	0.71
52:AC:125:ARG:HH11	79:A4:94:TYR:HB2	1.57	0.70
70:AW:154:LEU:HB3	81:A2:29:LEU:HG	1.74	0.70
9:8:50:LEU:HB2	89:Aw:39:U:H4'	1.74	0.69
79:A4:429:LEU:HA	79:A4:464:LEU:HD21	1.75	0.69
39:e:231:VAL:HG21	91:B:76:A:H61	1.57	0.69
34:z:108:LYS:O	34:z:112:LEU:HB2	1.93	0.68
79:A4:262:MET:HB3	79:A4:278:LEU:HD21	1.75	0.68
76:AY:290:ASN:HA	79:A4:446:LYS:HD3	1.75	0.68
79:A4:196:CYS:HB3	79:A4:265:GLY:HA3	1.75	0.68
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.77	0.67
38:d:150:LEU:HD13	38:d:153:ASN:HD22	1.58	0.67
77:AA:976:A:H5''	82:AQ:1:ACE:H1	1.77	0.67
38:d:91:PRO:HB2	38:d:94:ASP:HB2	1.77	0.67
69:AV:64:LYS:HG3	77:AA:1530:A:H4'	1.77	0.66
77:AA:944:U:H2'	77:AA:945:G:H8	1.59	0.66
73:A1:71:PRO:HB3	79:A4:78:VAL:HG21	1.76	0.66
54:AE:92:ASN:HB2	64:AP:117:MET:HE3	1.77	0.66
77:AA:773:U:H2'	77:AA:774:G:H8	1.59	0.66
35:G:143:VAL:HA	35:G:146:ILE:HG12	1.78	0.66
34:z:295:LEU:HB2	34:z:305:LEU:HD11	1.78	0.65
77:AA:1201:A:H2'	77:AA:1202:G:H8	1.61	0.65
79:A4:532:LEU:HD11	79:A4:555:ILE:HG21	1.79	0.65
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.77	0.65
56:AG:92:MET:HE3	56:AG:107:ALA:HB1	1.78	0.65
89:Aw:73:U:H5''	89:Aw:74:C:H5'	1.79	0.65
11:A:2727:C:H5''	89:Aw:76:A:H5'	1.79	0.65
12:C:211:ILE:HD12	35:G:143:VAL:HG12	1.77	0.65
18:J:85:PRO:HG2	45:l:77:ILE:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:A1:126:LEU:HD11	79:A4:70:VAL:HG13	1.79	0.65
11:A:2586:U:H2'	11:A:2587:G:H8	1.62	0.65
80:AX:273:THR:HG23	80:AX:316:LEU:HD13	1.79	0.65
38:d:57:MET:HE1	38:d:67:ILE:HD11	1.78	0.64
90:Ax:8:U:H5'	90:Ax:49:G:H5'	1.78	0.64
73:A1:86:ARG:HB3	73:A1:96:PRO:HB2	1.79	0.64
36:V:79:VAL:HG12	36:V:86:VAL:HG12	1.79	0.64
24:P:52:ASN:HB3	24:P:55:ASN:HB2	1.79	0.64
6:5:236:LEU:HD21	6:5:289:HIS:HD2	1.63	0.64
69:AV:66:PRO:HD3	77:AA:1529:A:H1'	1.80	0.64
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.80	0.64
16:H:163:THR:HG21	34:z:86:VAL:HG23	1.80	0.64
39:e:257:LYS:HD3	39:e:278:ASP:HB3	1.80	0.64
61:AM:53:SER:H	61:AM:67:ALA:HB3	1.62	0.64
6:5:283:TYR:HE1	86:s:152:GLN:HG2	1.62	0.63
80:AX:177:ARG:HB3	80:AX:288:ALA:HB2	1.80	0.63
12:C:239:LEU:HD11	12:C:256:CYS:HB2	1.79	0.63
69:AV:149:ASP:HA	69:AV:152:ILE:HG22	1.80	0.63
35:G:165:VAL:HG22	35:G:168:LEU:HD11	1.79	0.63
63:AO:104:PRO:HG2	63:AO:109:ARG:HG2	1.80	0.63
72:A0:5:LYS:HZ3	72:A0:7:ARG:HA	1.64	0.63
77:AA:1440:G:H2'	77:AA:1441:A:C8	2.34	0.63
58:AJ:72:LYS:HG3	77:AA:1557:A:H5''	1.81	0.63
35:t:64:ILE:HD12	35:t:67:LEU:HD12	1.80	0.63
77:AA:1201:A:H2'	77:AA:1202:G:C8	2.33	0.63
77:AA:1562:G:H1'	77:AA:1583:MA6:H2	1.81	0.63
69:AV:152:ILE:HD12	69:AV:185:VAL:HG22	1.81	0.62
69:AV:271:GLU:HA	69:AV:346:LYS:HE2	1.81	0.62
65:AR:157:VAL:HG22	65:AR:174:VAL:HG22	1.80	0.62
77:AA:663:A:H2'	77:AA:664:G:C8	2.35	0.62
79:A4:576:LEU:HB3	79:A4:599:PHE:HE1	1.63	0.62
77:AA:838:U:H2'	77:AA:839:A:H8	1.65	0.62
77:AA:1002:C:H2'	77:AA:1003:A:H8	1.63	0.62
73:A1:194:VAL:HB	73:A1:197:ARG:HB2	1.81	0.61
11:A:2055:U:H2'	11:A:2056:G:H8	1.65	0.61
9:8:136:ILE:HD13	84:f:173:ILE:HG13	1.83	0.61
9:8:192:TYR:HB3	84:f:132:ILE:HD11	1.82	0.61
12:C:185:LYS:HD2	12:C:258:LEU:HB3	1.81	0.61
34:z:181:THR:HA	34:z:184:ILE:HD12	1.81	0.61
69:AV:64:LYS:HE2	77:AA:1530:A:H5''	1.82	0.61
9:8:142:ALA:HA	39:e:274:ARG:HH21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AH:164:LEU:HD12	57:AH:165:PRO:HD2	1.82	0.61
11:A:2582:A:H2	77:AA:1560:U:H1'	1.64	0.61
34:z:103:VAL:HG21	34:z:267:ILE:HG21	1.82	0.61
44:k:18:VAL:HG11	44:k:34:LEU:HB2	1.83	0.61
69:AV:116:CYS:HA	69:AV:121:ALA:HB3	1.82	0.61
7:6:217:LEU:HD13	7:6:219:THR:HG23	1.82	0.61
89:Aw:23:A:H2'	89:Aw:24:A:H8	1.66	0.61
12:C:90:LEU:HG	12:C:153:LEU:HD22	1.81	0.60
36:V:55:TYR:HB2	36:V:133:ILE:HD11	1.84	0.60
77:AA:1365:A:H4'	77:AA:1389:G:H4'	1.83	0.60
18:J:117:VAL:HG21	18:J:145:ILE:HG13	1.83	0.60
38:d:208:VAL:HG22	38:d:253:THR:HG23	1.84	0.60
80:AX:101:VAL:HG22	80:AX:140:HIS:HE1	1.67	0.60
28:T:62:ARG:HE	38:d:230:ARG:HD2	1.66	0.59
77:AA:1132:U:H2'	77:AA:1133:C:C6	2.37	0.59
77:AA:1398:U:H2'	77:AA:1399:A:H8	1.67	0.59
76:AY:346:PRO:HD2	76:AY:392:ILE:HD11	1.84	0.59
77:AA:1025:A:H2'	77:AA:1026:A:C8	2.37	0.59
8:7:143:TRP:HE1	8:7:172:VAL:HG23	1.68	0.59
35:t:53:LEU:HB2	35:t:56:ALA:HB2	1.84	0.59
69:AV:70:LEU:HD21	69:AV:390:ILE:HD12	1.83	0.59
79:A4:392:ILE:HG13	79:A4:393:ILE:N	2.17	0.59
62:AN:21:LYS:HB3	77:AA:777:G:H5''	1.84	0.59
62:AN:95:VAL:HG23	62:AN:96:THR:HG23	1.84	0.59
77:AA:1132:U:H2'	77:AA:1133:C:H6	1.68	0.59
7:6:255:LEU:HD12	7:6:256:PRO:HD2	1.84	0.59
77:AA:1452:U:H2'	77:AA:1453:A:H8	1.66	0.59
77:AA:1239:C:H2'	77:AA:1240:A:H8	1.66	0.59
73:A1:272:ALA:HB1	80:AX:118:ALA:HB1	1.85	0.59
77:AA:1012:A:H2'	77:AA:1013:A:C8	2.38	0.59
31:X:20:ILE:HG22	87:OX:434:LEU:HD23	1.85	0.58
18:J:114:LEU:HB3	45:l:96:LEU:HD21	1.84	0.58
69:AV:50:LEU:HD22	69:AV:84:GLU:HG2	1.85	0.58
66:AS:71:ARG:HG2	66:AS:100:VAL:HG21	1.85	0.58
54:AE:96:HIS:HB3	54:AE:99:THR:HG23	1.84	0.58
69:AV:76:ILE:HD12	69:AV:112:TRP:HD1	1.68	0.58
11:A:3211:C:H4'	11:A:3212:C:H5	1.68	0.58
73:A1:53:LEU:HD12	79:A4:518:GLU:HG2	1.85	0.58
91:B:30:A:H2'	91:B:31:A:H8	1.68	0.58
77:AA:1578:A:H2'	77:AA:1579:C:C6	2.38	0.58
90:Ax:27:U:H3	90:Ax:42:G:H1	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:AA:730:A:H3'	77:AA:731:A:H8	1.69	0.58
77:AA:799:A:H2'	77:AA:800:C:C6	2.38	0.58
83:c:160:LEU:HD21	83:c:223:MET:HG3	1.85	0.58
21:M:177:ALA:HB1	21:M:203:ARG:HH12	1.68	0.58
77:AA:944:U:H2'	77:AA:945:G:C8	2.37	0.58
12:C:284:SER:HA	12:C:289:VAL:HG11	1.85	0.58
13:D:184:LEU:HD22	13:D:216:LEU:HD13	1.86	0.58
34:z:88:LEU:H	34:z:91:LEU:HD12	1.68	0.58
39:e:183:THR:HG23	39:e:186:GLY:N	2.18	0.58
80:AX:188:LEU:HD22	80:AX:226:VAL:HG23	1.86	0.57
9:8:52:LYS:HE3	89:Aw:38:C:H4'	1.85	0.57
17:I:154:LEU:HD12	17:I:164:MET:HE3	1.85	0.57
25:Q:69:VAL:HG12	25:Q:71:PRO:HD3	1.84	0.57
66:AS:51:VAL:HG13	81:A2:117:LEU:HD11	1.86	0.57
54:AE:94:VAL:HG12	77:AA:1033:U:H4'	1.86	0.57
11:A:2093:U:H2'	11:A:2094:G:C8	2.39	0.57
35:G:131:THR:HA	35:G:174:ALA:HA	1.86	0.57
53:AD:420:SER:HA	77:AA:929:A:H4'	1.86	0.57
69:AV:218:SER:HB2	69:AV:274:LYS:H	1.69	0.57
77:AA:839:A:H2'	77:AA:840:A:H8	1.69	0.57
77:AA:985:U:H2'	77:AA:986:G:H8	1.70	0.57
77:AA:1317:A:H3'	77:AA:1318:A:H8	1.70	0.57
1:0:138:ARG:HB3	11:A:2321:A:C8	2.40	0.57
79:A4:349:ALA:HB3	79:A4:378:LEU:HD21	1.87	0.57
79:A4:350:ARG:HA	79:A4:379:PHE:CE1	2.40	0.57
79:A4:562:GLN:HB3	79:A4:564:ILE:HG22	1.87	0.57
11:A:2099:U:H2'	11:A:2100:C:C6	2.39	0.57
17:I:197:LEU:HD22	35:u:76:LEU:HD12	1.86	0.57
39:e:172:ILE:HG21	91:B:76:A:C2	2.39	0.57
77:AA:1003:A:H2'	77:AA:1004:G:H8	1.70	0.57
79:A4:573:ALA:HB2	79:A4:604:LYS:HD3	1.85	0.57
77:AA:1528:A:H2'	77:AA:1529:A:H8	1.70	0.57
17:I:116:LEU:HG	17:I:121:ILE:HB	1.86	0.56
34:z:161:THR:HG23	34:z:230:ILE:HD12	1.86	0.56
72:A0:68:LEU:HD21	72:A0:80:VAL:HG21	1.87	0.56
72:A0:39:GLU:HG2	72:A0:40:THR:HG23	1.86	0.56
77:AA:1308:U:H2'	77:AA:1309:A:H8	1.70	0.56
77:AA:1589:C:H2'	77:AA:1590:A:C8	2.41	0.56
2:1:34:ARG:HD3	2:1:41:LEU:HD13	1.87	0.56
6:5:236:LEU:HD21	6:5:289:HIS:CD2	2.41	0.56
8:7:204:LYS:HE2	88:a:92:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:AV:231:LEU:HD12	69:AV:243:VAL:HG13	1.86	0.56
77:AA:740:G:H2'	77:AA:741:A:H8	1.70	0.56
77:AA:1012:A:H2	78:AI:185:GLY:HA2	1.70	0.56
77:AA:1239:C:H2'	77:AA:1240:A:C8	2.40	0.56
77:AA:1131:C:H2'	77:AA:1132:U:C6	2.40	0.56
77:AA:745:A:H3'	77:AA:746:A:H8	1.70	0.56
39:e:173:LEU:HD23	39:e:233:PHE:HD2	1.70	0.56
79:A4:400:LEU:HA	79:A4:403:LYS:HD3	1.88	0.56
12:C:246:LEU:HD21	12:C:251:LEU:HD22	1.88	0.56
77:AA:1042:U:H2'	77:AA:1043:C:C6	2.41	0.56
77:AA:1577:U:H2'	77:AA:1578:A:C8	2.41	0.56
77:AA:1583:MA6:O5'	77:AA:1583:MA6:H8	2.05	0.56
11:A:3199:U:H5''	11:A:3200:U:H4'	1.87	0.56
34:z:184:ILE:HD13	34:z:206:GLU:HB2	1.87	0.56
55:AF:129:ALA:HB1	55:AF:133:GLU:HB2	1.88	0.56
59:AK:75:ILE:HA	59:AK:78:LEU:HD12	1.88	0.56
86:s:137:LEU:HD21	86:s:422:VAL:HG11	1.88	0.56
2:1:19:ARG:HB2	2:1:62:ILE:HD11	1.87	0.56
7:6:327:VAL:HA	7:6:330:ILE:HD12	1.87	0.56
6:5:242:ARG:HA	6:5:245:ILE:HD12	1.88	0.56
39:e:265:LYS:HD3	91:B:76:A:H5'	1.88	0.56
6:5:283:TYR:CE1	86:s:152:GLN:HG2	2.40	0.55
13:D:216:LEU:HD11	13:D:224:ALA:HB1	1.87	0.55
39:e:168:GLN:HB3	102:B:101:VAL:N	2.21	0.55
57:AH:157:LEU:HD23	57:AH:160:ILE:HD11	1.88	0.55
63:AO:208:PRO:HG2	63:AO:213:LEU:HD21	1.88	0.55
77:AA:1034:U:H2'	77:AA:1035:U:H6	1.71	0.55
77:AA:1146:C:H2'	77:AA:1147:G:H8	1.72	0.55
11:A:2740:A:H2'	11:A:2741:A:C8	2.42	0.55
39:e:195:LEU:HD12	39:e:243:PHE:HZ	1.71	0.55
77:AA:1002:C:H2'	77:AA:1003:A:C8	2.41	0.55
86:s:142:LEU:HD13	86:s:422:VAL:HG21	1.88	0.55
18:J:25:ARG:HH12	45:l:56:LEU:HB3	1.71	0.55
56:AG:310:ARG:HA	56:AG:313:LEU:HD12	1.88	0.55
77:AA:960:C:H42	77:AA:1041:A:H2	1.54	0.55
77:AA:1349:U:H2'	77:AA:1350:G:C8	2.41	0.55
77:AA:1471:A:H2'	77:AA:1472:G:H8	1.69	0.55
12:C:92:VAL:HG22	12:C:97:PRO:HA	1.88	0.55
35:G:188:LEU:HA	35:G:191:VAL:HG12	1.89	0.55
57:AH:104:ILE:HG23	57:AH:148:LEU:HD11	1.89	0.55
80:AX:162:VAL:HG21	80:AX:267:ALA:HB1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:218:ILE:HG23	22:N:223:MET:HB2	1.88	0.55
77:AA:838:U:H2'	77:AA:839:A:C8	2.41	0.55
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.89	0.55
69:AV:117:LEU:HA	69:AV:122:GLN:OE1	2.07	0.55
72:A0:193:VAL:HG12	72:A0:196:ILE:HD11	1.88	0.55
79:A4:161:ILE:HG21	79:A4:190:SER:HB3	1.87	0.55
79:A4:309:PHE:HB2	79:A4:313:TRP:HZ3	1.71	0.55
86:s:119:PRO:HD3	86:s:371:CYS:SG	2.47	0.55
89:Aw:9:A:H1'	89:Aw:45:A:H2'	1.88	0.55
77:AA:1470:A:H2'	77:AA:1471:A:H8	1.71	0.55
80:AX:153:LEU:HD21	80:AX:247:LEU:HD13	1.89	0.55
83:c:93:VAL:HG11	83:c:119:LEU:HG	1.89	0.55
9:8:57:ASP:HB2	89:Aw:23:A:H1'	1.89	0.54
69:AV:387:VAL:HA	69:AV:390:ILE:HG22	1.89	0.54
81:A2:43:ALA:HB1	81:A2:46:ILE:HD11	1.88	0.54
89:Aw:62:C:H2'	89:Aw:63:A:C8	2.42	0.54
7:6:224:HIS:CE1	7:6:227:GLU:H	2.25	0.54
12:C:191:VAL:HG11	12:C:251:LEU:HD23	1.89	0.54
15:F:62:VAL:HG23	15:F:82:LEU:HB2	1.88	0.54
38:d:186:VAL:HG21	38:d:239:PRO:HB3	1.90	0.54
77:AA:1578:A:H2'	77:AA:1579:C:H6	1.72	0.54
9:8:55:LYS:HB2	89:Aw:24:A:H5'	1.89	0.54
69:AV:57:MET:HG2	69:AV:71:THR:HG21	1.89	0.54
69:AV:148:MET:HE1	69:AV:160:ALA:HB1	1.89	0.54
80:AX:179:ASP:HB3	80:AX:237:THR:HG21	1.90	0.54
89:Aw:54:U:H3'	89:Aw:55:A:H8	1.71	0.54
17:I:98:VAL:HG12	17:I:177:LEU:HD12	1.90	0.54
22:N:36:VAL:HG11	45:I:124:GLN:HB3	1.88	0.54
29:U:44:ILE:HG21	29:U:53:LEU:HD22	1.88	0.54
37:b:72:VAL:HG13	37:b:90:HIS:HB2	1.90	0.54
50:r:99:MET:HE1	50:r:115:ILE:HG22	1.89	0.54
53:AD:209:GLY:HA3	53:AD:213:GLU:HB2	1.90	0.54
56:AG:275:LYS:HG2	56:AG:280:LYS:HG2	1.89	0.54
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.89	0.54
79:A4:556:LYS:HD2	79:A4:595:MET:HE1	1.89	0.54
89:Aw:23:A:H2'	89:Aw:24:A:C8	2.42	0.54
11:A:1857:U:H2'	11:A:1858:G:C8	2.43	0.54
11:A:2553:G:H2'	11:A:2554:A:H8	1.73	0.54
85:p:133:LEU:HD21	85:p:157:MET:HE1	1.89	0.54
90:Ax:29:U:H2'	90:Ax:30:G:C8	2.43	0.54
11:A:1895:C:H2'	11:A:1896:U:H6	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2392:U:H2'	11:A:2394:A:H62	1.71	0.54
12:C:91:ALA:HB2	12:C:108:ILE:HD12	1.89	0.54
11:A:1862:U:H2'	11:A:1863:A:H8	1.72	0.54
19:K:60:MET:HE2	19:K:133:ILE:HD11	1.90	0.54
77:AA:705:C:H3'	77:AA:706:C:H6	1.73	0.54
11:A:3150:U:H2'	11:A:3151:A:H8	1.73	0.54
18:J:140:VAL:O	18:J:144:ILE:HG12	2.07	0.54
77:AA:1498:C:H2'	77:AA:1499:U:H6	1.73	0.54
90:Ax:70:C:H2'	90:Ax:71:U:C6	2.43	0.54
77:AA:773:U:H2'	77:AA:774:G:C8	2.41	0.53
77:AA:1175:G:H2'	77:AA:1176:G:C8	2.44	0.53
11:A:2545:U:H5''	11:A:2546:G:H5'	1.89	0.53
21:M:226:PRO:HG3	85:p:45:LEU:HD23	1.89	0.53
34:z:184:ILE:HG22	34:z:209:ARG:HH21	1.73	0.53
39:e:231:VAL:HG21	91:B:76:A:N6	2.22	0.53
59:AK:52:LEU:HD22	71:AZ:41:PRO:HG3	1.89	0.53
89:Aw:26:U:H2'	89:Aw:27:A:C8	2.43	0.53
15:F:175:LYS:HG2	15:F:273:LEU:HD13	1.89	0.53
55:AF:168:TYR:HB3	55:AF:236:LEU:HD13	1.90	0.53
69:AV:143:THR:HA	69:AV:146:LEU:HD12	1.90	0.53
77:AA:1042:U:H2'	77:AA:1043:C:H6	1.73	0.53
11:A:1895:C:H2'	11:A:1896:U:C6	2.43	0.53
13:D:109:PHE:HB3	13:D:204:ALA:HB3	1.90	0.53
74:A3:193:LYS:HB3	74:A3:196:LEU:HD23	1.90	0.53
77:AA:1471:A:H2'	77:AA:1472:G:C8	2.43	0.53
54:AE:26:ILE:HG22	54:AE:30:MET:HE2	1.91	0.53
77:AA:867:C:H2'	77:AA:870:C:H42	1.74	0.53
84:f:90:VAL:HG13	84:f:189:HIS:HB3	1.90	0.53
77:AA:872:G:H2'	77:AA:873:G:C8	2.43	0.53
77:AA:1129:U:H2'	77:AA:1130:G:H8	1.73	0.53
80:AX:181:PRO:HB2	80:AX:233:VAL:HG22	1.90	0.53
83:c:258:THR:HA	88:a:72:THR:HG22	1.91	0.53
89:Aw:40:C:H2'	89:Aw:41:A:C8	2.44	0.53
21:M:261:ASP:HB3	21:M:264:GLN:HB2	1.91	0.53
77:AA:872:G:H2'	77:AA:873:G:H8	1.72	0.53
79:A4:494:ILE:HD11	79:A4:527:LEU:HA	1.90	0.53
11:A:1952:U:H2'	11:A:1953:A:C8	2.43	0.53
55:AF:93:LYS:HE3	77:AA:1459:A:H5''	1.91	0.53
77:AA:914:A:H2'	77:AA:915:C:H6	1.72	0.53
8:7:204:LYS:HZ1	88:a:92:LEU:HB3	1.74	0.53
11:A:1952:U:H2'	11:A:1953:A:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:t:86:LEU:HD22	35:u:68:VAL:HG22	1.91	0.53
77:AA:914:A:H2'	77:AA:915:C:C6	2.44	0.53
91:B:23:A:H2'	91:B:24:G:C8	2.44	0.53
17:I:82:LEU:HB3	17:I:130:VAL:HG21	1.91	0.53
27:S:156:VAL:HG22	27:S:198:ILE:HG12	1.91	0.53
77:AA:970:A:H2'	77:AA:971:A:C8	2.45	0.53
17:I:200:LEU:HD13	35:u:76:LEU:HB3	1.91	0.52
52:AC:136:VAL:HG22	52:AC:153:LEU:HD22	1.91	0.52
77:AA:832:U:H2'	77:AA:833:A:H8	1.73	0.52
80:AX:222:LEU:HA	80:AX:225:VAL:HG12	1.90	0.52
5:4:103:MET:HE1	11:A:2952:U:H5'	1.91	0.52
11:A:2006:C:H2'	11:A:2007:U:C6	2.44	0.52
71:AZ:24:ARG:HH21	76:AY:348:ARG:HG3	1.74	0.52
9:8:92:LEU:HD13	49:q:162:GLU:HG3	1.92	0.52
25:Q:76:LEU:HD23	25:Q:279:GLU:HG2	1.91	0.52
36:V:153:ILE:HG12	87:OX:399:GLN:HG2	1.90	0.52
39:e:170:VAL:HG21	91:B:76:A:H5''	1.92	0.52
12:C:204:GLU:O	12:C:208:GLU:HG2	2.10	0.52
63:AO:193:LEU:HD12	65:AR:143:ALA:HA	1.90	0.52
64:AP:54:MET:HE2	66:AS:64:TRP:HB3	1.90	0.52
77:AA:672:A:H2'	77:AA:673:U:C6	2.44	0.52
79:A4:545:GLN:HE22	79:A4:585:ARG:HH21	1.56	0.52
11:A:2081:U:H2'	11:A:2082:G:C8	2.45	0.52
16:H:102:VAL:HB	16:H:105:VAL:HG22	1.92	0.52
81:A2:95:GLU:HB3	81:A2:100:LEU:HG	1.92	0.52
11:A:1868:G:H2'	21:M:40:PRO:HG3	1.92	0.52
51:AB:64:ASN:HA	51:AB:67:LEU:HD12	1.92	0.52
68:AU:64:ARG:HA	68:AU:67:VAL:HG12	1.90	0.52
77:AA:1007:G:H2'	77:AA:1008:A:C8	2.44	0.52
12:C:201:VAL:HG22	12:C:205:ARG:HH22	1.74	0.52
21:M:44:ARG:HG3	21:M:45:ARG:HG3	1.92	0.52
21:M:244:LEU:HD12	21:M:245:PRO:HD2	1.92	0.52
38:d:86:ASP:HB2	38:d:198:ARG:HG3	1.92	0.52
39:e:173:LEU:HD23	39:e:233:PHE:CD2	2.45	0.52
90:Ax:28:C:H2'	90:Ax:29:U:C6	2.43	0.52
34:z:76:PRO:HB2	34:z:93:PRO:HG2	1.91	0.52
77:AA:1034:U:H2'	77:AA:1035:U:C6	2.45	0.52
77:AA:1065:C:H2'	77:AA:1066:C:O4'	2.09	0.52
77:AA:1089:U:H2'	77:AA:1090:A:H8	1.73	0.52
11:A:2734:A:H2'	11:A:2735:G:H8	1.73	0.52
60:AL:209:LEU:HD13	74:A3:173:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:AA:738:A:H3'	77:AA:739:C:H6	1.74	0.52
11:A:2151:A:H2'	11:A:2152:A:C8	2.45	0.52
11:A:2584:C:H2'	11:A:2585:G:C8	2.45	0.52
17:I:163:GLU:HG3	17:I:166:ARG:HH22	1.75	0.52
57:AH:74:LYS:HB2	57:AH:177:LEU:HG	1.91	0.52
61:AM:101:PRO:HB3	68:AU:59:ARG:HB3	1.92	0.52
77:AA:911:U:H2'	77:AA:912:U:C6	2.45	0.52
16:H:216:TRP:HA	16:H:237:VAL:HB	1.92	0.51
70:AW:104:ILE:HG13	70:AW:114:ILE:HG13	1.92	0.51
77:AA:673:U:H2'	77:AA:674:U:C6	2.45	0.51
77:AA:847:G:H2'	77:AA:848:U:C6	2.45	0.51
79:A4:170:VAL:HG23	79:A4:247:ILE:HD11	1.92	0.51
86:s:145:VAL:HG21	86:s:187:LEU:HD11	1.92	0.51
12:C:189:ILE:HB	12:C:232:PHE:HB2	1.91	0.51
53:AD:103:LEU:HD11	53:AD:123:ARG:HB2	1.92	0.51
69:AV:202:ARG:HD2	69:AV:247:MET:HG3	1.92	0.51
77:AA:920:G:H2'	77:AA:921:U:C6	2.45	0.51
77:AA:1043:C:H2'	77:AA:1044:U:C6	2.46	0.51
11:A:2408:U:H2'	11:A:2409:A:H8	1.74	0.51
12:C:217:ASP:HB2	12:C:233:ILE:HB	1.92	0.51
58:AJ:80:CYS:HB3	58:AJ:94:PHE:HA	1.93	0.51
60:AL:165:LYS:HE3	77:AA:947:U:H5''	1.92	0.51
61:AM:114:ARG:HA	61:AM:117:GLU:HB3	1.91	0.51
79:A4:571:TRP:HE3	79:A4:576:LEU:HD21	1.74	0.51
9:8:133:ARG:HH12	91:B:27:C:H4'	1.75	0.51
12:C:168:LEU:HD23	12:C:279:LEU:HD11	1.92	0.51
16:H:176:MET:HE1	16:H:188:ILE:HD11	1.92	0.51
25:Q:182:ARG:HG3	25:Q:187:LEU:HD11	1.91	0.51
58:AJ:66:PHE:HE2	58:AJ:68:ARG:HE	1.57	0.51
77:AA:985:U:H2'	77:AA:986:G:C8	2.45	0.51
77:AA:1427:A:H2'	77:AA:1428:G:C8	2.45	0.51
17:I:140:TYR:HB3	17:I:143:LEU:HD12	1.91	0.51
34:z:219:PRO:HA	34:z:225:SER:HB2	1.92	0.51
50:r:71:PRO:HD2	50:r:107:LEU:HD23	1.92	0.51
80:AX:159:HIS:CD2	80:AX:267:ALA:HB2	2.45	0.51
11:A:1765:C:H5'	42:i:75:ARG:HH22	1.74	0.51
26:R:35:LYS:HD2	26:R:45:THR:HG21	1.92	0.51
53:AD:244:LEU:HD22	53:AD:343:LEU:HD23	1.92	0.51
64:AP:124:TYR:HE2	82:AQ:4:HIS:HB3	1.76	0.51
77:AA:1033:U:H2'	77:AA:1034:U:H6	1.76	0.51
9:8:160:GLU:HA	9:8:163:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:118:LEU:HD11	16:H:122:ARG:HH21	1.76	0.51
72:A0:99:ARG:HD3	77:AA:1526:U:H2'	1.91	0.51
6:5:165:GLN:NE2	6:5:175:THR:HG22	2.26	0.51
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.46	0.51
11:A:2727:C:H2'	11:A:2728:C:H6	1.76	0.51
11:A:2804:A:H2'	11:A:2805:A:H8	1.76	0.51
27:S:114:ILE:HD12	27:S:116:ILE:HD11	1.91	0.51
35:G:146:ILE:HG22	35:G:158:LEU:HB2	1.91	0.51
58:AJ:62:VAL:HA	58:AJ:83:VAL:HG12	1.92	0.51
77:AA:705:C:H3'	77:AA:706:C:C6	2.46	0.51
11:A:2409:A:H2'	11:A:2410:U:C6	2.46	0.51
11:A:2514:C:H2'	11:A:2515:U:H6	1.76	0.51
11:A:3054:G:H2'	11:A:3055:U:C6	2.46	0.51
61:AM:34:ILE:HG12	61:AM:87:MET:HE1	1.93	0.51
77:AA:916:C:H2'	77:AA:917:C:C6	2.46	0.51
77:AA:1114:U:H2'	77:AA:1115:U:C6	2.46	0.51
90:Ax:5:G:H2'	90:Ax:6:A:C8	2.46	0.51
90:Ax:6:A:H2'	90:Ax:7:A:C8	2.46	0.51
2:1:38:ARG:HH12	2:1:41:LEU:HD11	1.76	0.51
11:A:2727:C:H2'	11:A:2728:C:C6	2.46	0.51
14:E:107:MET:HE3	25:Q:145:LEU:HD12	1.93	0.51
34:z:160:PHE:HD2	34:z:199:ALA:HB2	1.76	0.51
35:G:134:LEU:HA	35:G:195:VAL:HA	1.93	0.51
48:o:15:ARG:HB3	48:o:18:ILE:HG12	1.93	0.51
55:AF:237:ALA:HB1	81:A2:46:ILE:HD12	1.91	0.51
69:AV:276:CYS:SG	69:AV:352:LEU:HD21	2.51	0.51
77:AA:659:U:H2'	77:AA:660:C:C6	2.46	0.51
77:AA:918:A:H4'	77:AA:920:G:H4'	1.93	0.51
77:AA:969:A:H2'	77:AA:970:A:H8	1.76	0.51
89:Aw:5:A:H2'	89:Aw:6:U:H6	1.76	0.51
19:K:94:GLN:O	19:K:98:ARG:HG2	2.11	0.50
77:AA:686:A:H2'	77:AA:687:G:C8	2.45	0.50
86:s:63:ILE:HA	86:s:66:TRP:CD1	2.45	0.50
9:8:125:LYS:HD3	91:B:29:C:H5''	1.93	0.50
13:D:237:LEU:HG	13:D:296:VAL:HG12	1.93	0.50
49:q:191:LYS:HA	49:q:194:LYS:HG2	1.93	0.50
77:AA:1232:A:H2	77:AA:1404:A:H5'	1.76	0.50
77:AA:1349:U:H2'	77:AA:1350:G:H8	1.75	0.50
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.93	0.50
25:Q:100:LEU:HD21	25:Q:286:ILE:HG12	1.93	0.50
77:AA:1173:C:H2'	77:AA:1174:U:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:A4:85:VAL:HG21	79:A4:97:PRO:HD2	1.92	0.50
79:A4:529:GLU:HB3	79:A4:533:MET:HE3	1.93	0.50
89:Aw:52:G:H3'	89:Aw:53:A:H8	1.76	0.50
72:A0:102:PRO:HB2	72:A0:109:LEU:HD12	1.93	0.50
77:AA:1559:G:H5'	89:Aw:38:C:H5	1.75	0.50
86:s:271:LEU:HD23	86:s:273:LEU:HD13	1.92	0.50
91:B:68:C:H2'	91:B:69:U:C6	2.47	0.50
6:5:55:LEU:HD11	31:X:163:ARG:HE	1.76	0.50
12:C:216:GLU:HB3	12:C:234:CYS:HA	1.93	0.50
15:F:123:GLY:HA3	15:F:142:ARG:HG2	1.92	0.50
17:I:96:ILE:HA	17:I:155:VAL:HG12	1.94	0.50
69:AV:49:CYS:HB3	69:AV:52:ASP:HB2	1.94	0.50
8:7:307:ARG:HD2	14:E:47:THR:HG21	1.93	0.50
66:AS:29:PRO:HG2	66:AS:32:PHE:HB2	1.94	0.50
69:AV:246:ASN:HA	72:A0:70:ARG:HH22	1.76	0.50
76:AY:306:LYS:HA	79:A4:67:LYS:HZ1	1.76	0.50
77:AA:1194:C:H2'	77:AA:1195:U:C6	2.47	0.50
11:A:2275:U:H5''	83:c:34:GLY:HA3	1.94	0.50
17:I:115:GLN:HA	17:I:118:LYS:HG3	1.94	0.50
28:T:107:GLY:HA2	28:T:110:ILE:HD12	1.93	0.50
39:e:61:LYS:HE2	39:e:155:ARG:HD2	1.93	0.50
77:AA:832:U:H2'	77:AA:833:A:C8	2.46	0.50
79:A4:462:PHE:HZ	79:A4:481:LEU:HB3	1.77	0.50
86:s:84:THR:HB	86:s:280:ASN:HB2	1.92	0.50
23:O:46:TRP:CD1	23:O:121:ALA:HB2	2.46	0.50
77:AA:659:U:H2'	77:AA:660:C:H6	1.75	0.50
51:AB:69:HIS:HB2	51:AB:72:PHE:HB2	1.94	0.50
57:AH:162:ARG:HH12	79:A4:71:LEU:HD11	1.77	0.50
61:AM:100:HIS:H	61:AM:103:MET:HE3	1.77	0.50
73:A1:45:GLU:HG2	73:A1:47:PRO:HD2	1.94	0.50
76:AY:294:LEU:HD13	76:AY:300:GLU:HG3	1.94	0.50
45:l:92:TYR:HB3	45:l:96:LEU:HD13	1.94	0.49
48:o:12:ILE:HG21	48:o:16:GLN:HA	1.94	0.49
77:AA:1265:C:H2'	77:AA:1266:A:H8	1.76	0.49
11:A:2318:A:H2'	11:A:2319:A:C8	2.47	0.49
17:I:47:LEU:HD22	22:N:226:ILE:HG12	1.92	0.49
18:J:113:THR:HG22	18:J:116:HIS:ND1	2.27	0.49
76:AY:385:ASP:O	76:AY:389:GLU:HG2	2.12	0.49
77:AA:839:A:H2'	77:AA:840:A:C8	2.47	0.49
77:AA:1244:C:H2'	77:AA:1245:U:C6	2.46	0.49
11:A:2086:A:H2'	11:A:2087:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:G:134:LEU:HB2	35:G:195:VAL:HG22	1.94	0.49
56:AG:87:HIS:O	56:AG:91:MET:HG2	2.12	0.49
56:AG:328:VAL:HG11	56:AG:348:MET:HG2	1.93	0.49
59:AK:115:ALA:HB2	59:AK:120:LEU:HD12	1.92	0.49
77:AA:1175:G:H2'	77:AA:1176:G:H8	1.75	0.49
81:A2:29:LEU:HD22	82:AQ:68:MET:HE2	1.93	0.49
11:A:2093:U:H2'	11:A:2094:G:H8	1.77	0.49
34:z:133:LYS:HG3	34:z:134:LYS:H	1.77	0.49
34:z:150:PHE:CE2	34:z:152:SER:HB3	2.47	0.49
34:z:296:ARG:HB3	34:z:302:GLY:HA2	1.93	0.49
38:d:208:VAL:HG23	38:d:252:LEU:HB2	1.93	0.49
77:AA:947:U:H2'	77:AA:948:U:H6	1.77	0.49
38:d:186:VAL:HB	38:d:219:ARG:HG2	1.94	0.49
77:AA:1502:A:H2'	77:AA:1503:G:O4'	2.13	0.49
77:AA:1523:A:H2'	77:AA:1524:A:C8	2.47	0.49
90:Ax:69:C:H2'	90:Ax:70:C:H6	1.77	0.49
52:AC:117:LEU:HD23	52:AC:151:VAL:HG22	1.94	0.49
80:AX:67:HIS:HB3	80:AX:98:CYS:HB3	1.93	0.49
4:3:175:ASP:HB3	4:3:178:GLN:HB2	1.94	0.49
34:z:243:ILE:HG21	34:z:278:VAL:HG12	1.94	0.49
77:AA:922:C:H2'	77:AA:923:A:C8	2.48	0.49
77:AA:1401:G:N2	77:AA:1403:A:H3'	2.28	0.49
9:8:201:GLN:HB3	84:f:201:ARG:HG3	1.93	0.49
11:A:2174:G:H4'	18:J:151:LEU:HD23	1.95	0.49
11:A:2894:U:H5''	11:A:2895:U:O4'	2.13	0.49
12:C:124:THR:HA	12:C:127:LYS:HB2	1.93	0.49
69:AV:34:TYR:HA	69:AV:372:ILE:HD11	1.93	0.49
77:AA:715:G:H2'	77:AA:716:U:C6	2.47	0.49
77:AA:868:C:H2'	77:AA:869:C:H6	1.78	0.49
89:Aw:40:C:H2'	89:Aw:41:A:H8	1.76	0.49
27:S:96:PHE:HB3	37:b:126:ILE:HD13	1.95	0.49
77:AA:970:A:H2'	77:AA:971:A:H8	1.76	0.49
89:Aw:16:A:N1	89:Aw:61:U:H5''	2.28	0.49
90:Ax:68:C:H2'	90:Ax:69:C:C6	2.48	0.49
6:5:336:LEU:HD21	6:5:362:THR:HG23	1.95	0.49
18:J:189:ALA:HA	18:J:192:LYS:HB2	1.94	0.49
39:e:213:TYR:HD2	91:B:76:A:H62	1.57	0.49
77:AA:661:C:H2'	77:AA:662:U:C6	2.48	0.49
77:AA:1177:C:H2'	77:AA:1178:G:C8	2.48	0.49
79:A4:89:PHE:CZ	79:A4:103:SER:HB2	2.47	0.49
79:A4:548:PHE:HB3	79:A4:582:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1935:A:C2	11:A:1936:A:H1'	2.47	0.48
55:AF:200:LEU:HB3	55:AF:202:PRO:HD2	1.95	0.48
64:AP:65:CYS:HB2	64:AP:68:CYS:SG	2.52	0.48
77:AA:833:A:H2'	77:AA:834:G:C8	2.47	0.48
77:AA:1003:A:H2'	77:AA:1004:G:C8	2.48	0.48
77:AA:1156:C:H2'	77:AA:1157:U:H6	1.78	0.48
77:AA:1441:A:H2	77:AA:1449:G:H22	1.60	0.48
90:Ax:68:C:H2'	90:Ax:69:C:H6	1.78	0.48
11:A:2483:U:H2'	11:A:2484:C:O4'	2.14	0.48
11:A:2804:A:H2'	11:A:2805:A:C8	2.48	0.48
12:C:211:ILE:HD13	35:G:147:LYS:HB2	1.95	0.48
12:C:241:GLN:HA	12:C:244:LYS:HE3	1.95	0.48
27:S:99:VAL:HG12	27:S:133:VAL:HG22	1.95	0.48
34:z:69:ILE:HA	34:z:72:ILE:HG12	1.94	0.48
34:z:127:LEU:HD22	34:z:290:VAL:HG13	1.95	0.48
56:AG:161:LEU:HD22	56:AG:209:LEU:HD21	1.95	0.48
77:AA:840:A:H2'	77:AA:841:A:H8	1.78	0.48
77:AA:968:U:H2'	77:AA:969:A:H8	1.77	0.48
77:AA:1021:U:H4'	77:AA:1022:A:H5'	1.95	0.48
77:AA:1032:C:H2'	77:AA:1033:U:H6	1.79	0.48
84:f:171:LEU:HD11	84:f:186:VAL:HG11	1.95	0.48
12:C:77:ARG:HG3	58:AJ:104:GLU:HG2	1.94	0.48
14:E:334:ASP:HB3	14:E:337:VAL:HG23	1.95	0.48
69:AV:68:SER:N	77:AA:1523:A:H5''	2.27	0.48
69:AV:114:ARG:HA	69:AV:117:LEU:HD12	1.93	0.48
84:f:91:LEU:HB2	84:f:159:ILE:HG13	1.94	0.48
84:f:171:LEU:HD13	84:f:174:ILE:HD11	1.94	0.48
85:p:57:THR:HA	85:p:60:ARG:HE	1.78	0.48
6:5:113:LEU:HD12	6:5:311:ALA:HB1	1.96	0.48
15:F:138:HIS:CD2	15:F:146:TRP:HE1	2.31	0.48
18:J:90:PHE:HB3	18:J:120:ILE:HG12	1.94	0.48
66:AS:104:THR:O	66:AS:108:LYS:HG2	2.14	0.48
77:AA:1399:A:H2'	77:AA:1400:U:C6	2.48	0.48
90:Ax:69:C:H2'	90:Ax:70:C:C6	2.48	0.48
16:H:171:ARG:HG3	16:H:234:PRO:HB2	1.96	0.48
34:z:198:VAL:HB	34:z:230:ILE:HG23	1.94	0.48
35:G:132:VAL:HB	35:G:195:VAL:HG11	1.95	0.48
77:AA:1066:C:H2'	77:AA:1067:A:C8	2.49	0.48
77:AA:1174:U:H2'	77:AA:1175:G:C8	2.48	0.48
77:AA:1177:C:H2'	77:AA:1178:G:H8	1.78	0.48
6:5:354:PHE:HB3	6:5:417:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3117:C:H2'	11:A:3118:U:H6	1.78	0.48
38:d:152:LEU:HD22	38:d:176:ILE:HD11	1.95	0.48
54:AE:71:PRO:HG2	54:AE:74:ALA:HB2	1.96	0.48
56:AG:390:LYS:HG2	94:AA:1782:SPD:H71	1.95	0.48
61:AM:110:LEU:O	61:AM:114:ARG:HG3	2.14	0.48
77:AA:1033:U:H2'	77:AA:1034:U:C6	2.47	0.48
77:AA:1407:U:H2'	77:AA:1408:A:C8	2.49	0.48
11:A:3142:A:H2'	11:A:3143:U:C6	2.49	0.48
15:F:53:LEU:HD11	15:F:271:ASP:HA	1.96	0.48
29:U:131:GLU:O	29:U:134:ARG:HD3	2.14	0.48
61:AM:96:PHE:HD1	72:A0:169:LEU:HD22	1.78	0.48
63:AO:205:TRP:CZ3	68:AU:55:VAL:HG21	2.48	0.48
67:AT:32:VAL:HG22	67:AT:76:LEU:HD22	1.96	0.48
77:AA:740:G:H2'	77:AA:741:A:C8	2.48	0.48
11:A:1936:A:H4'	11:A:1937:A:N7	2.27	0.48
11:A:2056:G:H2'	11:A:2057:C:H6	1.79	0.48
13:D:184:LEU:HD23	13:D:187:LEU:HD12	1.95	0.48
38:d:85:PHE:HZ	38:d:209:TYR:HB2	1.78	0.48
72:A0:51:PRO:HG3	77:AA:705:C:H5'	1.95	0.48
77:AA:739:C:H2'	77:AA:740:G:O4'	2.14	0.48
12:C:203:LEU:HD13	12:C:230:PHE:HE1	1.79	0.48
61:AM:93:LEU:HD13	65:AR:156:TYR:HE2	1.78	0.48
63:AO:123:LEU:HB3	63:AO:154:ILE:HG13	1.95	0.48
72:A0:99:ARG:HB3	72:A0:115:TRP:HB2	1.96	0.48
77:AA:1469:G:H2'	77:AA:1470:A:H8	1.79	0.48
79:A4:126:LYS:HA	79:A4:129:GLN:HG2	1.96	0.48
90:Ax:27:U:H2'	90:Ax:28:C:C6	2.49	0.48
11:A:1886:G:H1	42:i:61:GLY:HA3	1.78	0.48
11:A:2339:G:H21	11:A:2427:C:H5'	1.79	0.48
11:A:2668:A:H2'	11:A:2669:A:C8	2.49	0.48
11:A:3141:A:H2'	11:A:3142:A:C8	2.49	0.48
14:E:99:LEU:HD22	14:E:193:LEU:HB3	1.96	0.48
17:I:193:ASN:HA	17:I:196:LYS:HG2	1.96	0.48
29:U:110:LEU:HD12	32:Y:118:GLU:HG2	1.95	0.48
56:AG:357:THR:HG23	56:AG:360:GLU:H	1.78	0.48
60:AL:92:LEU:HD13	68:AU:160:LEU:HD11	1.96	0.48
77:AA:968:U:H2'	77:AA:969:A:C8	2.49	0.48
77:AA:1191:C:H2'	77:AA:1192:C:C6	2.49	0.48
79:A4:156:ALA:O	79:A4:160:ARG:HG2	2.13	0.48
11:A:2553:G:H2'	11:A:2554:A:C8	2.48	0.47
34:z:243:ILE:HG23	34:z:255:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:AA:986:G:H2'	77:AA:987:A:H8	1.79	0.47
80:AX:260:VAL:HB	80:AX:306:ILE:HG12	1.96	0.47
91:B:29:C:H2'	91:B:30:A:H8	1.79	0.47
11:A:1862:U:H2'	11:A:1863:A:C8	2.49	0.47
60:AL:209:LEU:HD12	74:A3:189:TRP:CE2	2.49	0.47
62:AN:73:ARG:HH21	77:AA:768:A:H5''	1.79	0.47
77:AA:661:C:H2'	77:AA:662:U:H6	1.79	0.47
77:AA:951:G:H2'	77:AA:952:A:H8	1.80	0.47
2:1:17:LEU:HB2	2:1:65:LEU:HD21	1.96	0.47
11:A:1737:A:H61	11:A:1760:G:H1'	1.79	0.47
11:A:2765:A:H1'	16:H:245:THR:HG22	1.96	0.47
12:C:191:VAL:HG11	12:C:251:LEU:HB3	1.96	0.47
56:AG:393:TRP:CD2	94:AA:1782:SPD:H31	2.49	0.47
69:AV:103:TYR:CZ	77:AA:1524:A:H4'	2.49	0.47
69:AV:322:THR:HG23	69:AV:325:SER:H	1.79	0.47
70:AW:103:ARG:HE	70:AW:139:ARG:HH21	1.61	0.47
77:AA:1056:A:H4'	77:AA:1588:G:N2	2.29	0.47
77:AA:1347:G:H2'	77:AA:1348:G:H8	1.79	0.47
79:A4:350:ARG:HA	79:A4:379:PHE:HE1	1.78	0.47
89:Aw:74:C:H3'	89:Aw:75:C:C6	2.49	0.47
11:A:1829:A:H2'	11:A:1830:G:H8	1.78	0.47
12:C:192:GLU:HA	12:C:227:ARG:HH12	1.79	0.47
17:I:102:VAL:HG22	17:I:174:LEU:HD13	1.96	0.47
69:AV:113:ILE:HD11	69:AV:137:ILE:HG12	1.96	0.47
77:AA:969:A:H2'	77:AA:970:A:C8	2.48	0.47
77:AA:1461:A:H4'	77:AA:1462:G:C8	2.48	0.47
84:f:175:GLN:HA	84:f:178:LEU:HD23	1.96	0.47
6:5:165:GLN:HG2	6:5:166:THR:HG23	1.96	0.47
11:A:1977:U:H2'	11:A:1978:A:H8	1.78	0.47
11:A:2741:A:H1'	11:A:2921:A:H1'	1.96	0.47
53:AD:140:LEU:HD11	53:AD:160:ARG:HE	1.79	0.47
54:AE:30:MET:HE1	68:AU:173:LEU:HD22	1.96	0.47
75:Az:8:U:H2'	75:Az:9:U:C6	2.49	0.47
77:AA:1379:A:H2'	77:AA:1380:G:C8	2.49	0.47
77:AA:1416:A:H2'	77:AA:1417:A:C8	2.49	0.47
77:AA:1495:C:H2'	77:AA:1496:U:C6	2.49	0.47
7:6:175:VAL:HG22	7:6:204:VAL:HG13	1.96	0.47
11:A:3144:A:H2'	11:A:3145:A:H8	1.80	0.47
14:E:50:ASP:HA	14:E:53:LEU:HG	1.96	0.47
38:d:110:GLU:O	38:d:114:LYS:HG2	2.15	0.47
77:AA:1138:G:H2'	77:AA:1139:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:206:TYR:HH	7:6:214:TRP:CD1	2.33	0.47
7:6:341:VAL:HG21	30:W:148:LEU:HD12	1.97	0.47
8:7:286:LEU:HD11	8:7:296:ARG:HB2	1.97	0.47
11:A:1939:G:O2'	11:A:1973:G:H4'	2.15	0.47
35:G:133:ARG:HD3	35:G:171:GLU:HG2	1.95	0.47
39:e:166:GLY:HA3	102:B:101:VAL:HB	1.97	0.47
39:e:272:VAL:HA	39:e:275:PHE:CE2	2.48	0.47
60:AL:126:GLU:HB3	60:AL:181:ILE:HD11	1.96	0.47
69:AV:70:LEU:HD22	69:AV:389:LEU:HG	1.96	0.47
73:A1:171:VAL:HG11	73:A1:219:TYR:HA	1.96	0.47
77:AA:1086:C:H2'	77:AA:1087:A:H8	1.78	0.47
77:AA:1362:G:H2'	77:AA:1363:C:C6	2.48	0.47
77:AA:1400:U:H2'	77:AA:1401:G:C8	2.49	0.47
77:AA:1408:A:H2'	77:AA:1409:A:H8	1.79	0.47
79:A4:517:LYS:HG2	79:A4:522:THR:HG23	1.97	0.47
11:A:2094:G:H2'	11:A:2095:U:H6	1.80	0.47
11:A:2930:U:H2'	11:A:2931:A:C8	2.50	0.47
23:O:52:MET:HE3	23:O:52:MET:HB3	1.79	0.47
53:AD:332:MET:HE3	53:AD:334:ALA:HB2	1.95	0.47
57:AH:72:LEU:HD21	79:A4:59:ILE:HG23	1.96	0.47
77:AA:1086:C:H2'	77:AA:1087:A:C8	2.49	0.47
77:AA:1560:U:H2'	77:AA:1561:C:C6	2.50	0.47
77:AA:1595:G:H2'	77:AA:1596:A:H8	1.80	0.47
79:A4:385:PRO:HB3	79:A4:387:LYS:HE3	1.97	0.47
83:c:79:LEU:HD13	83:c:214:PHE:HE2	1.79	0.47
11:A:1828:A:H4'	11:A:1829:A:C8	2.50	0.47
11:A:2677:A:H2'	11:A:2678:A:C8	2.49	0.47
12:C:207:LEU:HD22	35:G:158:LEU:HD13	1.97	0.47
26:R:91:VAL:HG11	43:j:24:GLY:HA3	1.96	0.47
46:m:55:LEU:HD23	46:m:63:THR:HG21	1.95	0.47
69:AV:148:MET:HE3	69:AV:185:VAL:HG21	1.96	0.47
77:AA:727:U:H2'	77:AA:728:C:O4'	2.15	0.47
77:AA:882:A:N3	77:AA:915:C:HI'	2.30	0.47
77:AA:1005:U:H4'	78:AI:87:HIS:CE1	2.49	0.47
77:AA:1071:U:H2'	77:AA:1072:G:C8	2.49	0.47
77:AA:1348:G:H2'	77:AA:1349:U:C6	2.50	0.47
80:AX:117:PHE:HB3	80:AX:303:GLY:HA2	1.97	0.47
85:p:110:TRP:H	85:p:110:TRP:CD1	2.33	0.47
11:A:2868:C:H2'	11:A:2869:A:O4'	2.15	0.47
55:AF:88:ASP:HB3	55:AF:91:ILE:HB	1.97	0.47
57:AH:155:VAL:HG13	73:A1:126:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
91:B:21:A:H61	91:B:46:A:H2'	1.79	0.47
11:A:1839:C:H2'	11:A:1840:C:C6	2.51	0.46
11:A:2549:C:N4	11:A:2562:U:H2'	2.30	0.46
46:m:69:ARG:HG3	46:m:70:GLU:HG2	1.95	0.46
59:AK:31:ASP:HB3	94:AA:1703:SPD:HN12	1.79	0.46
69:AV:263:MET:HG2	69:AV:341:LEU:HD11	1.96	0.46
77:AA:682:A:H2'	77:AA:683:G:C8	2.51	0.46
77:AA:686:A:H2'	77:AA:687:G:H8	1.79	0.46
77:AA:909:G:H2'	77:AA:910:A:H8	1.81	0.46
77:AA:1165:C:H2'	77:AA:1166:A:C8	2.49	0.46
11:A:3115:U:H2'	11:A:3116:C:C6	2.50	0.46
21:M:156:VAL:O	21:M:176:THR:HA	2.15	0.46
25:Q:201:ASP:HB3	25:Q:204:MET:HB3	1.97	0.46
77:AA:798:C:H2'	77:AA:799:A:C8	2.50	0.46
90:Ax:67:U:H2'	90:Ax:68:C:C6	2.51	0.46
11:A:3151:A:H4'	25:Q:146:GLY:O	2.15	0.46
38:d:269:TRP:CD1	38:d:269:TRP:H	2.33	0.46
49:q:184:LYS:O	49:q:188:LYS:HG2	2.15	0.46
35:t:85:LEU:HD23	35:u:68:VAL:HG21	1.97	0.46
77:AA:821:U:H2'	77:AA:822:G:H8	1.79	0.46
90:Ax:63:U:H2'	90:Ax:64:C:C6	2.51	0.46
11:A:1806:U:H4'	11:A:1807:U:H5'	1.98	0.46
11:A:1974:A:H5'	13:D:261:GLY:HA2	1.96	0.46
12:C:265:LYS:HB3	12:C:297:GLU:HB2	1.98	0.46
13:D:207:ILE:HG12	13:D:229:PRO:HD3	1.97	0.46
30:W:67:ILE:HG21	30:W:131:VAL:HG21	1.98	0.46
69:AV:99:PRO:HG3	72:A0:104:TYR:CZ	2.51	0.46
69:AV:228:TYR:HB3	69:AV:259:ALA:HB2	1.96	0.46
77:AA:738:A:H3'	77:AA:739:C:C6	2.51	0.46
77:AA:1148:A:H2'	77:AA:1149:G:C8	2.51	0.46
77:AA:1561:C:H2'	77:AA:1562:G:C8	2.51	0.46
79:A4:626:GLN:O	79:A4:630:VAL:HG23	2.15	0.46
80:AX:245:LYS:HD2	101:AX:503:GDP:H5'	1.96	0.46
11:A:2930:U:H2'	11:A:2931:A:H8	1.81	0.46
12:C:110:GLU:HA	12:C:113:ARG:HD3	1.97	0.46
12:C:136:LEU:HG	12:C:138:TYR:CE2	2.51	0.46
39:e:192:LEU:HA	39:e:195:LEU:HD23	1.97	0.46
40:g:109:VAL:HG13	40:g:146:THR:HG23	1.98	0.46
51:AB:180:ARG:HH21	53:AD:210:PRO:HB2	1.81	0.46
55:AF:240:ARG:HG3	55:AF:242:TRP:H	1.79	0.46
77:AA:682:A:H2'	77:AA:683:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:AA:1552:G:H2'	77:AA:1553:A:H8	1.79	0.46
79:A4:266:MET:HB3	79:A4:275:ALA:HB2	1.98	0.46
80:AX:56:PRO:HG3	80:AX:143:HIS:CG	2.51	0.46
80:AX:371:ALA:HB2	80:AX:398:LEU:HD21	1.96	0.46
88:a:92:LEU:HD23	88:a:95:ARG:HD2	1.96	0.46
6:5:333:ALA:HB1	6:5:363:ASP:HA	1.97	0.46
7:6:237:LEU:HD12	7:6:245:VAL:HG22	1.96	0.46
11:A:2757:A:H2'	11:A:2758:G:O4'	2.16	0.46
11:A:3115:U:H2'	11:A:3116:C:H6	1.81	0.46
19:K:67:PHE:HB3	19:K:71:LYS:HB2	1.97	0.46
27:S:183:LYS:HE2	27:S:185:ILE:HD11	1.97	0.46
33:Z:73:LYS:HB3	33:Z:116:LEU:HA	1.96	0.46
57:AH:101:GLU:HG3	73:A1:123:CYS:SG	2.56	0.46
58:AJ:55:ARG:HD3	58:AJ:58:LEU:HD21	1.96	0.46
73:A1:60:MET:HG2	79:A4:83:THR:HG21	1.97	0.46
74:A3:177:TRP:CD1	74:A3:178:LEU:HD12	2.51	0.46
77:AA:833:A:H2'	77:AA:834:G:H8	1.81	0.46
77:AA:871:A:H4'	77:AA:872:G:H5'	1.97	0.46
77:AA:1376:C:H4'	77:AA:1377:C:H5'	1.95	0.46
79:A4:462:PHE:HE2	79:A4:482:ILE:HG12	1.81	0.46
9:8:99:ARG:HG2	39:e:83:LEU:HB3	1.98	0.46
12:C:193:VAL:HG12	12:C:230:PHE:HE2	1.81	0.46
17:I:203:VAL:HA	17:I:206:GLU:HB2	1.97	0.46
23:O:44:ALA:HB3	23:O:49:VAL:HG23	1.98	0.46
39:e:124:TRP:CE2	46:m:72:ARG:HG2	2.51	0.46
51:AB:222:ILE:HD13	51:AB:236:VAL:HB	1.97	0.46
58:AJ:75:SER:HB3	77:AA:890:C:H1'	1.98	0.46
65:AR:172:ILE:HD12	65:AR:189:ARG:HG2	1.97	0.46
66:AS:89:ASN:HB3	66:AS:92:PHE:HB2	1.96	0.46
69:AV:205:GLY:HA2	69:AV:208:LEU:HD12	1.97	0.46
72:A0:11:ILE:HB	77:AA:806:C:C2	2.51	0.46
77:AA:716:U:H2'	77:AA:717:G:C8	2.51	0.46
77:AA:958:C:H4'	77:AA:959:C:O4'	2.16	0.46
11:A:2127:A:H4'	11:A:2251:A:C5	2.51	0.46
11:A:2748:A:H2'	11:A:2749:A:H8	1.81	0.46
12:C:99:PRO:HB3	12:C:109:LEU:HD12	1.97	0.46
69:AV:276:CYS:HA	69:AV:348:GLU:HB3	1.98	0.46
77:AA:1412:G:H2'	77:AA:1413:U:O4'	2.16	0.46
79:A4:316:ILE:HA	79:A4:319:LEU:HD12	1.98	0.46
12:C:110:GLU:HA	12:C:113:ARG:HH11	1.79	0.46
39:e:213:TYR:CE2	39:e:215:PHE:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AL:175:TYR:HB2	62:AN:89:GLY:HA3	1.97	0.46
77:AA:840:A:H2'	77:AA:841:A:C8	2.51	0.46
77:AA:877:G:H2'	77:AA:878:G:C8	2.51	0.46
77:AA:1485:G:H2'	77:AA:1486:B8T:O4'	2.16	0.46
77:AA:1592:U:H2'	77:AA:1593:U:C6	2.51	0.46
8:7:156:ARG:HH12	8:7:260:PHE:HB2	1.80	0.46
17:I:79:ILE:HG23	17:I:130:VAL:HG12	1.98	0.46
22:N:78:GLU:HG3	22:N:158:ARG:HH12	1.81	0.46
69:AV:246:ASN:HB2	72:A0:70:ARG:HH12	1.80	0.46
71:AZ:4:LEU:HB3	71:AZ:8:ALA:HB3	1.98	0.46
77:AA:1470:A:H2'	77:AA:1471:A:C8	2.50	0.46
79:A4:628:ILE:HD12	79:A4:631:VAL:HB	1.98	0.46
11:A:2049:U:H2'	11:A:2050:A:H8	1.81	0.45
11:A:2457:A:H3'	23:O:10:SER:HB2	1.98	0.45
11:A:2740:A:H2'	11:A:2741:A:H8	1.80	0.45
60:AL:86:ASP:HB3	60:AL:89:VAL:HG23	1.98	0.45
77:AA:853:C:H2'	77:AA:854:U:C6	2.51	0.45
77:AA:1439:A:H2'	77:AA:1440:G:H8	1.81	0.45
77:AA:1595:G:H2'	77:AA:1596:A:C8	2.51	0.45
89:Aw:66:U:H2'	89:Aw:67:U:C6	2.51	0.45
11:A:2598:A:H3'	11:A:2625:C:H42	1.80	0.45
77:AA:1006:U:H2'	77:AA:1007:G:C8	2.51	0.45
77:AA:1439:A:H2'	77:AA:1440:G:C8	2.51	0.45
77:AA:1464:G:H2'	77:AA:1465:C:C6	2.51	0.45
77:AA:1488:5MC:H2'	77:AA:1489:G:C8	2.50	0.45
9:8:48:GLU:HG3	75:Az:7:G:C8	2.52	0.45
11:A:2718:C:H2'	11:A:2991:U:H4'	1.98	0.45
11:A:2751:G:H2'	11:A:2752:C:C6	2.51	0.45
49:q:164:LEU:HD22	49:q:168:VAL:HG21	1.98	0.45
69:AV:163:VAL:O	69:AV:167:VAL:HG23	2.17	0.45
72:A0:167:PRO:HG2	72:A0:170:LEU:HB2	1.98	0.45
77:AA:672:A:H2'	77:AA:673:U:H6	1.80	0.45
77:AA:854:U:H2'	77:AA:855:A:C8	2.52	0.45
77:AA:1552:G:H2'	77:AA:1553:A:C8	2.51	0.45
79:A4:65:TRP:HD1	79:A4:66:ASP:O	1.99	0.45
89:Aw:36:C:H3'	89:Aw:37:A:H8	1.80	0.45
90:Ax:66:U:H2'	90:Ax:67:U:C6	2.52	0.45
11:A:2006:C:H2'	11:A:2007:U:H6	1.81	0.45
12:C:207:LEU:HG	12:C:218:VAL:HG21	1.99	0.45
46:m:54:VAL:HG11	46:m:68:TYR:HB3	1.99	0.45
72:A0:64:LEU:HD13	72:A0:134:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:AA:1195:U:H2'	77:AA:1196:A:C8	2.51	0.45
77:AA:1408:A:H2'	77:AA:1409:A:C8	2.51	0.45
79:A4:416:PHE:HB3	79:A4:457:TYR:CE2	2.52	0.45
80:AX:60:GLY:H	80:AX:63:HIS:HD2	1.64	0.45
90:Ax:51:A:H2'	90:Ax:52:G:C8	2.52	0.45
11:A:2111:C:H2'	11:A:2112:A:C8	2.52	0.45
16:H:193:PHE:HD1	16:H:197:LEU:HD12	1.82	0.45
34:z:293:ALA:O	34:z:304:LEU:HA	2.16	0.45
63:AO:183:ALA:HA	65:AR:183:LYS:HE2	1.99	0.45
63:AO:187:THR:HG21	65:AR:142:LEU:HD13	1.99	0.45
77:AA:852:A:H3'	77:AA:853:C:H6	1.81	0.45
77:AA:1085:C:H2'	77:AA:1086:C:H6	1.81	0.45
77:AA:1495:C:H2'	77:AA:1496:U:H6	1.81	0.45
77:AA:1577:U:H2'	77:AA:1578:A:H8	1.80	0.45
70:AW:88:PRO:HA	70:AW:91:GLN:HG2	1.99	0.45
72:A0:82:ARG:HB2	72:A0:85:TRP:CD2	2.51	0.45
77:AA:845:A:H2'	77:AA:846:A:C8	2.52	0.45
77:AA:862:A:H2'	77:AA:863:C:C6	2.51	0.45
77:AA:871:A:O3'	77:AA:872:G:H8	1.99	0.45
77:AA:980:U:H2'	77:AA:981:C:C6	2.52	0.45
77:AA:1452:U:H2'	77:AA:1453:A:C8	2.50	0.45
7:6:273:PHE:HB3	7:6:311:MET:HG2	1.99	0.45
11:A:2699:C:H2'	11:A:2700:G:H8	1.81	0.45
33:Z:70:THR:HG22	33:Z:97:PRO:HA	1.97	0.45
34:z:201:PRO:HA	34:z:204:MET:HB2	1.99	0.45
35:G:172:ILE:HG22	35:G:173:LYS:HG2	1.99	0.45
49:q:195:GLN:HB3	49:q:199:LYS:HZ1	1.81	0.45
53:AD:225:VAL:HG22	53:AD:243:VAL:HG22	1.98	0.45
58:AJ:94:PHE:CZ	58:AJ:96:PRO:HB3	2.52	0.45
77:AA:927:G:H2'	77:AA:928:A:C8	2.52	0.45
77:AA:1209:C:H2'	77:AA:1210:U:H6	1.82	0.45
7:6:161:LEU:HD23	7:6:300:THR:HG21	1.98	0.45
11:A:1829:A:H2'	11:A:1830:G:C8	2.51	0.45
11:A:2053:U:HO2'	11:A:2054:U:H6	1.62	0.45
18:J:88:SER:HA	18:J:151:LEU:HD11	1.98	0.45
21:M:274:VAL:HG11	49:q:75:LEU:HD13	1.99	0.45
34:z:99:VAL:HG22	34:z:305:LEU:HD13	1.98	0.45
59:AK:33:ARG:NE	77:AA:1236:C:H5''	2.32	0.45
59:AK:86:ARG:HG2	77:AA:1233:C:O2	2.17	0.45
69:AV:175:VAL:HG12	69:AV:177:SER:H	1.82	0.45
73:A1:320:LEU:HB2	73:A1:322:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:AY:384:LYS:HA	76:AY:387:LEU:HB2	1.99	0.45
77:AA:848:U:H2'	77:AA:849:U:C6	2.52	0.45
77:AA:1174:U:H2'	77:AA:1175:G:H8	1.81	0.45
77:AA:1397:U:H2'	77:AA:1398:U:C6	2.52	0.45
79:A4:352:PRO:O	79:A4:355:GLN:HG3	2.17	0.45
79:A4:377:ARG:NH2	79:A4:418:SER:HA	2.31	0.45
80:AX:152:ILE:HG23	80:AX:259:LEU:HD23	1.99	0.45
11:A:1750:G:H2'	11:A:1751:A:C8	2.51	0.45
11:A:1851:G:H2'	11:A:2693:A:N7	2.31	0.45
11:A:2747:U:H2'	11:A:2748:A:H8	1.81	0.45
16:H:174:VAL:HG12	16:H:192:HIS:HB3	1.97	0.45
71:AZ:56:HIS:O	71:AZ:60:GLU:HG3	2.17	0.45
77:AA:732:A:H2'	77:AA:733:U:C6	2.51	0.45
88:a:103:LEU:HD12	88:a:107:PRO:HB2	1.99	0.45
89:Aw:26:U:H2'	89:Aw:27:A:H8	1.82	0.45
10:9:130:LEU:HD13	32:Y:154:ARG:HA	1.98	0.45
11:A:2099:U:H2'	11:A:2100:C:H6	1.78	0.45
11:A:3124:U:H2'	11:A:3125:A:H8	1.82	0.45
11:A:3150:U:C2	11:A:3151:A:C8	3.05	0.45
29:U:27:GLN:HG3	29:U:43:ARG:HB2	1.99	0.45
36:V:147:SER:HB3	36:V:154:ILE:HD11	1.99	0.45
57:AH:135:GLU:HG3	59:AK:124:GLN:HG3	1.98	0.45
79:A4:295:ASN:HB3	79:A4:337:THR:HG21	1.99	0.45
61:AM:20:ARG:HB2	77:AA:839:A:H5''	1.98	0.44
12:C:107:ASN:O	12:C:110:GLU:HG3	2.16	0.44
39:e:159:LEU:HD12	39:e:254:TRP:CZ2	2.52	0.44
68:AU:66:THR:HG22	72:A0:164:VAL:HG21	2.00	0.44
77:AA:658:G:H2'	77:AA:659:U:H6	1.81	0.44
77:AA:746:A:H2'	77:AA:747:A:H8	1.82	0.44
83:c:228:LEU:HB2	83:c:307:PHE:CD2	2.51	0.44
90:Ax:5:G:H2'	90:Ax:6:A:H8	1.83	0.44
11:A:3038:U:H2'	11:A:3039:OMU:H6	1.99	0.44
35:G:130:PHE:HE2	35:G:178:LYS:HD2	1.82	0.44
57:AH:163:ASN:HB3	73:A1:114:LEU:HD11	1.99	0.44
58:AJ:51:PRO:HG3	58:AJ:122:LYS:HB3	2.00	0.44
77:AA:877:G:H2'	77:AA:878:G:H8	1.81	0.44
77:AA:981:C:H2'	77:AA:982:A:H8	1.81	0.44
77:AA:1006:U:H2'	77:AA:1007:G:H8	1.82	0.44
77:AA:1071:U:H2'	77:AA:1072:G:H8	1.80	0.44
77:AA:1496:U:H2'	77:AA:1497:C:C6	2.52	0.44
86:s:65:ARG:O	86:s:69:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:Ax:64:C:H2'	90:Ax:65:C:C6	2.52	0.44
91:B:43:G:H2'	91:B:44:A:C8	2.51	0.44
6:5:167:THR:HG21	86:s:281:HIS:CE1	2.53	0.44
11:A:2586:U:H2'	11:A:2587:G:C8	2.48	0.44
17:I:141:GLN:HG3	35:t:47:ALA:HB2	2.00	0.44
36:V:117:HIS:CE1	36:V:118:ARG:HG2	2.52	0.44
39:e:213:TYR:HD1	39:e:271:GLN:HG2	1.81	0.44
45:l:111:ASP:HB3	45:l:114:SER:HB3	1.99	0.44
77:AA:952:A:H2'	77:AA:953:U:C6	2.52	0.44
77:AA:980:U:H2'	77:AA:981:C:H6	1.81	0.44
80:AX:85:PRO:HA	80:AX:88:VAL:HG12	1.99	0.44
11:A:2728:C:H2'	11:A:2729:U:H6	1.81	0.44
43:j:88:LEU:HD23	43:j:88:LEU:HA	1.86	0.44
46:m:58:LYS:HZ1	46:m:64:ILE:HG23	1.83	0.44
52:AC:100:PHE:HB3	52:AC:103:CYS:HB2	1.99	0.44
61:AM:104:ILE:HG23	65:AR:147:ILE:HG12	2.00	0.44
69:AV:243:VAL:HG11	69:AV:255:TYR:CE2	2.53	0.44
73:A1:157:VAL:HG13	76:AY:315:ILE:HG13	1.98	0.44
77:AA:726:C:H2'	77:AA:727:U:C6	2.52	0.44
11:A:3158:A:H2'	11:A:3159:A:C8	2.52	0.44
34:z:293:ALA:HB3	34:z:305:LEU:HB2	1.98	0.44
52:AC:96:MET:HB2	52:AC:108:LEU:HD11	2.00	0.44
72:A0:91:GLU:HB2	72:A0:121:LYS:HA	1.99	0.44
77:AA:1450:C:H2'	77:AA:1451:U:C6	2.53	0.44
77:AA:1462:G:H2'	77:AA:1463:G:H8	1.83	0.44
89:Aw:62:C:H2'	89:Aw:63:A:H8	1.82	0.44
12:C:102:ASN:HB3	12:C:105:LEU:HB3	1.98	0.44
12:C:138:TYR:OH	12:C:161:GLN:HB2	2.18	0.44
18:J:56:ARG:HD3	18:J:80:ILE:HD11	2.00	0.44
35:G:132:VAL:HG12	35:G:197:LEU:HB3	1.98	0.44
35:u:85:LEU:HA	35:u:88:LYS:HG2	2.00	0.44
77:AA:1407:U:H2'	77:AA:1408:A:H8	1.83	0.44
80:AX:145:CYS:HB3	80:AX:150:TRP:HB2	1.99	0.44
80:AX:366:LEU:HD22	80:AX:398:LEU:HD22	2.00	0.44
90:Ax:55:U:H1'	90:Ax:58:A:N6	2.33	0.44
90:Ax:71:U:H2'	90:Ax:72:A:C8	2.52	0.44
12:C:268:LEU:HB3	12:C:272:ASP:HB2	1.98	0.44
49:q:187:ARG:HG2	90:Ax:53:G:OP1	2.17	0.44
56:AG:165:VAL:HG11	56:AG:224:LEU:HB3	1.99	0.44
58:AJ:95:ILE:HA	58:AJ:125:VAL:HB	2.00	0.44
63:AO:143:CYS:HB2	63:AO:146:GLN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AR:155:LYS:HB3	65:AR:177:PRO:HD3	1.99	0.44
69:AV:263:MET:HE1	69:AV:334:PHE:HD1	1.83	0.44
79:A4:471:ILE:HG12	79:A4:505:ARG:HG3	2.00	0.44
9:8:92:LEU:O	9:8:95:LEU:HG	2.18	0.44
11:A:2682:A:H4'	26:R:41:LEU:HD13	1.99	0.44
11:A:2812:U:H2'	11:A:2813:U:O4'	2.18	0.44
49:q:188:LYS:O	49:q:191:LYS:HG2	2.18	0.44
53:AD:114:ARG:HD3	77:AA:1326:A:C8	2.53	0.44
72:A0:171:ARG:O	72:A0:175:ILE:HG12	2.18	0.44
77:AA:822:G:H2'	77:AA:823:A:C8	2.53	0.44
77:AA:1080:A:H1'	77:AA:1082:A:N7	2.33	0.44
77:AA:1089:U:H2'	77:AA:1090:A:C8	2.52	0.44
77:AA:1161:A:H2'	77:AA:1162:A:H8	1.83	0.44
80:AX:56:PRO:HA	80:AX:59:HIS:ND1	2.33	0.44
80:AX:199:LEU:HD23	80:AX:223:GLY:HA2	1.98	0.44
39:e:213:TYR:HE2	91:B:76:A:N7	2.15	0.43
51:AB:148:ASN:HD22	51:AB:197:HIS:CD2	2.36	0.43
63:AO:82:LYS:HB3	77:AA:881:A:N6	2.32	0.43
69:AV:389:LEU:O	69:AV:392:ARG:HG2	2.18	0.43
77:AA:824:U:H2'	77:AA:825:U:C6	2.53	0.43
77:AA:1553:A:H2'	77:AA:1554:G:C8	2.53	0.43
79:A4:164:ARG:HA	79:A4:194:LEU:HD11	1.99	0.43
89:Aw:5:A:H2'	89:Aw:6:U:C6	2.53	0.43
5:4:96:PRO:HB2	11:A:3014:G:H5''	1.99	0.43
16:H:247:ARG:HG2	16:H:251:TRP:HE1	1.84	0.43
38:d:54:LYS:HE3	38:d:54:LYS:HB3	1.90	0.43
39:e:165:PHE:O	102:B:101:VAL:N	2.51	0.43
51:AB:203:PHE:HE1	70:AW:163:LEU:HD11	1.82	0.43
67:AT:102:ILE:HA	67:AT:105:ILE:HG12	2.00	0.43
69:AV:40:TRP:HE1	69:AV:111:THR:HG23	1.83	0.43
77:AA:726:C:H2'	77:AA:727:U:H6	1.83	0.43
77:AA:1209:C:H2'	77:AA:1210:U:C6	2.53	0.43
77:AA:1328:G:H2'	77:AA:1329:U:C6	2.53	0.43
79:A4:628:ILE:HD13	79:A4:650:MET:HE1	1.99	0.43
11:A:2697:G:H5'	94:A:3302:SPD:H31	1.99	0.43
11:A:2748:A:H2'	11:A:2749:A:C8	2.53	0.43
17:I:186:LEU:HA	35:t:51:ALA:HB2	2.00	0.43
49:q:138:GLN:O	49:q:141:GLU:HG3	2.18	0.43
52:AC:58:ALA:HB3	52:AC:60:HIS:CE1	2.53	0.43
56:AG:293:ILE:HB	56:AG:300:TYR:HB3	2.00	0.43
77:AA:1181:G:H2'	77:AA:1182:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:106:ARG:HG2	24:P:110:TRP:CE2	2.53	0.43
11:A:2455:U:H5'	23:O:47:ALA:HB3	1.99	0.43
11:A:3144:A:H2'	11:A:3145:A:C8	2.53	0.43
14:E:311:GLY:HA2	14:E:314:LEU:HD12	2.00	0.43
38:d:90:PRO:HB3	38:d:245:TYR:CE2	2.53	0.43
39:e:165:PHE:CE2	91:B:76:A:C2	3.06	0.43
57:AH:70:ASP:HA	79:A4:62:LYS:HE2	2.00	0.43
57:AH:137:ARG:HG3	59:AK:124:GLN:NE2	2.34	0.43
77:AA:1148:A:H2'	77:AA:1149:G:H8	1.83	0.43
77:AA:1162:A:H2'	77:AA:1163:C:C6	2.53	0.43
79:A4:298:ILE:HD13	79:A4:338:ILE:HG13	2.00	0.43
83:c:289:VAL:HG11	88:a:75:ILE:HG23	2.00	0.43
86:s:316:CYS:HB3	86:s:319:GLN:HB2	2.00	0.43
9:8:99:ARG:HE	39:e:89:LEU:HD11	1.82	0.43
9:8:191:ARG:HG2	84:f:135:LEU:HD21	2.00	0.43
11:A:2277:U:H2'	11:A:2278:A:H8	1.82	0.43
11:A:2776:G:H2'	11:A:2777:G:H8	1.83	0.43
15:F:82:LEU:HB3	15:F:87:PHE:CD2	2.53	0.43
19:K:20:LEU:HD22	19:K:141:LEU:HD13	2.00	0.43
27:S:143:LEU:HD22	27:S:204:LEU:HD21	2.00	0.43
53:AD:128:ARG:HD2	75:Az:18:A:C6	2.54	0.43
64:AP:65:CYS:SG	64:AP:100:CYS:HB3	2.58	0.43
75:Az:10:G:H5'	75:Az:11:U:OP2	2.19	0.43
77:AA:915:C:H2'	77:AA:916:C:C6	2.54	0.43
77:AA:998:A:H2'	77:AA:999:C:C6	2.53	0.43
77:AA:1353:A:H5'	77:AA:1354:A:H5'	2.01	0.43
77:AA:1506:U:H2'	77:AA:1507:A:C8	2.54	0.43
77:AA:1506:U:H2'	77:AA:1507:A:H8	1.83	0.43
77:AA:1542:U:H2'	77:AA:1543:U:C6	2.54	0.43
79:A4:308:LYS:HE3	79:A4:310:GLU:HB2	2.00	0.43
79:A4:440:LYS:HA	79:A4:440:LYS:HD2	1.88	0.43
79:A4:606:PRO:HG3	79:A4:611:LEU:HD21	2.00	0.43
80:AX:238:ASP:HB3	101:AX:503:GDP:HN22	1.82	0.43
20:L:32:ILE:HD11	20:L:103:ASN:HB3	1.99	0.43
35:u:75:THR:O	35:u:79:ILE:HG13	2.19	0.43
51:AB:223:VAL:HG11	51:AB:229:PRO:HB3	1.99	0.43
58:AJ:78:ARG:NH2	77:AA:894:C:H41	2.17	0.43
77:AA:1181:G:H2'	77:AA:1182:C:H6	1.82	0.43
77:AA:1440:G:H2'	77:AA:1441:A:H8	1.82	0.43
89:Aw:11:U:H2'	89:Aw:12:U:C6	2.54	0.43
90:Ax:63:U:H2'	90:Ax:64:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1975:U:H2'	11:A:1976:U:C6	2.54	0.43
11:A:2803:A:H2'	11:A:2804:A:O4'	2.18	0.43
11:A:3000:A:H2'	11:A:3001:G:C8	2.54	0.43
11:A:3139:G:H2'	11:A:3140:A:C8	2.53	0.43
18:J:82:ILE:HD12	18:J:82:ILE:HA	1.80	0.43
18:J:114:LEU:HD13	45:I:96:LEU:HD23	1.99	0.43
39:e:165:PHE:HE2	91:B:76:A:C2	2.36	0.43
54:AE:35:ILE:HD11	60:AL:91:ARG:HE	1.84	0.43
58:AJ:59:LYS:HE2	58:AJ:130:TYR:CZ	2.54	0.43
68:AU:61:GLN:HE21	72:A0:198:MET:HE1	1.83	0.43
77:AA:1161:A:H2'	77:AA:1162:A:C8	2.54	0.43
77:AA:1200:G:C2	77:AA:1201:A:C8	3.06	0.43
77:AA:1394:C:H2'	77:AA:1395:C:H6	1.84	0.43
79:A4:600:ARG:HA	79:A4:637:PHE:HZ	1.84	0.43
80:AX:244:LEU:HD22	80:AX:296:MET:HG3	1.99	0.43
3:2:92:HIS:HE2	11:A:1789:A:H5''	1.84	0.43
5:4:69:LYS:HB2	5:4:72:LEU:HD23	1.99	0.43
11:A:1911:C:H2'	11:A:1912:A:H8	1.82	0.43
11:A:2275:U:H2'	11:A:2276:C:C6	2.53	0.43
38:d:121:SER:O	38:d:125:ILE:HG13	2.18	0.43
39:e:198:ASN:HB3	39:e:243:PHE:CE1	2.54	0.43
54:AE:6:LEU:HD21	54:AE:8:LEU:HD13	2.00	0.43
66:AS:67:GLU:HB2	66:AS:100:VAL:HG11	2.01	0.43
73:A1:289:ILE:HD12	73:A1:319:LEU:HD11	2.01	0.43
77:AA:1156:C:H2'	77:AA:1157:U:C6	2.54	0.43
87:OX:427:LYS:HD2	87:OX:427:LYS:HA	1.86	0.43
90:Ax:50:G:H2'	90:Ax:51:A:C8	2.53	0.43
8:7:152:CYS:HB2	8:7:260:PHE:CD2	2.54	0.43
11:A:2461:A:H2'	11:A:2462:A:H8	1.84	0.43
16:H:244:LYS:HA	16:H:247:ARG:HH21	1.83	0.43
21:M:13:LEU:HD23	21:M:13:LEU:HA	1.80	0.43
34:z:292:ARG:HD2	34:z:304:LEU:HD13	2.01	0.43
57:AH:76:LEU:HB2	57:AH:145:LEU:HD12	2.01	0.43
63:AO:82:LYS:HD3	77:AA:881:A:H61	1.84	0.43
65:AR:271:MET:HE2	65:AR:271:MET:HB3	1.88	0.43
69:AV:225:LEU:HD13	69:AV:275:LEU:HD21	2.01	0.43
73:A1:299:LEU:HD23	73:A1:299:LEU:HA	1.83	0.43
77:AA:818:C:C2	77:AA:819:A:C8	3.07	0.43
77:AA:1373:U:H2'	77:AA:1374:A:C8	2.53	0.43
90:Ax:51:A:H2'	90:Ax:52:G:H8	1.83	0.43
6:5:289:HIS:O	6:5:343:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:254:LEU:HD22	8:7:263:VAL:HG22	2.01	0.43
9:8:117:LEU:HD11	39:e:69:GLU:HB3	2.01	0.43
11:A:2610:U:H2'	11:A:2611:C:C6	2.54	0.43
11:A:2807:U:H2'	11:A:2808:U:C6	2.53	0.43
11:A:2815:OMG:H1'	11:A:2815:OMG:HM23	1.75	0.43
19:K:99:ASP:HB3	19:K:102:ALA:HB2	2.01	0.43
36:V:199:MET:HE2	36:V:199:MET:HB3	1.92	0.43
56:AG:390:LYS:HG2	94:AA:1782:SPD:H92	2.01	0.43
62:AN:57:GLN:HG3	62:AN:84:ILE:HD11	2.01	0.43
76:AY:277:LEU:HD13	79:A4:164:ARG:HH12	1.83	0.43
76:AY:316:ASN:HB3	76:AY:319:ALA:HB2	2.01	0.43
77:AA:660:C:H1'	77:AA:1285:G:H21	1.83	0.43
77:AA:673:U:H2'	77:AA:674:U:H6	1.83	0.43
77:AA:884:U:H2'	77:AA:885:U:C6	2.54	0.43
77:AA:990:U:H2'	77:AA:991:G:O4'	2.19	0.43
79:A4:393:ILE:HA	79:A4:396:ILE:HG22	2.01	0.43
79:A4:545:GLN:HE22	79:A4:582:LEU:HD23	1.84	0.43
80:AX:56:PRO:HD2	80:AX:147:LYS:HG3	2.00	0.43
80:AX:60:GLY:H	80:AX:63:HIS:CD2	2.37	0.43
80:AX:242:ILE:HD11	101:AX:503:GDP:C4	2.54	0.43
91:B:25:C:H2'	91:B:26:A:H8	1.84	0.43
11:A:2584:C:H2'	11:A:2585:G:H8	1.83	0.42
11:A:2805:A:H2'	11:A:2806:U:C6	2.54	0.42
16:H:224:THR:HG23	16:H:230:THR:HG22	2.01	0.42
46:m:43:VAL:HB	84:f:101:THR:HG22	2.01	0.42
60:AL:112:MET:HE3	60:AL:119:PRO:HA	2.01	0.42
65:AR:329:LYS:HD2	65:AR:329:LYS:HA	1.89	0.42
70:AW:130:ASP:HB2	70:AW:133:LYS:HD3	2.01	0.42
77:AA:1078:A:H2'	77:AA:1079:G:C8	2.54	0.42
80:AX:121:ALA:HB1	80:AX:306:ILE:HG13	2.00	0.42
1:0:184:TRP:CD1	1:0:184:TRP:H	2.37	0.42
9:8:51:ARG:O	89:Aw:39:U:H5'	2.19	0.42
11:A:2588:C:H2'	11:A:2589:A:C8	2.53	0.42
11:A:2656:U:H4'	14:E:230:THR:OG1	2.19	0.42
53:AD:310:LYS:HB3	63:AO:130:HIS:ND1	2.34	0.42
6:5:177:CYS:HB3	6:5:178:PRO:HD3	2.01	0.42
11:A:3117:C:H2'	11:A:3118:U:C6	2.54	0.42
14:E:248:ILE:HG13	14:E:250:ARG:H	1.84	0.42
55:AF:172:VAL:HG12	55:AF:240:ARG:HD3	2.01	0.42
57:AH:77:SER:HB2	57:AH:173:THR:HB	2.02	0.42
63:AO:213:LEU:HB3	63:AO:217:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:AA:664:G:H2'	77:AA:665:C:C6	2.54	0.42
79:A4:166:VAL:HG12	79:A4:194:LEU:HG	2.00	0.42
89:Aw:51:U:H3'	89:Aw:52:G:H8	1.84	0.42
89:Aw:54:U:H3'	89:Aw:55:A:C8	2.53	0.42
90:Ax:22:A:H2'	90:Ax:23:A:H8	1.84	0.42
6:5:121:LEU:HD23	6:5:126:THR:HG23	2.02	0.42
11:A:1911:C:H2'	11:A:1912:A:C8	2.55	0.42
34:z:250:GLU:HB3	34:z:252:PHE:CE2	2.54	0.42
36:V:16:PRO:HD2	36:V:19:TYR:HB2	2.02	0.42
49:q:141:GLU:HA	49:q:144:GLU:HG3	2.01	0.42
51:AB:192:LEU:HD11	51:AB:220:VAL:HG23	2.00	0.42
63:AO:105:CYS:HB2	63:AO:142:VAL:HA	2.01	0.42
80:AX:105:ALA:O	80:AX:109:LEU:HG	2.19	0.42
11:A:2215:C:H2'	11:A:2216:A:O4'	2.20	0.42
11:A:2410:U:H2'	11:A:2411:U:C6	2.54	0.42
11:A:2692:G:OP1	48:o:15:ARG:HG3	2.20	0.42
32:Y:176:ILE:HG21	87:OX:430:TRP:CG	2.54	0.42
56:AG:285:VAL:HG22	56:AG:328:VAL:HG22	2.00	0.42
69:AV:340:LYS:HE3	69:AV:340:LYS:HB3	1.73	0.42
73:A1:67:PRO:HG3	73:A1:118:ALA:HB2	2.00	0.42
77:AA:1497:C:H2'	77:AA:1498:C:C6	2.54	0.42
77:AA:1510:U:H2'	77:AA:1511:C:C6	2.55	0.42
11:A:1970:G:H2'	11:A:1971:A:O4'	2.19	0.42
11:A:2275:U:H2'	11:A:2276:C:H6	1.84	0.42
18:J:70:ILE:HG12	18:J:80:ILE:HG22	2.01	0.42
69:AV:165:PHE:HA	69:AV:168:MET:HE3	2.02	0.42
77:AA:927:G:H2'	77:AA:928:A:H8	1.85	0.42
77:AA:983:C:H2'	77:AA:984:C:C6	2.54	0.42
77:AA:1044:U:H2'	77:AA:1045:G:O4'	2.20	0.42
79:A4:646:THR:O	79:A4:650:MET:HG2	2.19	0.42
80:AX:145:CYS:HB2	80:AX:259:LEU:HD22	2.02	0.42
83:c:93:VAL:HG22	83:c:180:LEU:HD12	2.02	0.42
11:A:2661:U:H2'	11:A:2662:A:C8	2.55	0.42
11:A:2847:C:H2'	11:A:2848:A:O4'	2.18	0.42
11:A:3089:A:H3'	11:A:3090:G:C5'	2.50	0.42
17:I:33:VAL:HG13	22:N:244:LYS:HB3	2.01	0.42
31:X:55:LYS:HB2	31:X:55:LYS:HE3	1.81	0.42
49:q:117:ARG:O	49:q:121:ILE:HG12	2.20	0.42
53:AD:100:LYS:HG2	77:AA:1262:C:H4'	2.02	0.42
54:AE:3:ARG:HD3	54:AE:69:TYR:CZ	2.55	0.42
57:AH:65:ILE:HG13	79:A4:63:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AJ:93:CYS:HB2	58:AJ:125:VAL:HG23	2.01	0.42
63:AO:235:MET:SD	65:AR:150:GLY:HA3	2.60	0.42
69:AV:81:SER:HB3	69:AV:84:GLU:HG3	2.02	0.42
77:AA:711:U:H5'	77:AA:712:C:C5	2.55	0.42
77:AA:867:C:H2'	77:AA:870:C:N4	2.34	0.42
77:AA:1007:G:H2'	77:AA:1008:A:H8	1.85	0.42
77:AA:1085:C:H2'	77:AA:1086:C:C6	2.54	0.42
86:s:371:CYS:SG	86:s:394:TRP:HB2	2.60	0.42
11:A:1718:A:H2'	11:A:1719:G:O4'	2.19	0.42
11:A:2053:U:OP2	48:o:79:THR:HG23	2.19	0.42
11:A:2060:A:C8	11:A:2079:C:C4	3.07	0.42
15:F:99:VAL:HG21	15:F:173:GLY:HA3	2.02	0.42
20:L:40:VAL:HG11	20:L:47:GLY:HA3	2.01	0.42
35:G:149:ILE:HG22	35:G:156:ILE:HD11	2.02	0.42
72:A0:136:TYR:CE1	77:AA:705:C:H2'	2.55	0.42
75:Az:21:A:H2'	75:Az:22:A:C4	2.55	0.42
77:AA:1231:A:H1'	77:AA:1236:C:N4	2.34	0.42
11:A:2575:U:H2'	11:A:2581:A:C2	2.55	0.42
12:C:213:ALA:HA	12:C:245:LYS:HE3	2.02	0.42
15:F:65:TRP:CD1	41:h:117:LEU:HD11	2.54	0.42
53:AD:401:VAL:HG21	67:AT:50:PHE:CE1	2.55	0.42
55:AF:228:LYS:HB3	55:AF:228:LYS:HE3	1.80	0.42
77:AA:658:G:H2'	77:AA:659:U:C6	2.55	0.42
79:A4:312:LYS:HD3	79:A4:312:LYS:HA	1.95	0.42
90:Ax:72:A:H3'	90:Ax:73:A:H8	1.85	0.42
7:6:37:ASN:HB3	84:f:62:LEU:HD21	2.02	0.42
19:K:45:PRO:HD2	37:b:130:TRP:CE2	2.54	0.42
50:r:78:LYS:HE2	97:r:201:FES:S2	2.60	0.42
52:AC:69:LEU:HD23	73:A1:107:LYS:HD3	2.01	0.42
57:AH:122:GLN:HG3	77:AA:1265:C:H4'	2.02	0.42
60:AL:209:LEU:HD22	74:A3:173:LEU:HD12	2.02	0.42
69:AV:120:ASP:HA	69:AV:122:GLN:HE22	1.85	0.42
70:AW:103:ARG:HE	70:AW:139:ARG:NH2	2.17	0.42
72:A0:61:GLU:HB3	72:A0:137:HIS:O	2.20	0.42
77:AA:822:G:H2'	77:AA:823:A:H8	1.84	0.42
77:AA:1236:C:H4'	77:AA:1237:A:O4'	2.20	0.42
77:AA:1371:U:H2'	77:AA:1372:C:C6	2.55	0.42
77:AA:1587:U:H2'	77:AA:1588:G:C8	2.42	0.42
79:A4:89:PHE:CE1	79:A4:97:PRO:HG3	2.55	0.42
80:AX:237:THR:HB	80:AX:289:LEU:HD21	2.01	0.42
90:Ax:61:C:H2'	90:Ax:62:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:158:ILE:HD11	6:5:382:LEU:HG	2.01	0.41
11:A:2408:U:H2'	11:A:2409:A:C8	2.54	0.41
11:A:2415:C:H3'	86:s:165:ARG:NH2	2.35	0.41
11:A:2552:U:C2	11:A:2553:G:C8	3.08	0.41
11:A:3044:A:H2'	11:A:3045:A:C8	2.55	0.41
11:A:3076:A:H2'	11:A:3077:C:C6	2.55	0.41
38:d:204:ASN:O	38:d:205:GLN:HG2	2.20	0.41
39:e:269:LEU:HA	39:e:272:VAL:HG12	2.02	0.41
61:AM:100:HIS:HD2	61:AM:102:MET:HB3	1.85	0.41
61:AM:101:PRO:HD3	68:AU:63:TYR:CG	2.55	0.41
72:A0:163:SER:HB3	72:A0:190:MET:HB3	2.01	0.41
75:Az:29:U:H2'	75:Az:30:A:C4	2.55	0.41
77:AA:663:A:H2'	77:AA:664:G:H8	1.82	0.41
77:AA:1082:A:H2'	77:AA:1083:C:C6	2.54	0.41
77:AA:1138:G:H2'	77:AA:1139:A:C8	2.54	0.41
77:AA:1171:A:H2'	77:AA:1172:C:O4'	2.20	0.41
77:AA:1504:U:H2'	77:AA:1505:A:C8	2.55	0.41
80:AX:82:GLY:HA2	80:AX:156:PRO:HA	2.02	0.41
11:A:2691:U:H2'	11:A:2692:G:C8	2.55	0.41
11:A:3142:A:H2'	11:A:3143:U:H6	1.85	0.41
11:A:3191:A:H4'	50:r:123:HIS:HB3	2.03	0.41
21:M:107:LEU:HD23	21:M:107:LEU:HA	1.91	0.41
22:N:101:HIS:CD2	22:N:184:PRO:HD3	2.55	0.41
38:d:93:GLY:HA2	38:d:96:ARG:HB3	2.02	0.41
38:d:201:SER:O	38:d:208:VAL:HG12	2.20	0.41
58:AJ:57:GLN:HB3	58:AJ:109:LEU:HD11	2.02	0.41
65:AR:128:MET:H	65:AR:128:MET:HG2	1.72	0.41
69:AV:263:MET:HE1	69:AV:334:PHE:CD1	2.55	0.41
75:Az:9:U:H2'	75:Az:10:G:O4'	2.20	0.41
77:AA:951:G:H2'	77:AA:952:A:C8	2.55	0.41
78:AI:176:THR:HB	82:AQ:11:THR:HG23	2.01	0.41
79:A4:292:TYR:HA	79:A4:295:ASN:ND2	2.35	0.41
79:A4:584:LEU:HB3	79:A4:613:GLU:OE1	2.19	0.41
83:c:259:ARG:HB2	83:c:271:PHE:HB2	2.01	0.41
84:f:96:THR:HB	84:f:152:THR:HG22	2.02	0.41
89:Aw:21:A:H61	89:Aw:46:A:H2'	1.85	0.41
90:Ax:72:A:H3'	90:Ax:73:A:C8	2.55	0.41
32:Y:202:LEU:HD23	32:Y:202:LEU:HA	1.89	0.41
49:q:188:LYS:HD3	49:q:191:LYS:HE2	2.02	0.41
67:AT:21:VAL:HG22	67:AT:103:ARG:HB2	2.02	0.41
69:AV:287:LEU:HD21	69:AV:331:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:AV:399:GLN:HG2	69:AV:402:GLN:HE21	1.84	0.41
77:AA:1043:C:H2'	77:AA:1044:U:H6	1.84	0.41
78:AI:166:ILE:HD13	78:AI:170:LEU:O	2.20	0.41
79:A4:302:VAL:HG11	79:A4:341:CYS:HB3	2.03	0.41
79:A4:466:CYS:SG	79:A4:496:LEU:HD22	2.60	0.41
2:1:16:ILE:HD11	2:1:34:ARG:CZ	2.49	0.41
12:C:119:LYS:HE2	12:C:119:LYS:HB2	1.77	0.41
12:C:234:CYS:SG	12:C:239:LEU:HA	2.60	0.41
16:H:208:LEU:HB3	16:H:209:PRO:HD2	2.02	0.41
35:G:150:LYS:HD2	35:G:158:LEU:HB3	2.03	0.41
57:AH:179:GLN:HG3	73:A1:147:PHE:CD1	2.55	0.41
77:AA:1012:A:C2	78:AI:185:GLY:HA2	2.52	0.41
79:A4:396:ILE:O	79:A4:399:GLU:HG3	2.20	0.41
86:s:332:LEU:HD23	86:s:332:LEU:HA	1.91	0.41
7:6:139:TRP:CE2	7:6:144:GLY:HA2	2.55	0.41
11:A:2491:C:H2'	11:A:2492:G:C8	2.55	0.41
11:A:3080:G:H2'	11:A:3081:A:H8	1.86	0.41
12:C:163:ASP:HB2	12:C:286:HIS:HE2	1.85	0.41
39:e:184:LEU:HD21	39:e:232:PHE:CG	2.55	0.41
35:u:74:LEU:HD23	35:u:79:ILE:HG12	2.03	0.41
57:AH:130:HIS:CE1	77:AA:1266:A:H5''	2.55	0.41
65:AR:286:ILE:HA	65:AR:289:ILE:HG22	2.02	0.41
77:AA:1191:C:H2'	77:AA:1192:C:H6	1.84	0.41
77:AA:1476:G:H2'	77:AA:1477:U:C6	2.55	0.41
82:AQ:66:MET:HE2	82:AQ:66:MET:HB3	1.95	0.41
6:5:236:LEU:HD23	6:5:236:LEU:HA	1.87	0.41
11:A:3150:U:H2'	11:A:3151:A:C8	2.54	0.41
18:J:20:ILE:HD13	18:J:20:ILE:HA	1.93	0.41
27:S:144:LEU:HB2	88:a:58:ILE:HB	2.03	0.41
34:z:127:LEU:HD22	34:z:290:VAL:HG22	2.03	0.41
35:G:180:GLU:O	35:G:183:LYS:HG3	2.20	0.41
53:AD:355:ARG:NH1	77:AA:1118:A:H4'	2.35	0.41
57:AH:79:LEU:HD11	57:AH:140:TYR:HB3	2.03	0.41
62:AN:12:TRP:HE3	62:AN:65:LEU:HD11	1.84	0.41
67:AT:161:GLY:HA2	67:AT:164:LYS:HB2	2.01	0.41
77:AA:946:U:H2'	77:AA:947:U:C6	2.56	0.41
77:AA:990:U:H3	77:AA:997:A:H61	1.69	0.41
77:AA:1169:G:H2'	77:AA:1170:G:H8	1.85	0.41
83:c:79:LEU:HD13	83:c:214:PHE:CE2	2.55	0.41
86:s:184:LEU:HD23	86:s:184:LEU:HA	1.89	0.41
7:6:199:ALA:HA	7:6:256:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2728:C:H2'	11:A:2729:U:C6	2.56	0.41
11:A:2750:U:H2'	11:A:2751:G:H8	1.85	0.41
12:C:84:LEU:HD11	12:C:117:MET:HE3	2.01	0.41
21:M:73:PRO:HG2	21:M:76:ILE:HB	2.02	0.41
24:P:88:HIS:HB2	91:B:24:G:OP2	2.21	0.41
24:P:130:ARG:HG3	24:P:164:ALA:HB1	2.03	0.41
49:q:174:ARG:HD3	49:q:174:ARG:HA	1.91	0.41
57:AH:181:PRO:O	57:AH:184:ILE:HG22	2.21	0.41
60:AL:67:PRO:HA	60:AL:68:PRO:HD3	1.94	0.41
62:AN:64:VAL:HG12	62:AN:84:ILE:HA	2.02	0.41
65:AR:138:ILE:HD11	65:AR:186:TRP:CE2	2.56	0.41
72:A0:178:ARG:O	72:A0:183:ASP:HB2	2.21	0.41
77:AA:1032:C:H2'	77:AA:1033:U:C6	2.56	0.41
77:AA:1195:U:H2'	77:AA:1196:A:H8	1.85	0.41
77:AA:1359:U:H2'	77:AA:1360:G:H8	1.85	0.41
79:A4:584:LEU:HD23	79:A4:589:THR:HG22	2.02	0.41
11:A:1936:A:H4'	11:A:1937:A:C8	2.55	0.41
11:A:2536:G:H2'	11:A:2537:G:C8	2.56	0.41
12:C:83:LYS:HD3	12:C:83:LYS:HA	1.86	0.41
34:z:150:PHE:HE2	34:z:152:SER:HB3	1.84	0.41
35:G:129:HIS:HA	35:G:176:VAL:O	2.21	0.41
40:g:90:ARG:HG3	40:g:91:MET:SD	2.61	0.41
67:AT:90:VAL:HA	67:AT:93:LYS:HD3	2.02	0.41
75:Az:27:C:C2	75:Az:28:U:H5	2.39	0.41
77:AA:676:G:H2'	77:AA:677:C:C6	2.56	0.41
77:AA:1397:U:H2'	77:AA:1398:U:H6	1.86	0.41
77:AA:1588:G:H2'	77:AA:1589:C:C6	2.56	0.41
84:f:169:ILE:H	84:f:169:ILE:HG12	1.70	0.41
7:6:138:GLU:HG2	24:P:114:LYS:NZ	2.35	0.41
7:6:233:LEU:HB2	7:6:298:PHE:CG	2.56	0.41
8:7:106:ALA:HB3	8:7:113:TRP:HB3	2.02	0.41
9:8:80:GLN:HA	9:8:201:GLN:HE22	1.86	0.41
11:A:1861:U:H2'	11:A:1862:U:C6	2.55	0.41
11:A:2786:U:H2'	11:A:2787:A:C8	2.56	0.41
11:A:3078:C:H2'	11:A:3079:G:H8	1.84	0.41
14:E:120:THR:HG21	14:E:289:VAL:HG22	2.02	0.41
27:S:101:PHE:HE1	43:j:49:TRP:HB3	1.85	0.41
35:G:146:ILE:CG2	35:G:158:LEU:HB2	2.51	0.41
38:d:160:LEU:O	38:d:164:VAL:HG22	2.21	0.41
38:d:266:VAL:HA	38:d:267:PRO:HD3	1.96	0.41
41:h:139:LYS:HA	41:h:139:LYS:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AD:141:TRP:HZ2	71:AZ:68:LEU:HB3	1.86	0.41
53:AD:415:GLN:HG2	67:AT:13:LEU:HD12	2.03	0.41
53:AD:415:GLN:HG2	67:AT:13:LEU:HB2	2.02	0.41
54:AE:42:LEU:HD12	54:AE:63:TYR:HB3	2.03	0.41
58:AJ:78:ARG:HD2	58:AJ:118:LEU:HD23	2.03	0.41
62:AN:17:VAL:HG12	62:AN:60:VAL:HA	2.03	0.41
72:A0:29:ARG:HG3	72:A0:105:THR:HG21	2.03	0.41
73:A1:105:LEU:HD23	73:A1:105:LEU:HA	1.91	0.41
77:AA:1122:A:H2'	77:AA:1123:C:C6	2.56	0.41
77:AA:1380:G:H1'	80:AX:163:LYS:HE2	2.03	0.41
77:AA:1394:C:H2'	77:AA:1395:C:C6	2.55	0.41
77:AA:1456:U:H2'	77:AA:1457:G:O4'	2.21	0.41
79:A4:339:LEU:HD22	79:A4:375:ILE:HD13	2.01	0.41
79:A4:606:PRO:HG3	79:A4:633:LEU:HD23	2.02	0.41
89:Aw:74:C:H3'	89:Aw:75:C:H6	1.85	0.41
90:Ax:54:U:H2'	90:Ax:55:U:O4'	2.21	0.41
8:7:199:LEU:HD21	8:7:283:VAL:HG23	2.03	0.41
9:8:180:PRO:HB3	39:e:153:LEU:HD13	2.03	0.41
11:A:1863:A:H2'	11:A:1864:A:C8	2.56	0.41
11:A:2101:C:H2'	11:A:2102:A:H8	1.85	0.41
11:A:2147:G:OP2	27:S:104:ARG:HD3	2.21	0.41
11:A:2802:A:H2'	11:A:2803:A:O4'	2.21	0.41
13:D:182:HIS:HB2	13:D:187:LEU:HD21	2.03	0.41
18:J:64:ILE:HD13	45:l:77:ILE:HG22	2.03	0.41
27:S:108:VAL:HB	27:S:195:ILE:HG13	2.03	0.41
34:z:184:ILE:HG12	34:z:207:LEU:HD13	2.02	0.41
53:AD:380:LEU:HD12	53:AD:381:PRO:HD2	2.01	0.41
73:A1:269:MET:HG2	80:AX:119:TYR:CG	2.56	0.41
77:AA:917:C:H2'	77:AA:918:A:C8	2.56	0.41
77:AA:1068:A:H5''	78:AI:190:LYS:HD3	2.03	0.41
77:AA:1372:C:H2'	77:AA:1373:U:C6	2.56	0.41
77:AA:1497:C:H2'	77:AA:1498:C:H6	1.85	0.41
77:AA:1560:U:H2'	77:AA:1561:C:H6	1.86	0.41
79:A4:157:LEU:HD11	79:A4:191:LEU:HD22	2.02	0.41
79:A4:307:GLU:HG2	79:A4:312:LYS:HE3	2.03	0.41
79:A4:373:HIS:HB2	79:A4:415:PHE:HA	2.03	0.41
84:f:94:HIS:HB2	84:f:185:SER:HB3	2.02	0.41
89:Aw:28:A:C2'	89:Aw:29:U:H5'	2.51	0.41
11:A:2049:U:H2'	11:A:2050:A:C8	2.55	0.40
21:M:19:LEU:HD13	48:o:95:LEU:HD12	2.04	0.40
34:z:128:ASP:HA	34:z:251:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:230:ARG:HE	38:d:230:ARG:HB2	1.74	0.40
51:AB:84:LEU:HD23	51:AB:248:LEU:HD21	2.02	0.40
63:AO:150:LEU:O	63:AO:154:ILE:HD12	2.21	0.40
67:AT:155:LEU:HD23	67:AT:155:LEU:HA	1.79	0.40
68:AU:57:MET:HE3	68:AU:57:MET:HB3	1.90	0.40
69:AV:82:ARG:HD3	69:AV:119:TYR:O	2.21	0.40
72:A0:116:GLY:N	72:A0:131:ILE:HD11	2.36	0.40
77:AA:667:U:H2'	77:AA:668:U:C6	2.56	0.40
77:AA:715:G:H2'	77:AA:716:U:H6	1.82	0.40
77:AA:1095:U:H2'	77:AA:1096:A:C8	2.56	0.40
4:3:127:ALA:HA	21:M:79:PRO:HD3	2.02	0.40
6:5:55:LEU:HD11	31:X:163:ARG:NE	2.35	0.40
9:8:181:PRO:HB3	46:m:60:ASP:HB2	2.02	0.40
11:A:1800:G:H1'	11:A:1805:A:N6	2.36	0.40
11:A:2109:A:C6	11:A:2946:A:C8	3.10	0.40
11:A:2536:G:H2'	11:A:2537:G:H8	1.86	0.40
12:C:163:ASP:CB	12:C:286:HIS:HE2	2.34	0.40
12:C:210:ALA:HA	12:C:246:LEU:HD12	2.03	0.40
18:J:25:ARG:HH12	45:l:56:LEU:HD23	1.86	0.40
18:J:29:ALA:HB2	18:J:53:PHE:HD2	1.86	0.40
18:J:69:LYS:HB2	18:J:81:LYS:HB2	2.03	0.40
27:S:120:LEU:HB3	27:S:122:LEU:HD12	2.02	0.40
35:G:185:LYS:HD2	35:G:188:LEU:HD11	2.03	0.40
40:g:91:MET:HB2	40:g:93:ASN:HD22	1.86	0.40
58:AJ:38:ARG:HH21	98:AA:1701:NAD:H3D	1.85	0.40
58:AJ:56:PRO:HD2	77:AA:826:A:C6	2.56	0.40
60:AL:206:LYS:HA	74:A3:173:LEU:HD11	2.02	0.40
61:AM:73:ILE:O	61:AM:77:ILE:HG12	2.21	0.40
65:AR:167:HIS:HB3	65:AR:193:ILE:HD13	2.01	0.40
75:Az:25:U:H2'	79:A4:489:HIS:CD2	2.55	0.40
77:AA:1509:U:H2'	77:AA:1510:U:C6	2.55	0.40
8:7:166:LEU:HD22	8:7:181:TYR:HE2	1.86	0.40
11:A:1924:U:H2'	11:A:1925:A:C8	2.57	0.40
11:A:2346:U:H2'	11:A:2347:C:C6	2.56	0.40
11:A:3201:A:H2'	11:A:3202:U:O4'	2.21	0.40
12:C:151:GLU:OE2	12:C:291:HIS:HB3	2.21	0.40
23:O:33:LEU:HD21	23:O:59:LEU:HD22	2.03	0.40
25:Q:87:THR:HG21	25:Q:91:LYS:HD2	2.03	0.40
25:Q:214:LYS:HE2	25:Q:214:LYS:HB2	1.91	0.40
34:z:97:TYR:HA	34:z:304:LEU:O	2.20	0.40
39:e:203:LYS:HB2	39:e:239:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:k:97:ARG:HA	44:k:97:ARG:HD3	1.93	0.40
68:AU:70:LEU:HD21	72:A0:167:PRO:HG3	2.03	0.40
72:A0:82:ARG:HB2	72:A0:85:TRP:CG	2.57	0.40
77:AA:675:A:H2'	77:AA:676:G:H8	1.86	0.40
77:AA:719:G:H2'	77:AA:720:U:O4'	2.21	0.40
77:AA:1203:C:H2'	77:AA:1204:C:H6	1.85	0.40
77:AA:1279:C:H2'	77:AA:1280:C:C6	2.57	0.40
77:AA:1399:A:H2'	77:AA:1400:U:H6	1.85	0.40
77:AA:1500:C:H2'	77:AA:1501:A:O4'	2.22	0.40
79:A4:375:ILE:HD12	79:A4:375:ILE:HA	1.88	0.40
7:6:279:ILE:HB	7:6:281:PHE:CE1	2.57	0.40
11:A:1884:G:H1'	11:A:1895:C:H1'	2.03	0.40
11:A:1938:A:O2'	11:A:1940:A:H5''	2.22	0.40
11:A:2751:G:H2'	11:A:2752:C:H6	1.87	0.40
11:A:3078:C:H2'	11:A:3079:G:C8	2.57	0.40
26:R:90:LEU:HD23	26:R:90:LEU:HA	1.86	0.40
28:T:57:LEU:HB2	28:T:60:GLU:HG3	2.03	0.40
35:G:137:ALA:HB2	35:G:168:LEU:HD12	2.03	0.40
54:AE:37:ARG:HG3	68:AU:167:PHE:CE1	2.57	0.40
61:AM:28:ASN:HB2	67:AT:155:LEU:HD12	2.04	0.40
77:AA:659:U:H1'	77:AA:1286:A:N3	2.36	0.40
77:AA:941:G:C6	77:AA:1109:A:C5	3.09	0.40
77:AA:1047:A:C5	77:AA:1158:U:H4'	2.56	0.40
79:A4:185:LEU:HD21	79:A4:255:ASN:HB3	2.03	0.40
91:B:29:C:C2	91:B:30:A:C8	3.10	0.40
2:1:13:SER:HB2	2:1:36:ARG:HH21	1.86	0.40
6:5:238:THR:HA	6:5:341:VAL:HG21	2.04	0.40
9:8:133:ARG:HA	9:8:136:ILE:HG22	2.04	0.40
11:A:1946:C:H2'	11:A:1947:C:C6	2.57	0.40
11:A:2196:A:O4'	11:A:2214:A:H1'	2.21	0.40
15:F:96:LEU:HD23	15:F:96:LEU:HA	1.96	0.40
17:I:124:LYS:HB2	17:I:153:LEU:HB2	2.04	0.40
22:N:183:LEU:HD23	22:N:183:LEU:HA	1.85	0.40
52:AC:125:ARG:NH1	79:A4:94:TYR:HB2	2.29	0.40
63:AO:213:LEU:HB3	63:AO:217:ARG:NH1	2.37	0.40
69:AV:85:ILE:HG21	69:AV:121:ALA:HB2	2.04	0.40
69:AV:128:THR:HG22	69:AV:135:TYR:CD2	2.55	0.40
70:AW:98:LYS:HA	70:AW:98:LYS:HD3	1.91	0.40
77:AA:911:U:H2'	77:AA:912:U:H6	1.85	0.40
77:AA:1203:C:H2'	77:AA:1204:C:C6	2.56	0.40
77:AA:1571:U:O2'	77:AA:1572:A:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
89:Aw:20:C:N4	89:Aw:56:A:H5'	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	108/188 (57%)	108 (100%)	0	0	100	100
2	1	54/65 (83%)	53 (98%)	1 (2%)	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	386 (98%)	6 (2%)	0	100	100
7	6	352/380 (93%)	344 (98%)	8 (2%)	0	100	100
8	7	292/338 (86%)	284 (97%)	8 (3%)	0	100	100
9	8	155/206 (75%)	149 (96%)	6 (4%)	0	100	100
10	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
12	C	221/297 (74%)	214 (97%)	7 (3%)	0	100	100
13	D	236/305 (77%)	229 (97%)	7 (3%)	0	100	100
14	E	303/348 (87%)	293 (97%)	10 (3%)	0	100	100
15	F	250/311 (80%)	250 (100%)	0	0	100	100
16	H	200/267 (75%)	192 (96%)	8 (4%)	0	100	100
17	I	179/261 (69%)	177 (99%)	2 (1%)	0	100	100
18	J	173/192 (90%)	171 (99%)	2 (1%)	0	100	100
19	K	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
20	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	M	289/296 (98%)	283 (98%)	6 (2%)	0	100	100
22	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
23	O	152/175 (87%)	147 (97%)	5 (3%)	0	100	100
24	P	142/180 (79%)	136 (96%)	6 (4%)	0	100	100
25	Q	224/292 (77%)	219 (98%)	5 (2%)	0	100	100
26	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
27	S	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
28	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
29	U	150/153 (98%)	146 (97%)	4 (3%)	0	100	100
30	W	114/148 (77%)	111 (97%)	3 (3%)	0	100	100
31	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
32	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
33	Z	120/161 (74%)	118 (98%)	2 (2%)	0	100	100
34	z	250/325 (77%)	231 (92%)	19 (8%)	0	100	100
35	G	70/198 (35%)	67 (96%)	3 (4%)	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%)	140 (95%)	8 (5%)	0	100	100
38	d	257/306 (84%)	239 (93%)	18 (7%)	0	100	100
39	e	236/279 (85%)	226 (96%)	10 (4%)	0	100	100
40	g	132/166 (80%)	131 (99%)	1 (1%)	0	100	100
41	h	108/158 (68%)	103 (95%)	5 (5%)	0	100	100
42	i	95/128 (74%)	95 (100%)	0	0	100	100
43	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
44	k	100/112 (89%)	99 (99%)	1 (1%)	0	100	100
45	l	80/138 (58%)	77 (96%)	3 (4%)	0	100	100
46	m	66/128 (52%)	63 (96%)	3 (4%)	0	100	100
48	o	92/102 (90%)	91 (99%)	1 (1%)	0	100	100
49	q	175/222 (79%)	175 (100%)	0	0	100	100
50	r	160/196 (82%)	157 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	AB	223/296 (75%)	215 (96%)	8 (4%)	0	100	100
52	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
53	AD	341/430 (79%)	332 (97%)	9 (3%)	0	100	100
54	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
55	AF	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
56	AG	323/396 (82%)	314 (97%)	9 (3%)	0	100	100
57	AH	138/201 (69%)	132 (96%)	5 (4%)	1 (1%)	18	50
58	AJ	106/138 (77%)	101 (95%)	5 (5%)	0	100	100
59	AK	99/128 (77%)	99 (100%)	0	0	100	100
60	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
61	AM	117/137 (85%)	114 (97%)	3 (3%)	0	100	100
62	AN	108/130 (83%)	103 (95%)	5 (5%)	0	100	100
63	AO	191/258 (74%)	187 (98%)	4 (2%)	0	100	100
64	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
65	AR	293/360 (81%)	287 (98%)	6 (2%)	0	100	100
66	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
67	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
68	AU	174/205 (85%)	174 (100%)	0	0	100	100
69	AV	358/414 (86%)	340 (95%)	18 (5%)	0	100	100
70	AW	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
71	AZ	98/106 (92%)	97 (99%)	1 (1%)	0	100	100
72	A0	213/217 (98%)	206 (97%)	7 (3%)	0	100	100
73	A1	277/323 (86%)	267 (96%)	10 (4%)	0	100	100
74	A3	68/199 (34%)	66 (97%)	2 (3%)	0	100	100
76	AY	117/395 (30%)	117 (100%)	0	0	100	100
78	AI	135/194 (70%)	129 (96%)	6 (4%)	0	100	100
79	A4	584/689 (85%)	570 (98%)	14 (2%)	0	100	100
80	AX	350/398 (88%)	334 (95%)	16 (5%)	0	100	100
81	A2	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
82	AQ	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
83	c	282/332 (85%)	276 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	f	153/212 (72%)	148 (97%)	5 (3%)	0	100	100
85	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
86	s	381/439 (87%)	372 (98%)	9 (2%)	0	100	100
87	OX	51/435 (12%)	48 (94%)	3 (6%)	0	100	100
88	a	99/142 (70%)	97 (98%)	2 (2%)	0	100	100
All	All	14871/19622 (76%)	14498 (98%)	372 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	AH	126	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	270/303 (89%)	270 (100%)	0	100	100
9	8	146/190 (77%)	146 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
12	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	246 (100%)	0	100	100
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	207/256 (81%)	207 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	k	83/89 (93%)	83 (100%)	0	100	100
45	l	76/116 (66%)	76 (100%)	0	100	100
46	m	61/113 (54%)	61 (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	AB	198/249 (80%)	198 (100%)	0	100	100
52	AC	115/143 (80%)	115 (100%)	0	100	100
53	AD	286/357 (80%)	286 (100%)	0	100	100
54	AE	104/107 (97%)	104 (100%)	0	100	100
55	AF	185/209 (88%)	185 (100%)	0	100	100
56	AG	285/342 (83%)	285 (100%)	0	100	100
57	AH	130/180 (72%)	130 (100%)	0	100	100
58	AJ	93/118 (79%)	93 (100%)	0	100	100
59	AK	91/113 (80%)	91 (100%)	0	100	100
60	AL	158/226 (70%)	158 (100%)	0	100	100
61	AM	97/113 (86%)	97 (100%)	0	100	100
62	AN	96/115 (84%)	96 (100%)	0	100	100
63	AO	174/230 (76%)	173 (99%)	1 (1%)	78	88
64	AP	88/123 (72%)	88 (100%)	0	100	100
65	AR	264/318 (83%)	264 (100%)	0	100	100
66	AS	116/164 (71%)	116 (100%)	0	100	100
67	AT	153/157 (98%)	153 (100%)	0	100	100
68	AU	152/174 (87%)	152 (100%)	0	100	100
69	AV	325/364 (89%)	325 (100%)	0	100	100
70	AW	87/158 (55%)	87 (100%)	0	100	100
71	AZ	90/95 (95%)	90 (100%)	0	100	100
72	A0	188/189 (100%)	188 (100%)	0	100	100
73	A1	257/291 (88%)	257 (100%)	0	100	100
74	A3	65/166 (39%)	65 (100%)	0	100	100
76	AY	110/357 (31%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	AI	105/147 (71%)	105 (100%)	0	100	100
79	A4	526/609 (86%)	526 (100%)	0	100	100
80	AX	311/351 (89%)	311 (100%)	0	100	100
81	A2	100/100 (100%)	100 (100%)	0	100	100
82	AQ	78/78 (100%)	78 (100%)	0	100	100
83	c	251/288 (87%)	251 (100%)	0	100	100
84	f	139/188 (74%)	139 (100%)	0	100	100
85	p	135/181 (75%)	135 (100%)	0	100	100
86	s	339/381 (89%)	339 (100%)	0	100	100
87	OX	49/372 (13%)	49 (100%)	0	100	100
88	a	99/133 (74%)	99 (100%)	0	100	100
All	All	13284/16932 (78%)	13283 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
63	AO	154	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	98	GLN
2	1	15	ASN
4	3	178	GLN
4	3	185	ASN
6	5	150	GLN
6	5	195	HIS
6	5	269	ASN
6	5	343	GLN
7	6	292	GLN
7	6	308	GLN
8	7	246	GLN
9	8	186	GLN
12	C	98	ASN
12	C	240	HIS
12	C	275	GLN
12	C	278	HIS

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Mol	Chain	Res	Type
12	C	281	GLN
13	D	168	HIS
15	F	103	GLN
16	H	196	ASN
16	H	254	GLN
17	I	119	HIS
18	J	84	GLN
18	J	186	GLN
19	K	9	GLN
20	L	48	ASN
21	M	30	ASN
21	M	53	HIS
21	M	114	GLN
22	N	86	ASN
27	S	140	ASN
28	T	103	ASN
28	T	127	ASN
29	U	27	GLN
31	X	4	HIS
31	X	93	ASN
32	Y	89	GLN
33	Z	126	GLN
33	Z	148	GLN
34	z	215	ASN
34	z	241	HIS
34	z	266	GLN
36	V	117	HIS
38	d	205	GLN
39	e	87	HIS
40	g	93	ASN
40	g	141	ASN
40	g	155	GLN
41	h	67	GLN
41	h	87	GLN
41	h	119	GLN
44	k	93	HIS
50	r	96	HIS
50	r	109	GLN
51	AB	201	ASN
53	AD	341	ASN
53	AD	360	GLN
53	AD	361	GLN

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Mol	Chain	Res	Type
53	AD	369	HIS
54	AE	56	GLN
54	AE	59	ASN
55	AF	113	GLN
55	AF	122	GLN
55	AF	207	HIS
56	AG	232	GLN
56	AG	384	GLN
59	AK	117	HIS
60	AL	118	ASN
60	AL	172	ASN
63	AO	169	GLN
64	AP	137	ASN
65	AR	86	ASN
66	AS	66	HIS
68	AU	31	HIS
68	AU	102	HIS
69	AV	215	GLN
69	AV	237	GLN
70	AW	135	GLN
72	A0	24	GLN
73	A1	231	HIS
73	A1	321	ASN
74	A3	158	GLN
74	A3	190	GLN
76	AY	295	GLN
78	AI	93	ASN
79	A4	545	GLN
79	A4	656	ASN
80	AX	81	HIS
80	AX	140	HIS
80	AX	148	GLN
80	AX	159	HIS
80	AX	190	ASN
80	AX	363	ASN
85	p	117	GLN
85	p	176	HIS
86	s	164	HIS
86	s	387	ASN
86	s	420	GLN
88	a	46	ASN
88	a	126	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1558 (99%)	261 (16%)	3 (0%)
75	Az	33/34 (97%)	13 (39%)	0
77	AA	953/954 (99%)	143 (15%)	0
89	Aw	64/76 (84%)	34 (53%)	0
90	Ax	67/76 (88%)	14 (20%)	0
91	B	70/72 (97%)	16 (22%)	0
All	All	2743/2770 (99%)	481 (17%)	3 (0%)

All (481) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1681	G
11	A	1689	C
11	A	1692	A
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1708	A
11	A	1709	G
11	A	1711	C
11	A	1713	A
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	1780	U
11	A	1805	A
11	A	1806	U
11	A	1807	U
11	A	1808	A
11	A	1809	U
11	A	1812	C
11	A	1817	C
11	A	1821	A
11	A	1827	C
11	A	1828	A
11	A	1829	A
11	A	1832	A
11	A	1836	A

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Mol	Chain	Res	Type
11	A	1844	A
11	A	1854	U
11	A	1856	A
11	A	1867	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	1903	C
11	A	1907	A
11	A	1909	A
11	A	1918	G
11	A	1937	A
11	A	1940	A
11	A	1958	G
11	A	1973	G
11	A	1985	G
11	A	1993	A
11	A	1994	A
11	A	2001	C
11	A	2003	A
11	A	2015	G
11	A	2022	G
11	A	2030	U
11	A	2036	C
11	A	2037	U
11	A	2039	A
11	A	2054	U
11	A	2055	U
11	A	2060	A
11	A	2070	C
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	2180	A
11	A	2181	A
11	A	2182	G
11	A	2184	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	2227	A
11	A	2228	A
11	A	2230	A
11	A	2233	U
11	A	2237	A
11	A	2241	A
11	A	2243	A
11	A	2245	A
11	A	2246	A
11	A	2262	C
11	A	2263	C
11	A	2284	C
11	A	2297	A
11	A	2300	G
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2345	G

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Mol	Chain	Res	Type
11	A	2350	A
11	A	2353	A
11	A	2357	C
11	A	2363	A
11	A	2369	A
11	A	2372	U
11	A	2374	A
11	A	2379	C
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	2427	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	2520	C
11	A	2521	A
11	A	2527	A
11	A	2540	C
11	A	2563	U
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	2606	U
11	A	2618	U
11	A	2625	C
11	A	2627	G
11	A	2630	U

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Mol	Chain	Res	Type
11	A	2633	A
11	A	2635	G
11	A	2654	U
11	A	2655	G
11	A	2656	U
11	A	2683	C
11	A	2686	G
11	A	2694	A
11	A	2696	A
11	A	2706	A
11	A	2709	A
11	A	2715	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	2745	A
11	A	2757	A
11	A	2762	C
11	A	2763	U
11	A	2765	A
11	A	2767	A
11	A	2768	A
11	A	2773	A
11	A	2780	C
11	A	2781	U
11	A	2782	A
11	A	2783	A
11	A	2786	U
11	A	2790	A
11	A	2810	G
11	A	2832	A
11	A	2833	A
11	A	2844	G
11	A	2847	C
11	A	2861	A
11	A	2864	U
11	A	2865	C
11	A	2885	U
11	A	2888	A

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Mol	Chain	Res	Type
11	A	2889	C
11	A	2893	A
11	A	2907	U
11	A	2913	A
11	A	2915	C
11	A	2916	G
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2928	C
11	A	2935	A
11	A	2956	A
11	A	2960	U
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	3022	G
11	A	3041	U
11	A	3053	A
11	A	3054	G
11	A	3060	C
11	A	3065	U
11	A	3086	U
11	A	3089	A
11	A	3090	G
11	A	3096	U
11	A	3100	U
11	A	3102	U
11	A	3108	U
11	A	3109	U
11	A	3110	C
11	A	3111	A
11	A	3112	A
11	A	3122	U
11	A	3150	U
11	A	3157	C

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Mol	Chain	Res	Type
11	A	3158	A
11	A	3162	C
11	A	3169	C
11	A	3172	C
11	A	3177	A
11	A	3180	A
11	A	3183	U
11	A	3189	C
11	A	3190	A
11	A	3199	U
11	A	3200	U
11	A	3207	A
11	A	3209	A
11	A	3210	C
11	A	3212	C
11	A	3217	A
11	A	3218	A
11	A	3220	A
11	A	3228	U
11	A	3229	U
11	A	3230	G
75	Az	0	U
75	Az	4	A
75	Az	11	U
75	Az	12	U
75	Az	13	U
75	Az	18	A
75	Az	19	A
75	Az	21	A
75	Az	22	A
75	Az	25	U
75	Az	26	A
75	Az	27	C
75	Az	30	A
77	AA	651	A
77	AA	680	U
77	AA	688	A
77	AA	704	U
77	AA	706	C
77	AA	712	C
77	AA	721	U
77	AA	737	C

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Mol	Chain	Res	Type
77	AA	738	A
77	AA	745	A
77	AA	753	A
77	AA	761	A
77	AA	766	G
77	AA	791	G
77	AA	794	U
77	AA	796	G
77	AA	822	G
77	AA	826	A
77	AA	828	C
77	AA	829	C
77	AA	830	U
77	AA	832	U
77	AA	835	C
77	AA	836	A
77	AA	860	A
77	AA	861	U
77	AA	868	C
77	AA	870	C
77	AA	871	A
77	AA	881	A
77	AA	889	G
77	AA	890	C
77	AA	893	G
77	AA	903	U
77	AA	904	C
77	AA	907	A
77	AA	919	A
77	AA	929	A
77	AA	930	G
77	AA	933	G
77	AA	938	A
77	AA	939	A
77	AA	942	A
77	AA	954	C
77	AA	959	C
77	AA	960	C
77	AA	961	U
77	AA	962	C
77	AA	967	A
77	AA	978	A

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Mol	Chain	Res	Type
77	AA	993	A
77	AA	1001	C
77	AA	1002	C
77	AA	1010	A
77	AA	1015	A
77	AA	1031	G
77	AA	1042	U
77	AA	1046	A
77	AA	1076	5MU
77	AA	1081	U
77	AA	1082	A
77	AA	1096	A
77	AA	1105	C
77	AA	1106	C
77	AA	1107	U
77	AA	1109	A
77	AA	1118	A
77	AA	1119	U
77	AA	1121	A
77	AA	1126	A
77	AA	1137	A
77	AA	1138	G
77	AA	1151	C
77	AA	1153	C
77	AA	1155	G
77	AA	1160	A
77	AA	1167	A
77	AA	1179	G
77	AA	1187	U
77	AA	1188	A
77	AA	1189	U
77	AA	1190	C
77	AA	1197	G
77	AA	1215	U
77	AA	1220	A
77	AA	1223	C
77	AA	1225	C
77	AA	1232	A
77	AA	1235	U
77	AA	1247	G
77	AA	1248	C
77	AA	1250	C

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Mol	Chain	Res	Type
77	AA	1251	A
77	AA	1261	C
77	AA	1271	C
77	AA	1273	G
77	AA	1284	U
77	AA	1290	C
77	AA	1291	U
77	AA	1292	A
77	AA	1318	A
77	AA	1326	A
77	AA	1327	G
77	AA	1330	C
77	AA	1343	A
77	AA	1344	U
77	AA	1353	A
77	AA	1354	A
77	AA	1355	G
77	AA	1356	A
77	AA	1376	C
77	AA	1378	C
77	AA	1387	A
77	AA	1390	A
77	AA	1405	C
77	AA	1443	U
77	AA	1466	C
77	AA	1478	A
77	AA	1481	C
77	AA	1482	A
77	AA	1519	A
77	AA	1522	U
77	AA	1525	C
77	AA	1526	U
77	AA	1527	A
77	AA	1528	A
77	AA	1533	C
77	AA	1535	U
77	AA	1537	C
77	AA	1538	G
77	AA	1539	C
77	AA	1540	A
77	AA	1551	G
77	AA	1557	A

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Mol	Chain	Res	Type
77	AA	1560	U
77	AA	1568	U
77	AA	1570	G
77	AA	1571	U
77	AA	1582	G
77	AA	1584	MA6
77	AA	1594	G
77	AA	1595	G
77	AA	1599	A
89	Aw	2	G
89	Aw	5	A
89	Aw	7	A
89	Aw	8	U
89	Aw	9	A
89	Aw	10	G
89	Aw	11	U
89	Aw	13	U
89	Aw	14	A
89	Aw	16	A
89	Aw	21	A
89	Aw	22	A
89	Aw	29	U
89	Aw	36	C
89	Aw	38	C
89	Aw	39	U
89	Aw	40	C
89	Aw	42	U
89	Aw	46	A
89	Aw	49	U
89	Aw	50	A
89	Aw	51	U
89	Aw	52	G
89	Aw	53	A
89	Aw	56	A
89	Aw	63	A
89	Aw	65	A
89	Aw	68	U
89	Aw	69	A
89	Aw	71	C
89	Aw	72	A
89	Aw	74	C
89	Aw	75	C

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Mol	Chain	Res	Type
89	Aw	76	A
90	Ax	2	A
90	Ax	25	C
90	Ax	37	A
90	Ax	40	C
90	Ax	41	A
90	Ax	42	G
90	Ax	43	A
90	Ax	44	A
90	Ax	49	G
90	Ax	56	C
90	Ax	57	A
90	Ax	61	C
90	Ax	73	A
90	Ax	76	A
91	B	8	U
91	B	10	2MG
91	B	16	C
91	B	19	C
91	B	21	A
91	B	45	G
91	B	46	A
91	B	54	C
91	B	55	U
91	B	56	U
91	B	58	A
91	B	59	A
91	B	64	A
91	B	69	U
91	B	72	G
91	B	76	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2194	U
11	A	2245	A
11	A	2484	C

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

13 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
77	B8T	AA	1486	96,77	19,22,23	0.41	0	25,31,34	0.31	0
11	OMG	A	2815	11,93	23,26,27	0.38	0	32,38,41	0.42	0
11	OMU	A	3039	11,93	19,22,23	0.33	0	25,31,34	0.74	1 (4%)
77	MA6	AA	1584	77	23,26,27	0.34	0	33,38,41	0.74	1 (3%)
91	1MA	B	9	91	21,25,26	0.38	0	30,37,40	0.65	0
77	MA6	AA	1583	77	23,26,27	0.34	0	33,38,41	0.72	1 (3%)
91	2MG	B	10	91	23,26,27	0.36	0	33,38,41	0.41	0
91	PSU	B	39	91	18,21,22	1.05	1 (5%)	21,30,33	0.72	0
11	PSU	A	3067	11	18,21,22	1.13	2 (11%)	21,30,33	0.80	1 (4%)
11	OMG	A	3040	11	23,26,27	0.35	0	32,38,41	0.45	0
77	5MU	AA	1076	77	19,22,23	0.38	0	27,32,35	0.59	0
11	1MA	A	2617	11	21,25,26	0.42	0	30,37,40	0.60	0
77	5MC	AA	1488	77	19,22,23	0.84	1 (5%)	26,32,35	0.52	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
77	B8T	AA	1486	96,77	-	0/7/27/28	0/2/2/2
11	OMG	A	2815	11,93	-	0/9/27/28	0/3/3/3
11	OMU	A	3039	11,93	-	0/9/27/28	0/2/2/2
77	MA6	AA	1584	77	-	1/11/29/30	0/3/3/3
91	1MA	B	9	91	-	1/7/25/26	0/3/3/3
77	MA6	AA	1583	77	-	0/11/29/30	0/3/3/3
91	2MG	B	10	91	-	0/9/27/28	0/3/3/3
91	PSU	B	39	91	-	0/7/25/26	0/2/2/2
11	PSU	A	3067	11	-	1/7/25/26	0/2/2/2
11	OMG	A	3040	11	-	0/9/27/28	0/3/3/3
77	5MU	AA	1076	77	-	4/7/25/26	0/2/2/2
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
77	5MC	AA	1488	77	-	0/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	B	39	PSU	C6-C5	3.65	1.39	1.35
11	A	3067	PSU	C6-C5	3.43	1.39	1.35
77	AA	1488	5MC	C5-C4	-3.33	1.41	1.44
11	A	3067	PSU	O4'-C1'	-2.75	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	AA	1584	MA6	C2-N1-C6	2.94	119.02	111.83
77	AA	1583	MA6	C2-N1-C6	2.94	119.02	111.83
11	A	3039	OMU	C2'-C1'-N1	-2.62	109.26	114.24
11	A	3067	PSU	O4'-C1'-C2'	2.40	108.47	105.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
77	AA	1076	5MU	O4'-C4'-C5'-O5'
77	AA	1076	5MU	C3'-C4'-C5'-O5'
77	AA	1584	MA6	C4'-C5'-O5'-P
77	AA	1076	5MU	C2'-C1'-N1-C6
77	AA	1076	5MU	C2'-C1'-N1-C2
11	A	3067	PSU	O4'-C4'-C5'-O5'
91	B	9	1MA	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	AA	1486	B8T	1	0
11	A	2815	OMG	1	0
11	A	3039	OMU	1	0
77	AA	1583	MA6	2	0
77	AA	1488	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 279 ligands modelled in this entry, 261 are monoatomic - leaving 18 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
99	SPM	AA	1702	-	13,13,13	0.16	0	12,12,12	0.25	0
94	SPD	A	3301	-	9,9,9	0.14	0	8,8,8	0.17	0
98	NAD	AA	1701	96	46,48,48	1.22	3 (6%)	64,73,73	0.85	4 (6%)
94	SPD	AA	1703	-	9,9,9	0.15	0	8,8,8	0.24	0
94	SPD	AA	1783	-	9,9,9	0.15	0	8,8,8	0.19	0
97	FES	AT	201	67,61	0,4,4	-	-	-	-	-
94	SPD	A	3472	-	9,9,9	0.14	0	8,8,8	0.34	0
95	PUT	A	3303	-	5,5,5	0.13	0	4,4,4	0.24	0
99	SPM	AA	1780	-	13,13,13	0.15	0	12,12,12	0.17	0
94	SPD	A	3302	-	9,9,9	0.15	0	8,8,8	0.20	0
97	FES	r	201	50,17	0,4,4	-	-	-	-	-
101	GDP	AX	503	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
94	SPD	A	3471	-	9,9,9	0.17	0	8,8,8	0.18	0
97	FES	AP	201	54,64	0,4,4	-	-	-	-	-
102	VAL	B	101	91	4,6,7	0.79	0	6,7,9	1.02	1 (16%)
94	SPD	AA	1782	-	9,9,9	0.14	0	8,8,8	0.16	0
100	ATP	AX	501	96	32,33,33	0.38	0	48,52,52	0.35	0
94	SPD	A	3473	-	9,9,9	0.17	0	8,8,8	0.23	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
99	SPM	AA	1702	-	-	0/11/11/11	-
94	SPD	A	3301	-	-	0/7/7/7	-
97	FES	AP	201	54,64	-	-	0/1/1/1
98	NAD	AA	1701	96	-	4/30/62/62	0/5/5/5
94	SPD	AA	1703	-	-	0/7/7/7	-
94	SPD	AA	1783	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
97	FES	AT	201	67,61	-	-	0/1/1/1
94	SPD	A	3472	-	-	1/7/7/7	-
95	PUT	A	3303	-	-	0/3/3/3	-
99	SPM	AA	1780	-	-	1/11/11/11	-
94	SPD	A	3302	-	-	1/7/7/7	-
101	GDP	AX	503	-	-	0/16/32/32	0/3/3/3
102	VAL	B	101	91	-	2/5/6/8	-
94	SPD	A	3471	-	-	0/7/7/7	-
97	FES	r	201	50,17	-	-	0/1/1/1
94	SPD	AA	1782	-	-	0/7/7/7	-
100	ATP	AX	501	96	-	0/22/38/38	0/3/3/3
94	SPD	A	3473	-	-	0/7/7/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
98	AA	1701	NAD	PA-O3	5.11	1.65	1.59
98	AA	1701	NAD	PN-O3	3.05	1.62	1.59
101	AX	503	GDP	C5-C4	3.04	1.47	1.38
98	AA	1701	NAD	O4D-C1D	-2.70	1.37	1.40
101	AX	503	GDP	C6-N1	-2.53	1.34	1.38
101	AX	503	GDP	C5-N7	-2.14	1.34	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
101	AX	503	GDP	C5-C4-N3	-5.87	119.05	128.39
101	AX	503	GDP	C2-N3-C4	4.76	120.50	112.30
101	AX	503	GDP	N9-C4-N3	4.36	134.68	125.95
101	AX	503	GDP	C6-C5-N7	3.18	136.08	130.29
101	AX	503	GDP	C4-C5-N7	-2.48	106.75	110.67
102	B	101	VAL	O-C-CA	-2.41	118.58	124.77
98	AA	1701	NAD	O7N-C7N-N7N	2.27	125.90	122.62
101	AX	503	GDP	C3'-C2'-C1'	2.25	105.73	101.46
98	AA	1701	NAD	O2A-PA-O1A	2.22	122.76	112.44
101	AX	503	GDP	O6-C6-C5	-2.11	120.95	126.53
98	AA	1701	NAD	O3-PA-O1A	-2.10	104.39	110.70
98	AA	1701	NAD	C3N-C7N-N7N	-2.06	115.20	117.74

There are no chirality outliers.

All (9) torsion outliers are listed below:

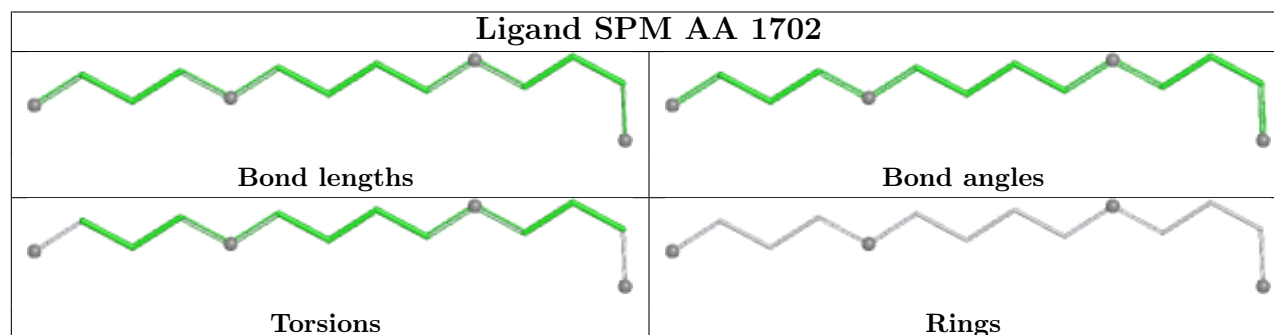
Mol	Chain	Res	Type	Atoms
102	B	101	VAL	O-C-CA-CB
102	B	101	VAL	C-CA-CB-CG2
98	AA	1701	NAD	O4D-C4D-C5D-O5D
98	AA	1701	NAD	C3D-C4D-C5D-O5D
94	A	3302	SPD	N1-C2-C3-C4
94	A	3472	SPD	C2-C3-C4-C5
98	AA	1701	NAD	C4N-C3N-C7N-N7N
98	AA	1701	NAD	C4N-C3N-C7N-O7N
99	AA	1780	SPM	C6-C7-C8-C9

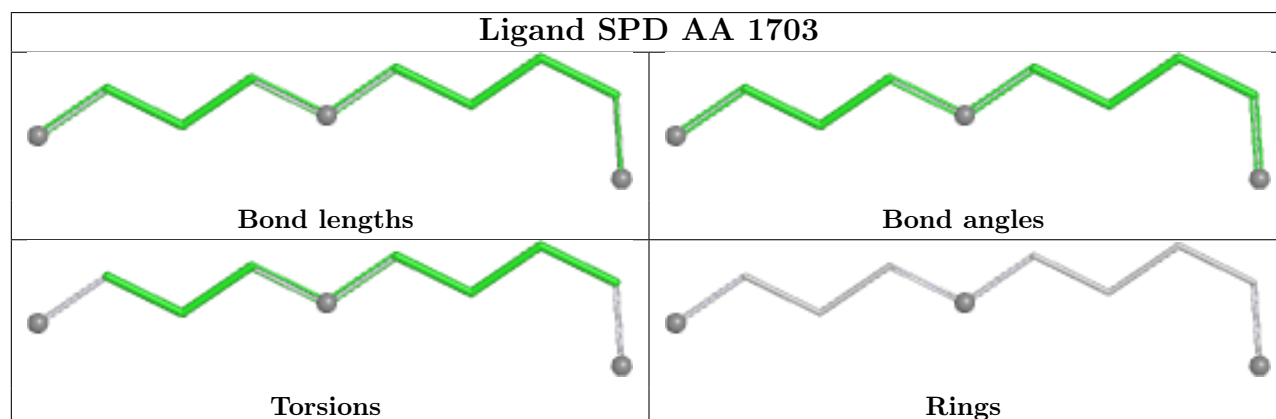
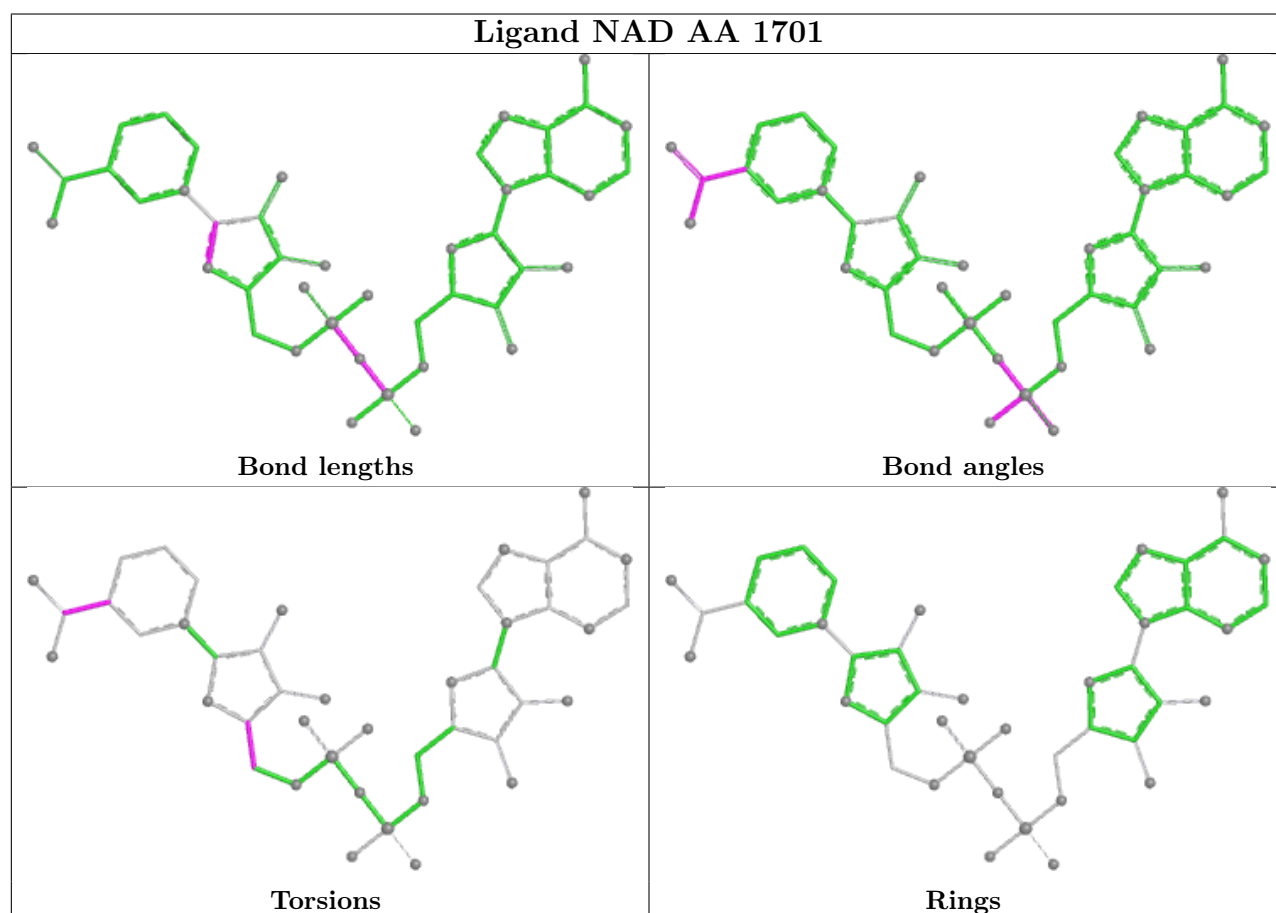
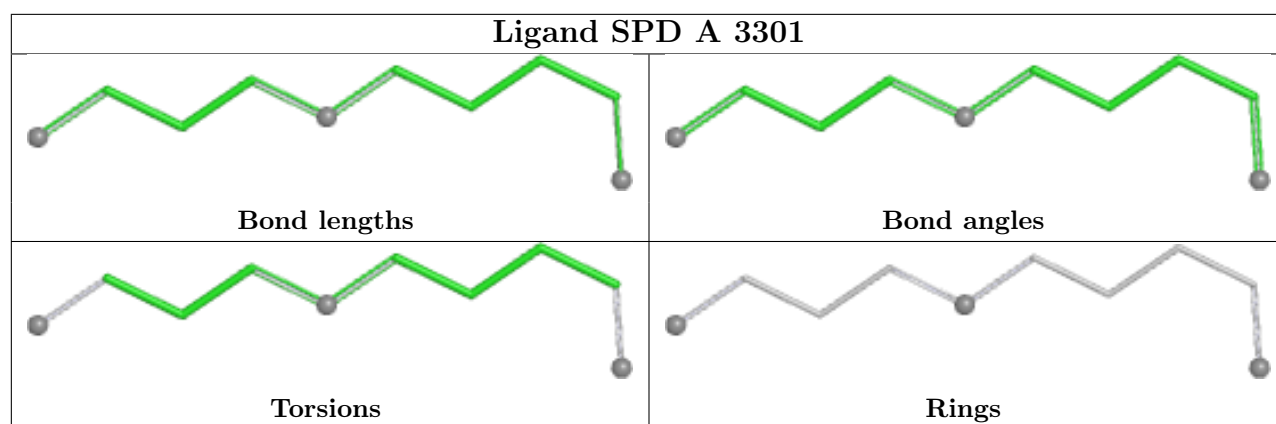
There are no ring outliers.

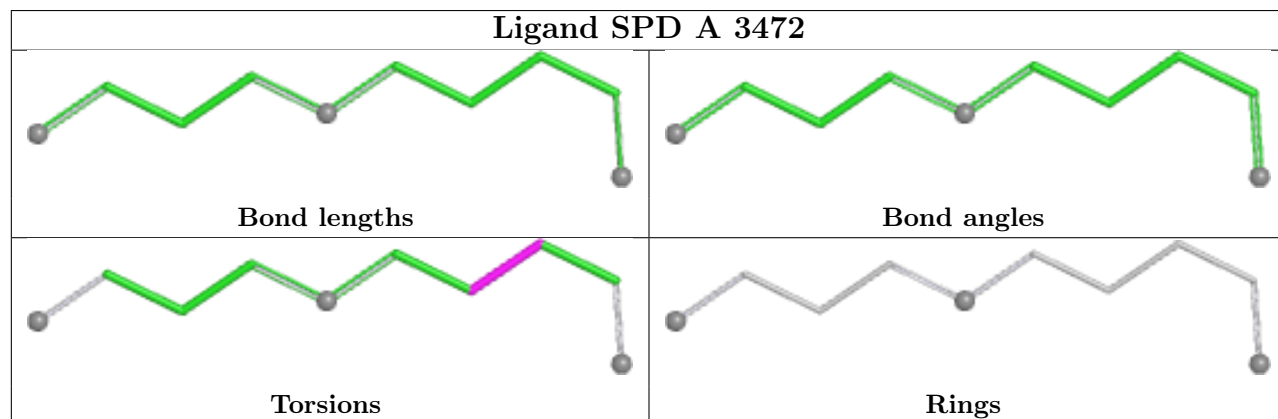
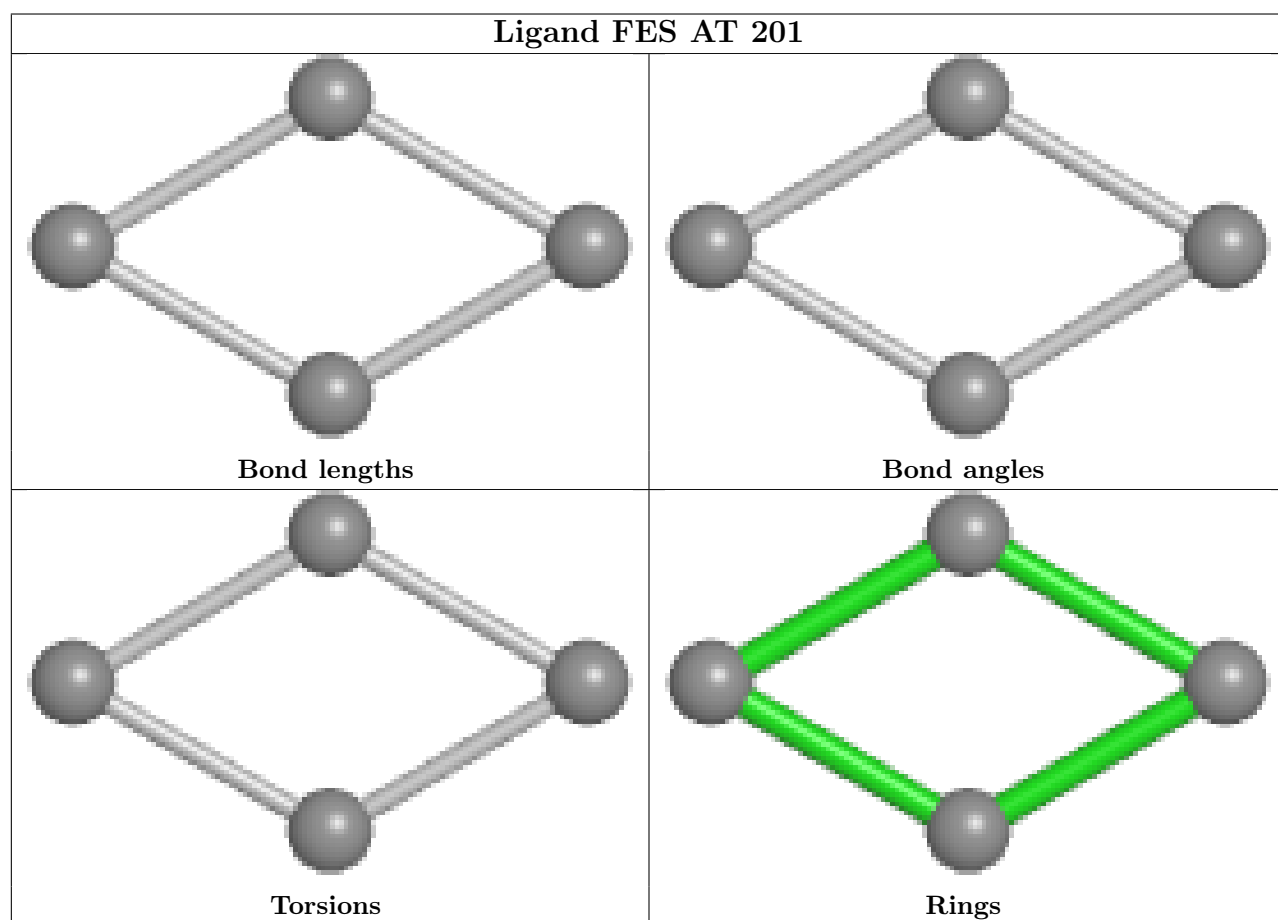
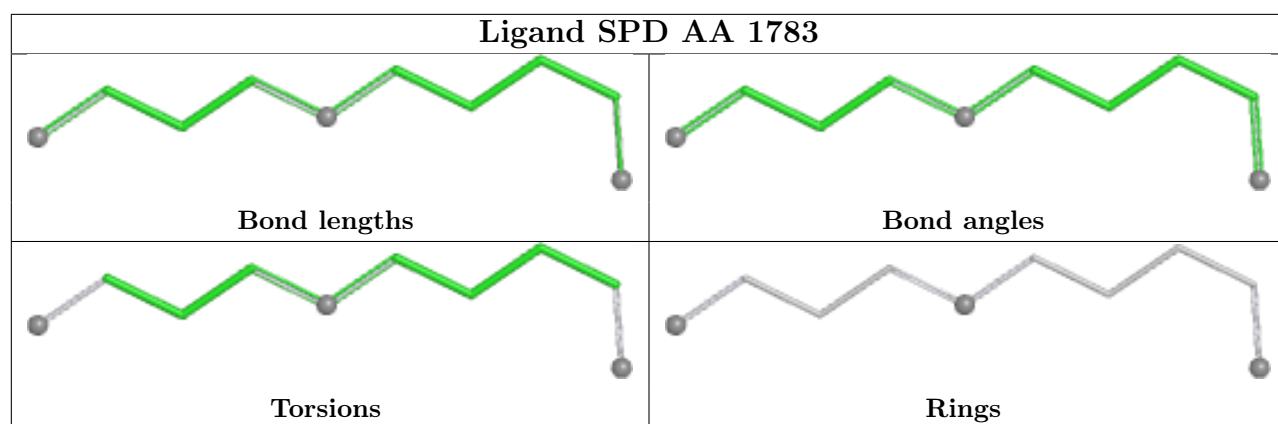
7 monomers are involved in 14 short contacts:

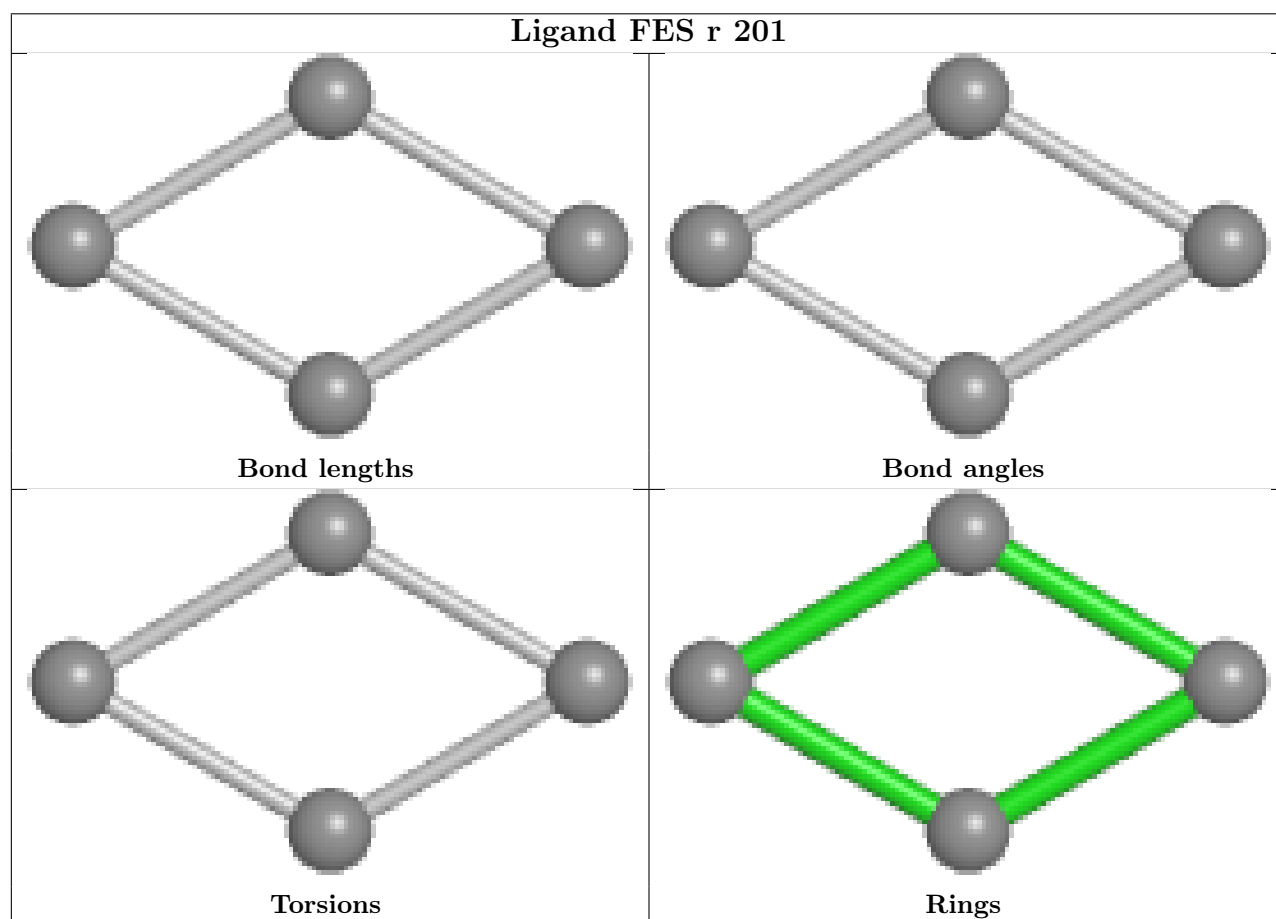
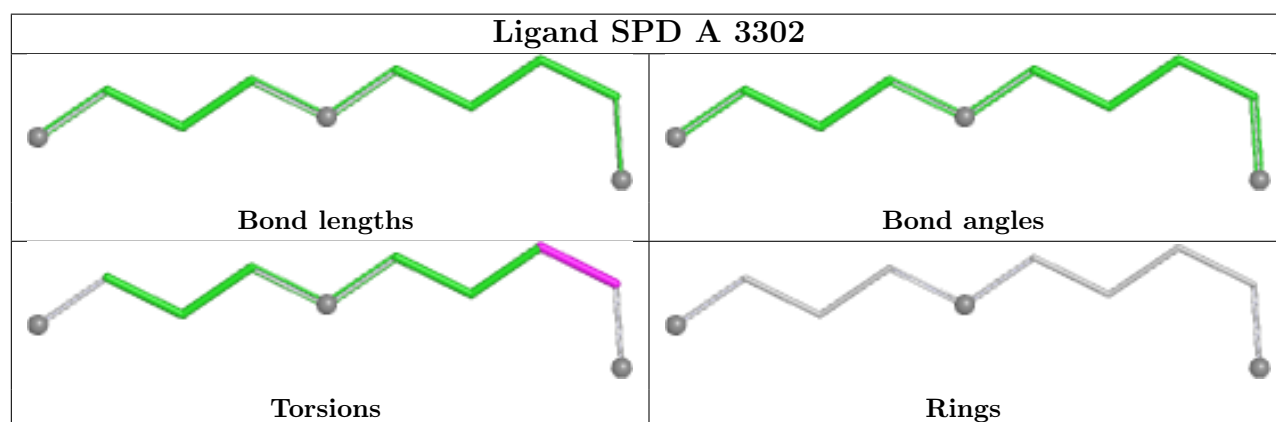
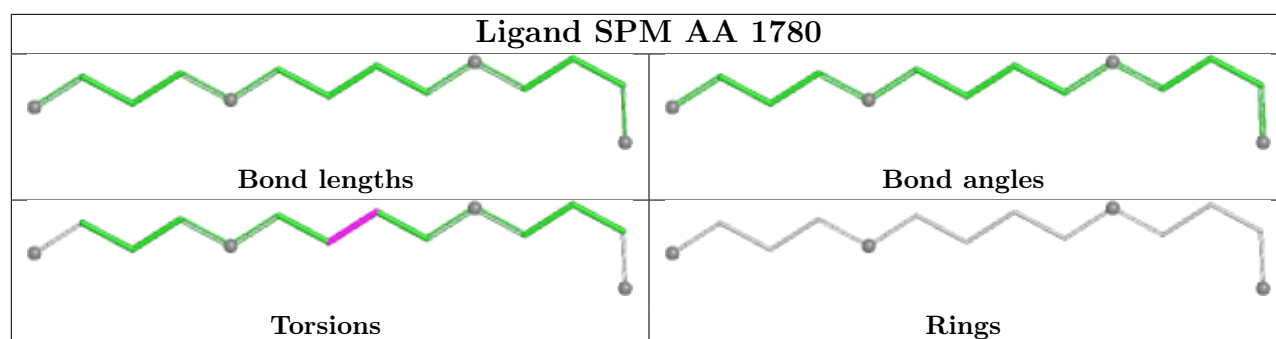
Mol	Chain	Res	Type	Clashes	Symm-Clashes
98	AA	1701	NAD	1	0
94	AA	1703	SPD	1	0
94	A	3302	SPD	1	0
97	r	201	FES	1	0
101	AX	503	GDP	3	0
102	B	101	VAL	4	0
94	AA	1782	SPD	3	0

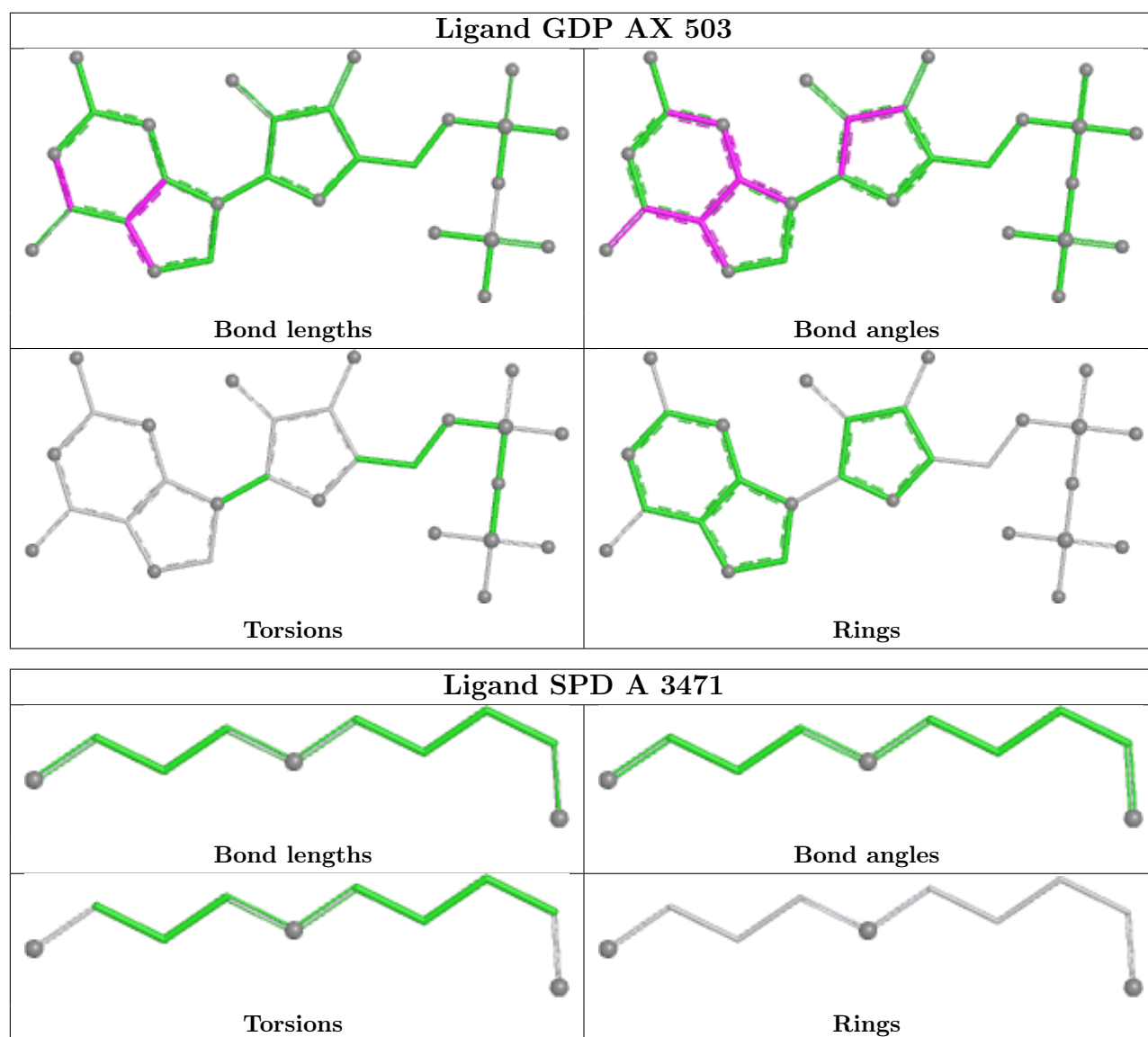
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

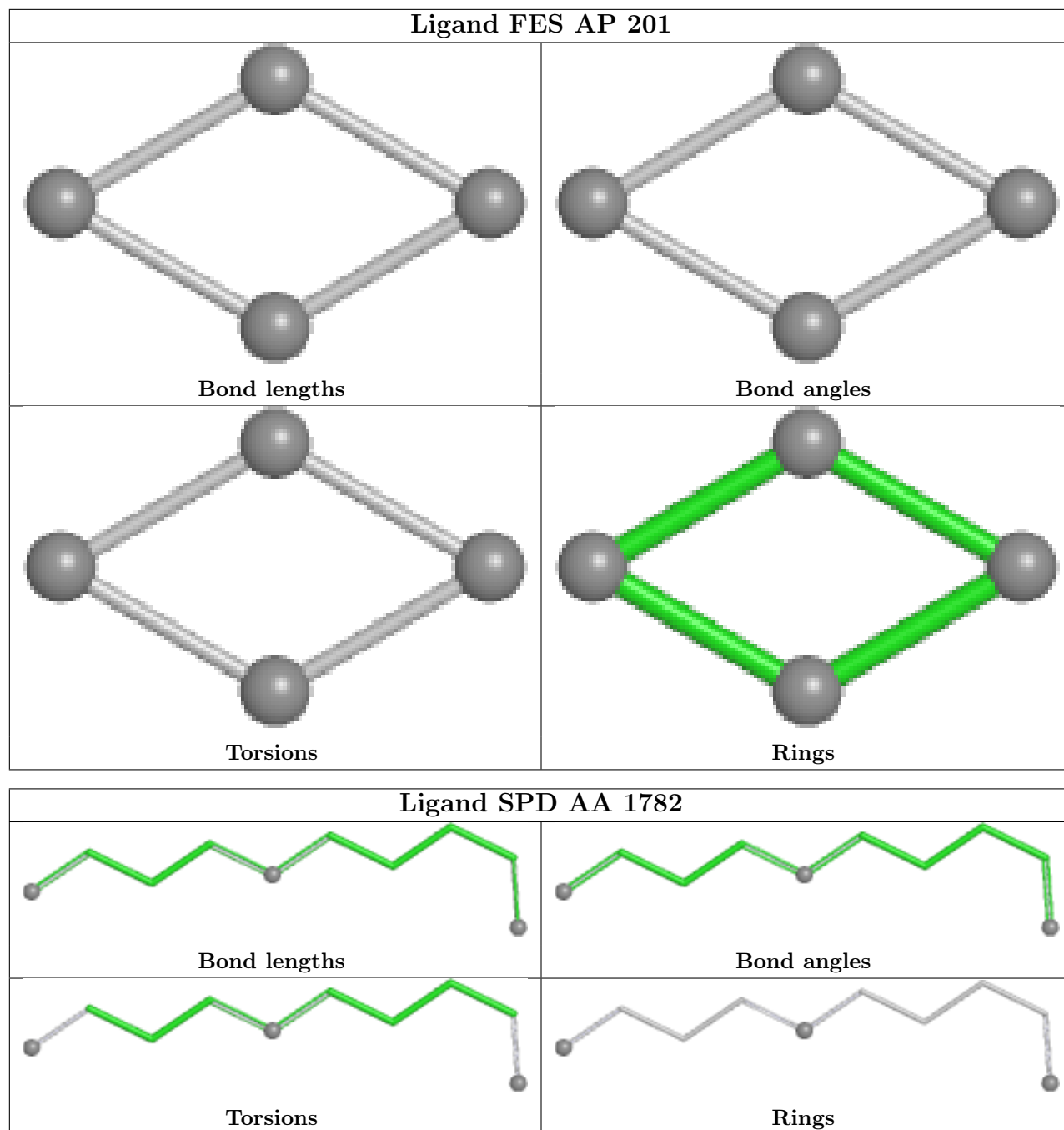


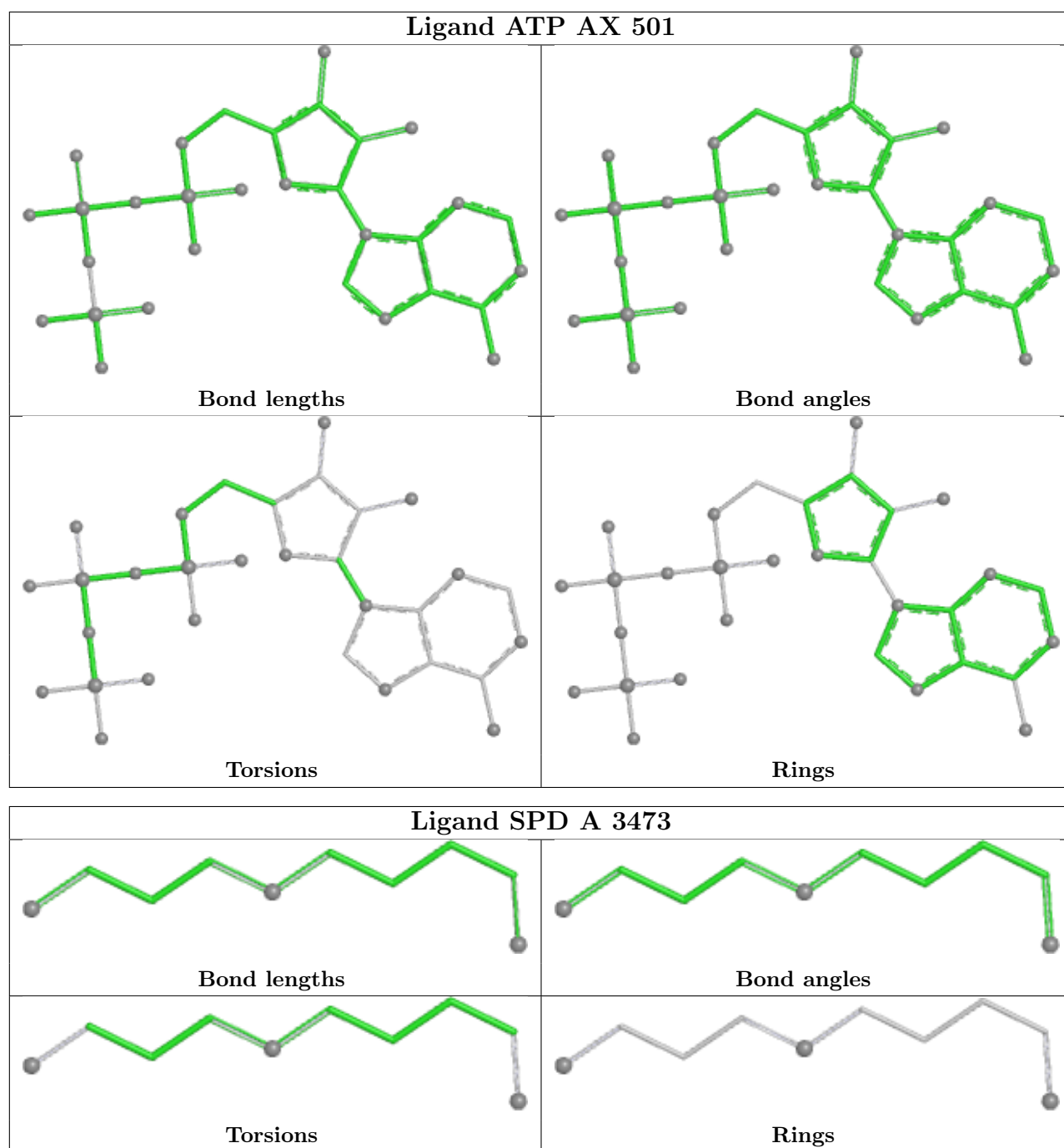












5.7 Other polymers [i](#)

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
11	A	1
91	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2357:C	O3'	2361:G	P	9.73
1	B	46:A	O3'	48:U	P	4.60

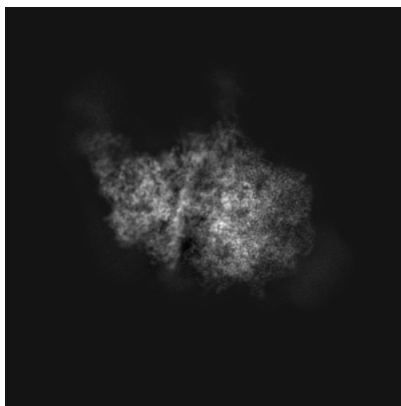
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71829. These allow visual inspection of the internal detail of the map and identification of artifacts.

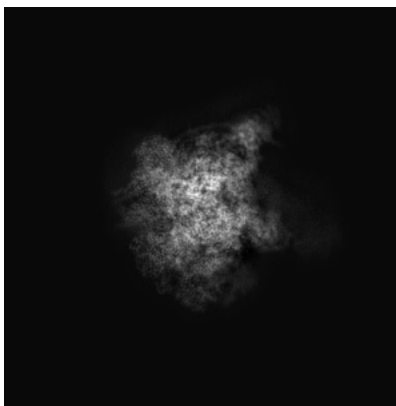
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

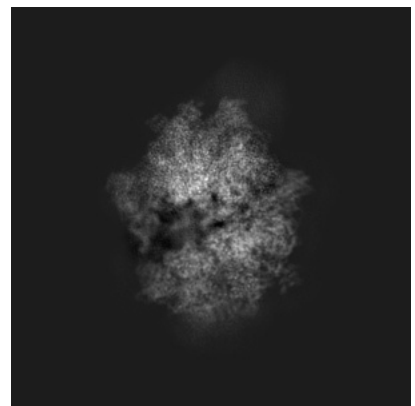
6.1.1 Primary map



X

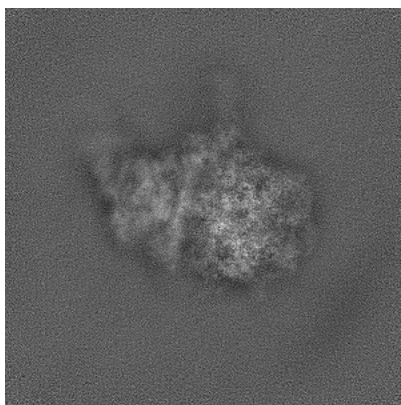


Y

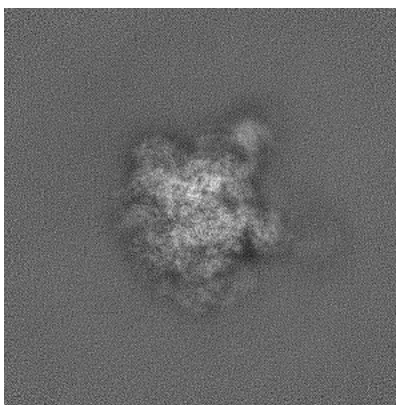


Z

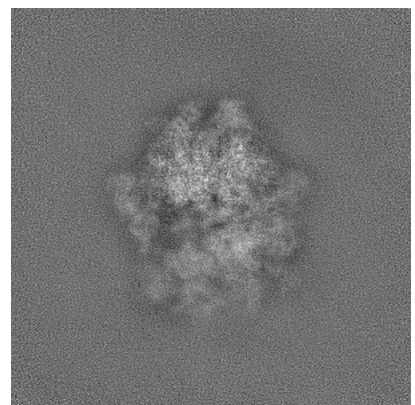
6.1.2 Raw map



X



Y

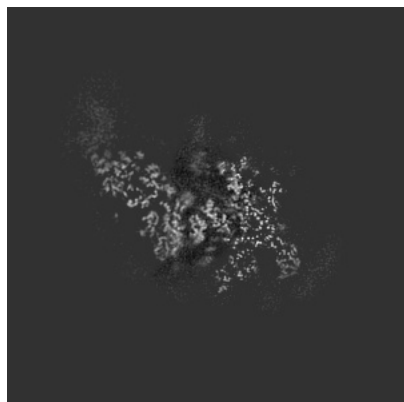


Z

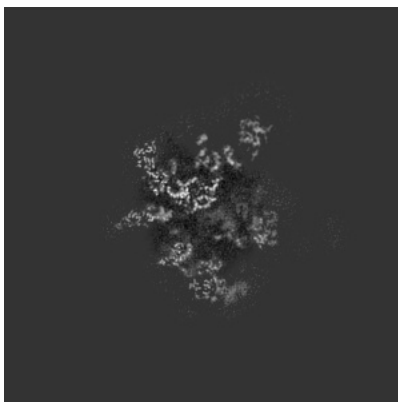
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

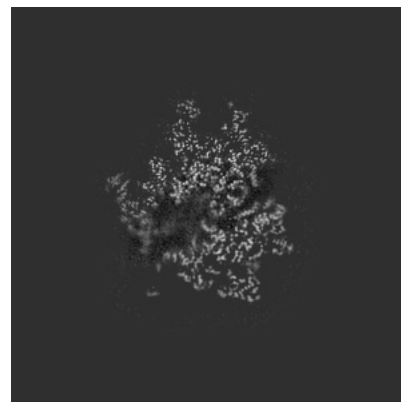
6.2.1 Primary map



X Index: 240

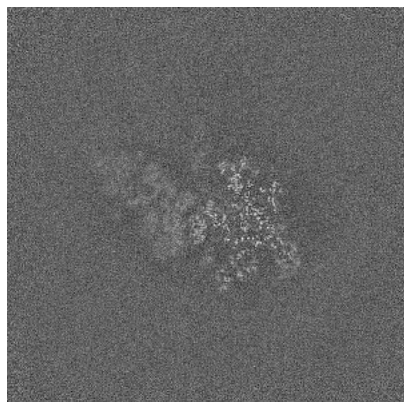


Y Index: 240

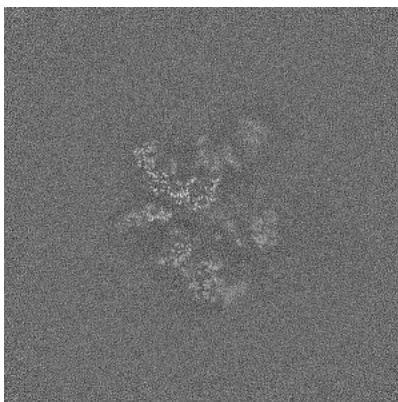


Z Index: 240

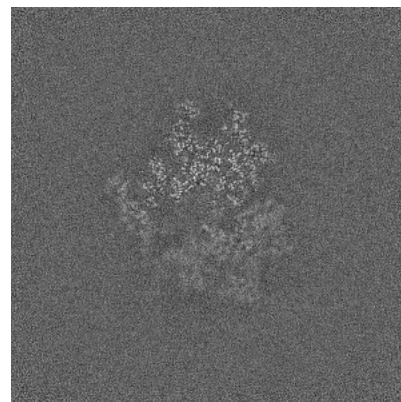
6.2.2 Raw map



X Index: 240



Y Index: 240

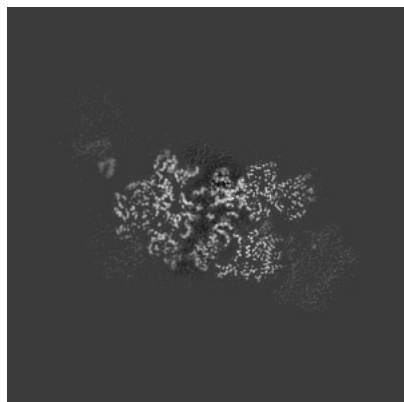


Z Index: 240

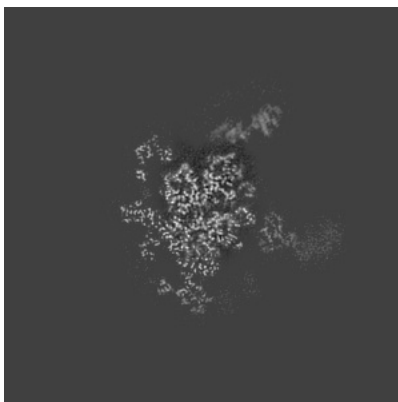
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

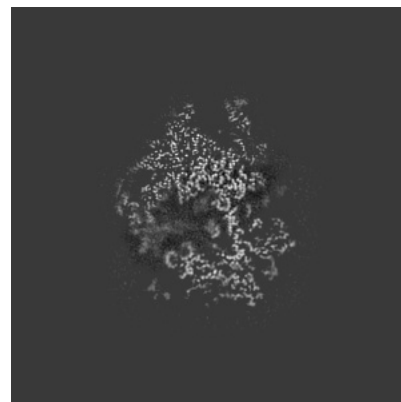
6.3.1 Primary map



X Index: 275

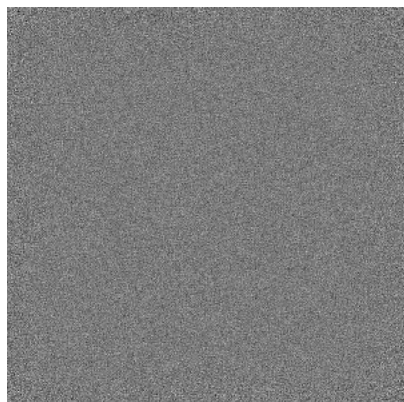


Y Index: 263

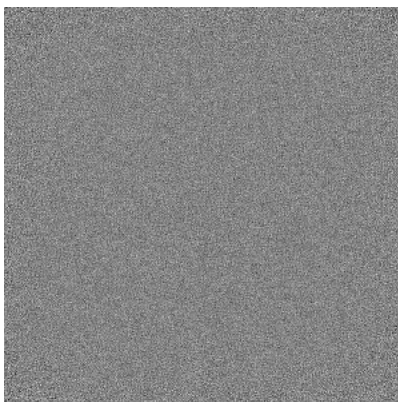


Z Index: 249

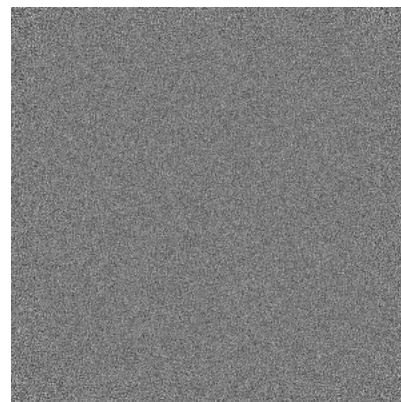
6.3.2 Raw map



X Index: 0



Y Index: 0

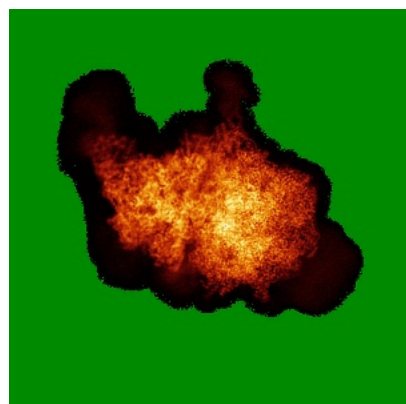


Z Index: 0

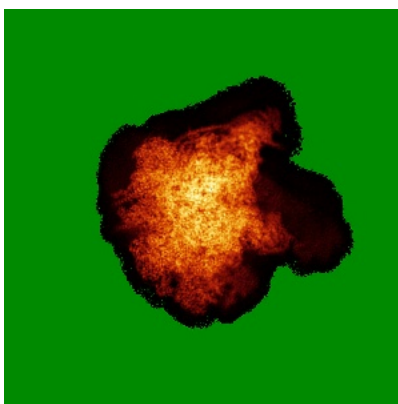
The images above show the largest variance slices of the map in three orthogonal directions.

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

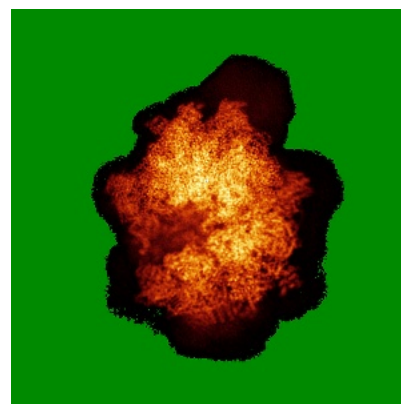
6.4.1 Primary map



X

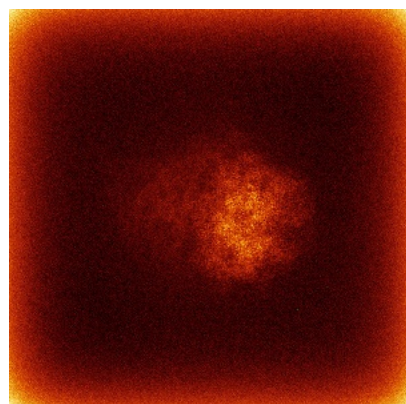


Y

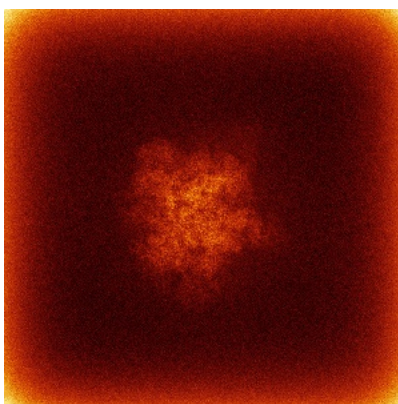


Z

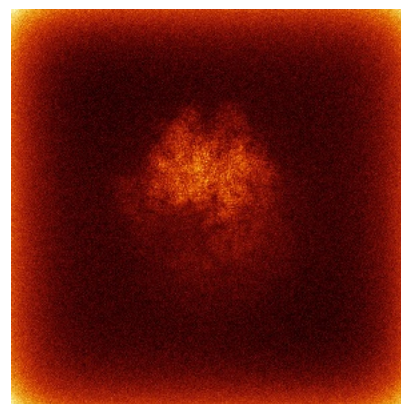
6.4.2 Raw map



X



Y

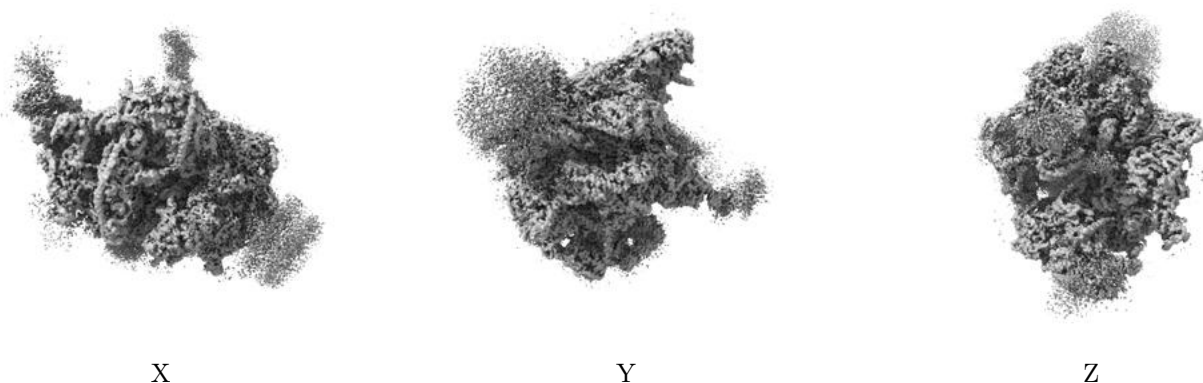


Z

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.

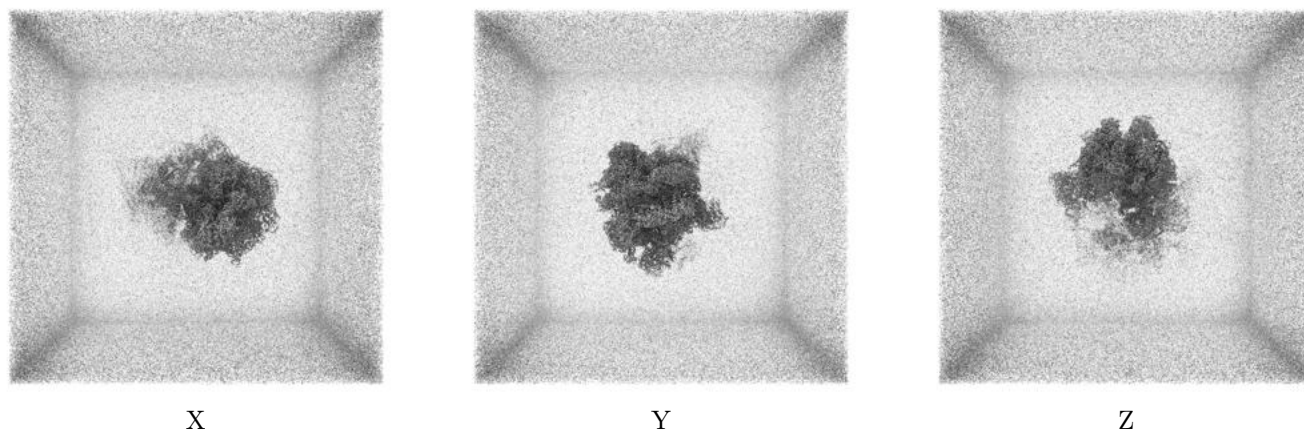
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

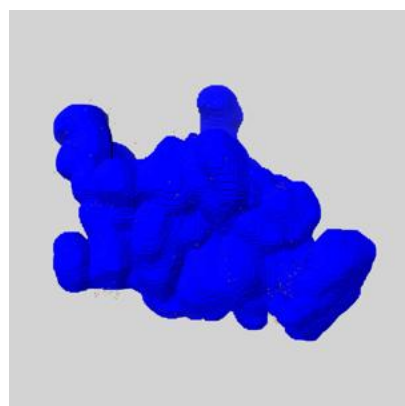
6.6 Mask visualisation [i](#)

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

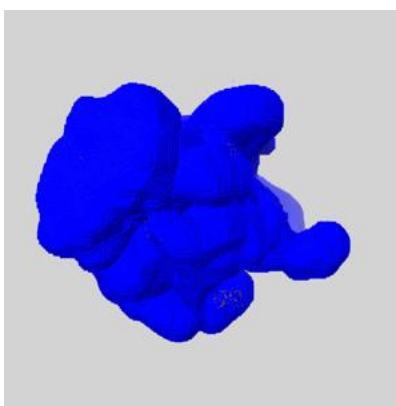
A mask typically either:

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

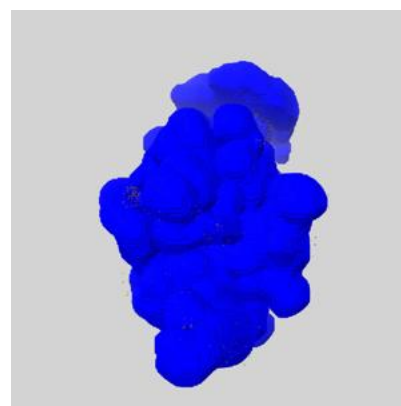
6.6.1 emd_71829_msk_1.map [i](#)



X



Y

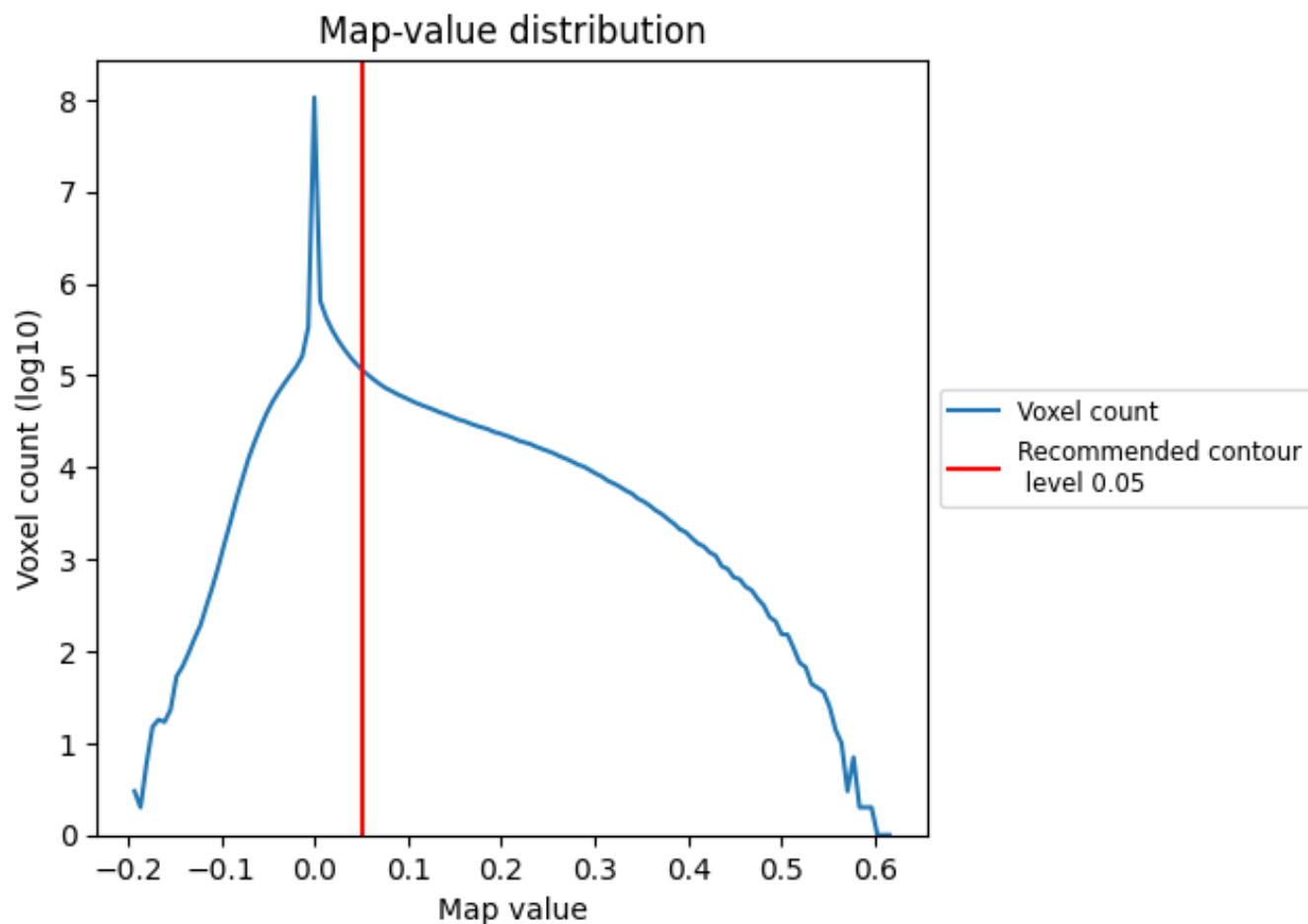


Z

7 Map analysis [i](#)

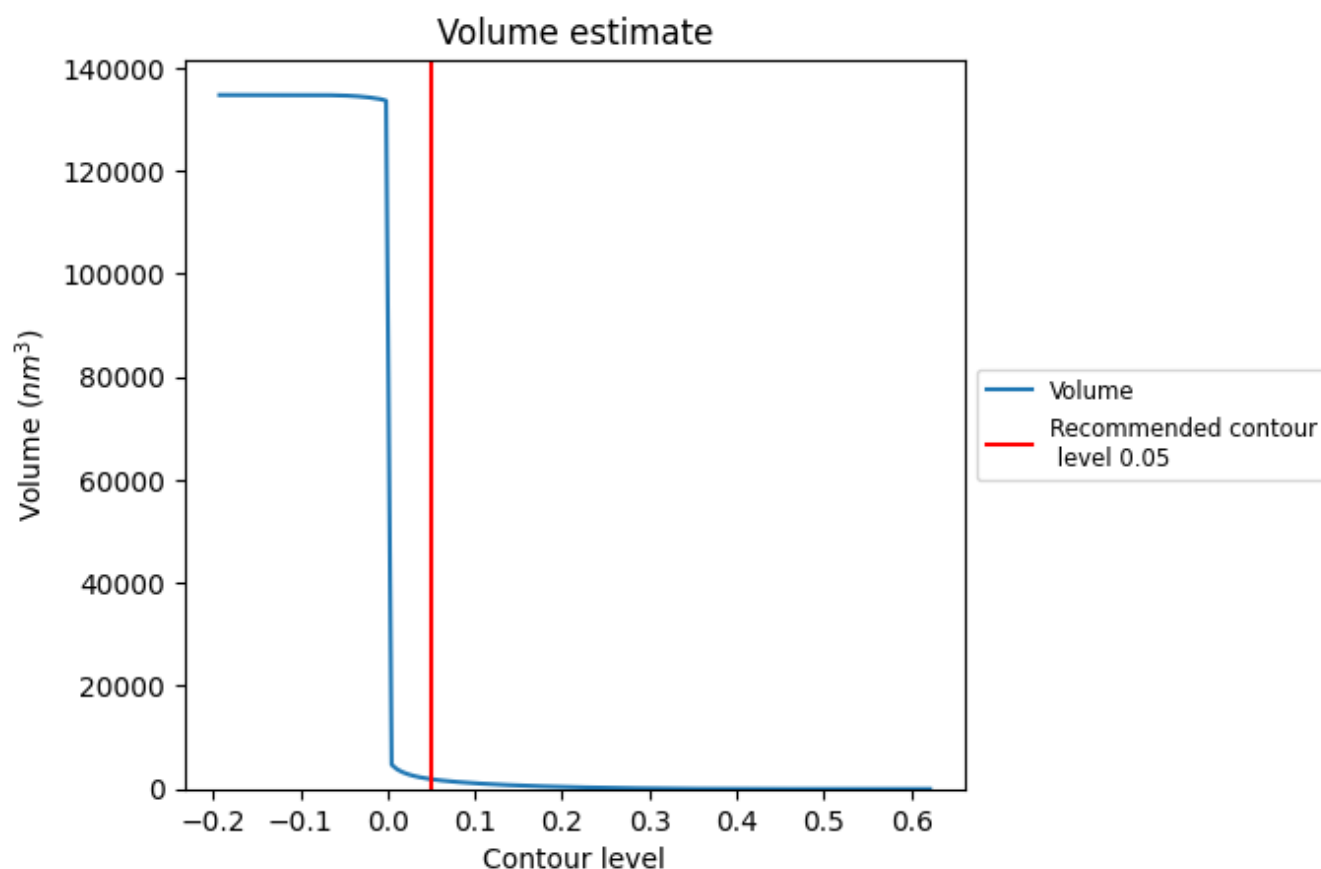
This section contains the results of statistical analysis of the map.

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.

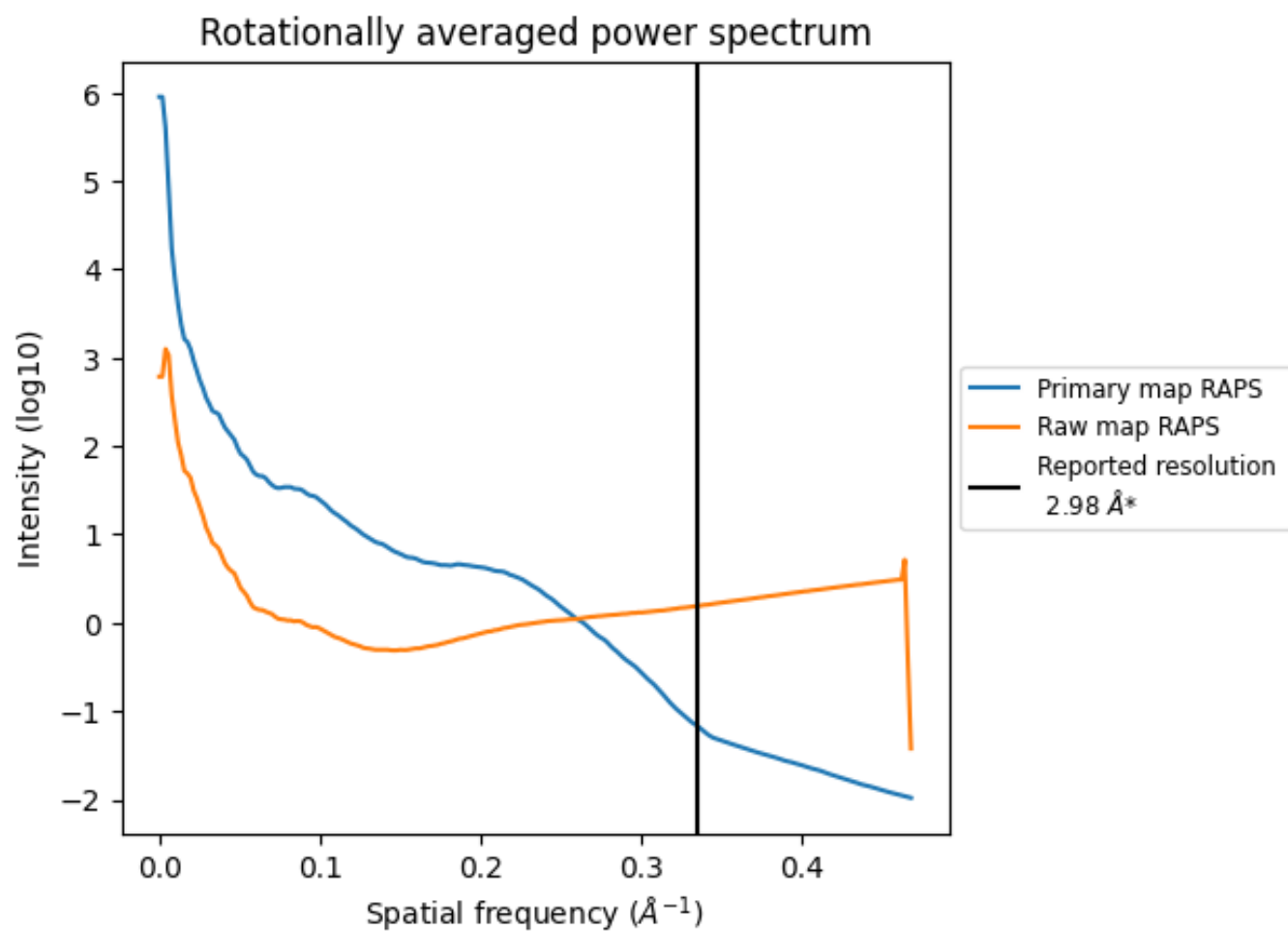
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1895 nm^3 ; this corresponds to an approximate mass of 1712 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 ⓘ

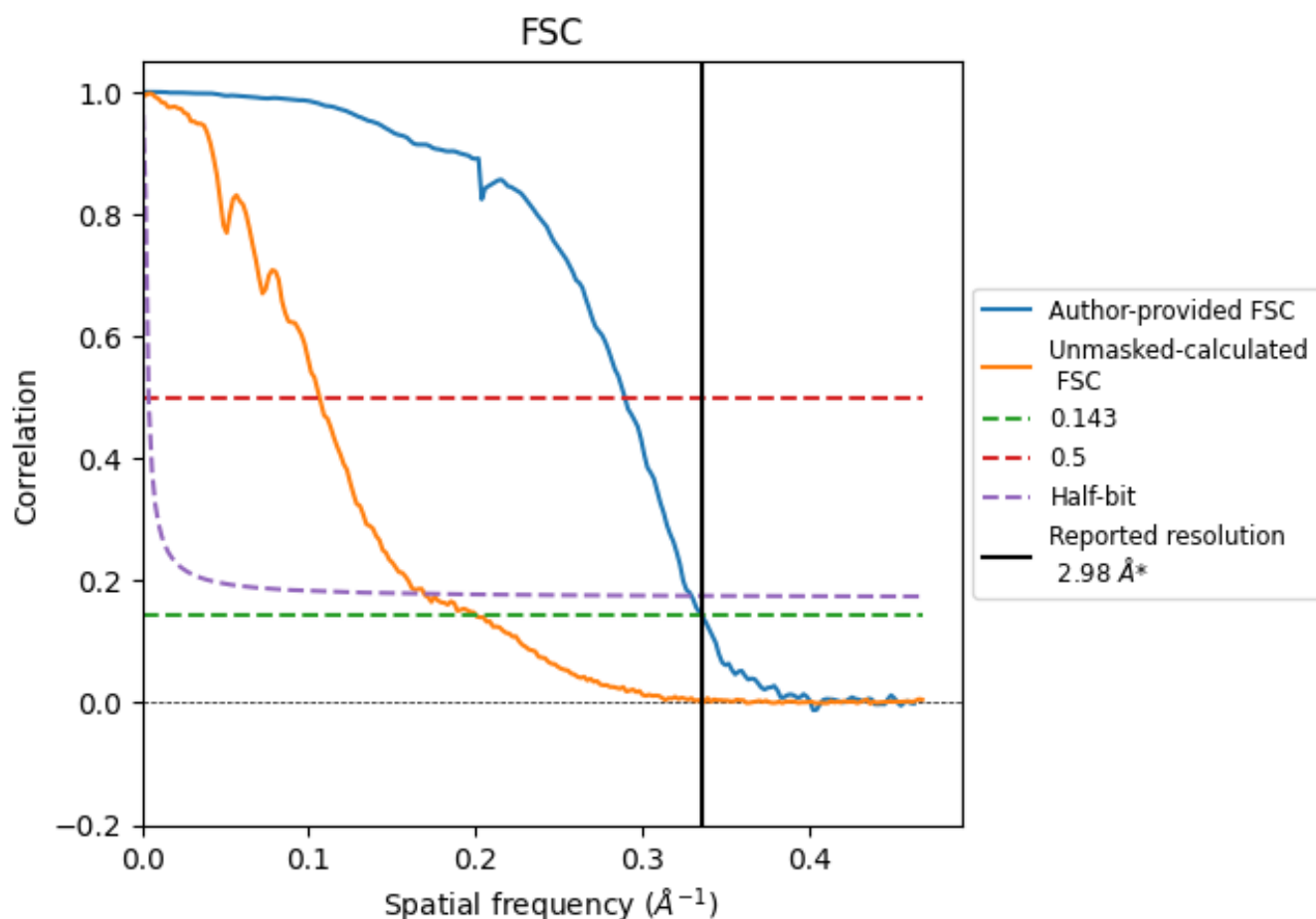


*Reported resolution corresponds to spatial frequency of 0.336 $\text{\AA}^{-1}$

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 0.336 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

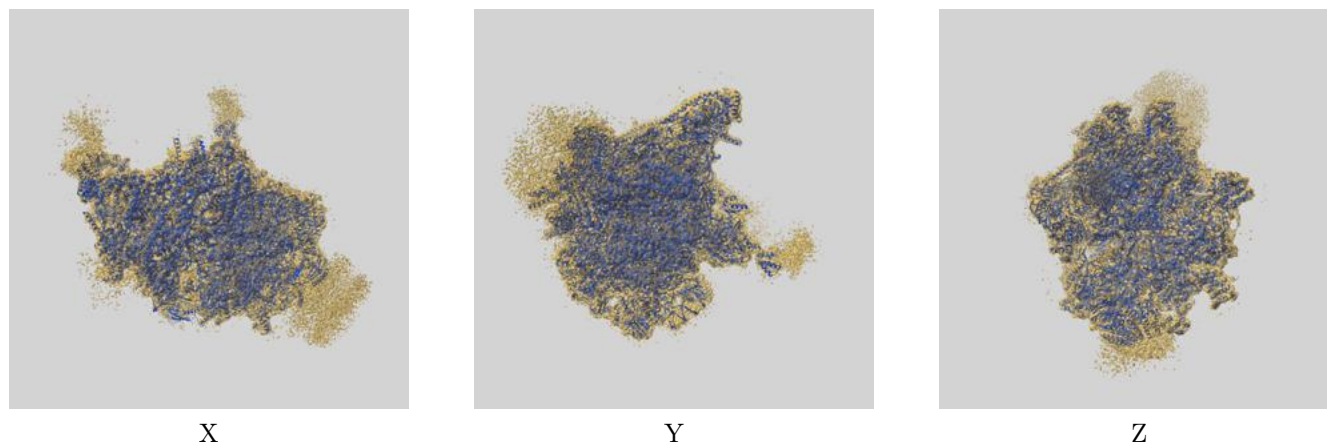
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.45	3.03
Unmasked-calculated*	4.99	9.39	5.91

*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 4.99 differs from the reported value 2.98 by more than 10 %

9 Map-model fit [i](#)

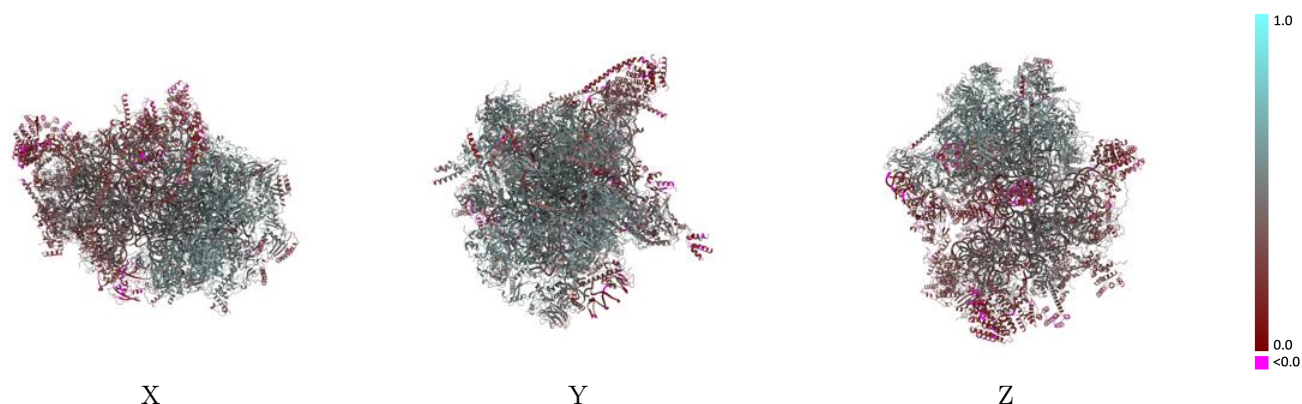
This section contains information regarding the fit between EMDB map EMD-71829 and PDB model 9PSM. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



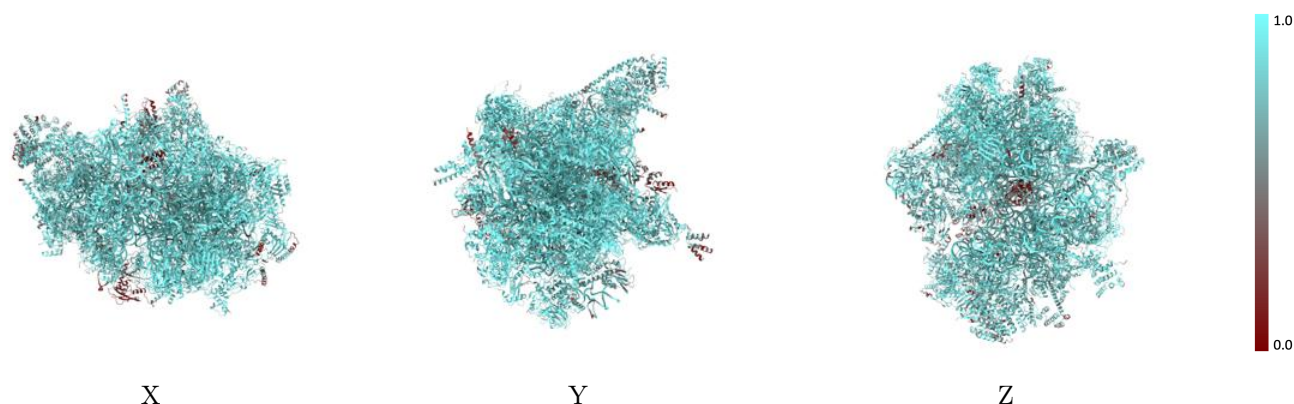
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



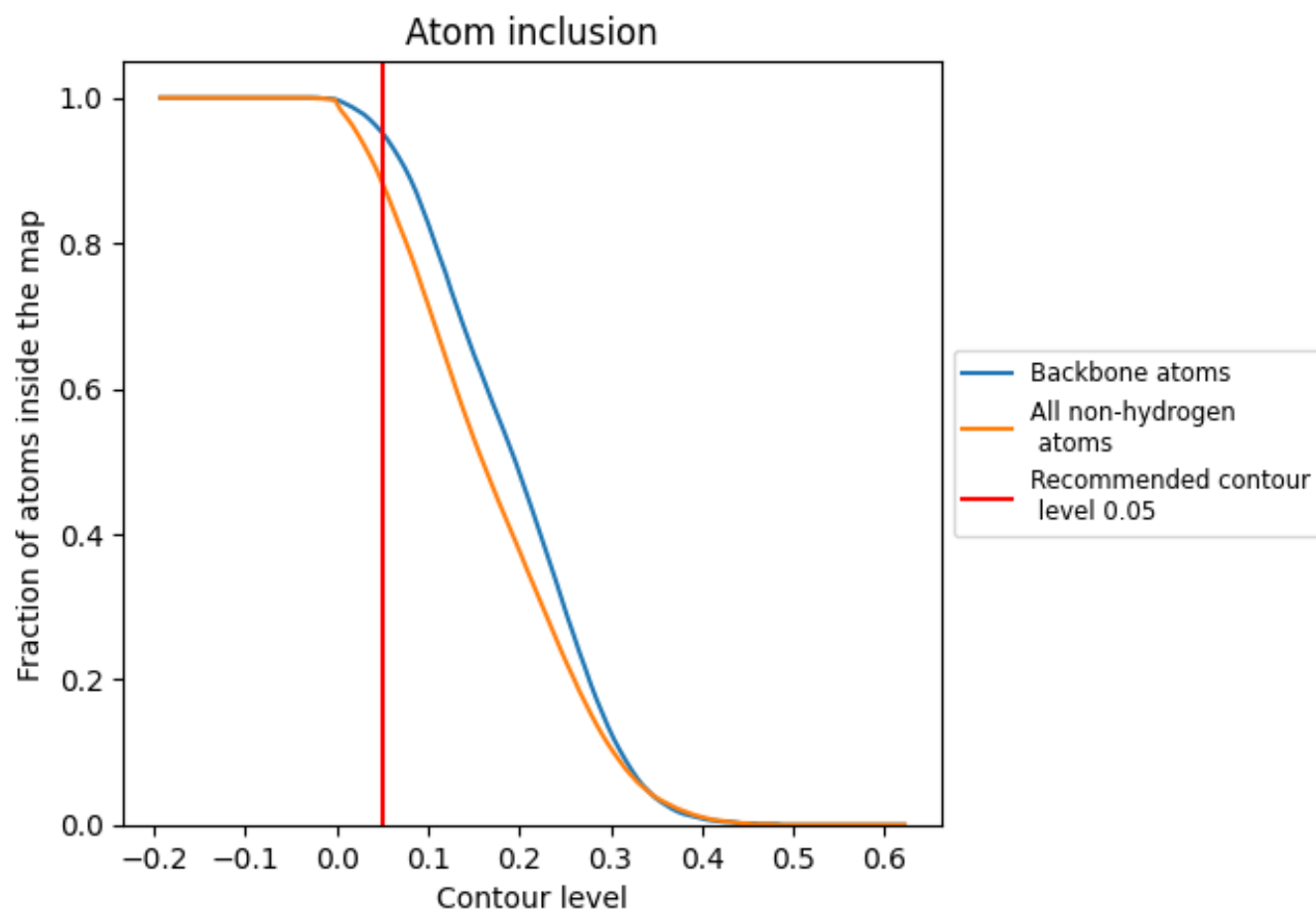
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.4190
0	 0.9250	 0.5300
1	 0.9250	 0.4850
2	 0.9860	 0.5770
3	 0.9780	 0.5780
4	 0.9450	 0.5540
5	 0.9240	 0.5160
6	 0.8930	 0.4710
7	 0.8920	 0.4670
8	 0.6860	 0.2340
9	 0.9180	 0.5120
A	 0.9750	 0.4950
A0	 0.8290	 0.2950
A1	 0.8030	 0.3120
A2	 0.8030	 0.3440
A3	 0.8740	 0.4040
A4	 0.7250	 0.2000
AA	 0.9860	 0.4130
AB	 0.8660	 0.3870
AC	 0.8600	 0.4110
AD	 0.8540	 0.3920
AE	 0.8500	 0.3670
AF	 0.8340	 0.3430
AG	 0.8230	 0.3470
AH	 0.8350	 0.3760
AI	 0.8660	 0.3760
AJ	 0.8420	 0.3990
AK	 0.8900	 0.3860
AL	 0.8380	 0.3560
AM	 0.8370	 0.3410
AN	 0.8590	 0.4040
AO	 0.8880	 0.3580
AP	 0.8590	 0.3790
AQ	 0.8700	 0.3830
AR	 0.8350	 0.3220



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Chain	Atom inclusion	Q-score
AS	 0.8450	 0.3470
AT	 0.8520	 0.3780
AU	 0.8260	 0.3050
AV	 0.7720	 0.2060
AW	 0.8390	 0.3760
AX	 0.8030	 0.2660
AY	 0.8120	 0.3130
AZ	 0.8310	 0.3290
Aw	 0.8350	 0.2130
Ax	 0.8990	 0.2390
Az	 0.8330	 0.2450
B	 0.8600	 0.2520
C	 0.4210	 0.2230
D	 0.9520	 0.5180
E	 0.9440	 0.5380
F	 0.9600	 0.5550
G	 0.2660	 0.1440
H	 0.5640	 0.2670
I	 0.8120	 0.4010
J	 0.7630	 0.3010
K	 0.9580	 0.5570
L	 0.9600	 0.5090
M	 0.9490	 0.5510
N	 0.9480	 0.5270
O	 0.9500	 0.5470
OX	 0.5590	 0.3070
P	 0.9130	 0.5020
Q	 0.9250	 0.5020
R	 0.9550	 0.5530
S	 0.9410	 0.5470
T	 0.9540	 0.5630
U	 0.8460	 0.4930
V	 0.8990	 0.4970
W	 0.9260	 0.5370
X	 0.9150	 0.5200
Y	 0.9330	 0.5390
Z	 0.9430	 0.5460
a	 0.8230	 0.4550
b	 0.9490	 0.5430
c	 0.9040	 0.5050
d	 0.7960	 0.4310
e	 0.7080	 0.2090

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Chain	Atom inclusion	Q-score
f	 0.7610	 0.3010
g	 0.9350	 0.5360
h	 0.9070	 0.4840
i	 0.9660	 0.5670
j	 0.8890	 0.4870
k	 0.8300	 0.4330
l	 0.8190	 0.3780
m	 0.8010	 0.2580
n	 0.7210	 0.3600
o	 0.9610	 0.5620
p	 0.8270	 0.4470
q	 0.8010	 0.3690
r	 0.9420	 0.5390
s	 0.9310	 0.5280
t	 0.5550	 0.2160
u	 0.4220	 0.1710
z	 0.2950	 0.0970