



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 05:49 PM UTC

PDB ID : 9PRX / pdb\_00009prx  
EMDB ID : EMD-71815  
Title : In situ structure of the human mitoribosome in the A-P state from TACO1-knockout cells  
Authors : Wang, S.; Xiong, Y.; Zhang, Y.  
Deposited on : 2025-07-24  
Resolution : 3.23 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

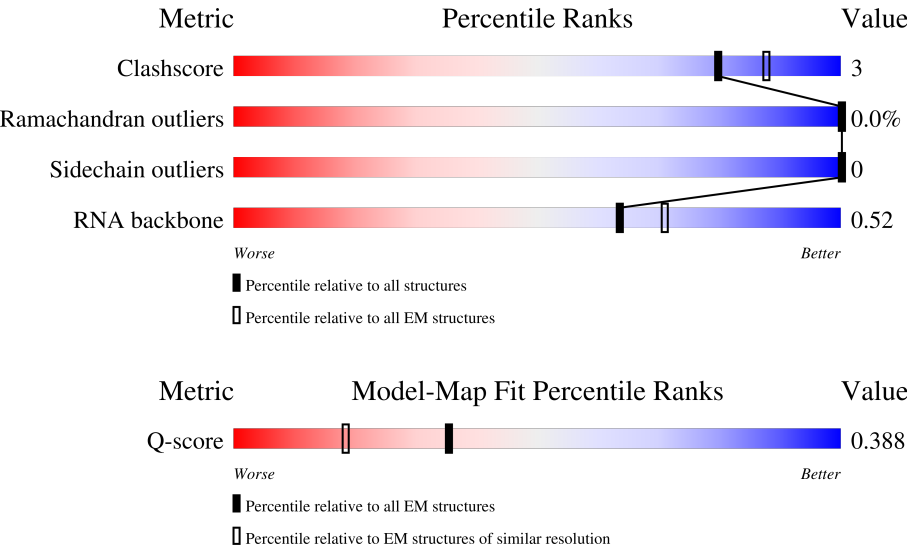
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.23 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	14612 ( 2.73 - 3.73 )

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

Mol	Chain	Length	Quality of chain
1	B	72	<div> <div>12%</div> <div>50%</div> <div>43%</div> <div>7%</div> </div>
2	0	188	<div> <div>58%</div> <div>41%</div> </div>
3	1	65	<div> <div>6%</div> <div>82%</div> <div>5%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	2	92	
5	3	188	
6	4	103	
7	5	423	
8	6	380	
9	7	338	
10	8	206	
11	9	137	
12	A	1558	
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	





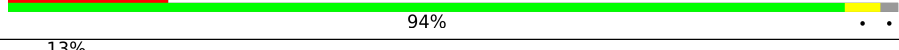

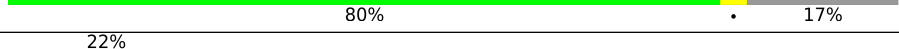
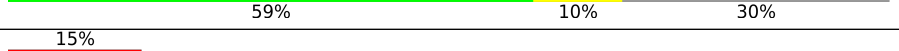
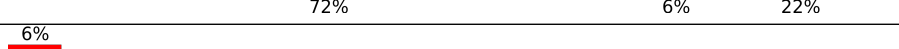
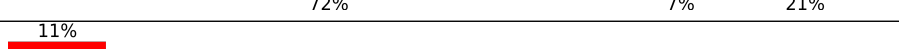
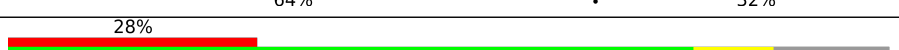

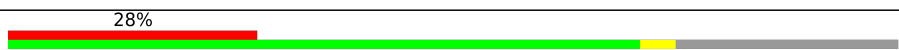

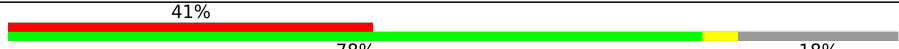

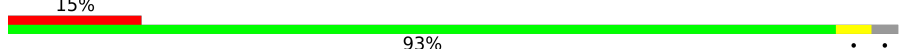



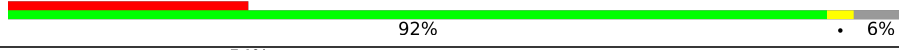




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Mol	Chain	Length	Quality of chain
29	U	153	
30	W	148	
31	X	256	
32	Y	250	
33	Z	161	
34	V	216	
35	b	215	
36	d	306	
37	e	279	
38	g	166	
39	h	158	
40	i	128	
41	j	123	
42	k	112	
43	l	138	
44	m	128	
45	n	43	
46	o	102	
47	q	222	
48	r	196	
49	t	198	
49	u	198	
50	c	332	
51	f	212	
52	p	206	

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Mol	Chain	Length	Quality of chain
53	s	439	
54	AB	296	
55	AC	167	
56	AD	430	
57	AE	125	
58	AF	242	
59	AG	396	
60	AH	201	
61	AJ	138	
62	AK	128	
63	AL	257	
64	AM	137	
65	AN	130	
66	AO	258	
67	AP	142	
68	AR	360	
69	AS	190	
70	AT	173	
71	AU	205	
72	AV	414	
73	AW	187	
74	AZ	106	
75	A0	217	
76	A1	323	
77	A3	199	

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Mol	Chain	Length	Quality of chain
78	Az	34	
79	AY	395	
80	AA	954	
81	AI	194	
82	OX	435	
83	a	142	
84	Ax	71	
85	Aw	76	
86	A4	689	
87	AX	398	
88	A2	118	
89	AQ	87	

## 2 Entry composition

There are 100 unique types of molecules in this entry. The entry contains 177884 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 RNA chain called mitochondrial tRNAVal.

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

- Molecule 2 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 3 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	56	Total	C	N	O	S	0	0
			464	296	89	77	2		

- Molecule 4 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 5 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 6 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 7 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 8 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 9 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 10 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	8	157	Total	C	N	O	S	0	0
			1327	844	235	246	2		

- Molecule 11 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 12 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	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 13 is a protein called 39S ribosomal protein L2, mitochondrial.



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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 20 is a protein called 39S ribosomal protein L14, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 34 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L49, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 42 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	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 43 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 45 is a protein called Nascent polypeptide.

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

- Molecule 46 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 47 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	t	46	Total	C	N	O	0	0
			354	228	56	70		
49	u	32	Total	C	N	O	0	0
			257	168	40	49		

- Molecule 50 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 52 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 54 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 55 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 56 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 58 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 60 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 61 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 62 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 63 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 64 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 65 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 66 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 67 is a protein called 28S ribosomal protein S18c, mitochondrial.



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

- Molecule 68 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 69 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 71 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 72 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 73 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 74 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 75 is a protein called Small ribosomal subunit protein mS34.

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

- Molecule 76 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 77 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 78 is a RNA chain called mRNA.

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

- Molecule 79 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 80 is a RNA chain called 12S mitochondrial rRNA.

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

- Molecule 81 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 82 is a protein called Mitochondrial inner membrane protein OXA1L.

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

- Molecule 83 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 84 is a RNA chain called P/P-tRNA.

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

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

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

- Molecule 86 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 87 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 88 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	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

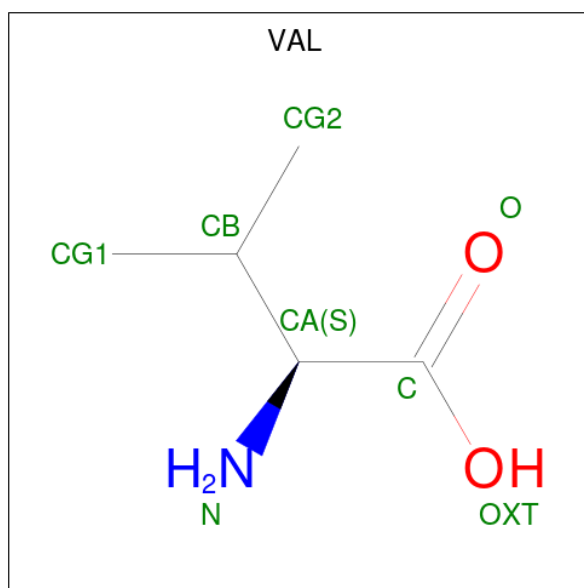
- Molecule 89 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	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 90 is VALINE (CCD ID: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



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

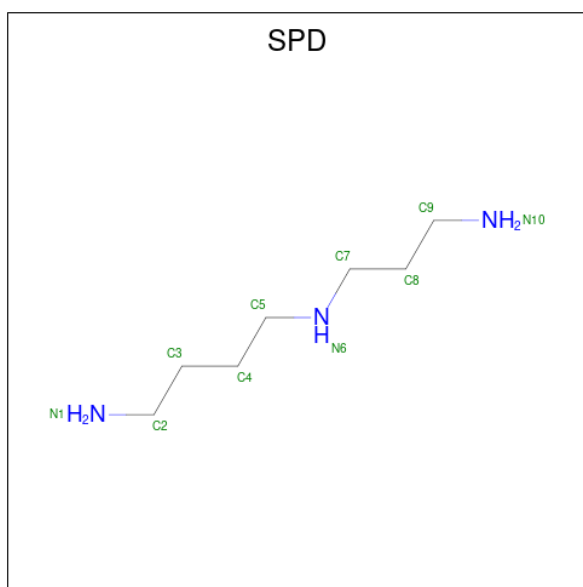
- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	0	1	Total 1	Zn 1	0
91	4	1	Total 1	Zn 1	0
91	AO	1	Total 1	Zn 1	0

- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K).

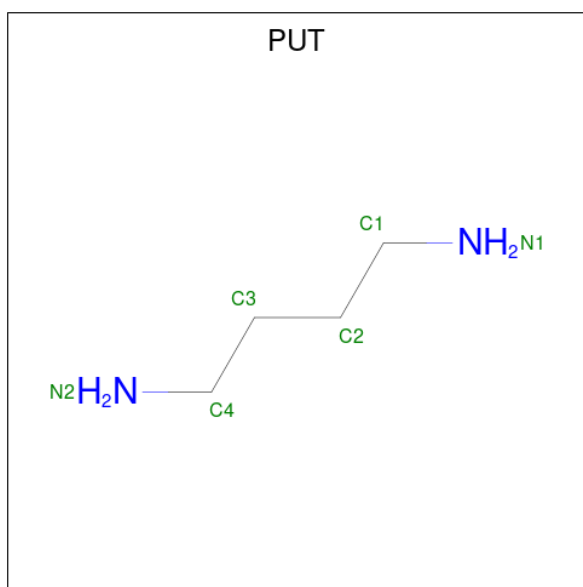
Mol	Chain	Residues	Atoms		AltConf
92	6	1	Total 1	K 1	0
92	A	29	Total 29	K 29	0
92	D	1	Total 1	K 1	0
92	M	2	Total 2	K 2	0
92	N	1	Total 1	K 1	0
92	W	1	Total 1	K 1	0
92	o	1	Total 1	K 1	0
92	AJ	1	Total 1	K 1	0
92	AA	17	Total 17	K 17	0

- Molecule 93 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 94 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



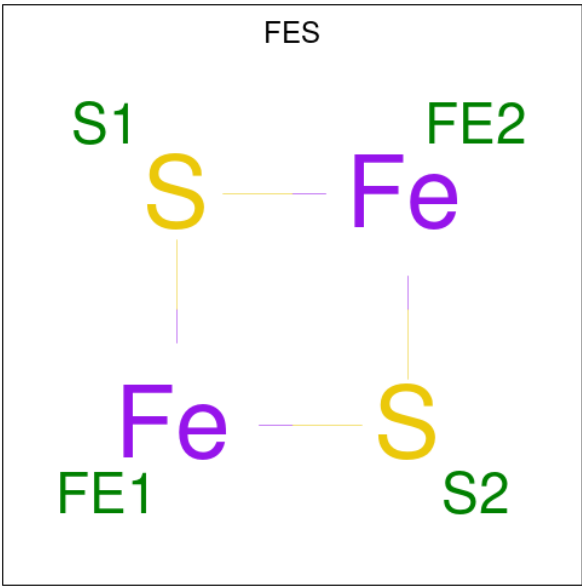
Mol	Chain	Residues	Atoms			AltConf
94	A	1	Total	C	N	0
			6	4	2	

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

Mol	Chain	Residues	Atoms		AltConf
95	A	136	Total	Mg	0
			136	136	
95	D	2	Total	Mg	0
			2	2	
95	E	1	Total	Mg	0
			1	1	
95	W	1	Total	Mg	0
			1	1	
95	g	1	Total	Mg	0
			1	1	
95	AB	1	Total	Mg	0
			1	1	
95	A3	1	Total	Mg	0
			1	1	
95	Az	1	Total	Mg	0
			1	1	
95	AA	59	Total	Mg	0
			59	59	
95	AX	1	Total	Mg	0
			1	1	

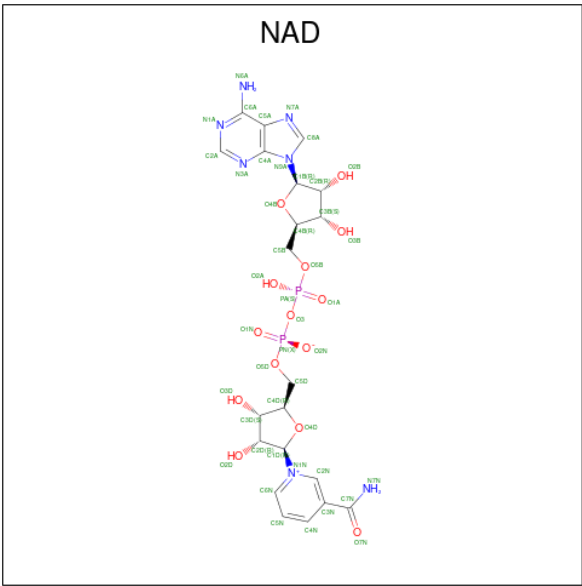
- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled

as "Ligand of Interest" by depositor).



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

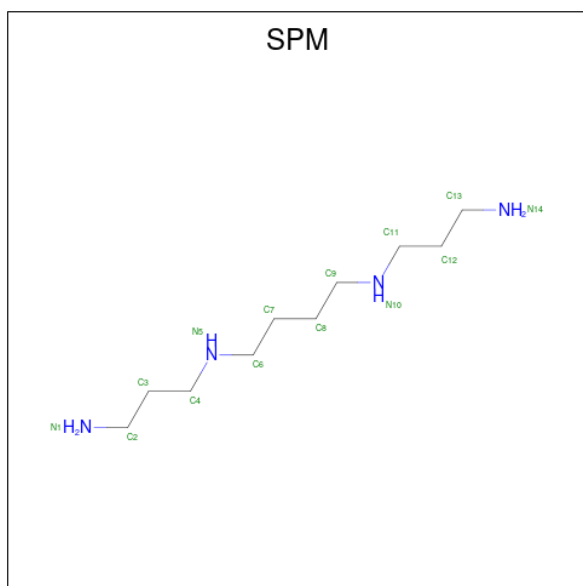
- Molecule 97 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by depositor).





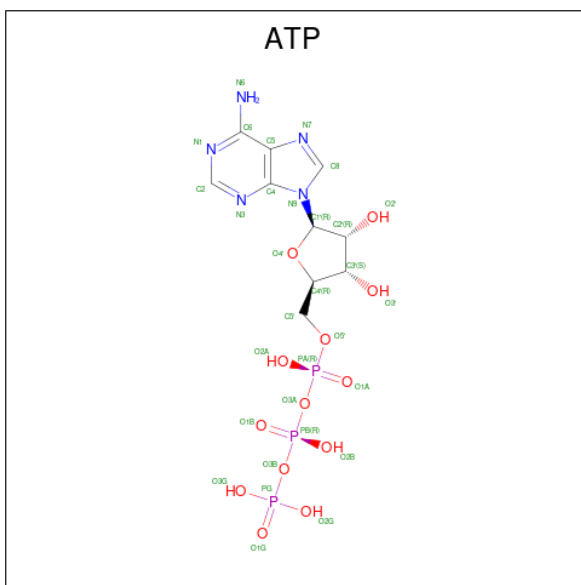
Mol	Chain	Residues	Atoms					AltConf
97	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 98 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ) (labeled as "Ligand of Interest" by depositor).



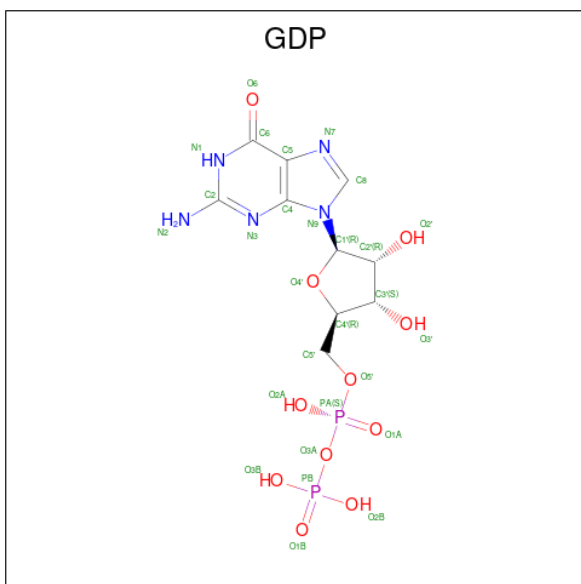
Mol	Chain	Residues	Atoms				AltConf
98	AA	1	Total	C	N		0
			14	10	4		
98	AA	1	Total	C	N		0
			14	10	4		

- Molecule 99 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
99	AX	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 100 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).

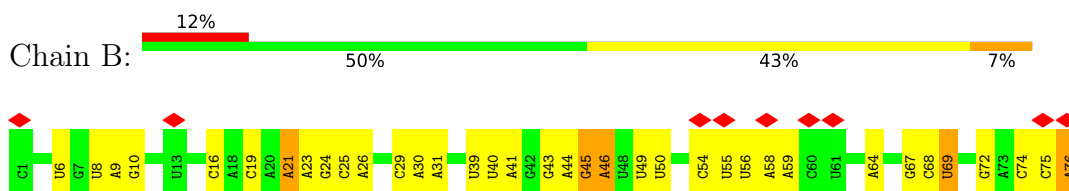


Mol	Chain	Residues	Atoms					AltConf
100	AX	1	Total 28	C 10	N 5	O 11	P 2	0

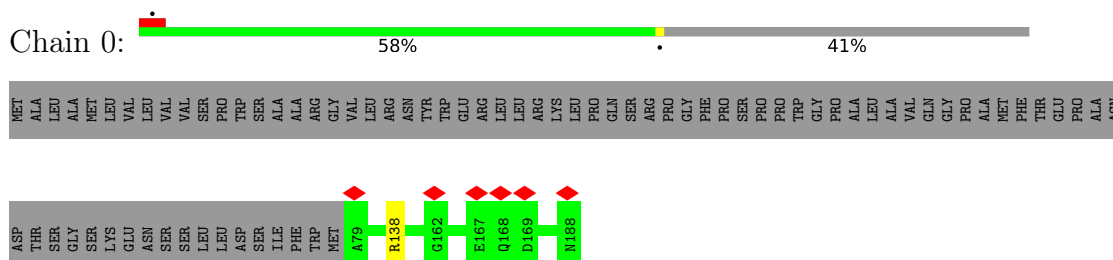
### 3 Residue-property plots [i](#)

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.

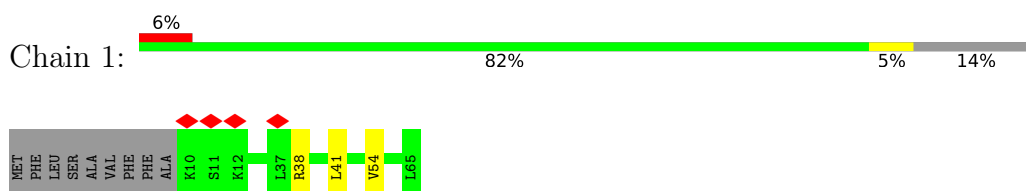
- Molecule 1: mitochondrial tRNAVal



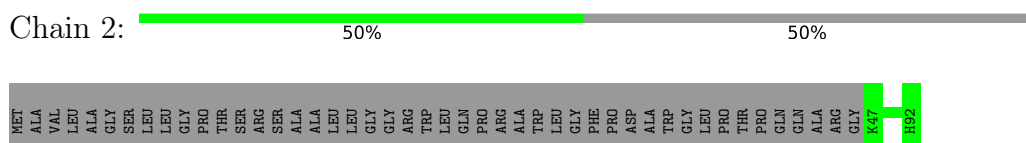
- Molecule 2: 39S ribosomal protein L32, mitochondrial



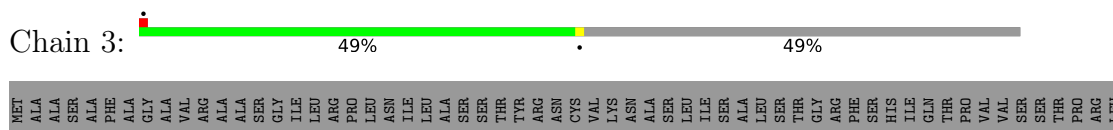
- Molecule 3: 39S ribosomal protein L33, mitochondrial

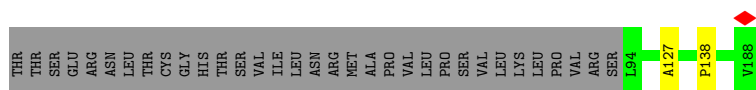


- Molecule 4: 39S ribosomal protein L34, mitochondrial

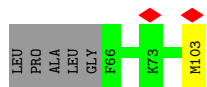
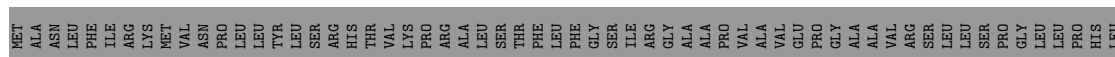


- Molecule 5: 39S ribosomal protein L35, mitochondrial

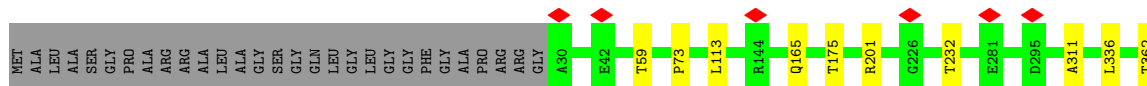
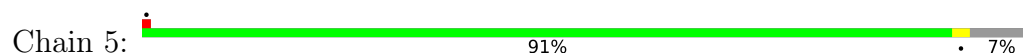




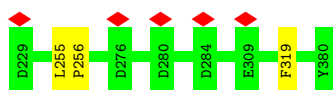
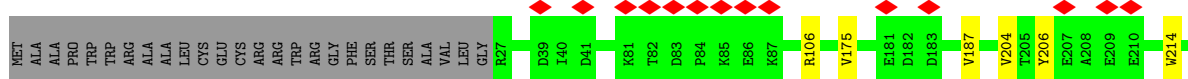
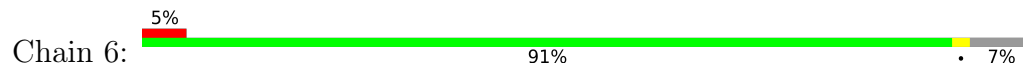
- Molecule 6: 39S ribosomal protein L36, mitochondrial



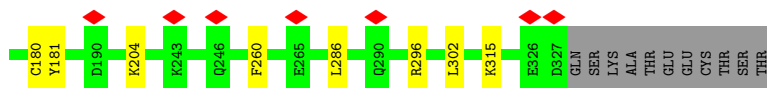
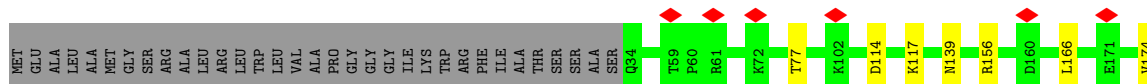
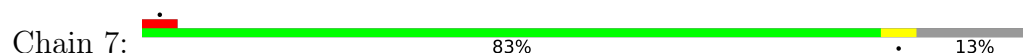
- Molecule 7: 39S ribosomal protein L37, mitochondrial



- Molecule 8: 39S ribosomal protein L38, mitochondrial

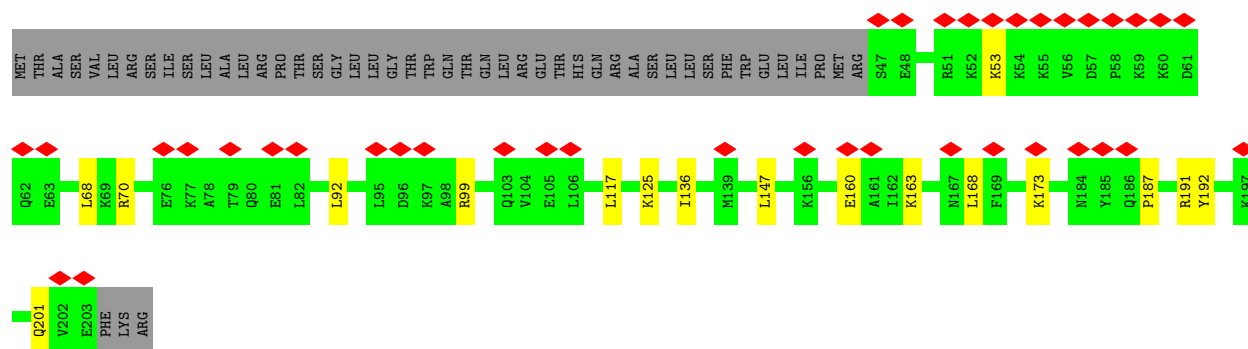


- Molecule 9: 39S ribosomal protein L39, mitochondrial

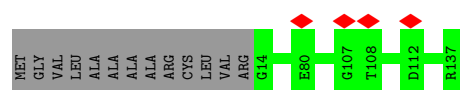


- Molecule 10: 39S ribosomal protein L40, mitochondrial

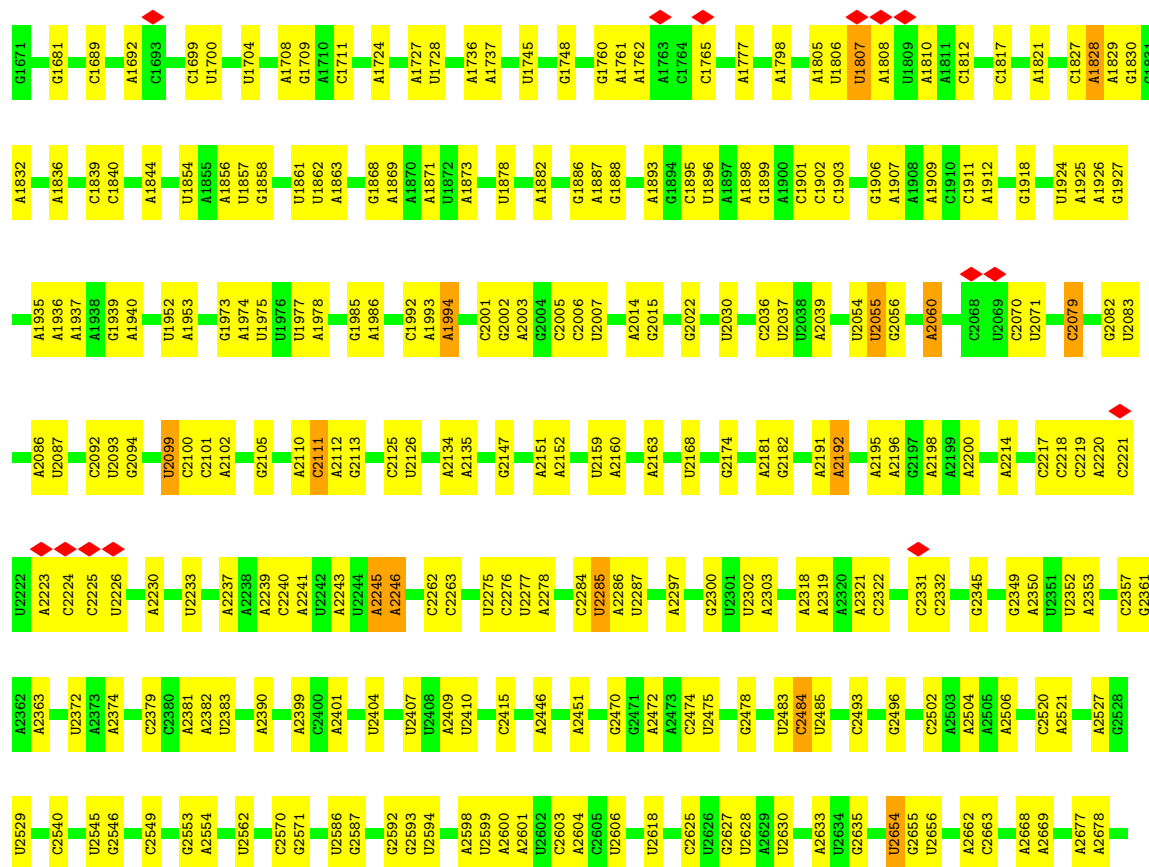


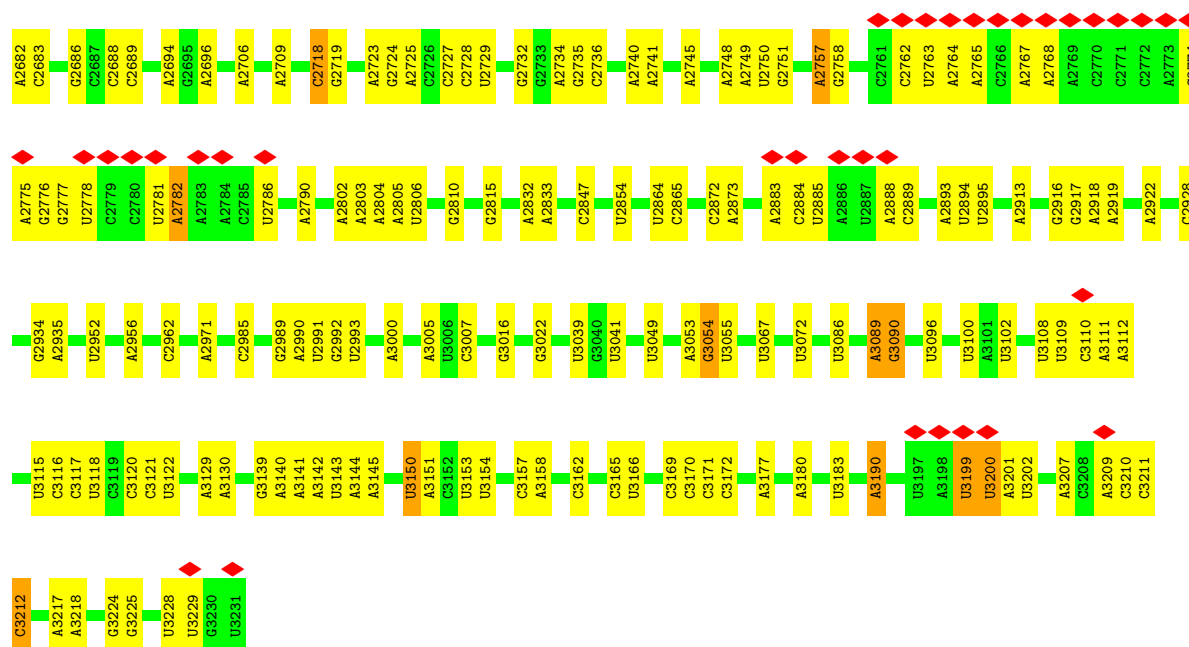


- Molecule 11: 39S ribosomal protein L41, mitochondrial

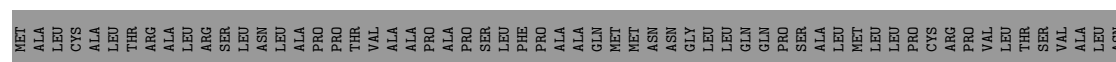
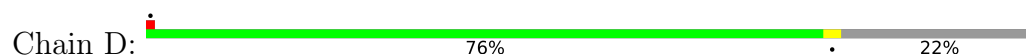


- Molecule 12: 16S mitochondrial rRNA

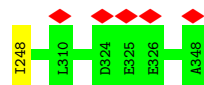
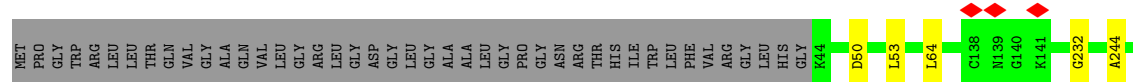
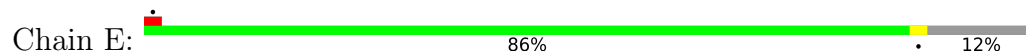




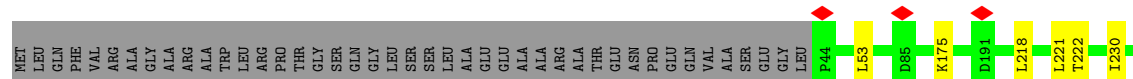
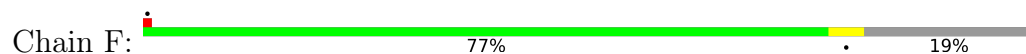
- Molecule 13: 39S ribosomal protein L2, mitochondrial



- Molecule 14: 39S ribosomal protein L3, mitochondrial



- Molecule 15: 39S ribosomal protein L4, mitochondrial




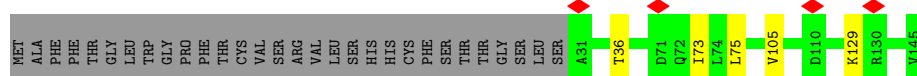


Chain K:  96%



- Molecule 20: 39S ribosomal protein L14, mitochondrial

Chain L:  76% 21%




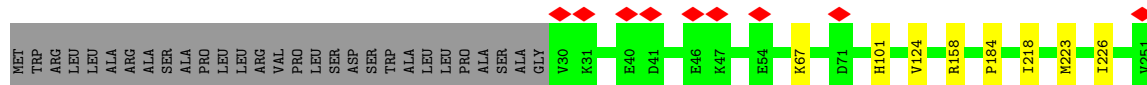
- Molecule 21: 39S ribosomal protein L15, mitochondrial

Chain M:  94% 5%




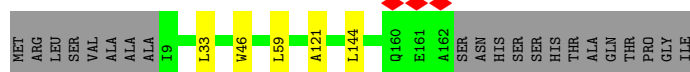
- Molecule 22: 39S ribosomal protein L16, mitochondrial

Chain N:  85% 12%




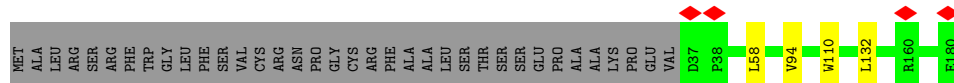
- Molecule 23: 39S ribosomal protein L17, mitochondrial

Chain O:  85% 12%




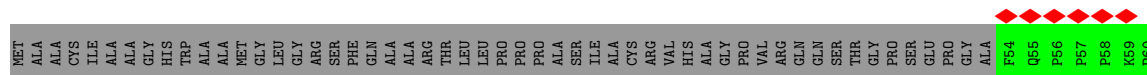
- Molecule 24: 39S ribosomal protein L18, mitochondrial

Chain P:  78% 20%



- Molecule 25: 39S ribosomal protein L19, mitochondrial

Chain Q:  8% 78% 18%



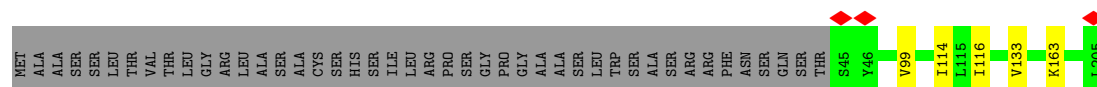
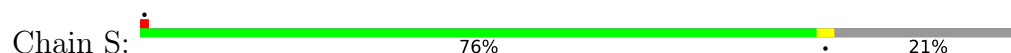




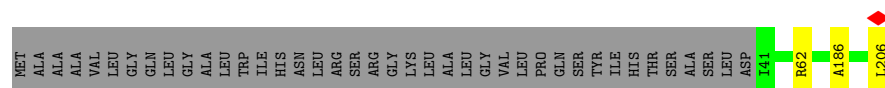
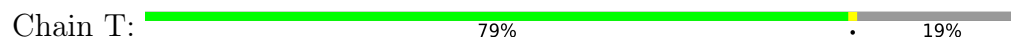
- Molecule 26: 39S ribosomal protein L20, mitochondrial



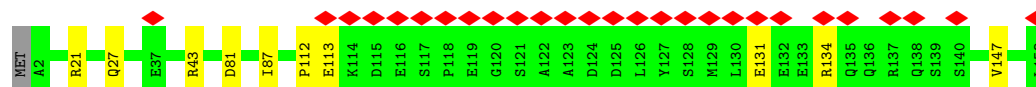
- Molecule 27: 39S ribosomal protein L21, mitochondrial



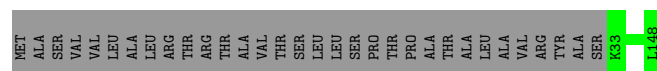
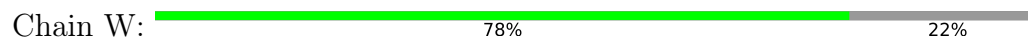
- Molecule 28: 39S ribosomal protein L22, mitochondrial



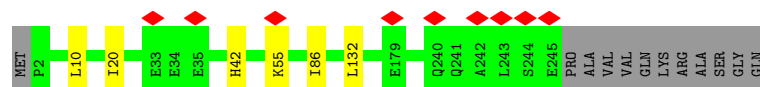
- Molecule 29: 39S ribosomal protein L23, mitochondrial



- Molecule 30: 39S ribosomal protein L27, mitochondrial



- Molecule 31: 39S ribosomal protein L28, mitochondrial



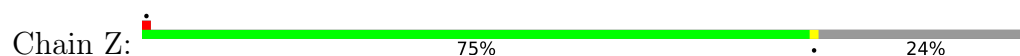
- Molecule 32: 39S ribosomal protein L47, mitochondrial



MET ALA ALA ALA GLY LEU ALA LEU LEU CYS ARG ARG VAL SER SER ALA LEU LYS SER ARG ARG ILE LEU THR PRO GLN VAL PRO ALA CYS THR GLY PHE LEU SER LEU PRO LYS SER THR PRO ASN VAL THR SER PHE HIS GLN TYR ARG LEU THR HIS THR SER

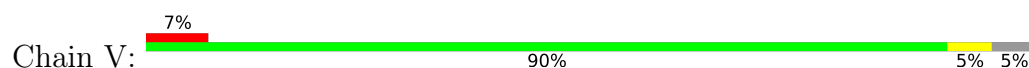
ARG LYS G53 E77 V146 I176 A242 E243 ALA GLN LYS SER SER LEU VAL

- Molecule 33: 39S ribosomal protein L30, mitochondrial



MET ALA GLY ILE LEU ARG LEU VAL VAL GLN TRP PRO PRO GLY ARG LEU GLN THR VAL THR LYS GLY VAL GLU SER LEU ILE CYS THR ASP TRP ILE ARG HIS K35 V99 Q156 LYS ALA HIS GLU SER

- Molecule 34: 39S ribosomal protein L24, mitochondrial



MET ARG LEU SER ALA LEU ALA LEU ALA ALA K12 V13 T14 H18 E52 Y55 E66 G67 K69 V79 I80 W85 V86 M102 D103 R128 I133 T138 E139 A140 G141 E142 A162 D163 E168 D181 Y216

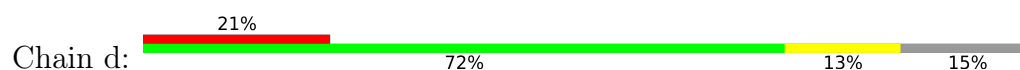
- Molecule 35: 39S ribosomal protein L43, mitochondrial



MET T2 D106 F119 R146 Q149 D150 P151 ALA PRO ALA ALA GLN ASP THR GLY LEU ARG LEU SER LEU ALA VAL VAL THR THR VAL CYS SER ALA

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

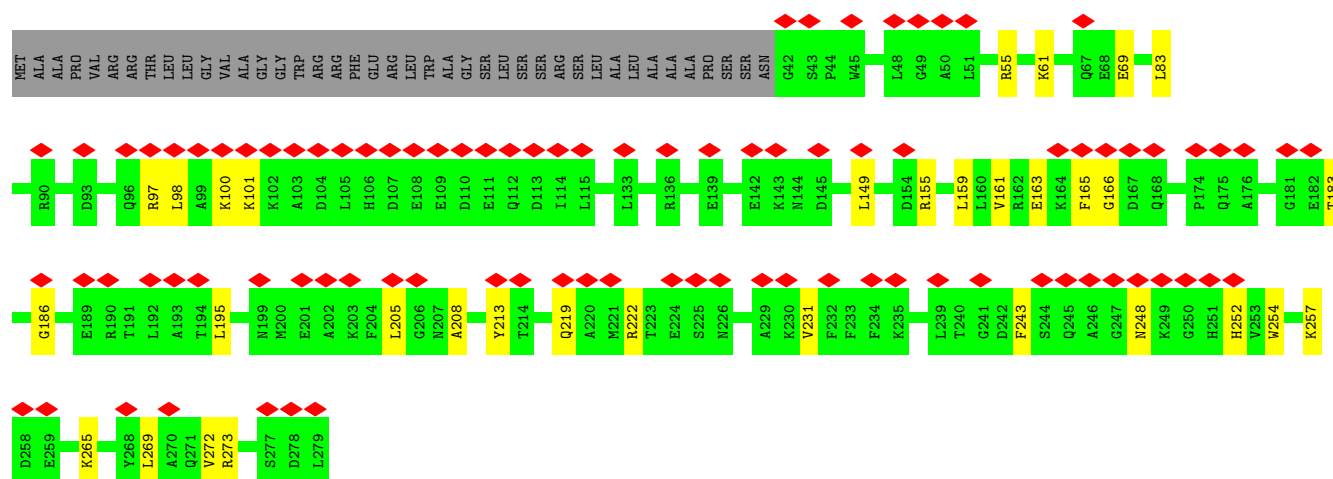
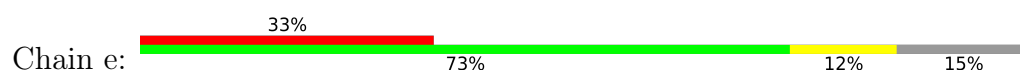
- Molecule 36: 39S ribosomal protein L45, mitochondrial



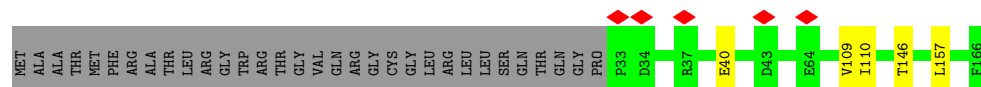
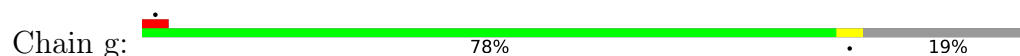
MET ALA ALA PRO ILE GLN GLY PHE SER CYS LEU SER ARG ARG PHE LEU LEU GLY TRP TRP PHE ARG GLN PRO VAL LEU VAL THR GLN SER ALA ALA ILE VAL PRO VAL ARG T37 K38 K39 R40 F41 T42 P43 P44 I45 Y46 Q47 P48 K49 F50 K51 T52 E53 K54 E55 F56 V66 I67 P68

P69 E70 K71 S72 D73 D86 A87 Y88 P89 P90 P91 E92 G93 D94 A95 R96 I97 S98 S99 L231 L100 S101 K102 E103 G104 L105 I106 I107 R108 T109 E110 R111 M112 K113 K114 S121 I122 R123 R124 I125 K126 D127 Y128 D129 A130 M131 P138 L160 V164 V186 E187 V194 V197

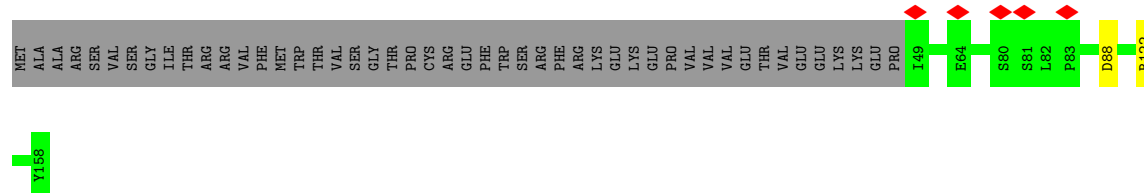
- Molecule 37: 39S ribosomal protein L46, mitochondrial



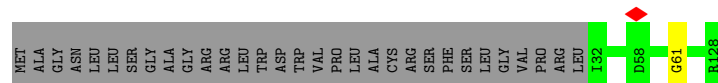
- Molecule 38: 39S ribosomal protein L49, mitochondrial



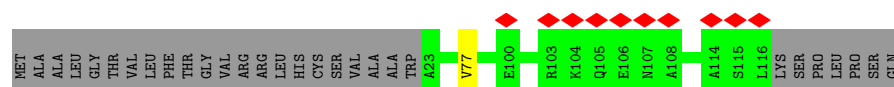
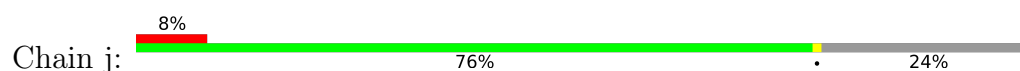
- Molecule 39: 39S ribosomal protein L50, mitochondrial



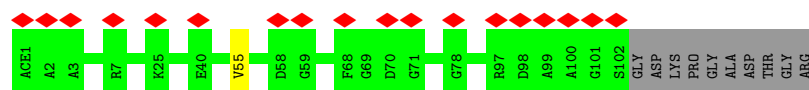
- Molecule 40: 39S ribosomal protein L51, mitochondrial



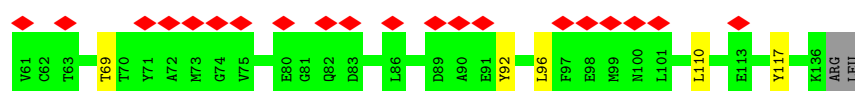
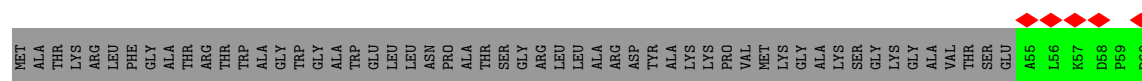
- Molecule 41: 39S ribosomal protein L52, mitochondrial



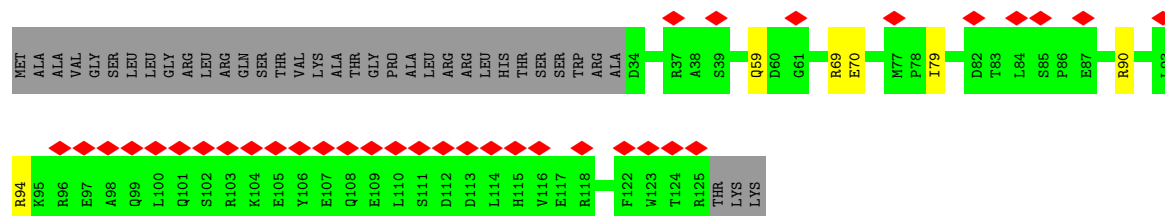
- Molecule 42: Large ribosomal subunit protein mL53



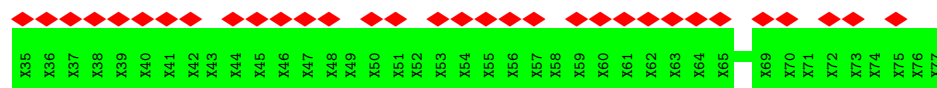
- Molecule 43: 39S ribosomal protein L54, mitochondrial



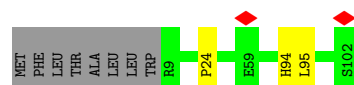
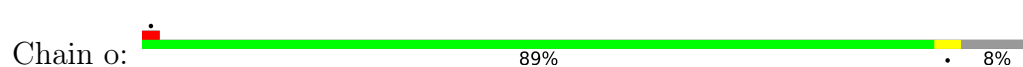
- Molecule 44: 39S ribosomal protein L55, mitochondrial



- Molecule 45: Nascent polypeptide



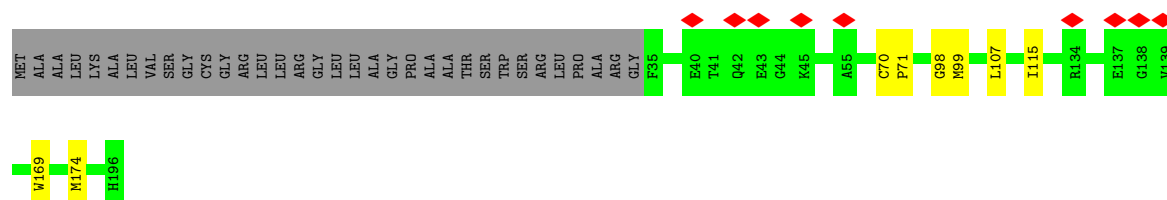
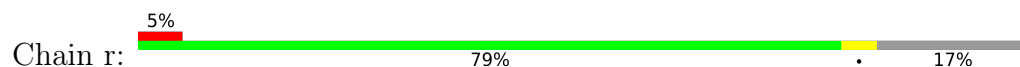
- Molecule 46: Ribosomal protein 63, mitochondrial



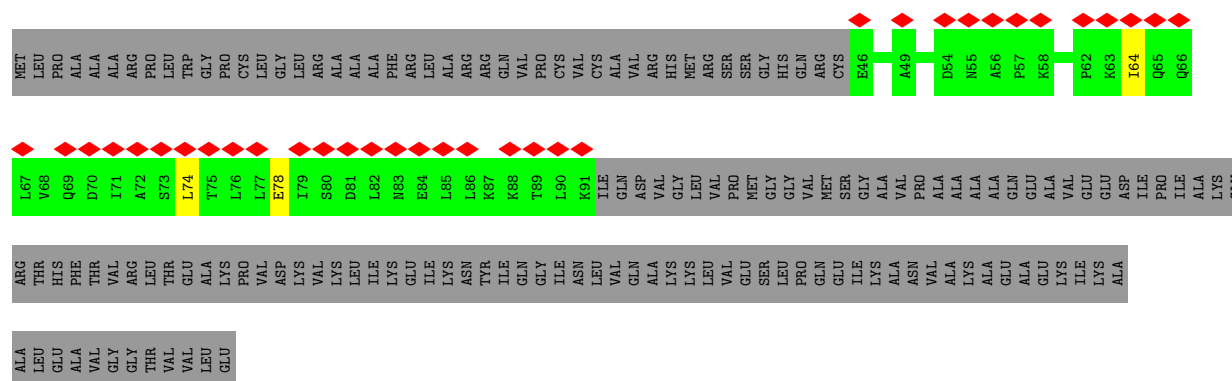
- Molecule 47: Growth arrest and DNA damage-inducible proteins-interacting protein 1



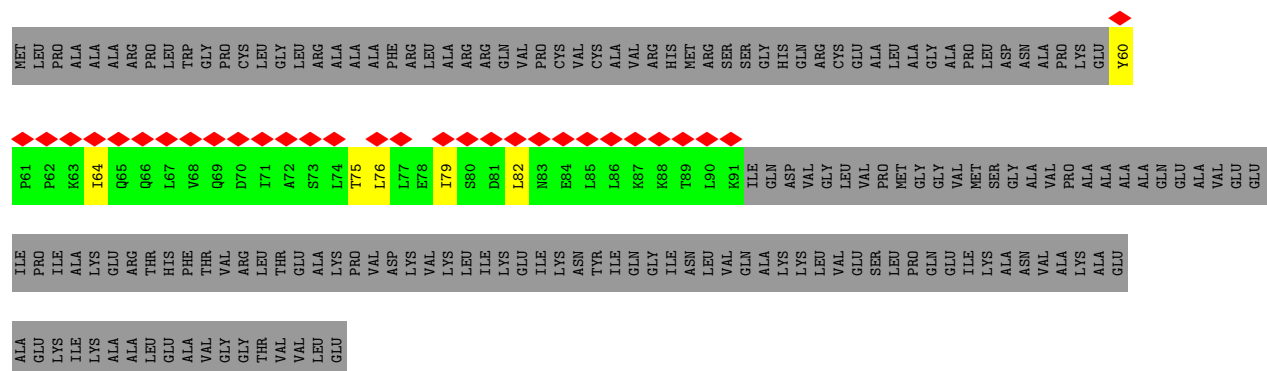
- Molecule 48: 39S ribosomal protein S18a, mitochondrial




- Molecule 49: 39S ribosomal protein L12, mitochondrial

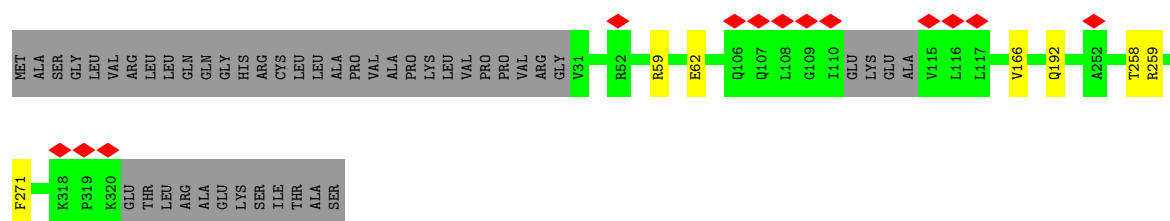


- Molecule 49: 39S ribosomal protein L12, mitochondrial



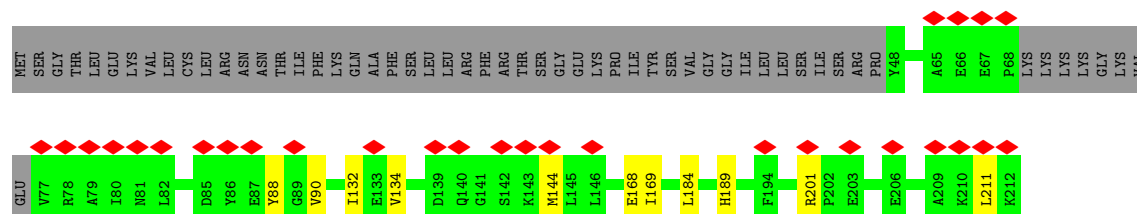
- Molecule 50: 39S ribosomal protein L44, mitochondrial

Chain c: 



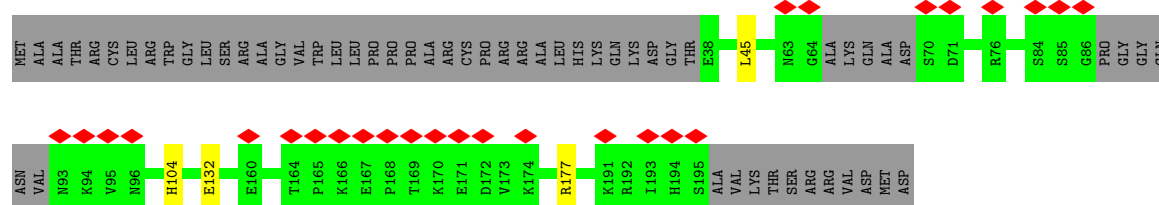
- Molecule 51: 39S ribosomal protein L48, mitochondrial

Chain f: 




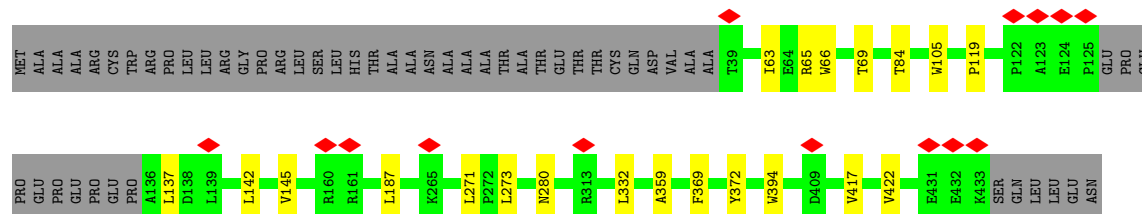
- Molecule 52: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p: 




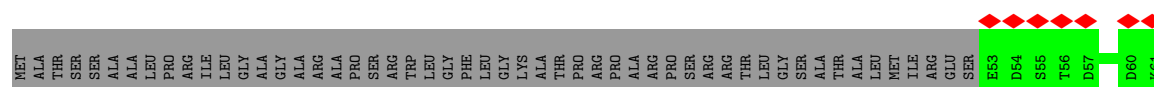
- Molecule 53: 39S ribosomal protein S30, mitochondrial

Chain s: 

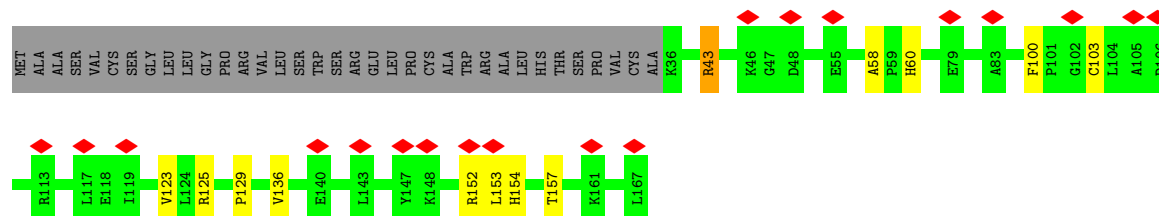


- Molecule 54: 28S ribosomal protein S2, mitochondrial

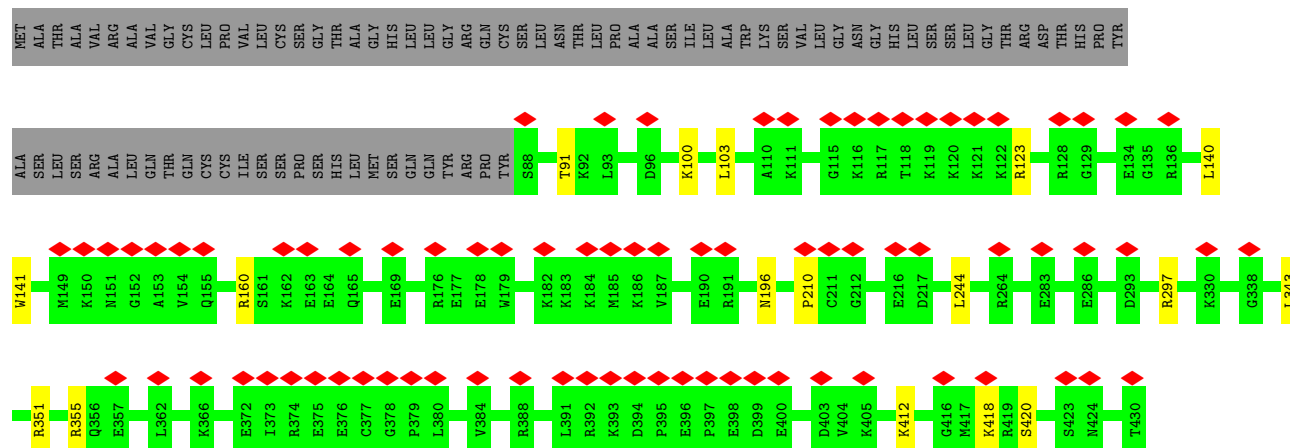
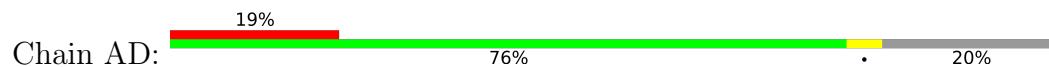
Chain AB: 



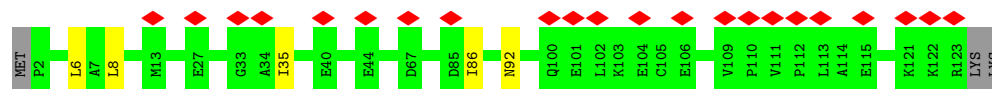
- Molecule 55: 28S ribosomal protein S24, mitochondrial



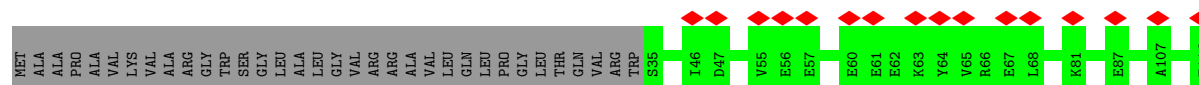
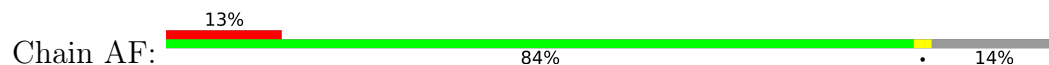
- Molecule 56: 28S ribosomal protein S5, mitochondrial

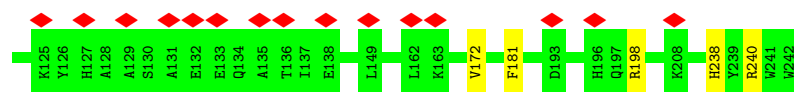


- Molecule 57: 28S ribosomal protein S6, mitochondrial



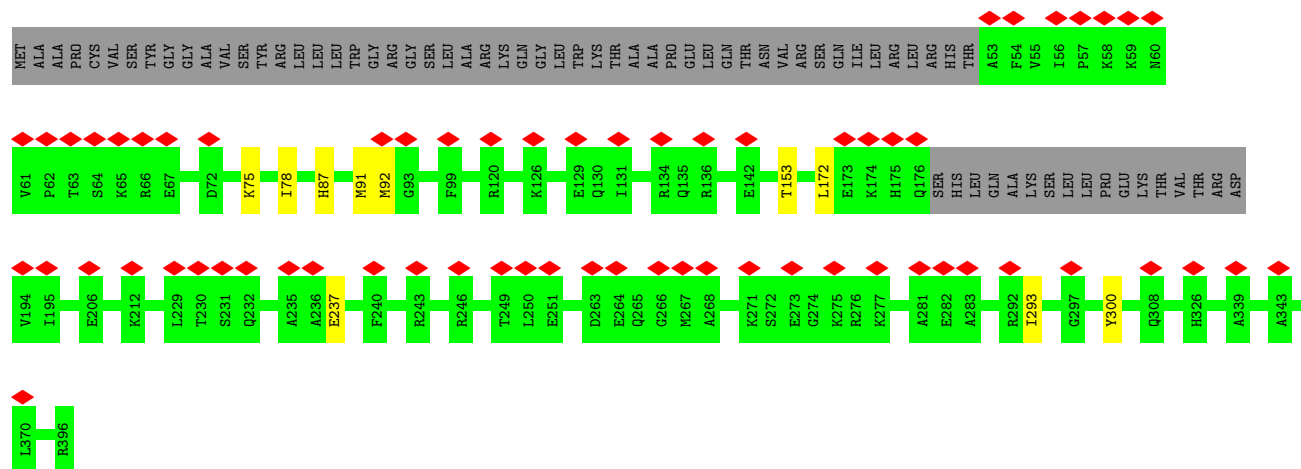
- Molecule 58: 28S ribosomal protein S7, mitochondrial





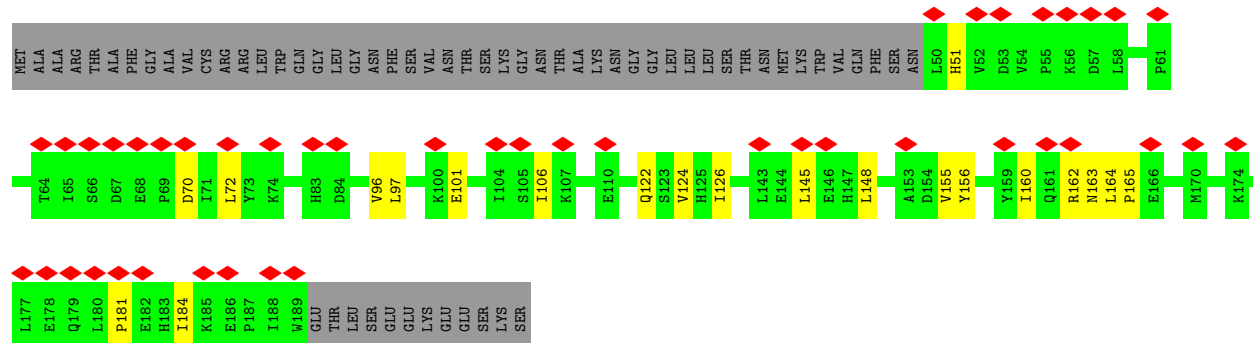
- Molecule 59: 28S ribosomal protein S9, mitochondrial

Chain AG: 16% 80% 17%



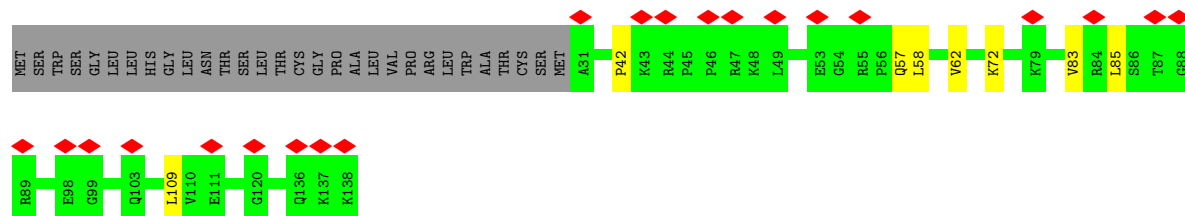
- Molecule 60: 28S ribosomal protein S10, mitochondrial

Chain AH: 22% 59% 10% 30%



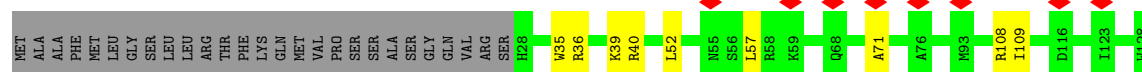
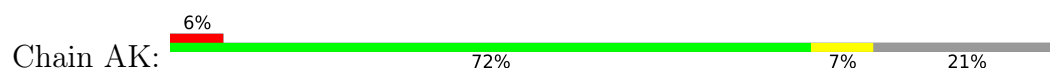
- Molecule 61: 28S ribosomal protein S12, mitochondrial

Chain AJ: 15% 72% 6% 22%

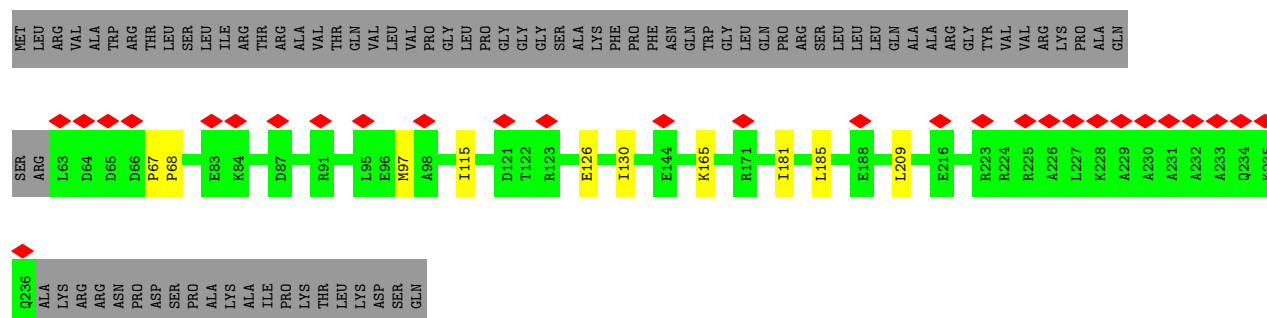


- Molecule 62: 28S ribosomal protein S14, mitochondrial

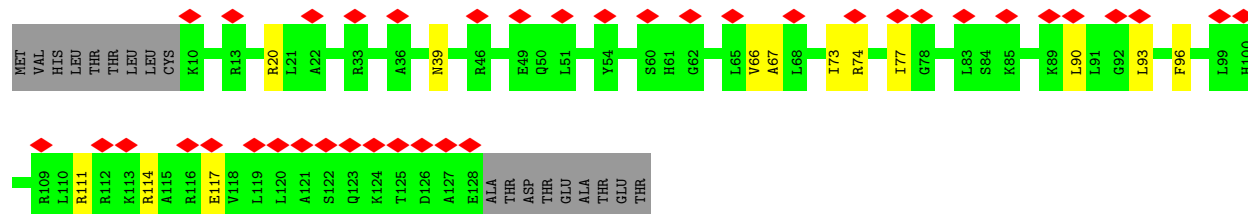
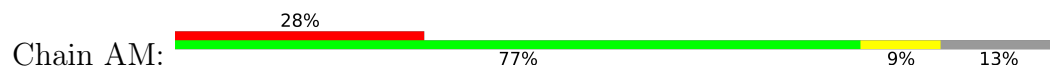




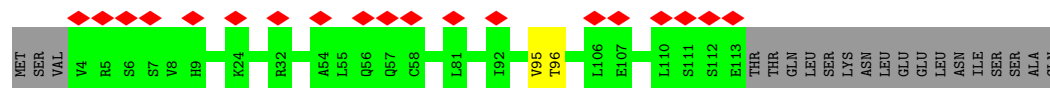
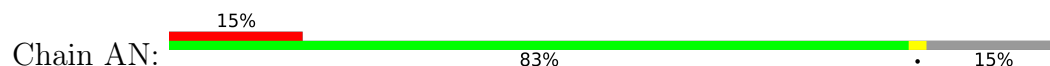
- Molecule 63: 28S ribosomal protein S15, mitochondrial



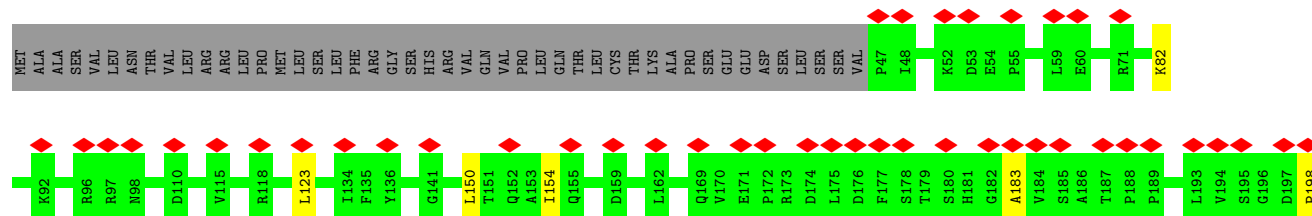
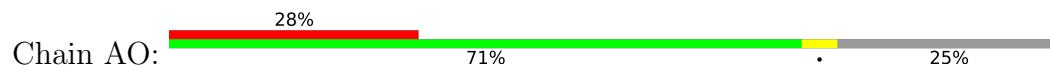
- Molecule 64: 28S ribosomal protein S16, mitochondrial



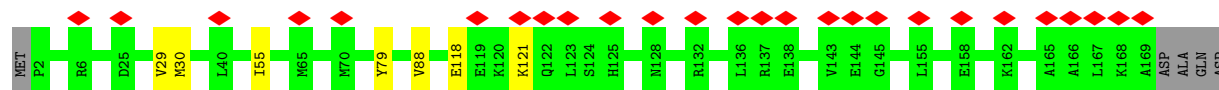
- Molecule 65: 28S ribosomal protein S17, mitochondrial



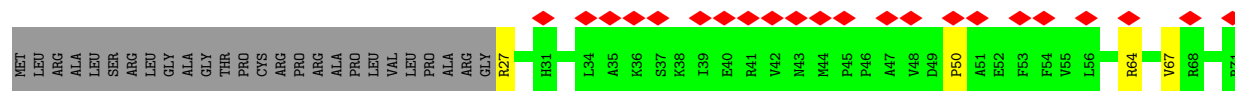
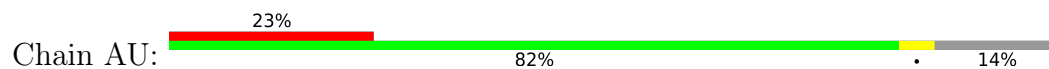
- Molecule 66: 28S ribosomal protein S18b, mitochondrial



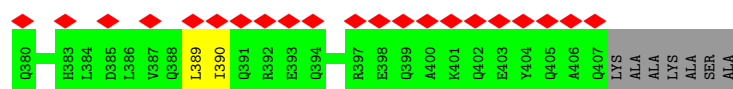
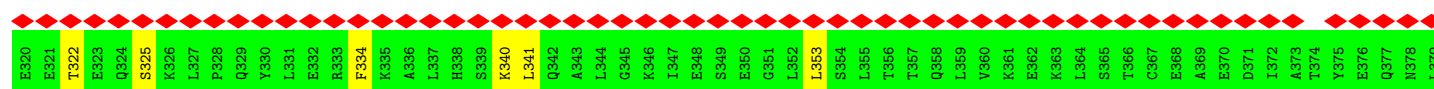
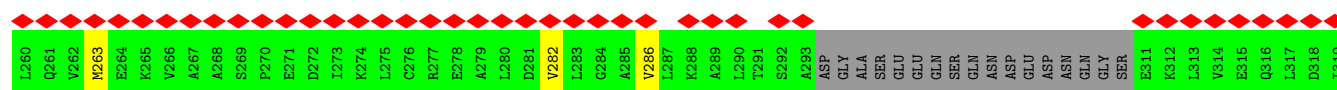
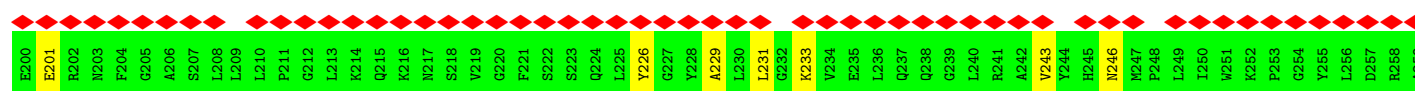
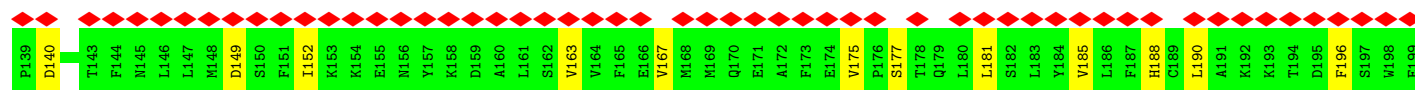
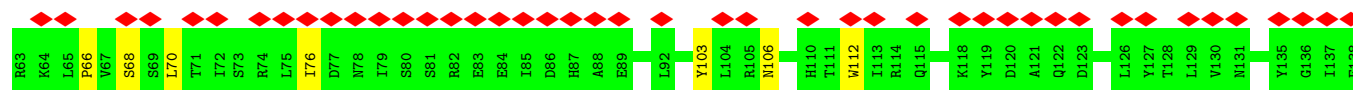
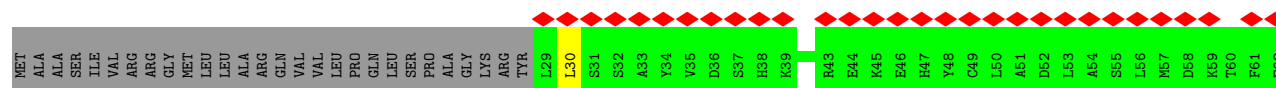
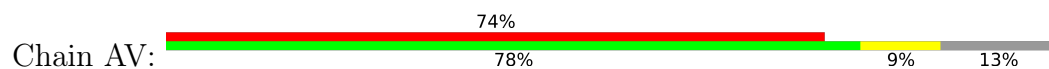




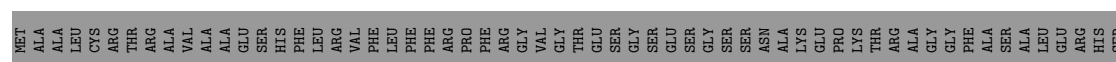
- Molecule 71: 28S ribosomal protein S26, mitochondrial

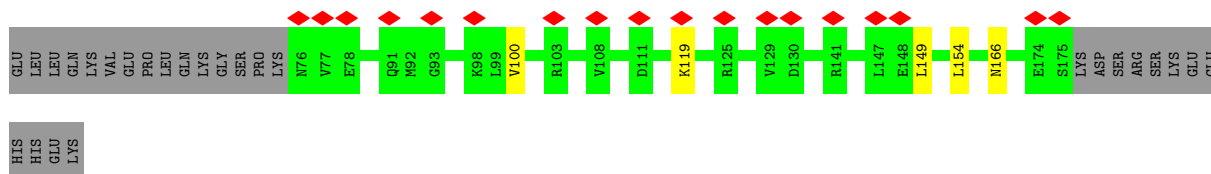


- Molecule 72: 28S ribosomal protein S27, mitochondrial



- Molecule 73: 28S ribosomal protein S28, mitochondrial

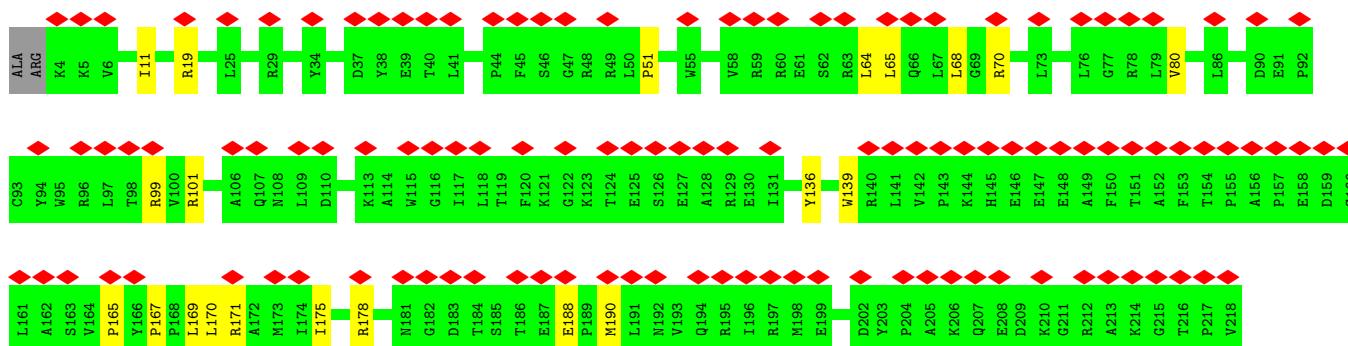
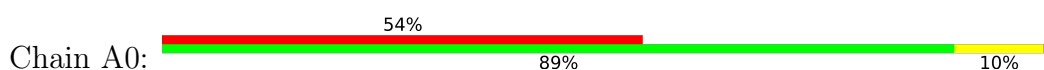




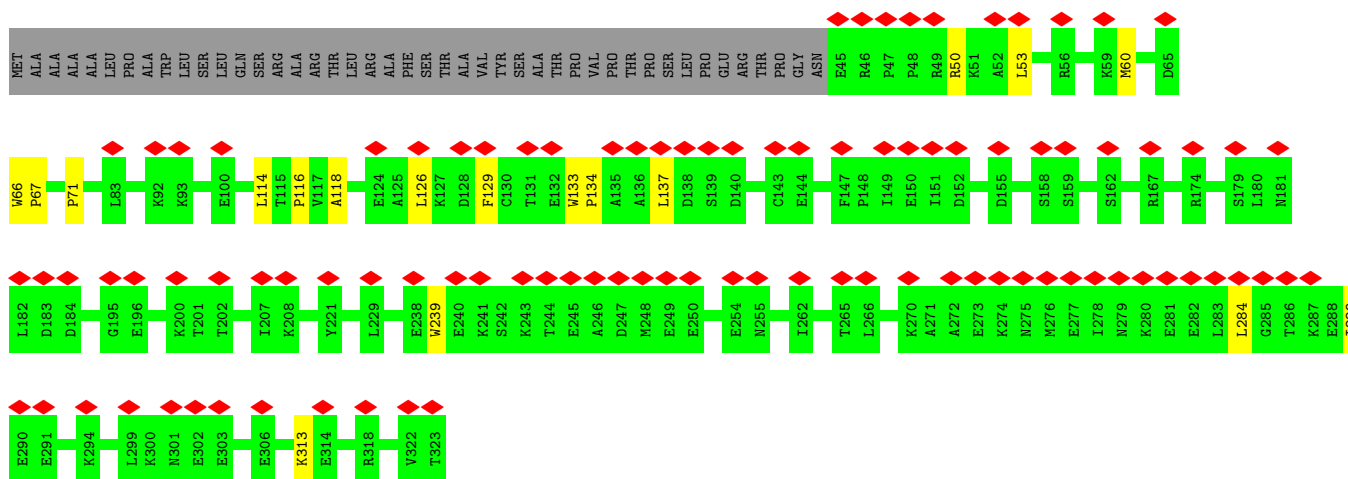
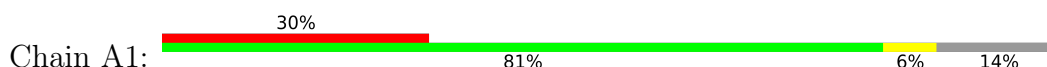
- Molecule 74: 28S ribosomal protein S33, mitochondrial



- Molecule 75: Small ribosomal subunit protein mS34



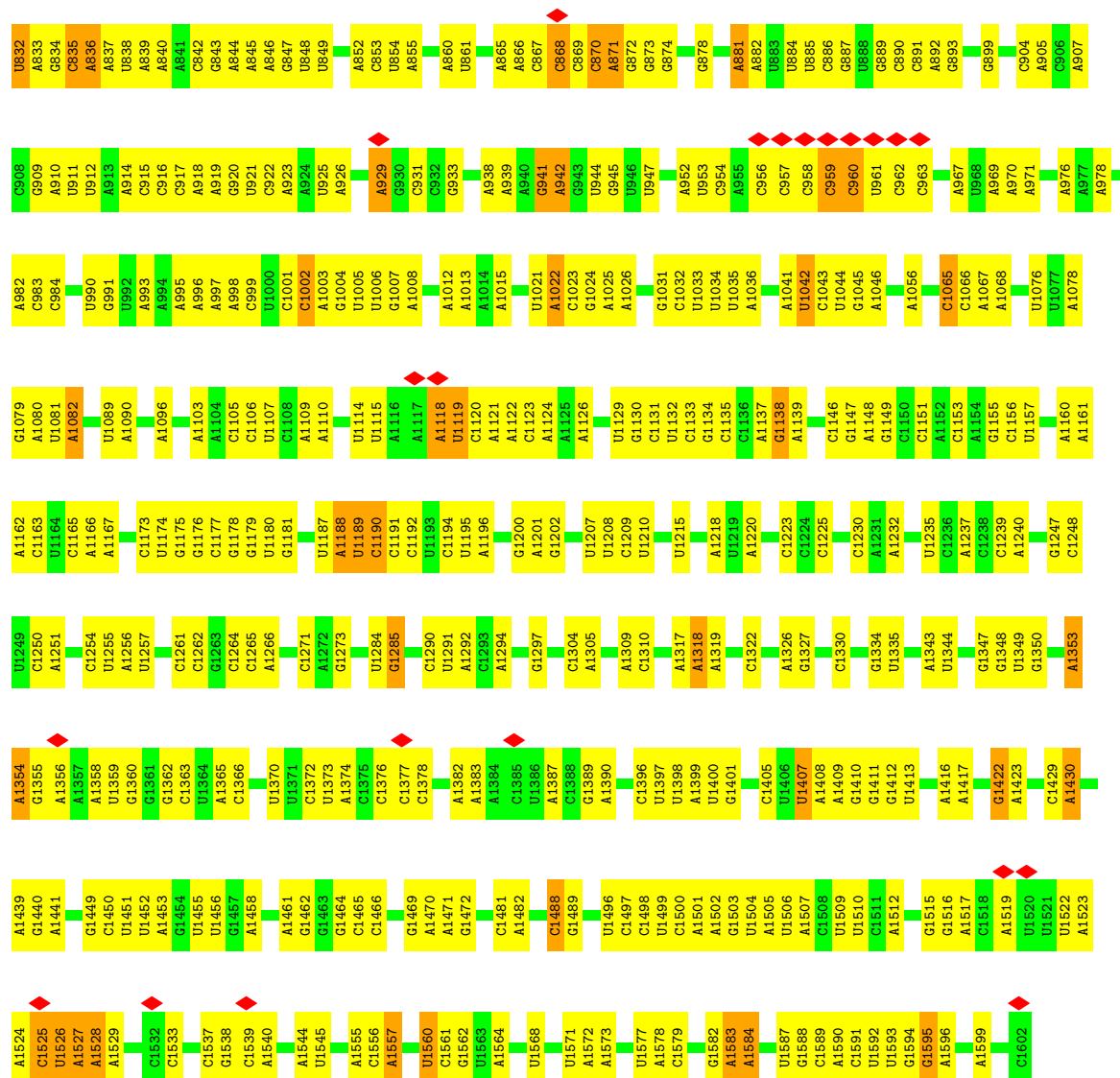
- Molecule 76: 28S ribosomal protein S35, mitochondrial



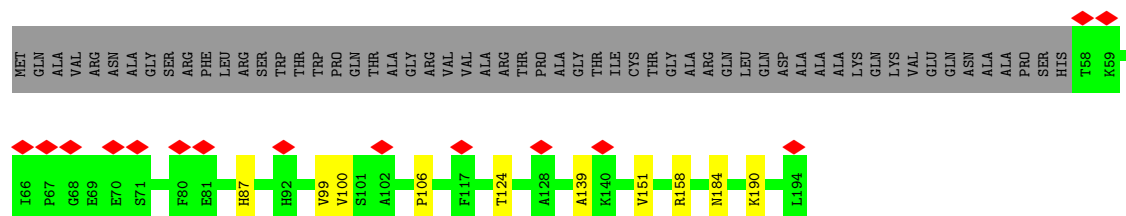
- Molecule 77: Aurora kinase A-interacting protein



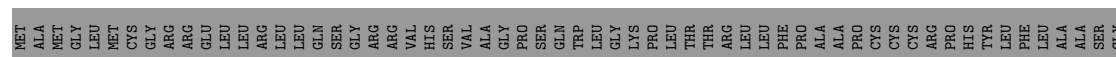




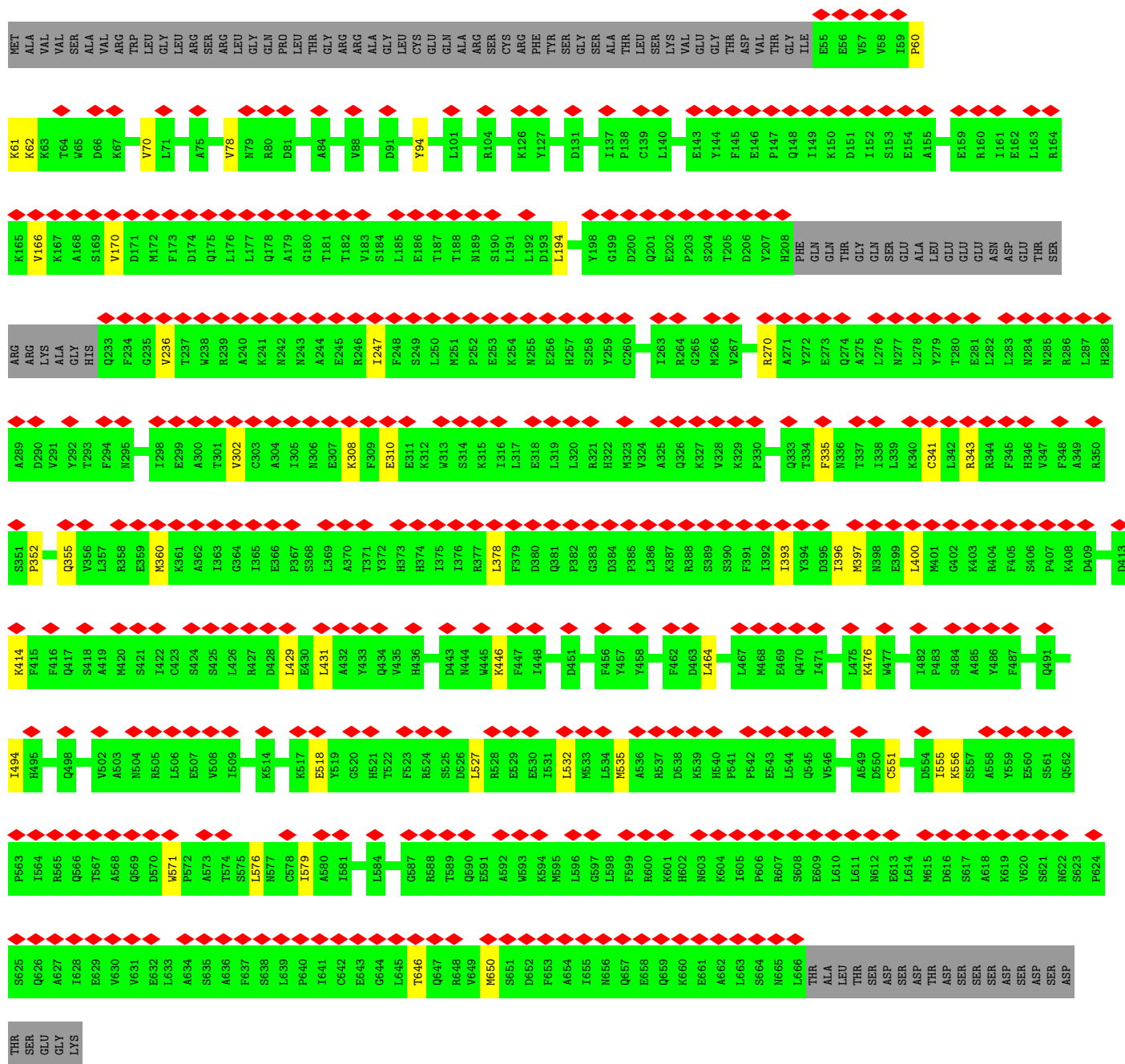
- Molecule 81: 28S ribosomal protein S11, mitochondrial



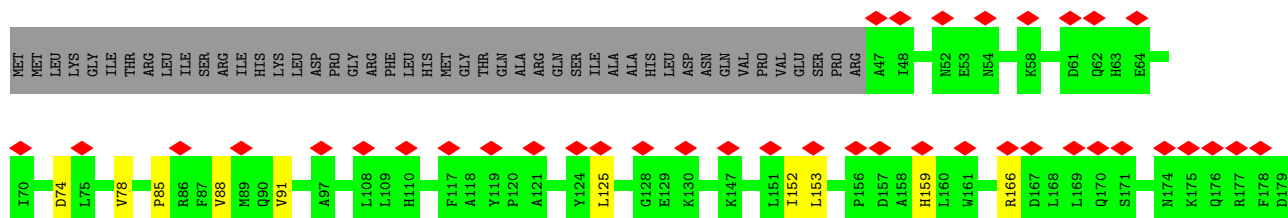
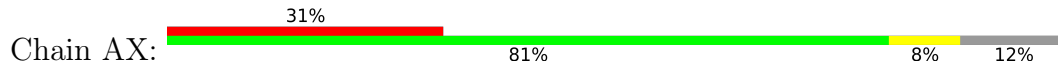
- Molecule 82: Mitochondrial inner membrane protein OXA1L



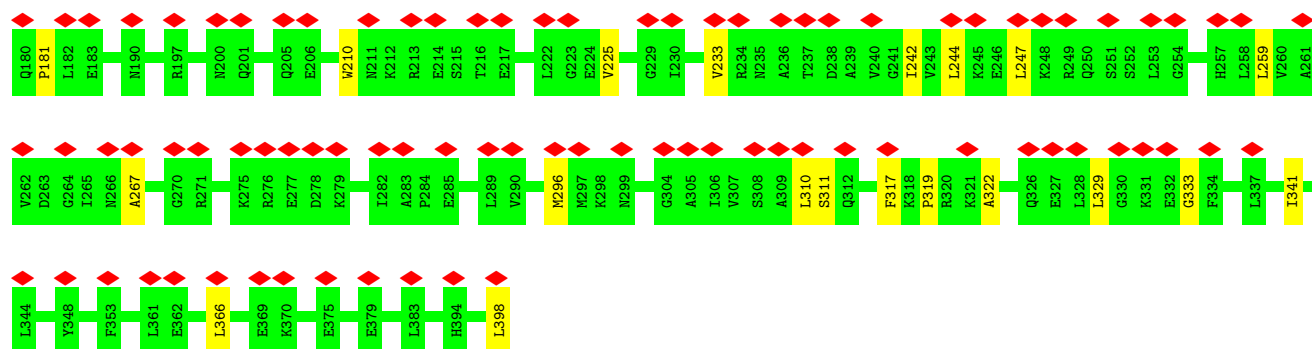




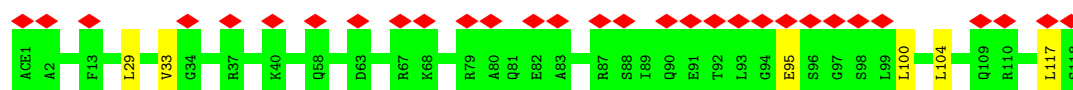
- Molecule 87: 28S ribosomal protein S29, mitochondrial



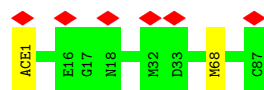




- Molecule 88: Small ribosomal subunit protein mS37



- Molecule 89: Small ribosomal subunit protein bS21m



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.151	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.027	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: B8T, ZN, MG, 5MC, MA6, 1MA, SPM, 5MU, ATP, FES, NAD, SPD, K, OMG, 2MG, PSU, PUT, GDP, ACE, OMU

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	B	0.16	0/1626	0.27	0/2523
2	0	0.16	0/913	0.24	0/1224
3	1	0.15	0/469	0.26	0/621
4	2	0.18	0/383	0.27	0/507
5	3	0.18	0/853	0.27	0/1136
6	4	0.17	0/350	0.27	0/461
7	5	0.16	0/3305	0.28	0/4502
8	6	0.14	0/3043	0.26	0/4140
9	7	0.15	0/2447	0.27	0/3310
10	8	0.13	0/1354	0.32	0/1819
11	9	0.15	0/1025	0.25	0/1379
12	A	0.20	0/36876	0.29	0/57402
13	D	0.17	0/1896	0.27	0/2549
14	E	0.17	0/2475	0.29	0/3355
15	F	0.18	0/2090	0.27	0/2842
16	H	0.13	0/1698	0.28	0/2292
17	I	0.15	0/1478	0.32	0/1999
18	J	0.15	0/1348	0.29	0/1813
19	K	0.18	0/1497	0.26	0/2031
20	L	0.15	0/905	0.26	0/1218
21	M	0.18	0/2381	0.27	0/3212
22	N	0.16	0/1833	0.24	0/2468
23	O	0.17	0/1283	0.27	0/1727
24	P	0.15	0/1199	0.25	0/1623
25	Q	0.15	0/2039	0.24	0/2750
26	R	0.18	0/1175	0.23	0/1572
27	S	0.18	0/1320	0.28	0/1789
28	T	0.17	0/1403	0.24	0/1886
29	U	0.18	0/1279	0.33	0/1730
30	W	0.18	0/926	0.25	0/1244
31	X	0.15	0/2099	0.24	0/2837

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.17	0/1593	0.24	0/2136
33	Z	0.17	0/1021	0.26	0/1378
34	V	0.15	0/1721	0.27	0/2333
35	b	0.17	0/1218	0.28	0/1649
36	d	0.16	0/2181	0.33	0/2949
37	e	0.14	0/1970	0.31	0/2658
38	g	0.16	0/1151	0.27	0/1569
39	h	0.13	0/918	0.23	0/1249
40	i	0.19	0/850	0.26	0/1135
41	j	0.16	0/760	0.24	0/1023
42	k	0.12	0/783	0.22	0/1057
43	l	0.12	0/707	0.27	0/960
44	m	0.12	0/805	0.31	0/1081
46	o	0.18	0/819	0.27	0/1097
47	q	0.15	0/1529	0.28	0/2055
48	r	0.16	0/1362	0.27	0/1846
49	t	0.15	0/358	0.33	0/486
49	u	0.19	0/259	0.38	0/350
50	c	0.15	0/2347	0.24	0/3171
51	f	0.16	0/1273	0.31	0/1716
52	p	0.14	0/1223	0.26	0/1641
53	s	0.16	0/3231	0.27	0/4389
54	AB	0.14	0/1871	0.26	0/2531
55	AC	0.14	0/1113	0.31	0/1505
56	AD	0.13	0/2783	0.25	0/3724
57	AE	0.13	0/989	0.26	0/1335
58	AF	0.12	0/1767	0.24	0/2373
59	AG	0.13	0/2746	0.25	0/3681
60	AH	0.15	0/1178	0.32	0/1598
61	AJ	0.13	0/855	0.26	0/1148
62	AK	0.13	0/880	0.25	0/1182
63	AL	0.12	0/1477	0.21	0/1974
64	AM	0.14	0/963	0.28	0/1295
65	AN	0.13	0/886	0.28	0/1199
66	AO	0.13	0/1648	0.29	0/2243
67	AP	0.13	0/798	0.24	0/1070
68	AR	0.11	0/2456	0.26	0/3317
69	AS	0.11	0/1138	0.21	0/1533
70	AT	0.12	0/1402	0.25	0/1883
71	AU	0.12	0/1510	0.25	0/2025
72	AV	0.15	0/3030	0.33	0/4093
73	AW	0.11	0/801	0.24	0/1079
74	AZ	0.13	0/857	0.29	0/1141

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	A0	0.12	0/1834	0.29	0/2484
76	A1	0.12	0/2313	0.28	0/3129
77	A3	0.15	0/636	0.28	0/839
78	Az	0.16	0/804	0.32	0/1248
79	AY	0.13	0/1040	0.25	0/1402
80	AA	0.16	0/22537	0.27	0/35085
81	AI	0.17	0/1039	0.33	1/1400 (0.1%)
82	OX	0.18	0/478	0.51	0/639
83	a	0.17	0/891	0.32	0/1208
84	Ax	0.16	0/1673	0.34	0/2602
85	Aw	0.14	0/1600	0.28	0/2476
86	A4	0.14	0/4877	0.32	0/6598
87	AX	0.14	0/2921	0.32	0/3954
88	A2	0.14	0/947	0.28	0/1266
89	AQ	0.13	0/754	0.23	0/1003
All	All	0.16	0/186539	0.28	1/265151 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
55	AC	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AI	184	ASN	N-CA-C	5.57	117.42	110.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
55	AC	43	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1524	0	779	14	0
2	0	898	0	916	1	0
3	1	464	0	511	2	0
4	2	377	0	406	0	0
5	3	832	0	883	2	0
6	4	342	0	361	1	0
7	5	3210	0	3206	5	0
8	6	2948	0	2841	5	0
9	7	2390	0	2397	11	0
10	8	1327	0	1368	19	0
11	9	997	0	987	0	0
12	A	33070	0	16797	129	0
13	D	1859	0	1920	6	0
14	E	2406	0	2415	4	0
15	F	2031	0	2065	6	0
16	H	1661	0	1734	6	0
17	I	1446	0	1532	8	0
18	J	1330	0	1407	10	0
19	K	1455	0	1452	4	0
20	L	890	0	941	4	0
21	M	2327	0	2394	10	0
22	N	1786	0	1817	5	0
23	O	1259	0	1294	3	0
24	P	1173	0	1165	3	0
25	Q	1990	0	2031	6	0
26	R	1154	0	1214	3	0
27	S	1293	0	1365	3	0
28	T	1369	0	1410	4	0
29	U	1248	0	1228	6	0
30	W	904	0	934	0	0
31	X	2044	0	2060	5	0
32	Y	1556	0	1597	2	0
33	Z	996	0	1044	1	0
34	V	1676	0	1687	6	0
35	b	1193	0	1191	3	0
36	d	2124	0	2125	25	0
37	e	1931	0	1916	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	g	1113	0	1097	3	0
39	h	895	0	881	1	0
40	i	828	0	857	1	0
41	j	745	0	746	1	0
42	k	774	0	784	1	0
43	l	688	0	674	3	0
44	m	791	0	796	5	0
45	n	215	0	53	0	0
46	o	798	0	804	3	0
47	q	1495	0	1492	15	0
48	r	1322	0	1348	6	0
49	t	354	0	377	2	0
49	u	257	0	283	4	0
50	c	2299	0	2320	4	0
51	f	1252	0	1269	11	0
52	p	1205	0	1223	3	0
53	s	3148	0	3131	12	0
54	AB	1828	0	1815	10	0
55	AC	1083	0	1088	11	0
56	AD	2731	0	2804	14	0
57	AE	972	0	1000	4	0
58	AF	1725	0	1769	4	0
59	AG	2688	0	2687	7	0
60	AH	1152	0	1183	18	0
61	AJ	839	0	887	5	0
62	AK	862	0	885	6	0
63	AL	1453	0	1540	8	0
64	AM	942	0	965	11	0
65	AN	868	0	928	1	0
66	AO	1592	0	1557	8	0
67	AP	781	0	806	1	0
68	AR	2409	0	2428	10	0
69	AS	1111	0	1115	5	0
70	AT	1371	0	1393	4	0
71	AU	1488	0	1499	7	0
72	AV	2969	0	2961	26	0
73	AW	789	0	802	4	0
74	AZ	839	0	858	3	0
75	A0	1787	0	1796	15	0
76	A1	2265	0	2294	15	0
77	A3	625	0	698	3	0
78	Az	719	0	359	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	AY	1010	0	957	4	0
80	AA	20260	0	10287	322	0
81	AI	1019	0	1059	6	0
82	OX	468	0	464	6	0
83	a	865	0	829	5	0
84	Ax	1498	0	766	4	0
85	Aw	1434	0	728	5	0
86	A4	4768	0	4766	32	0
87	AX	2849	0	2844	20	0
88	A2	935	0	971	5	0
89	AQ	744	0	758	2	0
90	B	7	0	8	1	0
91	0	1	0	0	0	0
91	4	1	0	0	0	0
91	AO	1	0	0	0	0
92	6	1	0	0	0	0
92	A	29	0	0	0	0
92	AA	17	0	0	0	0
92	AJ	1	0	0	0	0
92	D	1	0	0	0	0
92	M	2	0	0	0	0
92	N	1	0	0	0	0
92	W	1	0	0	0	0
92	o	1	0	0	0	0
93	A	40	0	76	0	0
93	AA	10	0	19	0	0
93	AG	10	0	19	0	0
93	O	10	0	19	0	0
94	A	6	0	12	0	0
95	A	136	0	0	0	0
95	A3	1	0	0	0	0
95	AA	59	0	0	0	0
95	AB	1	0	0	0	0
95	AX	1	0	0	0	0
95	Az	1	0	0	0	0
95	D	2	0	0	0	0
95	E	1	0	0	0	0
95	W	1	0	0	0	0
95	g	1	0	0	0	0
96	AP	4	0	0	0	0
96	AT	4	0	0	0	0
96	r	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
97	AA	44	0	26	0	0
98	AA	28	0	52	0	0
99	AX	31	0	12	0	0
100	AX	28	0	12	1	0
All	All	177884	0	150326	874	0

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

All (874) 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)
80:AA:1562:G:H1'	80:AA:1583:MA6:H2	1.64	0.79
28:T:62:ARG:HE	36:d:230:ARG:HD2	1.48	0.77
47:q:164:LEU:HB3	47:q:168:VAL:HG21	1.69	0.75
13:D:205:GLN:HA	13:D:208:ARG:HH21	1.52	0.73
37:e:183:THR:HG23	37:e:186:GLY:H	1.54	0.73
75:A0:99:ARG:HD3	80:AA:1526:U:H2'	1.69	0.72
80:AA:918:A:H4'	80:AA:920:G:H4'	1.73	0.71
80:AA:1365:A:H4'	80:AA:1389:G:H4'	1.74	0.69
82:OX:399:GLN:HE21	82:OX:401:PHE:HD1	1.42	0.68
80:AA:1002:C:H2'	80:AA:1003:A:H8	1.59	0.68
54:AB:167:HIS:HD1	59:AG:153:THR:HG22	1.59	0.68
80:AA:1201:A:H2'	80:AA:1202:G:H8	1.59	0.67
86:A4:556:LYS:HE3	86:A4:579:ILE:HD13	1.77	0.67
80:AA:941:G:H4'	80:AA:942:A:H5''	1.76	0.66
79:AY:338:LEU:HD11	79:AY:351:MET:HB3	1.75	0.66
80:AA:1440:G:H2'	80:AA:1441:A:C8	2.30	0.66
86:A4:397:MET:HG3	86:A4:431:LEU:HD11	1.78	0.66
80:AA:1528:A:H2'	80:AA:1529:A:H8	1.61	0.66
80:AA:976:A:H5''	89:AQ:1:ACE:H1	1.79	0.65
34:V:79:VAL:HG12	34:V:86:VAL:HG12	1.78	0.64
53:s:271:LEU:HD23	53:s:273:LEU:HD13	1.79	0.64
10:8:187:PRO:HG2	44:m:79:ILE:HD11	1.79	0.64
61:AJ:72:LYS:HG3	80:AA:1557:A:H5''	1.80	0.64
87:AX:153:LEU:HD21	87:AX:247:LEU:HD13	1.79	0.64
12:A:2545:U:H5''	12:A:2546:G:H5'	1.81	0.62
80:AA:1239:C:H2'	80:AA:1240:A:H8	1.65	0.62
12:A:2082:G:H2'	12:A:2083:U:O4'	2.00	0.62
25:Q:100:LEU:HD21	25:Q:286:ILE:HG12	1.80	0.62
54:AB:180:ARG:HH21	56:AD:210:PRO:HB2	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1201:A:H2'	80:AA:1202:G:C8	2.35	0.61
47:q:168:VAL:HG12	47:q:175:PHE:HB2	1.81	0.61
37:e:205:LEU:HB3	51:f:168:GLU:HB2	1.83	0.61
80:AA:745:A:H3'	80:AA:746:A:H8	1.66	0.60
76:A1:126:LEU:HD11	86:A4:70:VAL:HG13	1.81	0.60
80:AA:1515:G:H2'	80:AA:1516:G:H8	1.67	0.60
86:A4:170:VAL:HG23	86:A4:247:ILE:HD11	1.83	0.60
64:AM:20:ARG:HB2	80:AA:839:A:H5''	1.84	0.60
12:A:1857:U:H2'	12:A:1858:G:C8	2.37	0.59
63:AL:165:LYS:HE3	80:AA:947:U:H5''	1.84	0.59
80:AA:990:U:H3	80:AA:997:A:H61	1.50	0.59
72:AV:70:LEU:HD22	72:AV:389:LEU:HG	1.84	0.59
31:X:20:ILE:HG22	82:OX:434:LEU:HD23	1.83	0.59
72:AV:229:ALA:HB1	72:AV:286:VAL:HG11	1.83	0.59
80:AA:1440:G:H2'	80:AA:1441:A:H8	1.66	0.59
80:AA:1089:U:H2'	80:AA:1090:A:H8	1.66	0.59
60:AH:122:GLN:HG3	80:AA:1265:C:H4'	1.84	0.59
16:H:98:LEU:HD11	16:H:105:VAL:HG23	1.85	0.59
80:AA:1007:G:H2'	80:AA:1008:A:H8	1.68	0.59
80:AA:1006:U:H2'	80:AA:1007:G:H8	1.68	0.58
80:AA:1578:A:H2'	80:AA:1579:C:C6	2.38	0.58
8:6:187:VAL:HG13	8:6:319:PHE:HB3	1.85	0.58
76:A1:71:PRO:HB3	86:A4:78:VAL:HG21	1.85	0.58
80:AA:839:A:H2'	80:AA:840:A:H8	1.69	0.58
72:AV:66:PRO:HD3	80:AA:1529:A:H1'	1.86	0.58
75:A0:101:ARG:HH12	80:AA:1528:A:H4'	1.69	0.58
12:A:2006:C:H2'	12:A:2007:U:C6	2.39	0.58
80:AA:838:U:H2'	80:AA:839:A:H8	1.69	0.58
80:AA:1188:A:H4'	80:AA:1189:U:H5'	1.86	0.58
7:5:201:ARG:HB3	7:5:232:THR:HG22	1.84	0.58
87:AX:181:PRO:HB2	87:AX:233:VAL:HG22	1.87	0.57
65:AN:95:VAL:HG23	65:AN:96:THR:HG23	1.86	0.57
80:AA:663:A:H2'	80:AA:664:G:C8	2.39	0.57
80:AA:730:A:H3'	80:AA:731:A:H8	1.69	0.57
80:AA:1025:A:H2'	80:AA:1026:A:C8	2.40	0.57
8:6:175:VAL:HG22	8:6:204:VAL:HG22	1.87	0.57
18:J:121:ALA:HB2	18:J:144:ILE:HG13	1.87	0.57
80:AA:871:A:H4'	80:AA:872:G:H5'	1.85	0.57
85:Aw:9:A:H1'	85:Aw:45:A:H2'	1.87	0.57
82:OX:399:GLN:NE2	82:OX:401:PHE:HA	2.19	0.56
5:3:138:PRO:HG2	12:A:2854:U:H4'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:740:G:H2'	80:AA:741:A:H8	1.69	0.56
12:A:1994:A:H61	12:A:2736:C:H4'	1.71	0.56
84:Ax:40:A:H2'	84:Ax:41:A:C8	2.40	0.56
80:AA:1068:A:H5''	81:AI:190:LYS:HD3	1.87	0.56
80:AA:1002:C:H2'	80:AA:1003:A:C8	2.40	0.56
12:A:2134:A:H62	12:A:2135:A:H62	1.53	0.56
12:A:1862:U:H2'	12:A:1863:A:H8	1.71	0.56
80:AA:922:C:H2'	80:AA:923:A:C8	2.41	0.56
80:AA:1399:A:H2'	80:AA:1400:U:C6	2.41	0.56
37:e:213:TYR:HB3	37:e:231:VAL:HB	1.88	0.55
79:AY:290:ASN:HA	86:A4:446:LYS:HD3	1.88	0.55
17:I:47:LEU:HD22	22:N:226:ILE:HG12	1.88	0.55
80:AA:1416:A:H2'	80:AA:1417:A:C8	2.40	0.55
56:AD:244:LEU:HD22	56:AD:343:LEU:HD23	1.89	0.55
61:AJ:62:VAL:HA	61:AJ:83:VAL:HG12	1.88	0.55
12:A:2174:G:H4'	18:J:151:LEU:HD23	1.87	0.55
69:AS:51:VAL:HG13	88:A2:117:LEU:HD11	1.89	0.55
80:AA:1138:G:H2'	80:AA:1139:A:H8	1.71	0.55
80:AA:1470:A:H2'	80:AA:1471:A:H8	1.71	0.55
80:AA:1528:A:H2'	80:AA:1529:A:C8	2.39	0.55
36:d:108:ARG:HA	36:d:111:ARG:HD2	1.88	0.55
80:AA:1131:C:H2'	80:AA:1132:U:C6	2.42	0.55
8:6:206:TYR:HH	8:6:214:TRP:CD1	2.25	0.55
80:AA:1239:C:H2'	80:AA:1240:A:C8	2.41	0.55
20:L:75:LEU:HD11	20:L:105:VAL:HG21	1.88	0.55
87:AX:242:ILE:HD11	100:AX:503:GDP:C5	2.42	0.55
72:AV:70:LEU:HD21	72:AV:390:ILE:HD13	1.89	0.54
80:AA:1400:U:H2'	80:AA:1401:G:C8	2.42	0.54
85:Aw:68:U:H2'	85:Aw:69:A:C8	2.42	0.54
86:A4:429:LEU:HA	86:A4:464:LEU:HD21	1.89	0.54
19:K:60:MET:HE2	19:K:133:ILE:HD11	1.89	0.54
86:A4:308:LYS:HE3	86:A4:310:GLU:HB2	1.88	0.54
63:AL:209:LEU:HD13	77:A3:173:LEU:HD12	1.88	0.54
80:AA:1382:A:H5''	87:AX:166:ARG:HH21	1.71	0.54
12:A:2740:A:H2'	12:A:2741:A:C8	2.43	0.54
72:AV:149:ASP:HA	72:AV:152:ILE:HG22	1.89	0.54
80:AA:868:C:H2'	80:AA:869:C:H6	1.72	0.54
13:D:172:MET:HE1	57:AE:86:ILE:HG12	1.89	0.54
56:AD:420:SER:HA	80:AA:929:A:H4'	1.88	0.54
80:AA:1408:A:H2'	80:AA:1409:A:H8	1.72	0.54
21:M:28:LYS:HB3	46:o:94:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1065:C:H2'	80:AA:1066:C:O4'	2.06	0.54
80:AA:832:U:H2'	80:AA:833:A:H8	1.73	0.54
12:A:2740:A:H2'	12:A:2741:A:H8	1.72	0.54
18:J:140:VAL:O	18:J:144:ILE:HG12	2.08	0.54
1:B:23:A:H2'	1:B:24:G:C8	2.44	0.53
25:Q:148:THR:HG22	25:Q:165:GLU:HG2	1.89	0.53
63:AL:115:ILE:HG21	63:AL:181:ILE:HD13	1.90	0.53
27:S:163:LYS:HB2	35:b:106:ASP:HB3	1.90	0.53
80:AA:1012:A:H2'	80:AA:1013:A:C8	2.43	0.53
80:AA:1254:C:H4'	80:AA:1255:U:H5''	1.90	0.53
80:AA:1515:G:H2'	80:AA:1516:G:C8	2.43	0.53
36:d:208:VAL:HG22	36:d:253:THR:HG23	1.89	0.53
57:AE:92:ASN:HB2	67:AP:117:MET:HE3	1.91	0.53
62:AK:57:LEU:HD23	62:AK:71:ALA:HB2	1.90	0.53
80:AA:871:A:H1'	80:AA:872:G:C8	2.43	0.53
80:AA:686:A:H2'	80:AA:687:G:C8	2.43	0.53
80:AA:799:A:H2'	80:AA:800:C:C6	2.44	0.53
72:AV:68:SER:N	80:AA:1523:A:H5''	2.24	0.53
78:Az:28:U:H1'	86:A4:414:LYS:HG2	1.90	0.53
80:AA:838:U:H2'	80:AA:839:A:C8	2.43	0.53
12:A:1868:G:H2'	21:M:40:PRO:HG3	1.91	0.53
50:c:258:THR:HA	83:a:72:THR:HG22	1.91	0.53
74:AZ:10:ARG:HH12	76:A1:239:TRP:CD1	2.27	0.53
12:A:2718:C:H2'	12:A:2991:U:H4'	1.91	0.53
80:AA:1578:A:H2'	80:AA:1579:C:H6	1.72	0.53
53:s:63:ILE:HA	53:s:66:TRP:CD1	2.44	0.53
61:AJ:57:GLN:HB3	61:AJ:109:LEU:HD11	1.91	0.53
12:A:2409:A:H2'	12:A:2410:U:C6	2.44	0.53
60:AH:145:LEU:HB3	60:AH:148:LEU:HD11	1.90	0.53
80:AA:672:A:H2'	80:AA:673:U:C6	2.44	0.53
1:B:30:A:H2'	1:B:31:A:H8	1.73	0.52
72:AV:76:ILE:HD12	72:AV:112:TRP:HD1	1.73	0.52
80:AA:832:U:H2'	80:AA:833:A:C8	2.44	0.52
80:AA:1373:U:H2'	80:AA:1374:A:H8	1.74	0.52
10:8:99:ARG:HG2	37:e:83:LEU:HB3	1.90	0.52
12:A:2086:A:H2'	12:A:2087:U:C6	2.44	0.52
80:AA:702:C:H2'	80:AA:703:A:C8	2.45	0.52
80:AA:1376:C:H4'	80:AA:1377:C:H5'	1.90	0.52
68:AR:207:PRO:HB2	68:AR:209:ILE:HG22	1.90	0.52
72:AV:226:TYR:CZ	72:AV:282:VAL:HG11	2.45	0.52
80:AA:848:U:H2'	80:AA:849:U:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1348:G:H2'	80:AA:1349:U:C6	2.45	0.52
13:D:109:PHE:CE1	13:D:208:ARG:HD3	2.45	0.52
80:AA:839:A:H2'	80:AA:840:A:C8	2.44	0.52
80:AA:1066:C:H2'	80:AA:1067:A:C8	2.45	0.52
12:A:2734:A:H2'	12:A:2735:G:H8	1.73	0.52
80:AA:865:A:H2'	80:AA:866:A:C8	2.45	0.52
60:AH:70:ASP:HA	86:A4:62:LYS:HE3	1.91	0.52
80:AA:1416:A:H2'	80:AA:1417:A:H8	1.75	0.52
37:e:195:LEU:HD12	37:e:243:PHE:HZ	1.75	0.52
80:AA:659:U:H2'	80:AA:660:C:H6	1.75	0.52
6:4:103:MET:HE1	12:A:2952:U:H5'	1.92	0.52
60:AH:155:VAL:HG21	76:A1:129:PHE:HB3	1.91	0.52
72:AV:246:ASN:HB2	75:A0:70:ARG:HH12	1.75	0.51
80:AA:852:A:H3'	80:AA:853:C:H6	1.73	0.51
80:AA:1362:G:H2'	80:AA:1363:C:C6	2.44	0.51
2:0:138:ARG:HB3	12:A:2321:A:C8	2.45	0.51
10:8:160:GLU:HA	10:8:163:LYS:HE3	1.92	0.51
12:A:3211:C:H4'	12:A:3212:C:H5	1.75	0.51
80:AA:1042:U:H2'	80:AA:1043:C:H6	1.74	0.51
80:AA:1265:C:H2'	80:AA:1266:A:H8	1.74	0.51
10:8:92:LEU:HD13	47:q:162:GLU:HG3	1.92	0.51
80:AA:1595:G:H2'	80:AA:1596:A:C8	2.46	0.51
9:7:114:ASP:HB2	9:7:117:LYS:HB2	1.93	0.51
49:t:74:LEU:HD12	49:t:78:GLU:HB2	1.92	0.51
80:AA:659:U:H2'	80:AA:660:C:C6	2.46	0.51
80:AA:854:U:H2'	80:AA:855:A:C8	2.45	0.51
80:AA:998:A:H2'	80:AA:999:C:C6	2.45	0.51
75:A0:68:LEU:HD21	75:A0:80:VAL:HG21	1.91	0.51
80:AA:1129:U:H2'	80:AA:1130:G:H8	1.75	0.51
19:K:20:LEU:HD22	19:K:141:LEU:HD13	1.93	0.51
56:AD:196:ASN:HD22	80:AA:878:G:H4'	1.76	0.51
81:AI:100:VAL:HG12	81:AI:106:PRO:HA	1.93	0.51
10:8:173:LYS:HB3	51:f:184:LEU:HD23	1.93	0.51
13:D:207:ILE:HG12	13:D:229:PRO:HD3	1.93	0.51
55:AC:43:ARG:HD2	80:AA:1322:C:OP1	2.12	0.51
58:AF:172:VAL:HG12	58:AF:240:ARG:HD3	1.92	0.51
80:AA:1042:U:H2'	80:AA:1043:C:C6	2.46	0.51
80:AA:1469:G:H2'	80:AA:1470:A:H8	1.75	0.51
86:A4:532:LEU:HD11	86:A4:555:ILE:HG21	1.92	0.51
60:AH:163:ASN:HB3	76:A1:114:LEU:HD11	1.93	0.50
62:AK:36:ARG:HE	62:AK:40:ARG:HH22	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:821:U:H2'	80:AA:822:G:H8	1.76	0.50
80:AA:914:A:H2'	80:AA:915:C:C6	2.46	0.50
80:AA:833:A:H2'	80:AA:834:G:C8	2.46	0.50
80:AA:1439:A:H2'	80:AA:1440:G:H8	1.75	0.50
12:A:2099:U:H2'	12:A:2100:C:C6	2.46	0.50
66:AO:82:LYS:HB3	80:AA:881:A:N6	2.26	0.50
68:AR:142:LEU:HD21	68:AR:183:LYS:HE3	1.94	0.50
10:8:192:TYR:HB3	51:f:132:ILE:HD11	1.93	0.50
63:AL:209:LEU:HD12	77:A3:189:TRP:CE2	2.47	0.50
80:AA:1174:U:H2'	80:AA:1175:G:C8	2.47	0.50
1:B:29:C:H5''	10:8:125:LYS:HD3	1.92	0.50
7:5:165:GLN:NE2	7:5:175:THR:HG22	2.26	0.50
60:AH:124:VAL:HG13	80:AA:1264:C:H1'	1.93	0.50
80:AA:1132:U:H2'	80:AA:1133:C:C6	2.46	0.50
80:AA:1587:U:H2'	80:AA:1588:G:H8	1.76	0.50
86:A4:494:ILE:HD11	86:A4:527:LEU:HA	1.94	0.50
71:AU:64:ARG:HA	71:AU:67:VAL:HG12	1.93	0.50
80:AA:842:C:H2'	80:AA:843:G:C8	2.47	0.50
80:AA:1408:A:H2'	80:AA:1409:A:C8	2.47	0.50
12:A:1839:C:H2'	12:A:1840:C:C6	2.47	0.50
12:A:2662:A:H2'	12:A:2663:C:C6	2.47	0.50
72:AV:175:VAL:HG12	72:AV:177:SER:H	1.77	0.50
73:AW:149:LEU:HD11	73:AW:166:ASN:HB2	1.94	0.50
12:A:2553:G:H2'	12:A:2554:A:H8	1.77	0.49
80:AA:705:C:H3'	80:AA:706:C:H6	1.77	0.49
1:B:21:A:H61	1:B:46:A:H2'	1.77	0.49
80:AA:1194:C:H2'	80:AA:1195:U:C6	2.48	0.49
80:AA:1439:A:H2'	80:AA:1440:G:C8	2.48	0.49
36:d:219:ARG:HD3	36:d:239:PRO:HB2	1.93	0.49
80:AA:847:G:H2'	80:AA:848:U:C6	2.47	0.49
10:8:117:LEU:HD11	37:e:69:GLU:HB3	1.95	0.49
12:A:1911:C:H2'	12:A:1912:A:H8	1.76	0.49
56:AD:103:LEU:HD11	56:AD:123:ARG:HB2	1.94	0.49
80:AA:673:U:H2'	80:AA:674:U:C6	2.47	0.49
80:AA:872:G:H2'	80:AA:873:G:C8	2.47	0.49
9:7:302:LEU:HD23	23:O:144:LEU:HD23	1.94	0.49
12:A:2151:A:H2'	12:A:2152:A:C8	2.47	0.49
20:L:129:LYS:HE2	25:Q:125:TYR:OH	2.12	0.49
47:q:161:GLN:HG3	47:q:175:PHE:HE2	1.77	0.49
80:AA:818:C:H2'	80:AA:819:A:H8	1.77	0.49
80:AA:1359:U:H2'	80:AA:1360:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1589:C:H2'	80:AA:1590:A:C8	2.48	0.49
80:AA:1407:U:H2'	80:AA:1408:A:H8	1.77	0.49
80:AA:663:A:H2'	80:AA:664:G:H8	1.76	0.49
80:AA:1407:U:H2'	80:AA:1408:A:C8	2.48	0.49
80:AA:1450:C:H2'	80:AA:1451:U:C6	2.47	0.49
9:7:77:THR:HG23	36:d:283:PRO:HA	1.95	0.49
76:A1:53:LEU:HD12	86:A4:518:GLU:HG2	1.93	0.49
80:AA:1007:G:H2'	80:AA:1008:A:C8	2.47	0.49
80:AA:1583:MA6:O5'	80:AA:1583:MA6:H8	2.12	0.49
47:q:152:ARG:O	47:q:156:LEU:HG	2.13	0.49
80:AA:1317:A:H3'	80:AA:1318:A:H8	1.78	0.49
12:A:2529:U:OP2	13:D:208:ARG:HD2	2.13	0.49
64:AM:114:ARG:HA	64:AM:117:GLU:HB3	1.94	0.49
86:A4:343:ARG:HA	86:A4:378:LEU:HD13	1.95	0.49
12:A:2382:A:H2'	12:A:2383:U:C6	2.48	0.48
12:A:2662:A:H2'	12:A:2663:C:H6	1.78	0.48
16:H:98:LEU:HD23	16:H:129:ALA:HB2	1.95	0.48
28:T:206:LEU:HA	35:b:119:PHE:CE1	2.48	0.48
36:d:96:ARG:HG2	36:d:97:ILE:H	1.78	0.48
80:AA:916:C:H2'	80:AA:917:C:C6	2.48	0.48
87:AX:366:LEU:HD22	87:AX:398:LEU:HD22	1.95	0.48
29:U:81:ASP:HB3	29:U:87:ILE:HD11	1.95	0.48
33:Z:99:VAL:HG21	41:j:77:VAL:HG22	1.95	0.48
60:AH:164:LEU:HD12	60:AH:165:PRO:HD2	1.95	0.48
72:AV:103:TYR:CZ	80:AA:1524:A:H4'	2.48	0.48
80:AA:661:C:H2'	80:AA:662:U:C6	2.48	0.48
80:AA:990:U:H2'	80:AA:991:G:O4'	2.13	0.48
12:A:1977:U:H2'	12:A:1978:A:H8	1.78	0.48
12:A:2093:U:H2'	12:A:2094:G:C8	2.48	0.48
12:A:3089:A:H3'	12:A:3090:G:C5'	2.43	0.48
21:M:244:LEU:HD12	21:M:245:PRO:HD2	1.95	0.48
36:d:138:PRO:HG3	36:d:194:VAL:HG23	1.95	0.48
64:AM:114:ARG:HH22	66:AO:236:PRO:HD2	1.78	0.48
80:AA:872:G:H2'	80:AA:873:G:H8	1.79	0.48
80:AA:1173:C:H2'	80:AA:1174:U:C6	2.48	0.48
80:AA:1504:U:H2'	80:AA:1505:A:C8	2.48	0.48
34:V:102:MET:HE3	36:d:48:PRO:HG2	1.95	0.48
68:AR:288:GLN:HE22	68:AR:300:LEU:HD22	1.78	0.48
80:AA:868:C:H2'	80:AA:869:C:C6	2.48	0.48
80:AA:1033:U:H2'	80:AA:1034:U:C6	2.48	0.48
87:AX:159:HIS:HE1	87:AX:311:SER:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:2275:U:H2'	12:A:2276:C:C6	2.49	0.48
12:A:3115:U:H2'	12:A:3116:C:H6	1.79	0.48
36:d:217:HIS:CD2	36:d:243:LEU:HB2	2.48	0.48
55:AC:100:PHE:HB3	55:AC:103:CYS:HB2	1.95	0.48
9:7:204:LYS:HE3	83:a:92:LEU:HD22	1.94	0.48
34:V:55:TYR:HB2	34:V:133:ILE:HD11	1.95	0.48
38:g:110:ILE:HD11	38:g:157:LEU:HD13	1.95	0.48
80:AA:1180:U:H2'	80:AA:1181:G:H8	1.78	0.48
87:AX:152:ILE:HG12	87:AX:259:LEU:HD23	1.94	0.48
12:A:1952:U:H2'	12:A:1953:A:C8	2.49	0.48
80:AA:735:A:H2'	80:AA:736:C:O4'	2.13	0.48
80:AA:747:A:H2'	80:AA:748:G:C8	2.47	0.48
80:AA:798:C:H2'	80:AA:799:A:H8	1.79	0.48
12:A:3115:U:H2'	12:A:3116:C:C6	2.49	0.48
47:q:186:GLU:HA	47:q:189:ARG:HD2	1.95	0.48
76:A1:134:PRO:HG3	86:A4:60:PRO:HD3	1.95	0.48
80:AA:747:A:H2'	80:AA:748:G:H8	1.78	0.48
12:A:2757:A:H2'	12:A:2758:G:O4'	2.13	0.48
47:q:170:PRO:HA	47:q:175:PHE:CD1	2.48	0.48
56:AD:100:LYS:HG2	80:AA:1262:C:H4'	1.96	0.48
76:A1:134:PRO:HB2	76:A1:137:LEU:HD23	1.95	0.48
80:AA:1412:G:H2'	80:AA:1413:U:O4'	2.13	0.48
12:A:2060:A:C8	12:A:2079:C:C4	3.02	0.48
12:A:3054:G:H2'	12:A:3055:U:C6	2.49	0.48
36:d:38:LYS:HB3	36:d:40:ARG:HH12	1.77	0.48
73:AW:154:LEU:HB3	88:A2:29:LEU:HG	1.96	0.48
80:AA:969:A:H2'	80:AA:970:A:H8	1.79	0.48
80:AA:1175:G:H2'	80:AA:1176:G:C8	2.48	0.48
86:A4:302:VAL:HG21	86:A4:341:CYS:HB3	1.95	0.48
12:A:1829:A:H2'	12:A:1830:G:H8	1.79	0.47
14:E:50:ASP:HA	14:E:53:LEU:HG	1.95	0.47
80:AA:740:G:H2'	80:AA:741:A:C8	2.47	0.47
80:AA:1441:A:H2	80:AA:1449:G:H22	1.62	0.47
68:AR:157:VAL:HG22	68:AR:174:VAL:HG22	1.95	0.47
80:AA:914:A:H2'	80:AA:915:C:H6	1.79	0.47
80:AA:1035:U:H2'	80:AA:1036:A:H8	1.79	0.47
86:A4:352:PRO:O	86:A4:355:GLN:HG3	2.14	0.47
12:A:1952:U:H2'	12:A:1953:A:H8	1.78	0.47
53:s:142:LEU:HD13	53:s:422:VAL:HG21	1.96	0.47
53:s:332:LEU:HD13	53:s:372:TYR:HB2	1.95	0.47
54:AB:223:VAL:HG11	54:AB:229:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:798:C:H2'	80:AA:799:A:C8	2.49	0.47
80:AA:1470:A:H2'	80:AA:1471:A:C8	2.49	0.47
87:AX:319:PRO:HG2	87:AX:322:ALA:HB2	1.96	0.47
1:B:29:C:H2'	1:B:30:A:H8	1.79	0.47
12:A:2055:U:H2'	12:A:2056:G:H8	1.80	0.47
12:A:2748:A:H2'	12:A:2749:A:H8	1.80	0.47
17:I:197:LEU:HD22	49:u:76:LEU:HD12	1.95	0.47
80:AA:705:C:H3'	80:AA:706:C:C6	2.49	0.47
80:AA:800:C:H2'	80:AA:801:A:C8	2.50	0.47
87:AX:85:PRO:HA	87:AX:88:VAL:HG12	1.95	0.47
10:8:68:LEU:HD21	51:f:211:LEU:HB2	1.96	0.47
48:r:70:CYS:HB2	48:r:107:LEU:HA	1.95	0.47
72:AV:152:ILE:HD12	72:AV:185:VAL:HG22	1.95	0.47
80:AA:1078:A:H2'	80:AA:1079:G:C8	2.49	0.47
80:AA:1191:C:H2'	80:AA:1192:C:H6	1.80	0.47
86:A4:571:TRP:HE3	86:A4:576:LEU:HD21	1.80	0.47
80:AA:1191:C:H2'	80:AA:1192:C:C6	2.49	0.47
80:AA:1309:A:H2'	80:AA:1310:C:C6	2.49	0.47
1:B:68:C:H2'	1:B:69:U:C6	2.50	0.47
12:A:2598:A:H3'	12:A:2625:C:H42	1.79	0.47
12:A:2677:A:H2'	12:A:2678:A:C8	2.50	0.47
12:A:3150:U:C2	12:A:3151:A:C8	3.03	0.47
17:I:154:LEU:HD12	17:I:164:MET:HE3	1.96	0.47
18:J:113:THR:HG23	18:J:115:LYS:H	1.78	0.47
37:e:97:ARG:HA	37:e:100:LYS:HG2	1.96	0.47
60:AH:96:VAL:HA	60:AH:106:ILE:HD13	1.97	0.47
72:AV:196:PHE:HB3	72:AV:201:GLU:HG3	1.96	0.47
75:A0:136:TYR:CZ	80:AA:705:C:H2'	2.50	0.47
80:AA:884:U:H2'	80:AA:885:U:C6	2.50	0.47
80:AA:1021:U:H4'	80:AA:1022:A:H5'	1.95	0.47
80:AA:1044:U:H2'	80:AA:1045:G:O4'	2.14	0.47
10:8:201:GLN:HB3	51:f:201:ARG:HG3	1.96	0.47
12:A:1939:G:O2'	12:A:1973:G:H4'	2.15	0.47
12:A:2005:C:H2'	12:A:2006:C:C6	2.50	0.47
28:T:206:LEU:HA	35:b:119:PHE:HE1	1.78	0.47
36:d:88:TYR:OH	36:d:91:PRO:HD3	2.15	0.47
36:d:90:PRO:HB2	36:d:269:TRP:HZ2	1.79	0.47
54:AB:192:LEU:HD11	54:AB:220:VAL:HG23	1.96	0.47
64:AM:93:LEU:HD13	68:AR:156:TYR:HE2	1.80	0.47
75:A0:167:PRO:HG2	75:A0:170:LEU:HB2	1.97	0.47
80:AA:749:G:H2'	80:AA:750:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:AX:125:LEU:HD11	87:AX:310:LEU:HG	1.95	0.47
12:A:1935:A:C2	12:A:1936:A:H1'	2.50	0.47
12:A:2111:C:H2'	12:A:2112:A:C8	2.50	0.47
72:AV:103:TYR:HA	80:AA:1525:C:H5	1.79	0.47
80:AA:881:A:H2'	80:AA:882:A:C4	2.50	0.47
80:AA:944:U:H2'	80:AA:945:G:C8	2.50	0.47
88:A2:95:GLU:HB3	88:A2:100:LEU:HG	1.97	0.47
12:A:1911:C:H2'	12:A:1912:A:C8	2.50	0.46
47:q:141:GLU:HA	47:q:144:GLU:HG3	1.97	0.46
60:AH:162:ARG:HH11	79:AY:301:LEU:HD12	1.80	0.46
72:AV:30:LEU:HD23	72:AV:149:ASP:HB2	1.97	0.46
80:AA:1162:A:H2'	80:AA:1163:C:C6	2.50	0.46
80:AA:1175:G:H2'	80:AA:1176:G:H8	1.80	0.46
15:F:221:LEU:HG	15:F:222:THR:HG23	1.96	0.46
58:AF:238:HIS:CD2	81:AI:124:THR:HB	2.50	0.46
72:AV:322:THR:HG23	72:AV:325:SER:H	1.80	0.46
80:AA:1066:C:H2'	80:AA:1067:A:H8	1.80	0.46
80:AA:1374:A:H5''	87:AX:317:PHE:CE1	2.50	0.46
12:A:2101:C:H2'	12:A:2102:A:H8	1.79	0.46
72:AV:30:LEU:HD21	72:AV:181:LEU:HD22	1.96	0.46
12:A:2894:U:H5''	12:A:2895:U:O4'	2.15	0.46
39:h:88:ASP:HA	39:h:122:ARG:HD2	1.97	0.46
80:AA:686:A:H2'	80:AA:687:G:H8	1.80	0.46
80:AA:1488:5MC:H2'	80:AA:1489:G:C8	2.50	0.46
54:AB:155:ILE:HG12	54:AB:196:LEU:HD13	1.96	0.46
76:A1:67:PRO:HG3	76:A1:118:ALA:HB2	1.96	0.46
80:AA:660:C:H1'	80:AA:1285:G:H21	1.80	0.46
80:AA:915:C:H2'	80:AA:916:C:C6	2.50	0.46
80:AA:920:G:H2'	80:AA:921:U:C6	2.50	0.46
81:AI:99:VAL:HG11	81:AI:139:ALA:HB2	1.97	0.46
87:AX:244:LEU:HD22	87:AX:296:MET:HG3	1.97	0.46
12:A:1737:A:H61	12:A:1760:G:H1'	1.81	0.46
12:A:2275:U:H2'	12:A:2276:C:H6	1.80	0.46
12:A:2668:A:H2'	12:A:2669:A:C8	2.51	0.46
62:AK:52:LEU:HD22	74:AZ:41:PRO:HG3	1.98	0.46
1:B:76:A:H8	37:e:265:LYS:HZ3	1.64	0.46
12:A:2553:G:H2'	12:A:2554:A:C8	2.51	0.46
36:d:204:ASN:O	36:d:205:GLN:HG2	2.15	0.46
71:AU:27:ARG:HB2	80:AA:712:C:H42	1.81	0.46
80:AA:1455:U:H2'	80:AA:1456:U:C6	2.51	0.46
12:A:1828:A:H4'	12:A:1829:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:M:261:ASP:HB3	21:M:264:GLN:HB2	1.98	0.46
53:s:137:LEU:HD21	53:s:422:VAL:HG11	1.97	0.46
66:AO:208:PRO:HG2	66:AO:213:LEU:HD21	1.97	0.46
68:AR:323:GLU:H	68:AR:326:ASN:HB2	1.80	0.46
79:AY:351:MET:HE3	79:AY:380:PHE:HE2	1.79	0.46
80:AA:1138:G:H2'	80:AA:1139:A:C8	2.50	0.46
87:AX:88:VAL:HA	87:AX:91:VAL:HG22	1.97	0.46
37:e:55:ARG:HG3	37:e:149:LEU:HD22	1.96	0.46
80:AA:661:C:H2'	80:AA:662:U:H6	1.80	0.46
80:AA:1110:A:H61	80:AA:1131:C:H42	1.64	0.46
80:AA:1452:U:H2'	80:AA:1453:A:H8	1.81	0.46
12:A:2277:U:H2'	12:A:2278:A:H8	1.81	0.46
12:A:3139:G:H2'	12:A:3140:A:C8	2.51	0.46
12:A:3224:G:H2'	12:A:3225:G:H8	1.80	0.46
31:X:10:LEU:HD22	47:q:45:LEU:HD12	1.97	0.46
47:q:147:GLN:O	47:q:150:LYS:HG3	2.16	0.46
80:AA:873:G:H2'	80:AA:874:G:C8	2.51	0.46
80:AA:1056:A:H4'	80:AA:1588:G:N2	2.30	0.46
64:AM:67:ALA:HB2	68:AR:196:TYR:CZ	2.51	0.45
10:8:136:ILE:HD11	51:f:169:ILE:HG23	1.98	0.45
17:I:116:LEU:HG	17:I:121:ILE:HB	1.98	0.45
18:J:113:THR:HG22	18:J:116:HIS:ND1	2.31	0.45
37:e:269:LEU:HA	37:e:272:VAL:HG12	1.98	0.45
60:AH:51:HIS:HE1	86:A4:476:LYS:HG3	1.82	0.45
69:AS:134:ARG:HG2	69:AS:136:GLY:H	1.80	0.45
80:AA:1119:U:H2'	80:AA:1120:C:O4'	2.15	0.45
80:AA:1502:A:H2'	80:AA:1503:G:O4'	2.16	0.45
87:AX:225:VAL:HG21	87:AX:242:ILE:HG21	1.98	0.45
12:A:1886:G:H1	40:i:61:GLY:HA3	1.82	0.45
28:T:186:ALA:HB2	83:a:108:MET:HG3	1.98	0.45
64:AM:66:VAL:HG11	64:AM:90:LEU:HD11	1.98	0.45
80:AA:1398:U:H2'	80:AA:1399:A:H8	1.82	0.45
80:AA:1471:A:H2'	80:AA:1472:G:H8	1.82	0.45
8:6:255:LEU:HD12	8:6:256:PRO:HD2	1.98	0.45
49:t:64:ILE:HD11	49:u:82:LEU:HB2	1.98	0.45
70:AT:118:GLU:HA	70:AT:121:LYS:HD3	1.99	0.45
12:A:1974:A:H5'	13:D:261:GLY:HA2	1.98	0.45
36:d:52:THR:HG23	36:d:55:GLU:H	1.80	0.45
72:AV:163:VAL:O	72:AV:167:VAL:HG23	2.17	0.45
75:A0:11:ILE:HB	80:AA:806:C:C2	2.52	0.45
80:AA:845:A:H2'	80:AA:846:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:A4:166:VAL:HG12	86:A4:194:LEU:HG	1.99	0.45
1:B:43:G:H2'	1:B:44:A:C8	2.50	0.45
12:A:2470:G:H4'	20:L:36:THR:HG23	1.98	0.45
17:I:163:GLU:HG3	17:I:166:ARG:HH22	1.81	0.45
80:AA:956:C:H2'	80:AA:957:C:O4'	2.17	0.45
80:AA:960:C:H42	80:AA:1041:A:H2	1.63	0.45
80:AA:983:C:H2'	80:AA:984:C:C6	2.52	0.45
80:AA:1033:U:H2'	80:AA:1034:U:H6	1.81	0.45
80:AA:1358:A:H2'	80:AA:1359:U:C6	2.52	0.45
82:OX:399:GLN:NE2	82:OX:401:PHE:HD1	2.13	0.45
84:Ax:3:U:H2'	84:Ax:4:A:C8	2.51	0.45
12:A:2006:C:H2'	12:A:2007:U:H6	1.80	0.45
12:A:2483:U:H2'	12:A:2484:C:O4'	2.17	0.45
12:A:2586:U:H2'	12:A:2587:G:H8	1.82	0.45
37:e:219:GLN:HA	37:e:222:ARG:HB2	1.98	0.45
55:AC:136:VAL:HG22	55:AC:153:LEU:HD22	1.98	0.45
59:AG:87:HIS:O	59:AG:91:MET:HG2	2.17	0.45
66:AO:150:LEU:O	66:AO:154:ILE:HD12	2.16	0.45
80:AA:1506:U:H2'	80:AA:1507:A:C8	2.52	0.45
12:A:1925:A:H2'	12:A:1926:A:C8	2.52	0.45
36:d:160:LEU:O	36:d:164:VAL:HG22	2.17	0.45
37:e:98:LEU:HG	37:e:101:LYS:HE3	1.98	0.45
53:s:84:THR:HB	53:s:280:ASN:HB2	1.99	0.45
60:AH:124:VAL:HG12	62:AK:109:ILE:HG12	1.97	0.45
80:AA:1382:A:H2'	80:AA:1383:A:O4'	2.17	0.45
72:AV:190:LEU:HD11	72:AV:226:TYR:CZ	2.52	0.45
75:A0:64:LEU:HD12	75:A0:139:TRP:CD2	2.52	0.45
88:A2:29:LEU:HD22	89:AQ:68:MET:HE2	1.98	0.45
9:7:315:LYS:HD2	14:E:64:LEU:HD21	1.99	0.45
34:V:168:GLU:HB3	82:OX:374:MET:HE1	1.99	0.45
46:o:24:PRO:HG2	48:r:169:TRP:HB2	1.99	0.45
56:AD:91:THR:HB	80:AA:1334:G:H5'	1.98	0.45
59:AG:293:ILE:HB	59:AG:300:TYR:HB3	1.99	0.45
80:AA:886:C:H2'	80:AA:887:G:C8	2.52	0.45
80:AA:1080:A:H1'	80:AA:1082:A:N7	2.31	0.45
80:AA:1422:G:H2'	80:AA:1423:A:C8	2.52	0.45
9:7:166:LEU:HB3	9:7:181:TYR:HE2	1.82	0.44
12:A:1745:U:H5''	31:X:55:LYS:HD3	1.98	0.44
56:AD:140:LEU:HD11	56:AD:160:ARG:NE	2.32	0.44
72:AV:231:LEU:HD12	72:AV:243:VAL:HG13	2.00	0.44
80:AA:1353:A:H5'	80:AA:1354:A:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:2110:A:H5'	22:N:67:LYS:HE3	1.99	0.44
37:e:248:ASN:HD22	37:e:252:HIS:HE1	1.64	0.44
57:AE:35:ILE:HD12	63:AL:97:MET:HE2	1.99	0.44
59:AG:75:LYS:HA	59:AG:78:ILE:HD12	1.98	0.44
75:A0:165:PRO:HG3	75:A0:190:MET:HE2	1.99	0.44
80:AA:1506:U:H2'	80:AA:1507:A:H8	1.82	0.44
86:A4:61:LYS:HA	86:A4:61:LYS:HD3	1.76	0.44
12:A:2134:A:N6	12:A:2135:A:H62	2.16	0.44
12:A:3151:A:H4'	25:Q:146:GLY:O	2.17	0.44
48:r:99:MET:HE1	48:r:115:ILE:HG22	2.00	0.44
55:AC:152:ARG:HE	55:AC:154:HIS:CE1	2.35	0.44
80:AA:653:G:H2'	80:AA:654:U:O4'	2.18	0.44
80:AA:727:U:H2'	80:AA:728:C:O4'	2.17	0.44
80:AA:730:A:H3'	80:AA:731:A:C8	2.52	0.44
80:AA:1041:A:H8	80:AA:1041:A:P	2.40	0.44
80:AA:1256:A:H2'	80:AA:1257:U:C6	2.53	0.44
80:AA:1509:U:H2'	80:AA:1510:U:C6	2.52	0.44
84:Ax:22:U:C2	84:Ax:23:A:C8	3.05	0.44
18:J:161:SER:HA	43:l:69:THR:HG21	1.99	0.44
64:AM:73:ILE:O	64:AM:77:ILE:HG12	2.17	0.44
75:A0:171:ARG:HE	75:A0:188:GLU:HG2	1.82	0.44
80:AA:745:A:H3'	80:AA:746:A:C8	2.51	0.44
80:AA:786:G:H2'	80:AA:787:C:C6	2.53	0.44
80:AA:1023:C:H2'	80:AA:1024:G:C8	2.53	0.44
80:AA:1561:C:H2'	80:AA:1562:G:C8	2.52	0.44
87:AX:242:ILE:HD13	87:AX:242:ILE:HA	1.82	0.44
10:8:192:TYR:HE1	51:f:134:VAL:HG22	1.81	0.44
12:A:1761:A:H2'	12:A:1762:A:C8	2.52	0.44
12:A:2728:C:H2'	12:A:2729:U:H6	1.82	0.44
15:F:284:TYR:HD2	15:F:288:LEU:HD12	1.81	0.44
60:AH:145:LEU:HD11	60:AH:156:TYR:CE2	2.52	0.44
80:AA:776:A:O3'	80:AA:777:G:H8	2.00	0.44
80:AA:1005:U:H4'	81:AI:87:HIS:CE1	2.52	0.44
80:AA:1089:U:H2'	80:AA:1090:A:C8	2.51	0.44
80:AA:1156:C:H2'	80:AA:1157:U:H6	1.83	0.44
80:AA:1496:U:H2'	80:AA:1497:C:C6	2.53	0.44
12:A:2318:A:H2'	12:A:2319:A:C8	2.53	0.44
29:U:27:GLN:HG3	29:U:43:ARG:HB2	2.00	0.44
61:AJ:42:PRO:HD3	80:AA:931:C:C2	2.53	0.44
80:AA:715:G:H2'	80:AA:716:U:C6	2.52	0.44
12:A:2549:C:N4	12:A:2562:U:H2'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:e:159:LEU:HD12	37:e:254:TRP:CH2	2.53	0.44
60:AH:72:LEU:HD12	76:A1:133:TRP:CZ3	2.52	0.44
80:AA:922:C:H2'	80:AA:923:A:H8	1.82	0.44
81:AI:151:VAL:HG21	81:AI:158:ARG:HG3	1.99	0.44
12:A:2472:A:H62	12:A:2654:U:H3	1.65	0.44
12:A:3142:A:H2'	12:A:3143:U:C6	2.53	0.44
17:I:101:ASN:HB3	17:I:150:HIS:HB3	2.00	0.44
21:M:19:LEU:HD13	46:o:95:LEU:HD12	1.99	0.44
36:d:221:THR:HG22	36:d:239:PRO:HA	1.99	0.44
80:AA:952:A:H2'	80:AA:953:U:C6	2.53	0.44
86:A4:335:PHE:CG	86:A4:360:MET:HE2	2.53	0.44
1:B:74:C:H2'	1:B:75:C:O4'	2.17	0.44
12:A:2776:G:H2'	12:A:2777:G:H8	1.82	0.44
12:A:2805:A:H2'	12:A:2806:U:C6	2.53	0.44
66:AO:183:ALA:HA	68:AR:183:LYS:HE2	1.99	0.44
80:AA:667:U:H2'	80:AA:668:U:C6	2.52	0.44
80:AA:1177:C:H2'	80:AA:1178:G:C8	2.53	0.44
80:AA:1572:A:H2'	80:AA:1573:A:C8	2.53	0.44
12:A:2245:A:H4'	12:A:2246:A:OP1	2.17	0.43
12:A:2815:OMG:H1'	12:A:2815:OMG:HM23	1.80	0.43
53:s:145:VAL:HG21	53:s:187:LEU:HD11	1.99	0.43
80:AA:658:G:H2'	80:AA:659:U:H6	1.82	0.43
80:AA:696:U:H2'	80:AA:697:G:C8	2.53	0.43
80:AA:867:C:H2'	80:AA:870:C:H42	1.83	0.43
21:M:44:ARG:HG3	21:M:45:ARG:HG3	2.00	0.43
43:l:92:TYR:HB3	43:l:96:LEU:HD13	1.99	0.43
54:AB:142:ILE:HG12	54:AB:192:LEU:HD23	2.00	0.43
60:AH:51:HIS:CE1	86:A4:476:LYS:HG3	2.53	0.43
69:AS:126:LEU:HD21	69:AS:132:LEU:HB2	2.00	0.43
80:AA:853:C:H2'	80:AA:854:U:C6	2.53	0.43
80:AA:982:A:H2'	80:AA:983:C:C6	2.53	0.43
80:AA:1174:U:H2'	80:AA:1175:G:H8	1.82	0.43
80:AA:1309:A:H2'	80:AA:1310:C:H6	1.83	0.43
80:AA:1544:A:H2'	80:AA:1545:U:C6	2.53	0.43
86:A4:397:MET:HE3	86:A4:397:MET:HB3	1.87	0.43
86:A4:446:LYS:HB3	86:A4:446:LYS:HE3	1.82	0.43
88:A2:33:VAL:HG21	88:A2:104:LEU:HD23	2.00	0.43
10:8:136:ILE:HD11	51:f:169:ILE:CG2	2.48	0.43
12:A:2285:U:H2'	12:A:2286:A:H8	1.82	0.43
12:A:3143:U:H2'	12:A:3144:A:H8	1.84	0.43
12:A:3144:A:H2'	12:A:3145:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:88:SER:HA	18:J:151:LEU:HD11	1.99	0.43
44:m:90:ARG:HE	44:m:94:ARG:HG3	1.82	0.43
50:c:259:ARG:HB2	50:c:271:PHE:HB2	2.00	0.43
66:AO:213:LEU:HD13	71:AU:50:PRO:HB2	2.00	0.43
80:AA:739:C:H2'	80:AA:740:G:O4'	2.18	0.43
80:AA:1165:C:H2'	80:AA:1166:A:C8	2.53	0.43
80:AA:1334:G:H2'	80:AA:1335:U:O4'	2.17	0.43
80:AA:1527:A:H2'	80:AA:1528:A:O4'	2.18	0.43
80:AA:1555:A:H2'	80:AA:1556:C:O4'	2.19	0.43
5:3:127:ALA:HA	21:M:79:PRO:HD3	2.00	0.43
12:A:3117:C:H2'	12:A:3118:U:H6	1.83	0.43
47:q:175:PHE:CD1	47:q:179:LEU:HD23	2.53	0.43
54:AB:141:ILE:HG23	54:AB:165:TYR:CE1	2.54	0.43
56:AD:141:TRP:HZ2	74:AZ:68:LEU:HB3	1.84	0.43
56:AD:355:ARG:NH1	80:AA:1118:A:H4'	2.33	0.43
64:AM:74:ARG:HG3	71:AU:74:PHE:CD1	2.54	0.43
70:AT:30:MET:HE1	70:AT:55:ILE:HG21	1.99	0.43
80:AA:915:C:H2'	80:AA:916:C:H6	1.83	0.43
80:AA:1372:C:H2'	80:AA:1373:U:C6	2.54	0.43
10:8:187:PRO:HG3	44:m:59:GLN:HA	2.01	0.43
12:A:1906:G:H2'	12:A:2014:A:H61	1.83	0.43
12:A:3165:C:H2'	12:A:3166:U:C6	2.53	0.43
29:U:131:GLU:O	29:U:134:ARG:HG3	2.18	0.43
37:e:183:THR:HG23	37:e:186:GLY:N	2.27	0.43
47:q:164:LEU:HD13	47:q:168:VAL:HG11	1.99	0.43
53:s:105:TRP:CG	53:s:271:LEU:HD13	2.53	0.43
54:AB:148:ASN:HD22	54:AB:197:HIS:CD2	2.37	0.43
80:AA:1207:U:H2'	80:AA:1208:U:H6	1.83	0.43
80:AA:1497:C:H2'	80:AA:1498:C:C6	2.54	0.43
12:A:2727:C:H2'	12:A:2728:C:H6	1.84	0.43
27:S:114:ILE:HD12	27:S:116:ILE:HD11	1.99	0.43
34:V:80:ILE:HB	34:V:85:TRP:HB2	1.99	0.43
55:AC:125:ARG:HH11	86:A4:94:TYR:HB2	1.83	0.43
72:AV:188:HIS:CD2	72:AV:353:LEU:HG	2.54	0.43
80:AA:1146:C:H2'	80:AA:1147:G:H8	1.84	0.43
80:AA:1148:A:H2'	80:AA:1149:G:C8	2.53	0.43
80:AA:1304:C:H2'	80:AA:1305:A:O4'	2.18	0.43
80:AA:1498:C:H2'	80:AA:1499:U:H6	1.84	0.43
16:H:120:ARG:HD3	31:X:132:LEU:HD13	2.00	0.43
17:I:140:TYR:HB3	17:I:143:LEU:HD12	1.99	0.43
23:O:33:LEU:HD21	23:O:59:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AO:123:LEU:HD13	66:AO:154:ILE:HG13	2.00	0.43
80:AA:681:U:H2'	80:AA:682:A:H8	1.84	0.43
80:AA:1503:G:H2'	80:AA:1504:U:C6	2.54	0.43
12:A:1924:U:H2'	12:A:1925:A:C8	2.54	0.43
21:M:137:GLY:HA3	21:M:157:GLN:HG2	2.00	0.43
43:l:110:LEU:HB3	43:l:117:TYR:HB2	1.99	0.43
47:q:117:ARG:O	47:q:121:ILE:HG12	2.19	0.43
53:s:369:PHE:HZ	53:s:417:VAL:HG13	1.83	0.43
61:AJ:58:LEU:HB3	61:AJ:85:LEU:HD12	2.00	0.43
64:AM:96:PHE:HD1	75:A0:169:LEU:HD22	1.83	0.43
64:AM:111:ARG:HD2	64:AM:114:ARG:HH21	1.84	0.43
10:8:168:LEU:HD23	51:f:88:TYR:HE2	1.83	0.43
12:A:2748:A:H2'	12:A:2749:A:C8	2.53	0.43
12:A:2804:A:H2'	12:A:2805:A:H8	1.84	0.43
16:H:102:VAL:HG22	16:H:128:LEU:HD23	2.00	0.43
22:N:101:HIS:CD2	22:N:184:PRO:HD3	2.54	0.43
37:e:61:LYS:HE2	37:e:155:ARG:HD2	2.01	0.43
37:e:163:GLU:HB3	37:e:165:PHE:CE2	2.54	0.43
80:AA:873:G:H2'	80:AA:874:G:H8	1.83	0.43
80:AA:1349:U:H2'	80:AA:1350:G:C8	2.53	0.43
87:AX:159:HIS:CD2	87:AX:267:ALA:HB2	2.53	0.43
12:A:2302:U:H2'	12:A:2303:A:C8	2.54	0.43
44:m:69:ARG:HG3	44:m:70:GLU:HG2	2.01	0.43
54:AB:167:HIS:ND1	59:AG:153:THR:HG22	2.32	0.43
80:AA:891:C:H2'	80:AA:892:A:O4'	2.19	0.43
80:AA:1209:C:H2'	80:AA:1210:U:C6	2.53	0.43
80:AA:1430:A:N1	80:AA:1458:A:H5''	2.34	0.43
80:AA:1577:U:H2'	80:AA:1578:A:C8	2.53	0.43
9:7:139:ASN:HB3	9:7:174:VAL:HG21	2.00	0.42
12:A:2802:A:H2'	12:A:2803:A:O4'	2.19	0.42
59:AG:92:MET:HG3	76:A1:116:PRO:HD2	2.00	0.42
60:AH:97:LEU:O	60:AH:101:GLU:HG3	2.19	0.42
80:AA:995:A:H2'	80:AA:996:A:O4'	2.19	0.42
20:L:73:ILE:HD11	20:L:105:VAL:HG11	2.02	0.42
27:S:99:VAL:HG12	27:S:133:VAL:HG22	2.01	0.42
49:u:75:THR:O	49:u:79:ILE:HG13	2.19	0.42
53:s:119:PRO:HG3	53:s:394:TRP:CD2	2.54	0.42
80:AA:911:U:H2'	80:AA:912:U:C6	2.54	0.42
80:AA:1505:A:H2'	80:AA:1506:U:C6	2.55	0.42
1:B:25:C:H2'	1:B:26:A:H8	1.85	0.42
12:A:3141:A:H2'	12:A:3142:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AD:297:ARG:HH21	80:AA:1120:C:H5'	1.84	0.42
80:AA:664:G:H2'	80:AA:665:C:C6	2.53	0.42
80:AA:684:U:H2'	80:AA:685:A:H8	1.85	0.42
80:AA:746:A:H2'	80:AA:747:A:H8	1.85	0.42
80:AA:1003:A:H2'	80:AA:1004:G:H8	1.84	0.42
3:1:38:ARG:HH12	3:1:41:LEU:HD11	1.85	0.42
10:8:191:ARG:NH2	51:f:144:MET:HG3	2.35	0.42
12:A:2688:C:H2'	12:A:2689:C:C6	2.54	0.42
12:A:2728:C:H2'	12:A:2729:U:C6	2.54	0.42
36:d:186:VAL:HG21	36:d:239:PRO:HB3	2.01	0.42
80:AA:958:C:H4'	80:AA:959:C:O4'	2.19	0.42
80:AA:1177:C:H2'	80:AA:1178:G:H8	1.83	0.42
12:A:1861:U:H2'	12:A:1862:U:C6	2.54	0.42
12:A:2803:A:H2'	12:A:2804:A:O4'	2.19	0.42
15:F:218:LEU:HD23	15:F:260:VAL:HB	2.02	0.42
18:J:175:LEU:HA	18:J:178:GLN:HG3	2.01	0.42
37:e:257:LYS:HE2	37:e:273:ARG:HE	1.84	0.42
52:p:104:HIS:HA	52:p:132:GLU:HA	2.01	0.42
9:7:156:ARG:HH12	9:7:260:PHE:HB2	1.84	0.42
22:N:218:ILE:HG23	22:N:223:MET:HB2	2.02	0.42
24:P:58:LEU:HA	52:p:177:ARG:NH2	2.35	0.42
32:Y:176:ILE:HG21	82:OX:430:TRP:CG	2.55	0.42
36:d:121:SER:O	36:d:125:ILE:HG13	2.18	0.42
72:AV:233:LYS:HB2	72:AV:286:VAL:HG21	2.01	0.42
80:AA:1560:U:H2'	80:AA:1561:C:H6	1.85	0.42
80:AA:1588:G:H2'	80:AA:1589:C:C6	2.55	0.42
12:A:1895:C:H2'	12:A:1896:U:C6	2.54	0.42
12:A:2092:C:H2'	12:A:2093:U:C6	2.55	0.42
12:A:2302:U:H2'	12:A:2303:A:H8	1.83	0.42
14:E:244:ALA:HB1	14:E:248:ILE:HD11	2.02	0.42
25:Q:76:LEU:HD23	25:Q:279:GLU:HG2	2.01	0.42
58:AF:198:ARG:CZ	80:AA:1383:A:H2'	2.50	0.42
76:A1:313:LYS:HG3	87:AX:341:ILE:HG23	2.02	0.42
80:AA:959:C:H3'	80:AA:960:C:O4'	2.19	0.42
87:AX:210:TRP:HZ2	87:AX:225:VAL:HG23	1.83	0.42
1:B:49:U:H2'	1:B:50:U:C6	2.54	0.42
7:5:336:LEU:HD21	7:5:362:THR:HG23	2.01	0.42
10:8:53:LYS:NZ	85:Aw:40:C:H5''	2.35	0.42
12:A:2286:A:H2'	12:A:2287:U:C6	2.55	0.42
24:P:94:VAL:HG23	24:P:132:LEU:HD21	2.00	0.42
47:q:176:GLN:HA	47:q:179:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:AT:88:VAL:HG22	71:AU:109:ASN:HD21	1.85	0.42
71:AU:64:ARG:HH12	80:AA:844:A:H4'	1.85	0.42
80:AA:776:A:H4'	80:AA:777:G:H5'	2.02	0.42
85:Aw:74:C:H3'	85:Aw:75:C:C6	2.54	0.42
12:A:1806:U:H4'	12:A:1807:U:H5'	2.02	0.42
12:A:3190:A:H2	48:r:98:GLY:HA2	1.85	0.42
19:K:94:GLN:O	19:K:98:ARG:HG2	2.20	0.42
22:N:124:VAL:HG12	22:N:158:ARG:HE	1.85	0.42
38:g:109:VAL:HG13	38:g:146:THR:HG23	2.02	0.42
55:AC:129:PRO:HG3	76:A1:50:ARG:HE	1.84	0.42
56:AD:140:LEU:HD11	56:AD:160:ARG:HE	1.84	0.42
60:AH:156:TYR:O	60:AH:160:ILE:HG12	2.19	0.42
70:AT:29:VAL:HB	70:AT:79:TYR:HB2	2.02	0.42
75:A0:51:PRO:HG3	80:AA:705:C:H5'	2.01	0.42
80:AA:672:A:H2'	80:AA:673:U:H6	1.82	0.42
80:AA:865:A:H2'	80:AA:866:A:H8	1.82	0.42
80:AA:1396:C:H2'	80:AA:1397:U:C6	2.55	0.42
86:A4:646:THR:O	86:A4:650:MET:HG2	2.20	0.42
1:B:9:1MA:N3	1:B:45:G:H2'	2.34	0.42
1:B:40:U:H2'	1:B:41:A:C8	2.55	0.42
12:A:2682:A:H4'	26:R:41:LEU:HD13	2.01	0.42
12:A:2778:U:P	12:A:2782:A:H61	2.43	0.42
12:A:3153:U:H2'	12:A:3154:U:C6	2.55	0.42
26:R:97:LEU:HD22	26:R:101:VAL:HG11	2.01	0.42
80:AA:774:G:H2'	80:AA:775:C:C6	2.54	0.42
12:A:2734:A:H2'	12:A:2735:G:C8	2.54	0.41
12:A:2750:U:H2'	12:A:2751:G:H8	1.84	0.41
15:F:175:LYS:HG2	15:F:273:LEU:HD13	2.02	0.41
16:H:106:GLY:HA2	16:H:158:LYS:HB2	2.01	0.41
55:AC:123:VAL:HG23	55:AC:157:THR:HG22	2.02	0.41
71:AU:197:VAL:HG11	71:AU:199:ARG:HE	1.85	0.41
72:AV:106:ASN:HD21	72:AV:140:ASP:HB3	1.85	0.41
76:A1:284:LEU:HA	76:A1:289:ILE:HG21	2.00	0.41
80:AA:749:G:H2'	80:AA:750:G:C8	2.54	0.41
80:AA:990:U:H3	80:AA:997:A:N6	2.16	0.41
12:A:1862:U:H2'	12:A:1863:A:C8	2.51	0.41
12:A:1953:A:OP1	14:E:232:GLY:HA2	2.19	0.41
12:A:3199:U:H5''	12:A:3200:U:H4'	2.01	0.41
23:O:46:TRP:CD1	23:O:121:ALA:HB2	2.55	0.41
48:r:71:PRO:HD2	48:r:107:LEU:HD23	2.02	0.41
51:f:90:VAL:HG13	51:f:189:HIS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AC:60:HIS:ND1	80:AA:1319:A:H5''	2.35	0.41
80:AA:818:C:H2'	80:AA:819:A:C8	2.54	0.41
80:AA:834:G:H2'	80:AA:835:C:O4'	2.20	0.41
80:AA:1006:U:H2'	80:AA:1007:G:C8	2.51	0.41
80:AA:1497:C:H2'	80:AA:1498:C:H6	1.85	0.41
1:B:6:U:H3	1:B:67:G:H1	1.68	0.41
36:d:106:ILE:O	36:d:110:GLU:HG2	2.21	0.41
36:d:226:ASP:HB3	36:d:232:MET:SD	2.60	0.41
55:AC:58:ALA:HB3	55:AC:60:HIS:CE1	2.55	0.41
62:AK:35:TRP:NE1	62:AK:39:LYS:HD2	2.36	0.41
72:AV:340:LYS:HE3	72:AV:340:LYS:HB3	1.85	0.41
80:AA:1022:A:H2'	80:AA:1023:C:H6	1.85	0.41
80:AA:1043:C:H2'	80:AA:1044:U:C6	2.55	0.41
80:AA:1161:A:H2'	80:AA:1162:A:C8	2.55	0.41
80:AA:1188:A:H2'	80:AA:1429:C:OP2	2.19	0.41
85:Aw:26:U:H2'	85:Aw:27:A:C8	2.55	0.41
86:A4:535:MET:HE1	86:A4:551:CYS:HB3	2.01	0.41
87:AX:74:ASP:O	87:AX:78:VAL:HG12	2.20	0.41
7:5:113:LEU:HD12	7:5:311:ALA:HB1	2.01	0.41
21:M:281:LYS:HD2	38:g:40:GLU:OE1	2.20	0.41
80:AA:833:A:H2'	80:AA:834:G:H8	1.84	0.41
80:AA:1023:C:H2'	80:AA:1024:G:H8	1.86	0.41
90:B:101:VAL:HG22	37:e:166:GLY:HA3	2.02	0.41
9:7:180:CYS:HB2	9:7:296:ARG:HG3	2.02	0.41
12:A:3129:A:H2'	12:A:3130:A:C8	2.56	0.41
19:K:71:LYS:HG2	48:r:174:MET:SD	2.60	0.41
29:U:147:VAL:HG22	36:d:232:MET:HE2	2.02	0.41
56:AD:412:LYS:HG2	56:AD:418:LYS:HB2	2.01	0.41
59:AG:172:LEU:HD11	59:AG:237:GLU:HG2	2.03	0.41
80:AA:738:A:H3'	80:AA:739:C:H6	1.85	0.41
80:AA:836:A:H2'	80:AA:837:A:H8	1.85	0.41
80:AA:1592:U:H2'	80:AA:1593:U:C6	2.54	0.41
17:I:188:ARG:HD3	42:k:55:VAL:HB	2.02	0.41
18:J:159:LEU:HD21	18:J:164:LEU:HD13	2.01	0.41
21:M:226:PRO:HG3	52:p:45:LEU:HD23	2.03	0.41
26:R:141:ILE:HG22	83:a:51:LEU:HD12	2.03	0.41
36:d:40:ARG:HA	36:d:40:ARG:HD3	1.83	0.41
50:c:59:ARG:HB2	50:c:62:GLU:HG2	2.02	0.41
63:AL:130:ILE:HG12	63:AL:185:LEU:HD11	2.02	0.41
80:AA:1123:C:H2'	80:AA:1124:A:O4'	2.21	0.41
80:AA:1348:G:H2'	80:AA:1349:U:H6	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1399:A:H2'	80:AA:1400:U:H6	1.83	0.41
80:AA:1523:A:H2'	80:AA:1524:A:C8	2.55	0.41
53:s:65:ARG:O	53:s:69:THR:HG23	2.20	0.41
55:AC:43:ARG:HA	55:AC:43:ARG:HD3	1.88	0.41
57:AE:6:LEU:HD21	57:AE:8:LEU:HD13	2.03	0.41
63:AL:126:GLU:HB3	63:AL:181:ILE:HD11	2.03	0.41
80:AA:757:A:H4'	80:AA:758:U:H5''	2.01	0.41
80:AA:1207:U:H5''	80:AA:1218:A:H61	1.85	0.41
3:1:54:VAL:HG13	47:q:128:MET:HE2	2.02	0.41
7:5:59:THR:HB	7:5:73:PRO:HG3	2.02	0.41
12:A:1898:A:H2'	12:A:1899:G:H8	1.86	0.41
12:A:3170:C:N4	12:A:3171:C:H41	2.18	0.41
53:s:332:LEU:HD21	53:s:359:ALA:HB2	2.02	0.41
75:A0:175:ILE:HG22	75:A0:178:ARG:NH1	2.35	0.41
80:AA:700:A:H4'	80:AA:701:G:O5'	2.20	0.41
80:AA:753:A:H2'	80:AA:754:A:H8	1.85	0.41
80:AA:1180:U:H2'	80:AA:1181:G:C8	2.55	0.41
80:AA:1373:U:H2'	80:AA:1374:A:C8	2.53	0.41
80:AA:1461:A:H4'	80:AA:1462:G:N7	2.35	0.41
80:AA:1500:C:H2'	80:AA:1501:A:O4'	2.21	0.41
9:7:286:LEU:HD11	9:7:296:ARG:HB2	2.01	0.41
12:A:1798:A:H62	36:d:37:THR:HA	1.86	0.41
12:A:1829:A:H2'	12:A:1830:G:C8	2.56	0.41
12:A:2474:C:H2'	12:A:2475:U:O4'	2.21	0.41
12:A:2774:C:H2'	12:A:2775:A:C5	2.56	0.41
12:A:2872:C:H2'	12:A:2873:A:O4'	2.21	0.41
29:U:112:PRO:N	29:U:113:GLU:HA	2.36	0.41
36:d:197:VAL:HG13	36:d:212:ILE:HG12	2.03	0.41
37:e:159:LEU:HD21	37:e:161:VAL:HG13	2.03	0.41
49:u:60:TYR:N	49:u:64:ILE:HD11	2.36	0.41
50:c:166:VAL:HG11	50:c:192:GLN:HG3	2.02	0.41
60:AH:124:VAL:HA	62:AK:108:ARG:HH12	1.86	0.41
80:AA:658:G:H2'	80:AA:659:U:C6	2.56	0.41
80:AA:715:G:H2'	80:AA:716:U:H6	1.86	0.41
80:AA:827:A:H5'	80:AA:828:C:C5	2.55	0.41
80:AA:970:A:H2'	80:AA:971:A:C8	2.56	0.41
80:AA:1114:U:H2'	80:AA:1115:U:C6	2.56	0.41
80:AA:1134:G:H2'	80:AA:1135:C:O4'	2.21	0.41
80:AA:1347:G:H2'	80:AA:1348:G:H8	1.85	0.41
80:AA:1365:A:H2'	80:AA:1366:C:C6	2.56	0.41
80:AA:1397:U:H2'	80:AA:1398:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:A4:236:VAL:HG22	86:A4:270:ARG:HG3	2.02	0.41
86:A4:397:MET:HA	86:A4:400:LEU:HG	2.03	0.41
12:A:2192:A:O2'	18:J:135:VAL:HG11	2.21	0.41
12:A:2352:U:H3	12:A:2361:G:H1	1.69	0.41
12:A:2764:A:C4	16:H:252:LEU:HD21	2.56	0.41
15:F:218:LEU:HD13	15:F:230:ILE:HD11	2.03	0.41
31:X:42:HIS:CG	31:X:86:ILE:HD11	2.56	0.41
44:m:59:GLN:OE1	44:m:79:ILE:HG13	2.21	0.41
58:AF:181:PHE:CE2	80:AA:1194:C:H5''	2.56	0.41
66:AO:198:PRO:HB2	66:AO:203:TYR:HB2	2.03	0.41
68:AR:155:LYS:HB3	68:AR:177:PRO:HD3	2.03	0.41
68:AR:213:GLU:HG2	68:AR:214:ASN:N	2.36	0.41
80:AA:757:A:H62	80:AA:783:A:H1'	1.86	0.41
80:AA:795:A:H3'	80:AA:796:G:O4'	2.21	0.41
80:AA:944:U:H2'	80:AA:945:G:H8	1.85	0.41
80:AA:1471:A:H2'	80:AA:1472:G:C8	2.56	0.41
87:AX:329:LEU:HB3	87:AX:333:GLY:HA3	2.02	0.41
12:A:2239:A:H2'	12:A:2240:C:C6	2.56	0.40
36:d:187:GLU:HG2	36:d:219:ARG:HB3	2.03	0.40
54:AB:239:ASN:HD21	73:AW:119:LYS:HG3	1.86	0.40
64:AM:39:ASN:OD1	80:AA:840:A:H5''	2.21	0.40
72:AV:263:MET:HE1	72:AV:334:PHE:HD1	1.85	0.40
75:A0:19:ARG:HG3	80:AA:808:C:H5'	2.03	0.40
80:AA:1122:A:H2'	80:AA:1123:C:C6	2.57	0.40
80:AA:1200:G:C2	80:AA:1201:A:C8	3.09	0.40
80:AA:1349:U:H2'	80:AA:1350:G:H8	1.87	0.40
10:8:70:ARG:NH1	84:Ax:46:U:H5'	2.37	0.40
10:8:147:LEU:HD21	37:e:208:ALA:HB1	2.03	0.40
29:U:21:ARG:NH1	32:Y:146:VAL:HG11	2.35	0.40
56:AD:351:ARG:HD2	56:AD:355:ARG:CZ	2.51	0.40
69:AS:20:VAL:HG21	69:AS:28:LYS:HG2	2.03	0.40
76:A1:60:MET:HE1	76:A1:66:TRP:HZ3	1.86	0.40
80:AA:746:A:H2'	80:AA:747:A:C8	2.56	0.40
80:AA:909:G:H2'	80:AA:910:A:H8	1.86	0.40
80:AA:925:U:H2'	80:AA:926:A:H8	1.87	0.40
80:AA:1034:U:H2'	80:AA:1035:U:C6	2.56	0.40
80:AA:1035:U:H2'	80:AA:1036:A:C8	2.56	0.40
80:AA:1195:U:H2'	80:AA:1196:A:C8	2.55	0.40
80:AA:1237:A:H1'	80:AA:1254:C:O2	2.21	0.40
80:AA:1590:A:H2'	80:AA:1591:C:C6	2.57	0.40
86:A4:393:ILE:HA	86:A4:396:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6:106:ARG:HG2	24:P:110:TRP:CE2	2.56	0.40
12:A:3201:A:H2'	12:A:3202:U:O4'	2.22	0.40
25:Q:69:VAL:HG12	25:Q:71:PRO:HD3	2.03	0.40
75:A0:65:LEU:HD23	75:A0:68:LEU:HB2	2.02	0.40
80:AA:871:A:O3'	80:AA:872:G:H8	2.04	0.40
80:AA:1032:C:H2'	80:AA:1033:U:H6	1.86	0.40
80:AA:1464:G:H2'	80:AA:1465:C:C6	2.56	0.40
9:7:204:LYS:HE3	83:a:92:LEU:HD13	2.04	0.40
12:A:2727:C:H2'	12:A:2728:C:C6	2.57	0.40
12:A:3120:C:H2'	12:A:3121:C:O4'	2.21	0.40
15:F:53:LEU:HD11	15:F:271:ASP:HA	2.04	0.40
34:V:138:THR:HG23	34:V:140:ALA:N	2.37	0.40
63:AL:67:PRO:HA	63:AL:68:PRO:HD3	2.00	0.40
72:AV:263:MET:HG2	72:AV:341:LEU:HD11	2.02	0.40
80:AA:925:U:H2'	80:AA:926:A:C8	2.56	0.40
80:AA:1190:C:H2'	80:AA:1191:C:H6	1.86	0.40
80:AA:1410:G:H2'	80:AA:1411:G:C8	2.56	0.40
80:AA:1561:C:H2'	80:AA:1562:G:H8	1.87	0.40
12:A:2093:U:H2'	12:A:2094:G:H8	1.85	0.40
12:A:2217:C:H2'	12:A:2218:C:O4'	2.22	0.40
55:AC:125:ARG:NH1	86:A4:94:TYR:HB2	2.37	0.40
60:AH:181:PRO:HD2	60:AH:184:ILE:HG21	2.03	0.40
69:AS:85:PHE:HB2	73:AW:100:VAL:HG12	2.03	0.40
77:A3:177:TRP:CD1	77:A3:178:LEU:HD12	2.57	0.40
80:AA:969:A:H2'	80:AA:970:A:C8	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	0	108/188 (57%)	108 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1	54/65 (83%)	54 (100%)	0	0	100	100
4	2	44/92 (48%)	44 (100%)	0	0	100	100
5	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
6	4	36/103 (35%)	36 (100%)	0	0	100	100
7	5	392/423 (93%)	382 (97%)	10 (3%)	0	100	100
8	6	352/380 (93%)	345 (98%)	7 (2%)	0	100	100
9	7	292/338 (86%)	282 (97%)	10 (3%)	0	100	100
10	8	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
11	9	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
13	D	236/305 (77%)	230 (98%)	5 (2%)	1 (0%)	30	60
14	E	303/348 (87%)	294 (97%)	9 (3%)	0	100	100
15	F	250/311 (80%)	248 (99%)	2 (1%)	0	100	100
16	H	200/267 (75%)	194 (97%)	6 (3%)	0	100	100
17	I	179/261 (69%)	179 (100%)	0	0	100	100
18	J	173/192 (90%)	173 (100%)	0	0	100	100
19	K	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
20	L	113/145 (78%)	110 (97%)	3 (3%)	0	100	100
21	M	289/296 (98%)	279 (96%)	10 (4%)	0	100	100
22	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
23	O	152/175 (87%)	148 (97%)	4 (3%)	0	100	100
24	P	142/180 (79%)	139 (98%)	3 (2%)	0	100	100
25	Q	237/292 (81%)	233 (98%)	4 (2%)	0	100	100
26	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
27	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
28	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
29	U	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
30	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
31	X	242/256 (94%)	239 (99%)	3 (1%)	0	100	100
32	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
33	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
34	V	203/216 (94%)	202 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	b	148/215 (69%)	143 (97%)	5 (3%)	0	100	100
36	d	257/306 (84%)	240 (93%)	17 (7%)	0	100	100
37	e	236/279 (85%)	227 (96%)	9 (4%)	0	100	100
38	g	132/166 (80%)	131 (99%)	1 (1%)	0	100	100
39	h	108/158 (68%)	103 (95%)	5 (5%)	0	100	100
40	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
41	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
42	k	100/112 (89%)	100 (100%)	0	0	100	100
43	l	80/138 (58%)	78 (98%)	2 (2%)	0	100	100
44	m	90/128 (70%)	88 (98%)	2 (2%)	0	100	100
46	o	92/102 (90%)	92 (100%)	0	0	100	100
47	q	175/222 (79%)	175 (100%)	0	0	100	100
48	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
49	t	44/198 (22%)	44 (100%)	0	0	100	100
49	u	30/198 (15%)	30 (100%)	0	0	100	100
50	c	282/332 (85%)	281 (100%)	1 (0%)	0	100	100
51	f	153/212 (72%)	147 (96%)	6 (4%)	0	100	100
52	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
53	s	381/439 (87%)	374 (98%)	7 (2%)	0	100	100
54	AB	223/296 (75%)	217 (97%)	6 (3%)	0	100	100
55	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
56	AD	341/430 (79%)	332 (97%)	9 (3%)	0	100	100
57	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
58	AF	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
59	AG	323/396 (82%)	316 (98%)	7 (2%)	0	100	100
60	AH	138/201 (69%)	132 (96%)	5 (4%)	1 (1%)	18	50
61	AJ	106/138 (77%)	105 (99%)	1 (1%)	0	100	100
62	AK	99/128 (77%)	99 (100%)	0	0	100	100
63	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
64	AM	117/137 (85%)	114 (97%)	3 (3%)	0	100	100
65	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	AO	191/258 (74%)	186 (97%)	5 (3%)	0	100	100
67	AP	95/142 (67%)	95 (100%)	0	0	100	100
68	AR	293/360 (81%)	286 (98%)	7 (2%)	0	100	100
69	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
70	AT	166/173 (96%)	166 (100%)	0	0	100	100
71	AU	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
72	AV	358/414 (86%)	345 (96%)	13 (4%)	0	100	100
73	AW	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
74	AZ	98/106 (92%)	97 (99%)	1 (1%)	0	100	100
75	A0	213/217 (98%)	205 (96%)	8 (4%)	0	100	100
76	A1	277/323 (86%)	267 (96%)	10 (4%)	0	100	100
77	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
79	AY	117/395 (30%)	116 (99%)	1 (1%)	0	100	100
81	AI	135/194 (70%)	128 (95%)	7 (5%)	0	100	100
82	OX	51/435 (12%)	47 (92%)	4 (8%)	0	100	100
83	a	99/142 (70%)	98 (99%)	1 (1%)	0	100	100
86	A4	584/689 (85%)	570 (98%)	14 (2%)	0	100	100
87	AX	350/398 (88%)	338 (97%)	12 (3%)	0	100	100
88	A2	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
89	AQ	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
All	All	14367/18802 (76%)	14068 (98%)	297 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	AH	126	ILE
13	D	207	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	
2	0	99/164 (60%)	99 (100%)	0	100	100
3	1	53/60 (88%)	53 (100%)	0	100	100
4	2	40/72 (56%)	40 (100%)	0	100	100
5	3	88/166 (53%)	88 (100%)	0	100	100
6	4	37/89 (42%)	37 (100%)	0	100	100
7	5	353/368 (96%)	353 (100%)	0	100	100
8	6	313/332 (94%)	313 (100%)	0	100	100
9	7	270/303 (89%)	270 (100%)	0	100	100
10	8	146/190 (77%)	146 (100%)	0	100	100
11	9	104/112 (93%)	104 (100%)	0	100	100
13	D	192/245 (78%)	192 (100%)	0	100	100
14	E	260/290 (90%)	260 (100%)	0	100	100
15	F	219/262 (84%)	219 (100%)	0	100	100
16	H	182/228 (80%)	182 (100%)	0	100	100
17	I	165/232 (71%)	165 (100%)	0	100	100
18	J	138/150 (92%)	138 (100%)	0	100	100
19	K	155/155 (100%)	155 (100%)	0	100	100
20	L	98/124 (79%)	98 (100%)	0	100	100
21	M	246/249 (99%)	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	221/256 (86%)	221 (100%)	0	100	100
26	R	118/126 (94%)	118 (100%)	0	100	100
27	S	146/180 (81%)	146 (100%)	0	100	100
28	T	146/176 (83%)	146 (100%)	0	100	100
29	U	134/135 (99%)	134 (100%)	0	100	100
30	W	94/119 (79%)	94 (100%)	0	100	100
31	X	220/229 (96%)	220 (100%)	0	100	100
32	Y	163/223 (73%)	163 (100%)	0	100	100
33	Z	113/147 (77%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	V	183/191 (96%)	183 (100%)	0	100	100
35	b	132/186 (71%)	132 (100%)	0	100	100
36	d	237/274 (86%)	237 (100%)	0	100	100
37	e	207/236 (88%)	207 (100%)	0	100	100
38	g	124/148 (84%)	124 (100%)	0	100	100
39	h	104/148 (70%)	104 (100%)	0	100	100
40	i	86/110 (78%)	86 (100%)	0	100	100
41	j	74/97 (76%)	74 (100%)	0	100	100
42	k	83/89 (93%)	83 (100%)	0	100	100
43	l	76/116 (66%)	76 (100%)	0	100	100
44	m	85/113 (75%)	85 (100%)	0	100	100
46	o	80/87 (92%)	80 (100%)	0	100	100
47	q	153/178 (86%)	153 (100%)	0	100	100
48	r	147/169 (87%)	147 (100%)	0	100	100
49	t	40/158 (25%)	40 (100%)	0	100	100
49	u	31/158 (20%)	31 (100%)	0	100	100
50	c	251/288 (87%)	251 (100%)	0	100	100
51	f	139/188 (74%)	139 (100%)	0	100	100
52	p	135/181 (75%)	135 (100%)	0	100	100
53	s	339/381 (89%)	339 (100%)	0	100	100
54	AB	198/249 (80%)	198 (100%)	0	100	100
55	AC	115/143 (80%)	115 (100%)	0	100	100
56	AD	286/357 (80%)	286 (100%)	0	100	100
57	AE	104/107 (97%)	104 (100%)	0	100	100
58	AF	185/209 (88%)	185 (100%)	0	100	100
59	AG	285/342 (83%)	285 (100%)	0	100	100
60	AH	130/180 (72%)	130 (100%)	0	100	100
61	AJ	93/118 (79%)	93 (100%)	0	100	100
62	AK	91/113 (80%)	91 (100%)	0	100	100
63	AL	158/226 (70%)	158 (100%)	0	100	100
64	AM	97/113 (86%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	AN	96/115 (84%)	96 (100%)	0	100	100
66	AO	174/230 (76%)	174 (100%)	0	100	100
67	AP	88/123 (72%)	88 (100%)	0	100	100
68	AR	264/318 (83%)	264 (100%)	0	100	100
69	AS	116/164 (71%)	116 (100%)	0	100	100
70	AT	153/157 (98%)	153 (100%)	0	100	100
71	AU	152/174 (87%)	152 (100%)	0	100	100
72	AV	325/364 (89%)	325 (100%)	0	100	100
73	AW	87/158 (55%)	87 (100%)	0	100	100
74	AZ	90/95 (95%)	90 (100%)	0	100	100
75	A0	188/189 (100%)	188 (100%)	0	100	100
76	A1	257/291 (88%)	257 (100%)	0	100	100
77	A3	65/166 (39%)	65 (100%)	0	100	100
79	AY	110/357 (31%)	110 (100%)	0	100	100
81	AI	105/147 (71%)	105 (100%)	0	100	100
82	OX	49/372 (13%)	49 (100%)	0	100	100
83	a	99/133 (74%)	99 (100%)	0	100	100
86	A4	526/609 (86%)	526 (100%)	0	100	100
87	AX	311/351 (89%)	311 (100%)	0	100	100
88	A2	100/100 (100%)	100 (100%)	0	100	100
89	AQ	78/78 (100%)	78 (100%)	0	100	100
All	All	12843/16242 (79%)	12843 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
8	6	200	GLN
8	6	295	GLN
8	6	373	HIS
9	7	287	GLN
10	8	103	GLN
10	8	186	GLN

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Mol	Chain	Res	Type
13	D	156	ASN
13	D	168	HIS
14	E	72	GLN
14	E	137	ASN
15	F	103	GLN
16	H	196	ASN
17	I	36	HIS
17	I	119	HIS
17	I	142	ASN
21	M	114	GLN
22	N	210	GLN
25	Q	132	GLN
25	Q	209	GLN
28	T	127	ASN
29	U	27	GLN
31	X	4	HIS
31	X	177	HIS
32	Y	88	GLN
34	V	117	HIS
35	b	25	GLN
35	b	123	ASN
36	d	47	GLN
37	e	106	HIS
37	e	212	HIS
37	e	248	ASN
38	g	73	GLN
38	g	93	ASN
40	i	120	HIS
42	k	19	GLN
42	k	72	HIS
43	l	67	GLN
43	l	124	GLN
46	o	96	ASN
47	q	60	GLN
47	q	139	GLN
48	r	79	HIS
48	r	109	GLN
48	r	112	HIS
50	c	192	GLN
51	f	61	HIS
52	p	117	GLN
52	p	194	HIS

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Mol	Chain	Res	Type
53	s	420	GLN
54	AB	201	ASN
56	AD	130	GLN
56	AD	196	ASN
56	AD	341	ASN
56	AD	424	ASN
57	AE	56	GLN
57	AE	57	GLN
58	AF	113	GLN
61	AJ	37	HIS
61	AJ	106	GLN
61	AJ	134	HIS
63	AL	77	GLN
63	AL	108	GLN
63	AL	172	ASN
64	AM	28	ASN
64	AM	61	HIS
64	AM	75	HIS
66	AO	181	HIS
67	AP	71	HIS
68	AR	76	GLN
69	AS	66	HIS
69	AS	97	GLN
70	AT	69	ASN
72	AV	106	ASN
73	AW	135	GLN
75	A0	26	ASN
77	A3	158	GLN
79	AY	285	GLN
79	AY	378	ASN
81	AI	104	ASN
83	a	126	HIS
86	A4	201	GLN
86	A4	274	GLN
87	AX	66	GLN
87	AX	159	HIS
87	AX	176	GLN
87	AX	190	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	70/72 (97%)	16 (22%)	0
12	A	1556/1558 (99%)	254 (16%)	2 (0%)
78	Az	33/34 (97%)	12 (36%)	0
80	AA	953/954 (99%)	153 (16%)	0
84	Ax	70/71 (98%)	16 (22%)	0
85	Aw	64/76 (84%)	21 (32%)	0
All	All	2746/2765 (99%)	472 (17%)	2 (0%)

All (472) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	8	U
1	B	10	2MG
1	B	16	C
1	B	19	C
1	B	21	A
1	B	45	G
1	B	46	A
1	B	54	C
1	B	55	U
1	B	56	U
1	B	58	A
1	B	59	A
1	B	64	A
1	B	69	U
1	B	72	G
1	B	76	A
12	A	1681	G
12	A	1689	C
12	A	1692	A
12	A	1699	C
12	A	1700	U
12	A	1704	U
12	A	1708	A
12	A	1709	G
12	A	1711	C
12	A	1724	A
12	A	1727	A
12	A	1728	U
12	A	1736	A
12	A	1748	G
12	A	1765	C
12	A	1777	A

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Mol	Chain	Res	Type
12	A	1805	A
12	A	1807	U
12	A	1808	A
12	A	1810	A
12	A	1812	C
12	A	1817	C
12	A	1821	A
12	A	1827	C
12	A	1828	A
12	A	1832	A
12	A	1836	A
12	A	1844	A
12	A	1854	U
12	A	1856	A
12	A	1869	A
12	A	1871	A
12	A	1873	A
12	A	1878	U
12	A	1882	A
12	A	1887	A
12	A	1888	G
12	A	1893	A
12	A	1901	C
12	A	1902	C
12	A	1903	C
12	A	1907	A
12	A	1909	A
12	A	1918	G
12	A	1927	G
12	A	1937	A
12	A	1940	A
12	A	1975	U
12	A	1985	G
12	A	1986	A
12	A	1992	C
12	A	1993	A
12	A	1994	A
12	A	2001	C
12	A	2002	G
12	A	2003	A
12	A	2015	G
12	A	2022	G

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Mol	Chain	Res	Type
12	A	2030	U
12	A	2036	C
12	A	2037	U
12	A	2039	A
12	A	2054	U
12	A	2055	U
12	A	2060	A
12	A	2070	C
12	A	2071	U
12	A	2079	C
12	A	2099	U
12	A	2105	G
12	A	2111	C
12	A	2113	G
12	A	2125	C
12	A	2126	U
12	A	2147	G
12	A	2159	U
12	A	2160	A
12	A	2163	A
12	A	2168	U
12	A	2181	A
12	A	2182	G
12	A	2191	A
12	A	2192	A
12	A	2195	A
12	A	2196	A
12	A	2198	A
12	A	2200	A
12	A	2214	A
12	A	2219	C
12	A	2220	A
12	A	2221	C
12	A	2223	A
12	A	2224	C
12	A	2225	C
12	A	2226	U
12	A	2230	A
12	A	2233	U
12	A	2237	A
12	A	2241	A
12	A	2243	A

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Mol	Chain	Res	Type
12	A	2245	A
12	A	2246	A
12	A	2262	C
12	A	2263	C
12	A	2284	C
12	A	2285	U
12	A	2297	A
12	A	2300	G
12	A	2322	C
12	A	2331	C
12	A	2332	C
12	A	2345	G
12	A	2349	G
12	A	2350	A
12	A	2353	A
12	A	2357	C
12	A	2363	A
12	A	2372	U
12	A	2374	A
12	A	2379	C
12	A	2381	A
12	A	2390	A
12	A	2399	A
12	A	2401	A
12	A	2404	U
12	A	2407	U
12	A	2415	C
12	A	2446	A
12	A	2451	A
12	A	2478	G
12	A	2485	U
12	A	2493	C
12	A	2496	G
12	A	2502	C
12	A	2504	A
12	A	2506	A
12	A	2520	C
12	A	2521	A
12	A	2527	A
12	A	2540	C
12	A	2570	C
12	A	2571	G

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Mol	Chain	Res	Type
12	A	2592	G
12	A	2593	G
12	A	2594	U
12	A	2599	U
12	A	2600	A
12	A	2601	A
12	A	2603	C
12	A	2604	A
12	A	2606	U
12	A	2618	U
12	A	2627	G
12	A	2628	U
12	A	2630	U
12	A	2633	A
12	A	2635	G
12	A	2654	U
12	A	2655	G
12	A	2656	U
12	A	2683	C
12	A	2686	G
12	A	2694	A
12	A	2696	A
12	A	2706	A
12	A	2709	A
12	A	2718	C
12	A	2719	G
12	A	2723	A
12	A	2724	G
12	A	2725	A
12	A	2732	G
12	A	2745	A
12	A	2757	A
12	A	2762	C
12	A	2763	U
12	A	2765	A
12	A	2767	A
12	A	2768	A
12	A	2781	U
12	A	2782	A
12	A	2786	U
12	A	2790	A
12	A	2810	G

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Mol	Chain	Res	Type
12	A	2832	A
12	A	2833	A
12	A	2847	C
12	A	2864	U
12	A	2865	C
12	A	2883	A
12	A	2884	C
12	A	2885	U
12	A	2888	A
12	A	2889	C
12	A	2893	A
12	A	2913	A
12	A	2916	G
12	A	2917	G
12	A	2918	A
12	A	2919	A
12	A	2922	A
12	A	2928	C
12	A	2934	G
12	A	2935	A
12	A	2956	A
12	A	2962	C
12	A	2971	A
12	A	2985	C
12	A	2989	G
12	A	2990	A
12	A	2992	G
12	A	2993	U
12	A	3000	A
12	A	3005	A
12	A	3007	C
12	A	3016	G
12	A	3022	G
12	A	3041	U
12	A	3049	U
12	A	3053	A
12	A	3054	G
12	A	3072	U
12	A	3086	U
12	A	3089	A
12	A	3090	G
12	A	3096	U

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Mol	Chain	Res	Type
12	A	3100	U
12	A	3102	U
12	A	3108	U
12	A	3109	U
12	A	3110	C
12	A	3111	A
12	A	3112	A
12	A	3122	U
12	A	3150	U
12	A	3157	C
12	A	3158	A
12	A	3162	C
12	A	3169	C
12	A	3172	C
12	A	3177	A
12	A	3180	A
12	A	3183	U
12	A	3190	A
12	A	3199	U
12	A	3200	U
12	A	3207	A
12	A	3209	A
12	A	3210	C
12	A	3212	C
12	A	3217	A
12	A	3218	A
12	A	3228	U
12	A	3229	U
78	Az	0	U
78	Az	4	A
78	Az	11	U
78	Az	12	U
78	Az	13	U
78	Az	18	A
78	Az	21	A
78	Az	22	A
78	Az	25	U
78	Az	26	A
78	Az	27	C
78	Az	30	A
80	AA	651	A
80	AA	680	U

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Mol	Chain	Res	Type
80	AA	687	G
80	AA	688	A
80	AA	700	A
80	AA	704	U
80	AA	721	U
80	AA	722	C
80	AA	735	A
80	AA	737	C
80	AA	738	A
80	AA	745	A
80	AA	753	A
80	AA	757	A
80	AA	761	A
80	AA	766	G
80	AA	783	A
80	AA	791	G
80	AA	794	U
80	AA	796	G
80	AA	826	A
80	AA	828	C
80	AA	830	U
80	AA	832	U
80	AA	835	C
80	AA	836	A
80	AA	860	A
80	AA	861	U
80	AA	868	C
80	AA	870	C
80	AA	871	A
80	AA	881	A
80	AA	889	G
80	AA	890	C
80	AA	893	G
80	AA	899	G
80	AA	904	C
80	AA	905	A
80	AA	907	A
80	AA	919	A
80	AA	929	A
80	AA	933	G
80	AA	938	A
80	AA	939	A

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Mol	Chain	Res	Type
80	AA	941	G
80	AA	942	A
80	AA	954	C
80	AA	959	C
80	AA	960	C
80	AA	961	U
80	AA	962	C
80	AA	963	C
80	AA	967	A
80	AA	978	A
80	AA	993	A
80	AA	1001	C
80	AA	1002	C
80	AA	1015	A
80	AA	1022	A
80	AA	1031	G
80	AA	1042	U
80	AA	1046	A
80	AA	1065	C
80	AA	1076	5MU
80	AA	1081	U
80	AA	1082	A
80	AA	1096	A
80	AA	1103	A
80	AA	1105	C
80	AA	1106	C
80	AA	1107	U
80	AA	1109	A
80	AA	1118	A
80	AA	1119	U
80	AA	1121	A
80	AA	1126	A
80	AA	1137	A
80	AA	1138	G
80	AA	1151	C
80	AA	1153	C
80	AA	1155	G
80	AA	1160	A
80	AA	1167	A
80	AA	1179	G
80	AA	1187	U
80	AA	1188	A

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Mol	Chain	Res	Type
80	AA	1189	U
80	AA	1190	C
80	AA	1215	U
80	AA	1220	A
80	AA	1223	C
80	AA	1225	C
80	AA	1230	C
80	AA	1232	A
80	AA	1235	U
80	AA	1247	G
80	AA	1248	C
80	AA	1250	C
80	AA	1251	A
80	AA	1261	C
80	AA	1271	C
80	AA	1273	G
80	AA	1284	U
80	AA	1285	G
80	AA	1290	C
80	AA	1291	U
80	AA	1292	A
80	AA	1294	A
80	AA	1297	G
80	AA	1318	A
80	AA	1326	A
80	AA	1327	G
80	AA	1330	C
80	AA	1343	A
80	AA	1344	U
80	AA	1353	A
80	AA	1354	A
80	AA	1355	G
80	AA	1356	A
80	AA	1370	U
80	AA	1378	C
80	AA	1387	A
80	AA	1390	A
80	AA	1405	C
80	AA	1407	U
80	AA	1422	G
80	AA	1430	A
80	AA	1466	C

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Mol	Chain	Res	Type
80	AA	1481	C
80	AA	1482	A
80	AA	1512	A
80	AA	1517	A
80	AA	1519	A
80	AA	1522	U
80	AA	1525	C
80	AA	1526	U
80	AA	1527	A
80	AA	1528	A
80	AA	1533	C
80	AA	1537	C
80	AA	1538	G
80	AA	1539	C
80	AA	1540	A
80	AA	1557	A
80	AA	1560	U
80	AA	1564	A
80	AA	1568	U
80	AA	1571	U
80	AA	1582	G
80	AA	1584	MA6
80	AA	1594	G
80	AA	1595	G
80	AA	1599	A
84	Ax	13	U
84	Ax	16	A
84	Ax	17	U
84	Ax	18	A
84	Ax	22	U
84	Ax	43	A
84	Ax	44	U
84	Ax	47	U
84	Ax	48	G
84	Ax	51	U
84	Ax	52	A
84	Ax	56	C
84	Ax	61	C
84	Ax	63	G
84	Ax	65	A
84	Ax	71	A
85	Aw	9	A

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Mol	Chain	Res	Type
85	Aw	13	U
85	Aw	14	A
85	Aw	15	A
85	Aw	16	A
85	Aw	21	A
85	Aw	46	A
85	Aw	49	U
85	Aw	50	A
85	Aw	51	U
85	Aw	52	G
85	Aw	53	A
85	Aw	56	A
85	Aw	63	A
85	Aw	65	A
85	Aw	68	U
85	Aw	69	A
85	Aw	71	C
85	Aw	72	A
85	Aw	74	C
85	Aw	75	C

All (2) RNA pucker outliers are listed below:

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

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

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	$\# Z  > 2$
12	OMG	A	3040	12,85	23,26,27	0.35	0	32,38,41	0.40	0
12	PSU	A	3067	12	18,21,22	1.11	2 (11%)	21,30,33	0.79	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	OMG	A	2815	84,92,12	23,26,27	0.34	0	32,38,41	0.41	0
80	B8T	AA	1486	95,80	19,22,23	0.39	0	25,31,34	0.33	0
1	2MG	B	10	1	23,26,27	0.36	0	33,38,41	0.40	0
80	5MC	AA	1488	80	19,22,23	0.80	1 (5%)	26,32,35	0.50	0
12	OMU	A	3039	92,12	19,22,23	0.31	0	25,31,34	0.74	1 (4%)
80	5MU	AA	1076	80	19,22,23	0.36	0	27,32,35	0.58	0
12	1MA	A	2617	12	21,25,26	0.39	0	30,37,40	0.59	0
80	MA6	AA	1583	80	23,26,27	0.34	0	33,38,41	0.73	1 (3%)
1	1MA	B	9	1	21,25,26	0.38	0	30,37,40	0.67	0
1	PSU	B	39	1	18,21,22	1.03	1 (5%)	21,30,33	0.72	0
80	MA6	AA	1584	80	23,26,27	0.31	0	33,38,41	0.74	1 (3%)

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
12	OMG	A	3040	12,85	-	0/9/27/28	0/3/3/3
12	PSU	A	3067	12	-	1/7/25/26	0/2/2/2
12	OMG	A	2815	84,92,12	-	0/9/27/28	0/3/3/3
80	B8T	AA	1486	95,80	-	0/7/27/28	0/2/2/2
1	2MG	B	10	1	-	0/9/27/28	0/3/3/3
80	5MC	AA	1488	80	-	0/7/25/26	0/2/2/2
12	OMU	A	3039	92,12	-	0/9/27/28	0/2/2/2
80	5MU	AA	1076	80	-	5/7/25/26	0/2/2/2
12	1MA	A	2617	12	-	0/7/25/26	0/3/3/3
80	MA6	AA	1583	80	-	0/11/29/30	0/3/3/3
1	1MA	B	9	1	-	0/7/25/26	0/3/3/3
1	PSU	B	39	1	-	0/7/25/26	0/2/2/2
80	MA6	AA	1584	80	-	1/11/29/30	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	3067	PSU	C6-C5	3.57	1.39	1.35
1	B	39	PSU	C6-C5	3.55	1.39	1.35
80	AA	1488	5MC	C5-C4	-3.16	1.41	1.44
12	A	3067	PSU	O4'-C1'	-2.63	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	AA	1583	MA6	C2-N1-C6	2.93	118.98	111.83
80	AA	1584	MA6	C2-N1-C6	2.92	118.97	111.83
12	A	3039	OMU	C2'-C1'-N1	-2.81	108.90	114.24
12	A	3067	PSU	O4'-C1'-C2'	2.26	108.28	105.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	AA	1076	5MU	O4'-C4'-C5'-O5'
80	AA	1076	5MU	C3'-C4'-C5'-O5'
80	AA	1076	5MU	C4'-C5'-O5'-P
80	AA	1584	MA6	C4'-C5'-O5'-P
12	A	3067	PSU	O4'-C4'-C5'-O5'
80	AA	1076	5MU	C2'-C1'-N1-C6
80	AA	1076	5MU	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	2815	OMG	1	0
80	AA	1488	5MC	1	0
80	AA	1583	MA6	2	0
1	B	9	1MA	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 278 ligands modelled in this entry, 261 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
93	SPD	A	3301	95	9,9,9	0.14	0	8,8,8	0.17	0
96	FES	AP	201	67,57	0,4,4	-	-	-		
93	SPD	A	3302	-	9,9,9	0.15	0	8,8,8	0.18	0
98	SPM	AA	1702	-	13,13,13	0.17	0	12,12,12	0.26	0
99	ATP	AX	501	95	32,33,33	0.52	0	48,52,52	0.33	0
98	SPM	AA	1779	-	13,13,13	0.16	0	12,12,12	0.21	0
93	SPD	AG	401	-	9,9,9	0.14	0	8,8,8	0.18	0
93	SPD	A	3469	-	9,9,9	0.16	0	8,8,8	0.39	0
93	SPD	AA	1703	-	9,9,9	0.16	0	8,8,8	0.22	0
93	SPD	A	3470	-	9,9,9	0.15	0	8,8,8	0.31	0
96	FES	AT	201	70,64	0,4,4	-	-	-		
93	SPD	O	301	-	9,9,9	0.16	0	8,8,8	0.18	0
96	FES	r	201	17,48	0,4,4	-	-	-		
94	PUT	A	3303	-	5,5,5	0.14	0	4,4,4	0.22	0
90	VAL	B	101	1	4,6,7	0.82	0	6,7,9	1.09	1 (16%)
97	NAD	AA	1701	95	46,48,48	1.18	3 (6%)	64,73,73	0.79	2 (3%)
100	GDP	AX	503	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPD	A	3301	95	-	0/7/7/7	-
98	SPM	AA	1702	-	-	0/11/11/11	-
93	SPD	A	3302	-	-	2/7/7/7	-
99	ATP	AX	501	95	-	0/22/38/38	0/3/3/3
96	FES	AP	201	67,57	-	-	0/1/1/1
98	SPM	AA	1779	-	-	2/11/11/11	-
93	SPD	AG	401	-	-	1/7/7/7	-
93	SPD	A	3469	-	-	0/7/7/7	-
93	SPD	AA	1703	-	-	2/7/7/7	-
93	SPD	A	3470	-	-	1/7/7/7	-
96	FES	AT	201	70,64	-	-	0/1/1/1
93	SPD	O	301	-	-	1/7/7/7	-
96	FES	r	201	17,48	-	-	0/1/1/1
94	PUT	A	3303	-	-	0/3/3/3	-
90	VAL	B	101	1	-	0/5/6/8	-
97	NAD	AA	1701	95	-	3/30/62/62	0/5/5/5
100	GDP	AX	503	-	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AA	1701	NAD	PA-O3	5.10	1.65	1.59
100	AX	503	GDP	C5-C4	3.18	1.47	1.38
97	AA	1701	NAD	PN-O3	3.16	1.62	1.59
97	AA	1701	NAD	O4D-C1D	-2.60	1.37	1.40
100	AX	503	GDP	C6-N1	-2.45	1.34	1.38
100	AX	503	GDP	C5-N7	-2.07	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
100	AX	503	GDP	C5-C4-N3	-6.10	118.69	128.39
100	AX	503	GDP	C2-N3-C4	4.90	120.73	112.30
100	AX	503	GDP	N9-C4-N3	4.56	135.07	125.95
100	AX	503	GDP	C6-C5-N7	3.12	135.97	130.29
100	AX	503	GDP	C4-C5-N7	-2.51	106.70	110.67
100	AX	503	GDP	C3'-C2'-C1'	2.49	106.17	101.46
90	B	101	VAL	O-C-CA	-2.34	118.75	124.77
97	AA	1701	NAD	O3-PA-O1A	-2.26	103.90	110.70
97	AA	1701	NAD	O2A-PA-O1A	2.16	122.51	112.44
100	AX	503	GDP	O6-C6-C5	-2.08	121.05	126.53

There are no chirality outliers.

All (15) torsion outliers are listed below:

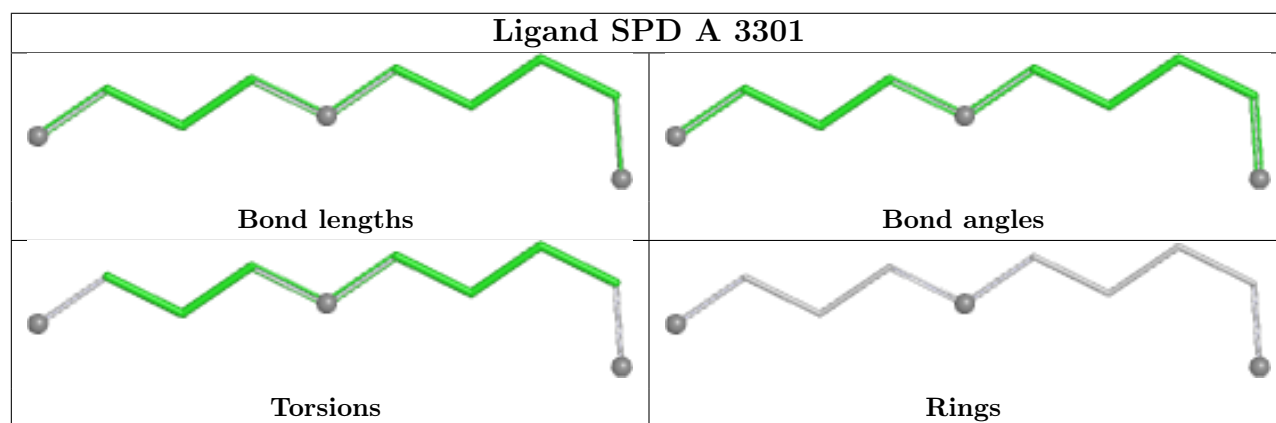
Mol	Chain	Res	Type	Atoms
93	A	3302	SPD	C2-C3-C4-C5
100	AX	503	GDP	C5'-O5'-PA-O3A
100	AX	503	GDP	C5'-O5'-PA-O1A
100	AX	503	GDP	C5'-O5'-PA-O2A
93	A	3470	SPD	C2-C3-C4-C5
98	AA	1779	SPM	N5-C6-C7-C8
97	AA	1701	NAD	C4N-C3N-C7N-N7N
93	O	301	SPD	C8-C7-N6-C5
98	AA	1779	SPM	C12-C11-N10-C9
97	AA	1701	NAD	C4N-C3N-C7N-O7N
93	AA	1703	SPD	C2-C3-C4-C5
93	A	3302	SPD	N1-C2-C3-C4
97	AA	1701	NAD	O4D-C4D-C5D-O5D
93	AA	1703	SPD	N1-C2-C3-C4
93	AG	401	SPD	C8-C7-N6-C5

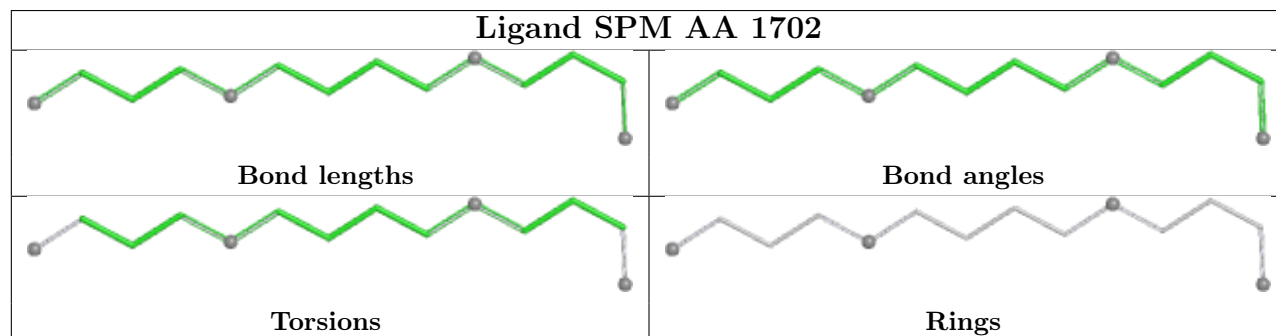
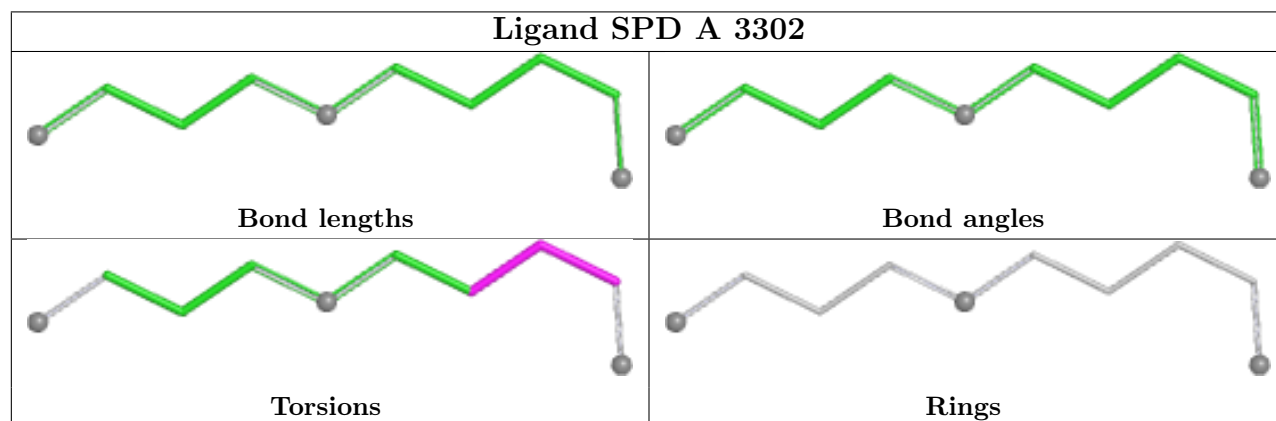
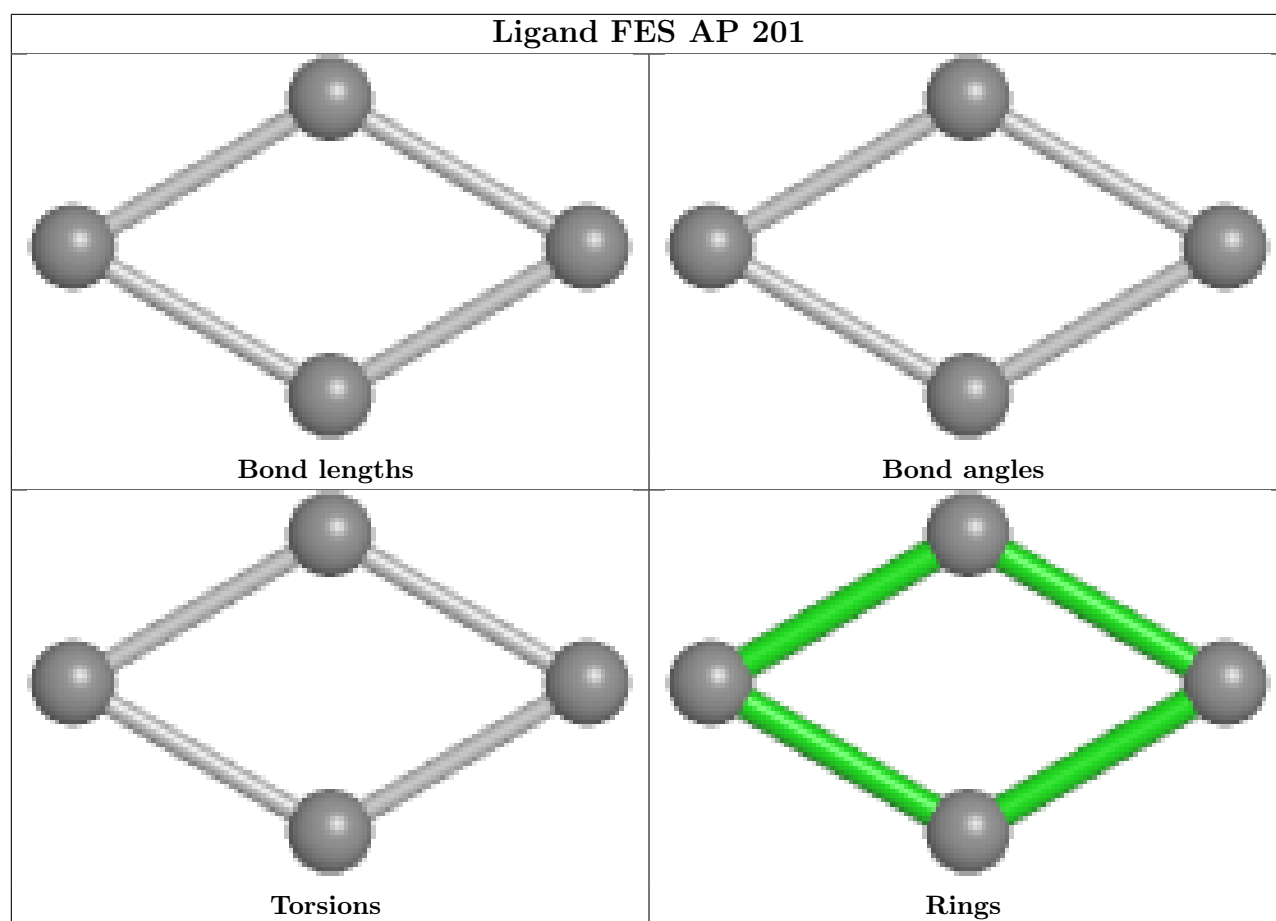
There are no ring outliers.

2 monomers are involved in 2 short contacts:

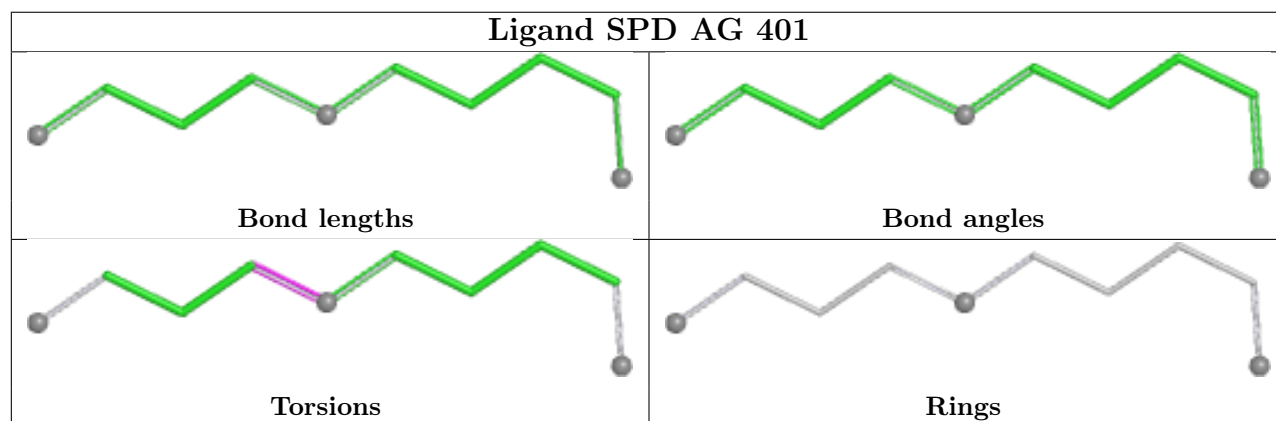
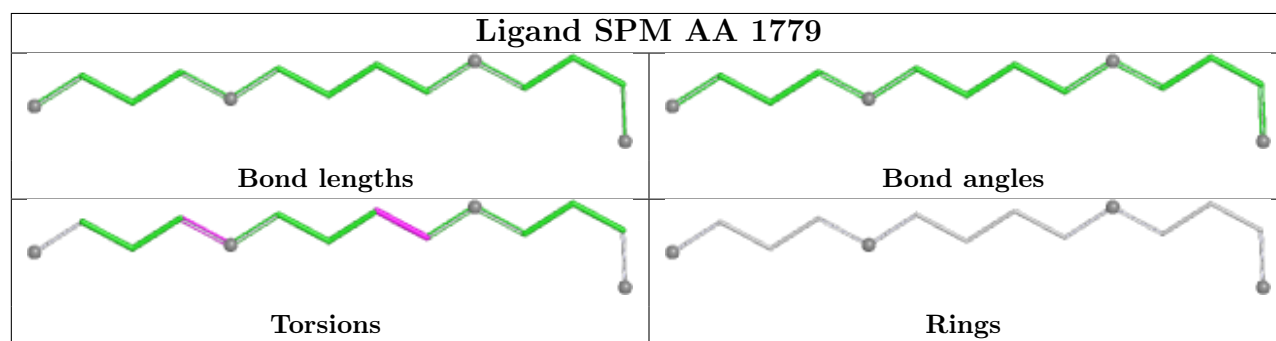
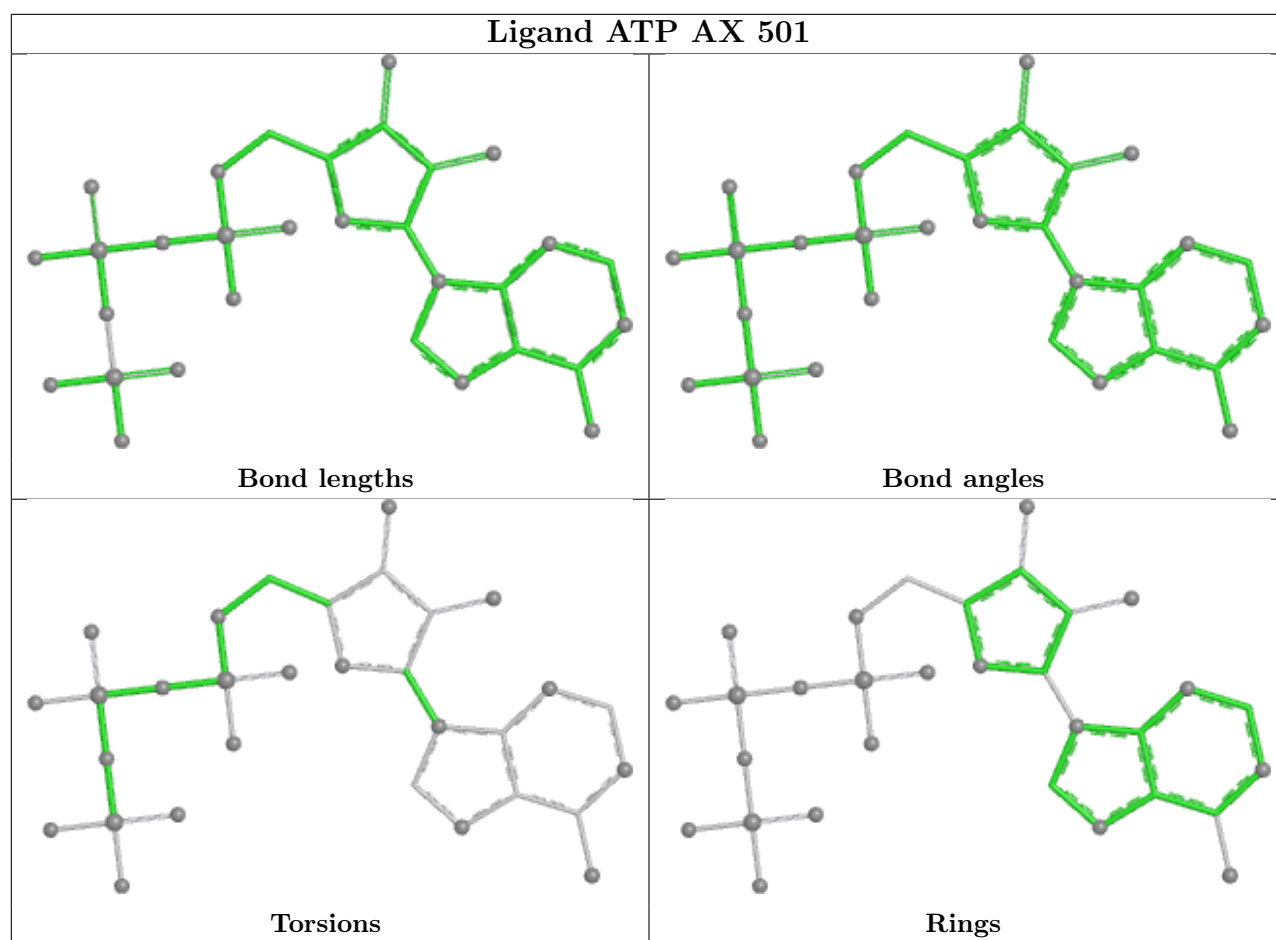
Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	B	101	VAL	1	0
100	AX	503	GDP	1	0

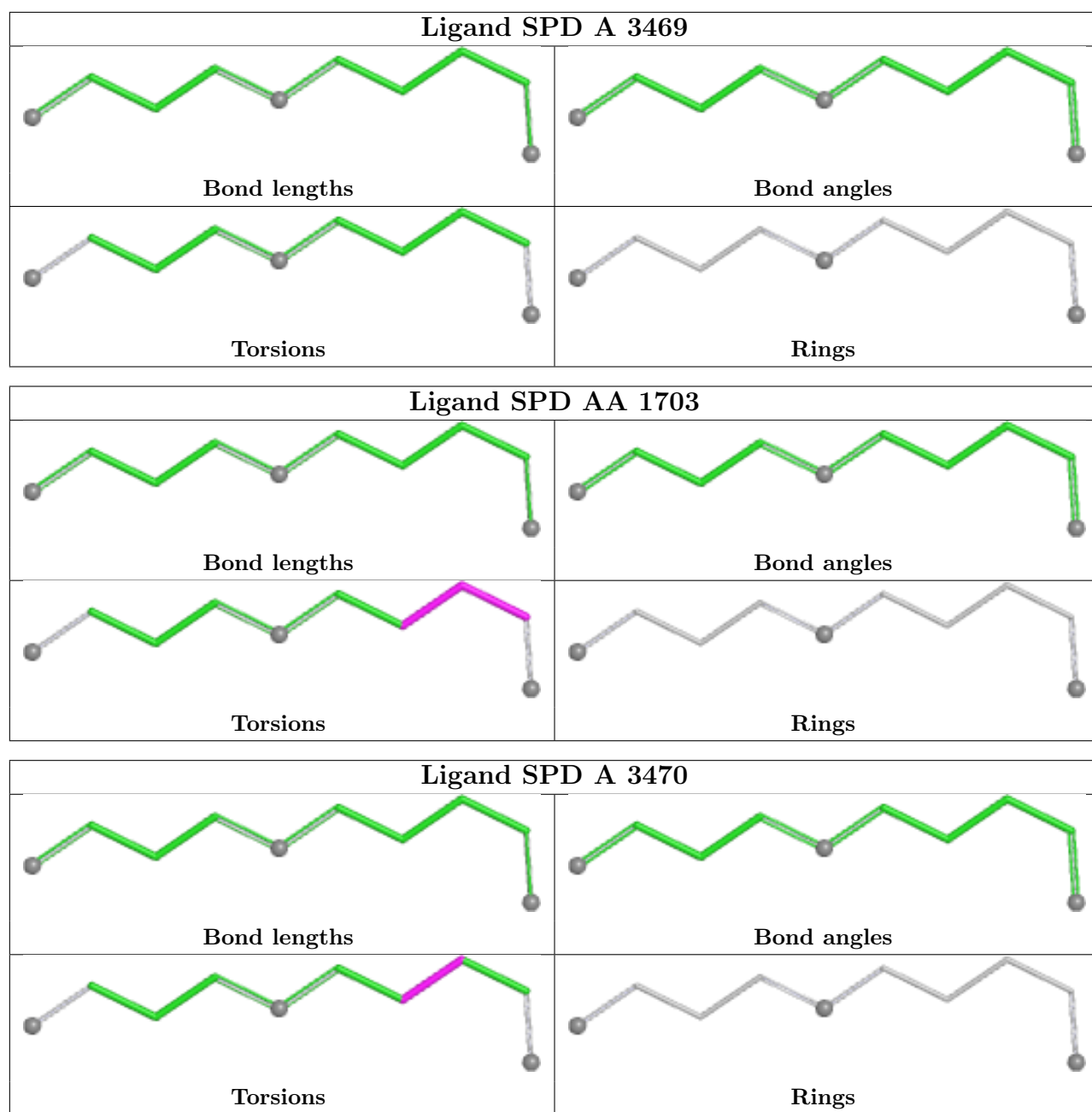
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

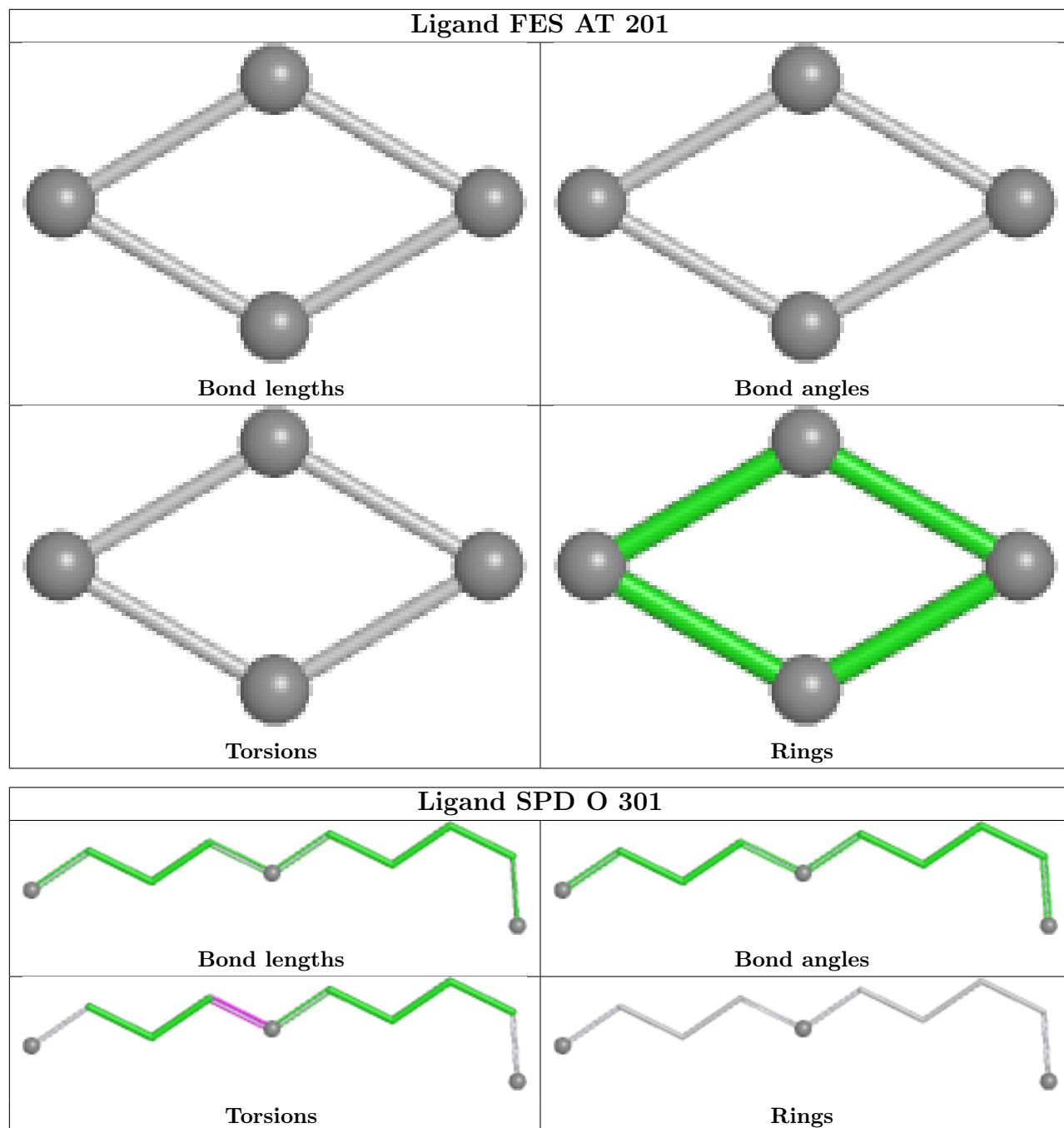


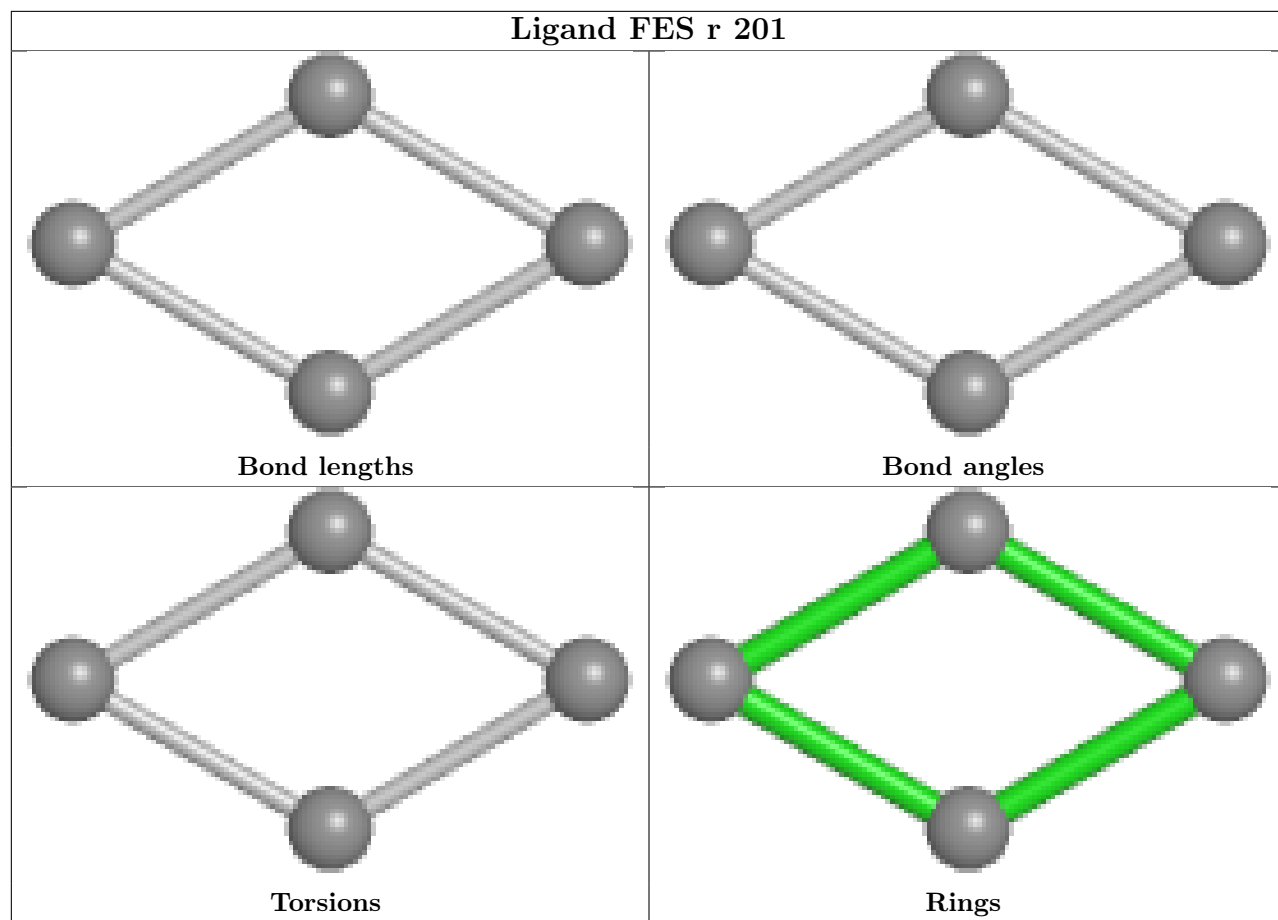




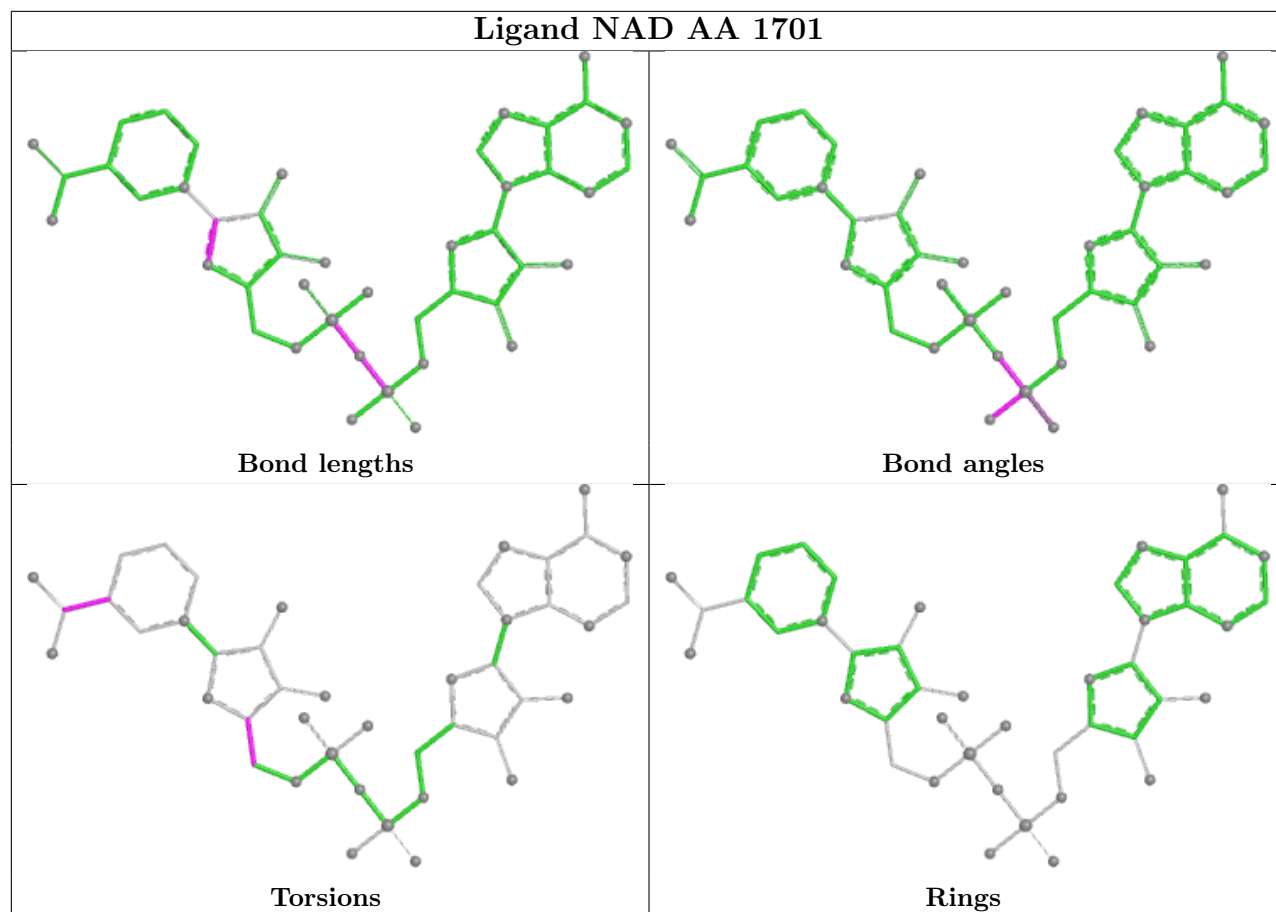




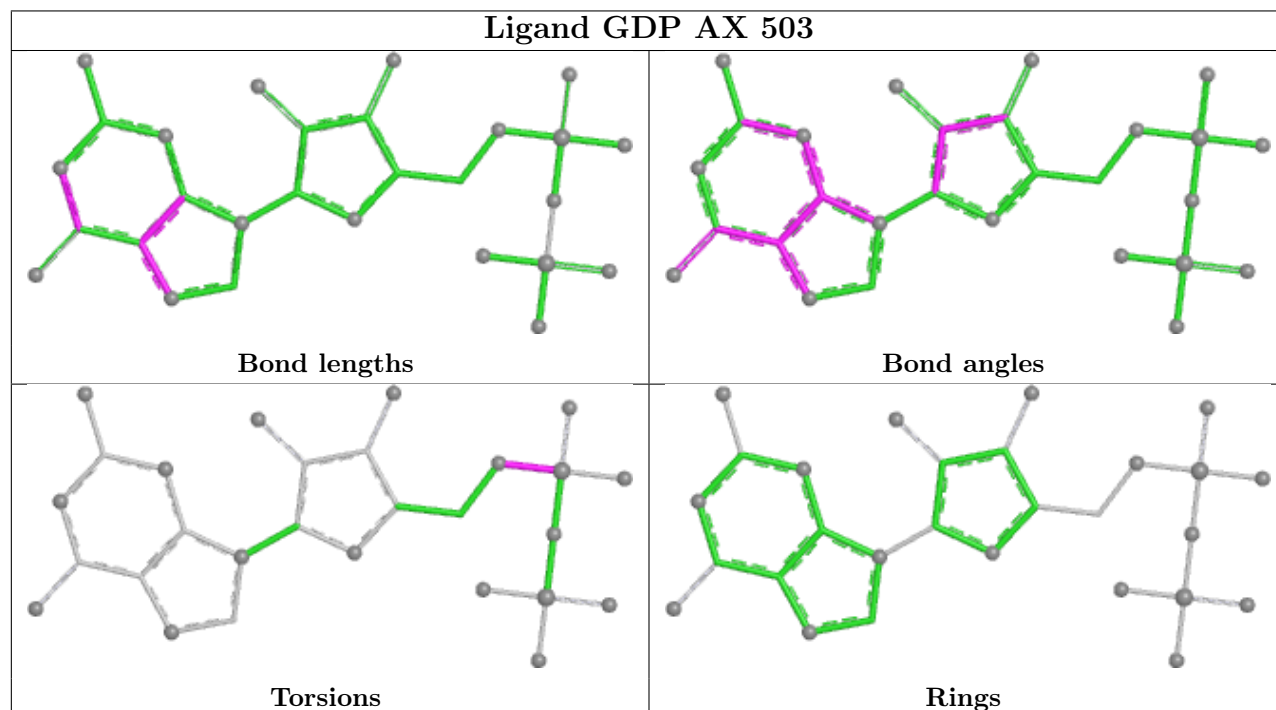




## Ligand NAD AA 1701



## Ligand GDP AX 503



## 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
12	A	1
1	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	8.79
1	B	46:A	O3'	48:U	P	4.60

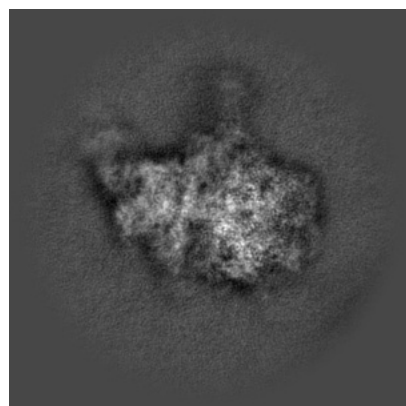
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71815. These allow visual inspection of the internal detail of the map and identification of artifacts.

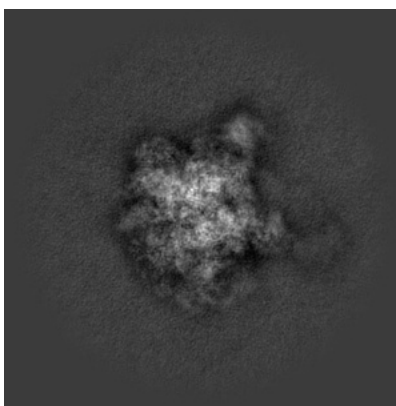
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

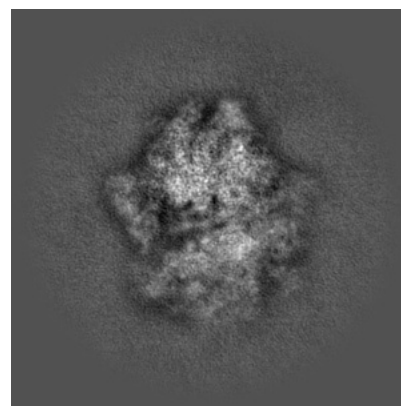
#### 6.1.1 Primary map



X

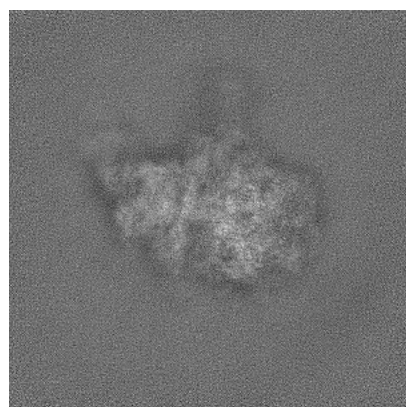


Y

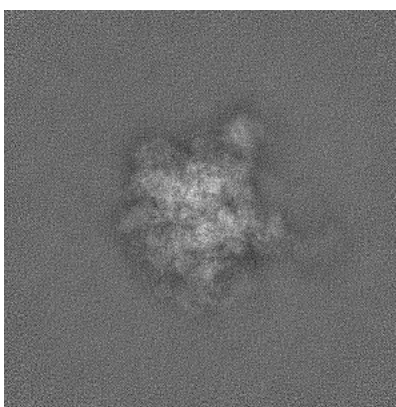


Z

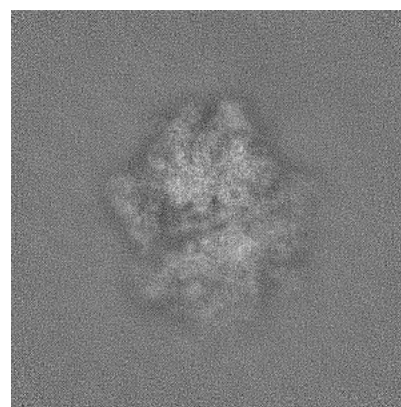
#### 6.1.2 Raw map



X



Y



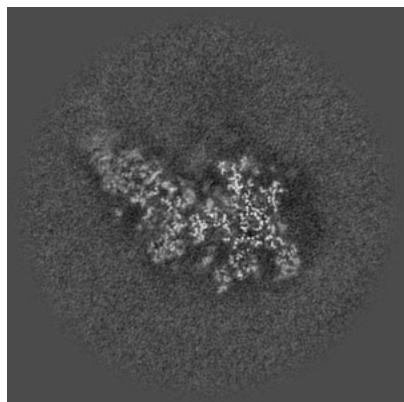
Z

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

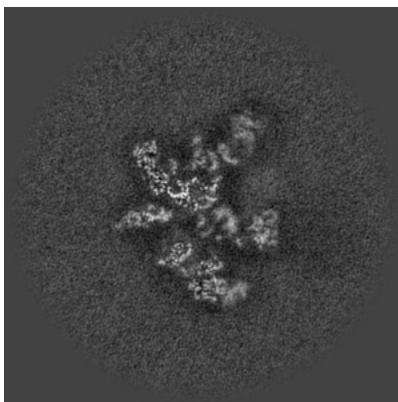


## 6.2 Central slices [i](#)

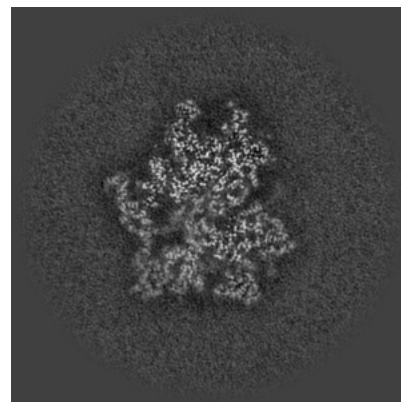
### 6.2.1 Primary map



X Index: 240

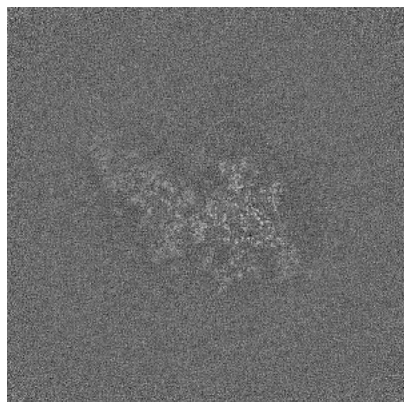


Y Index: 240

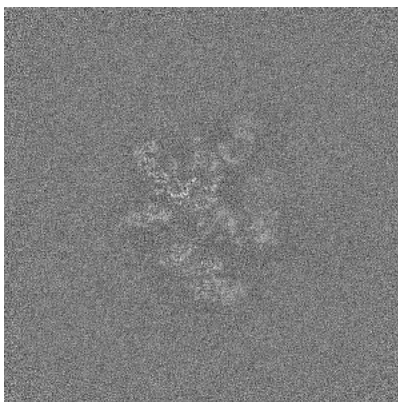


Z Index: 240

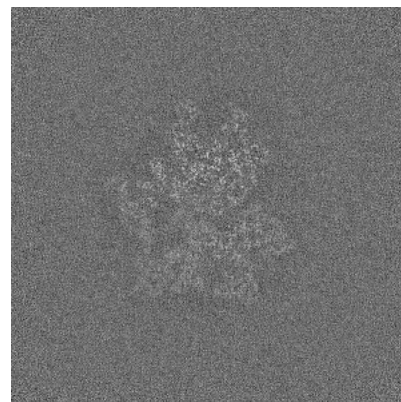
### 6.2.2 Raw map



X Index: 240



Y Index: 240



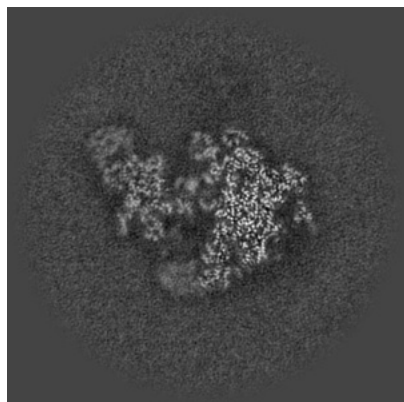
Z Index: 240

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

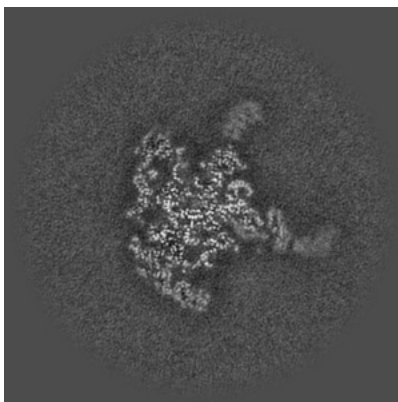


## 6.3 Largest variance slices [i](#)

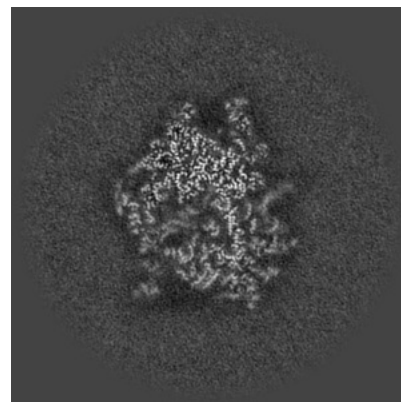
### 6.3.1 Primary map



X Index: 223

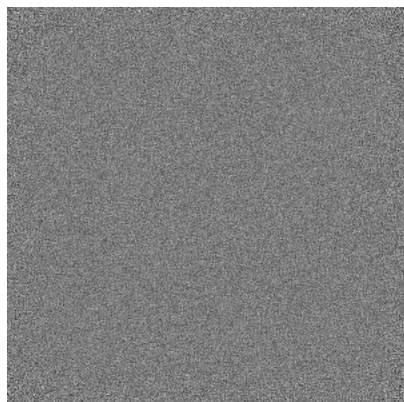


Y Index: 274

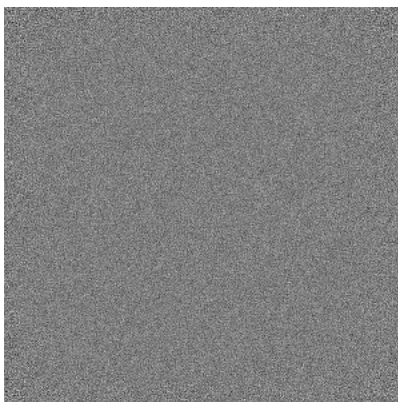


Z Index: 249

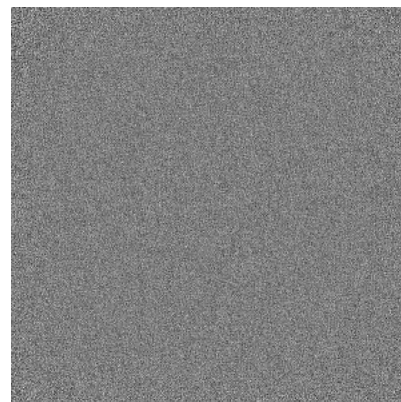
### 6.3.2 Raw map



X Index: 0



Y Index: 0

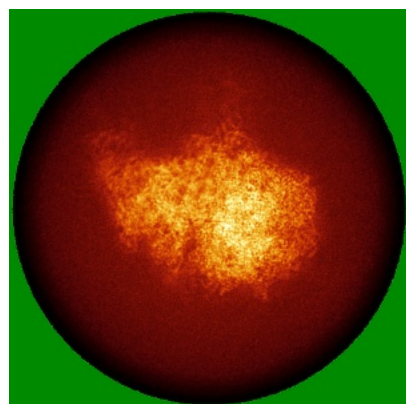


Z Index: 0

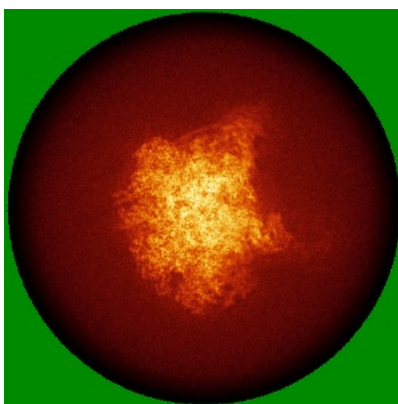
The images above show the largest variance slices of the map in three orthogonal directions.

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

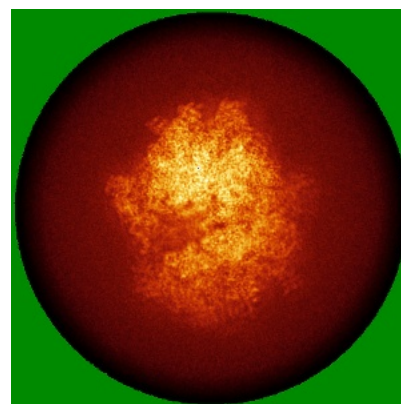
### 6.4.1 Primary map



X

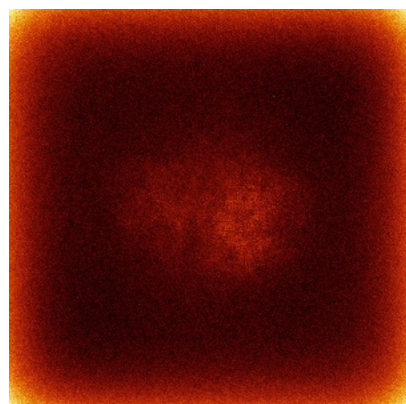


Y

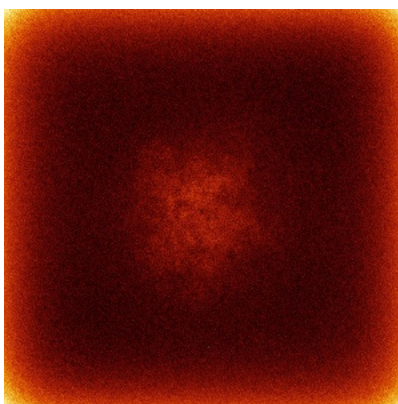


Z

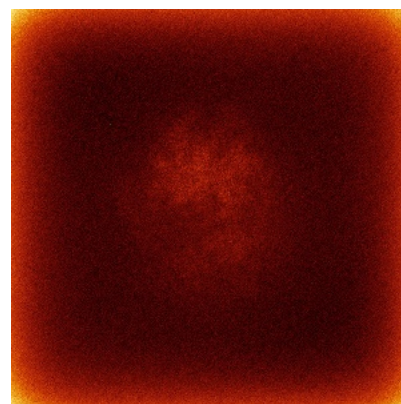
### 6.4.2 Raw map



X



Y

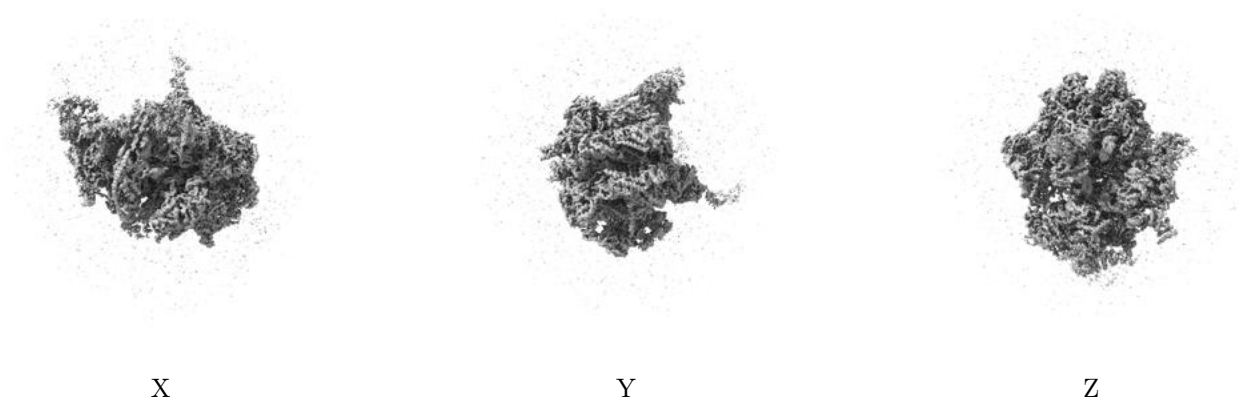


Z

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.

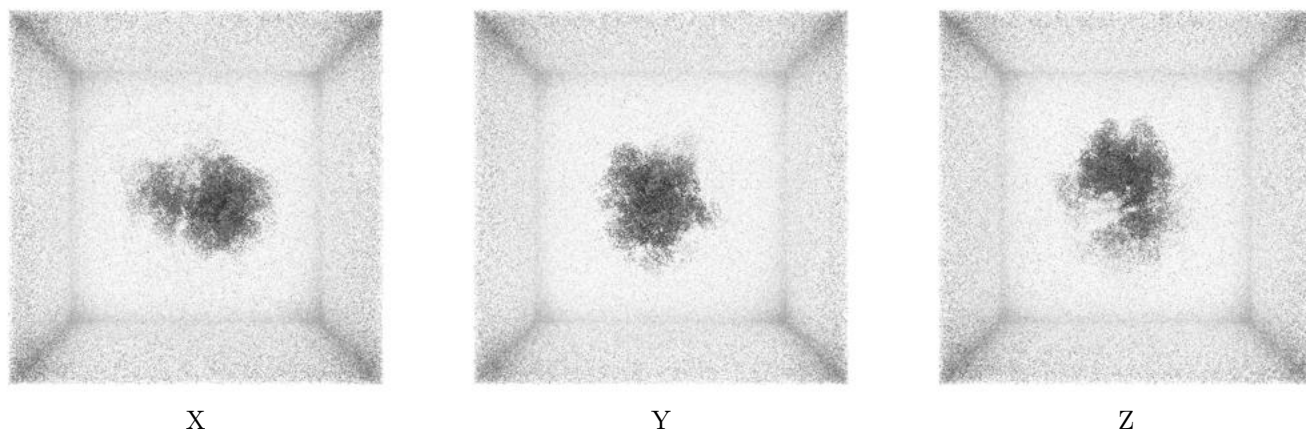
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.027. 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.

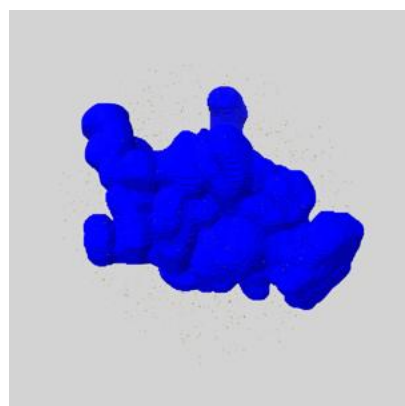
## 6.6 Mask visualisation [i](#)

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

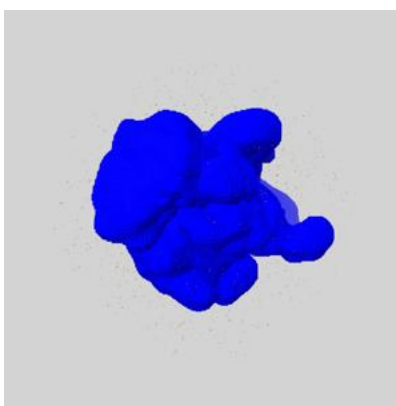
A mask typically either:

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

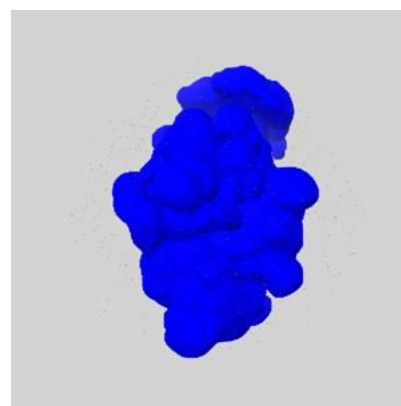
### 6.6.1 emd\_71815\_msk\_1.map [i](#)



X



Y



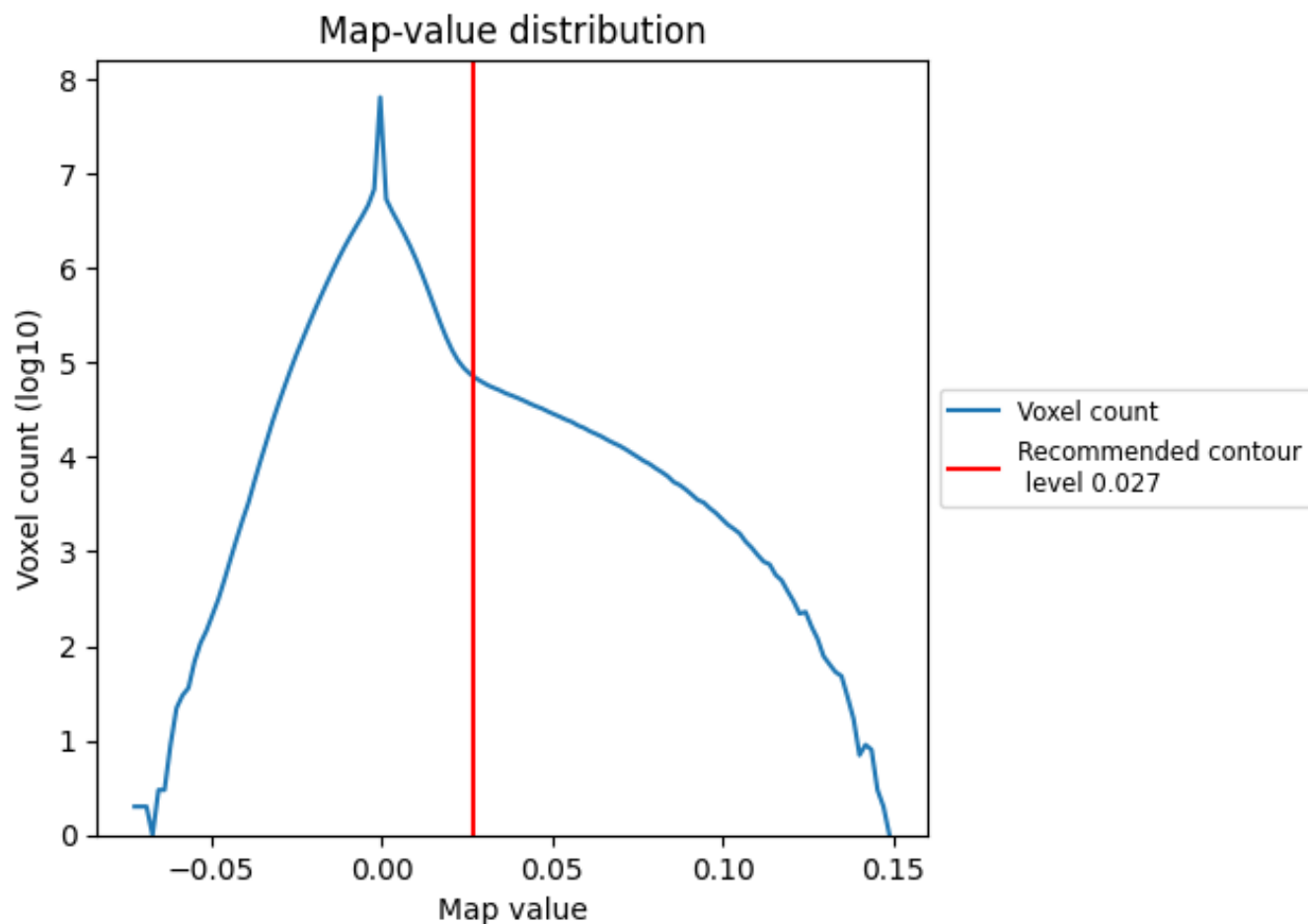
Z



## 7 Map analysis [i](#)

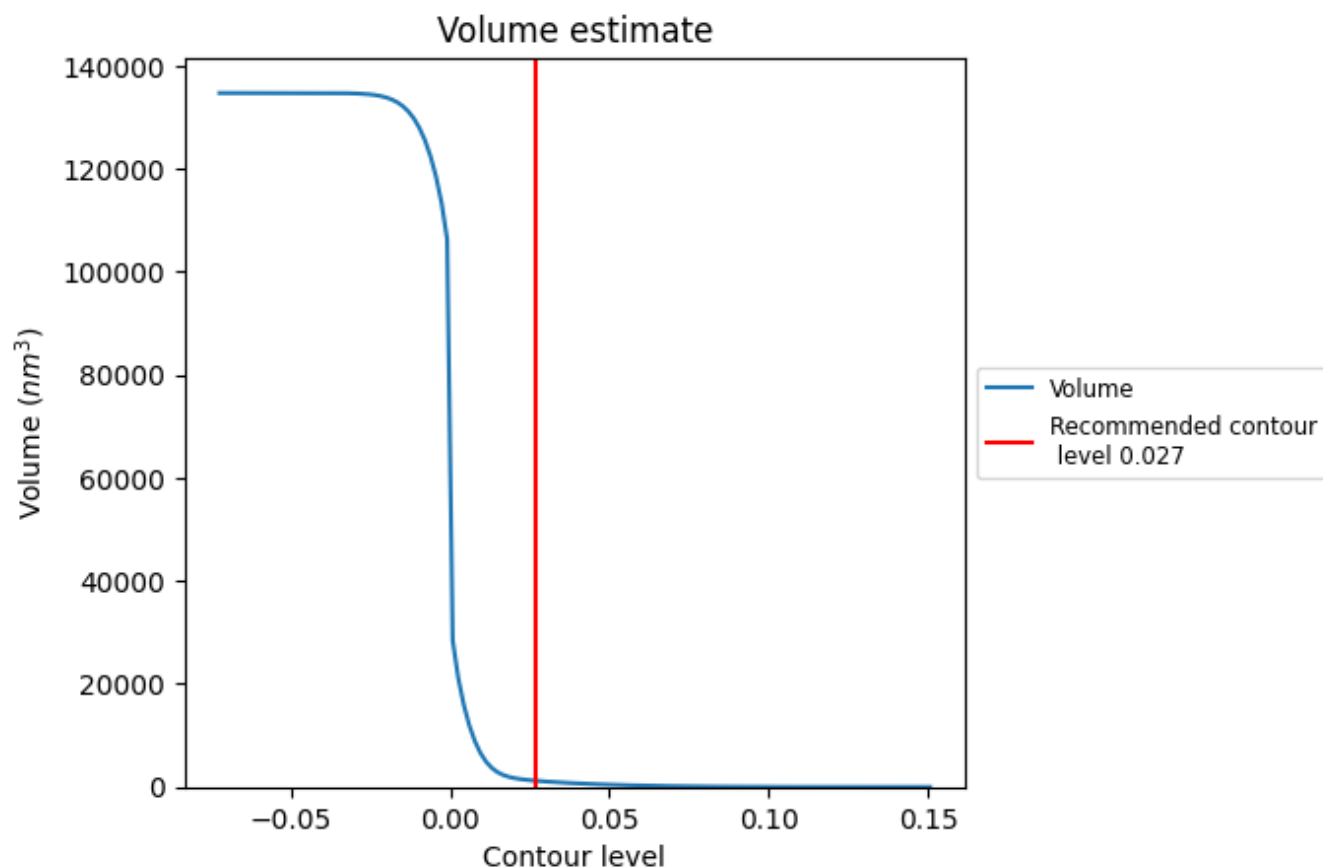
This section contains the results of statistical analysis of the map.

### 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.

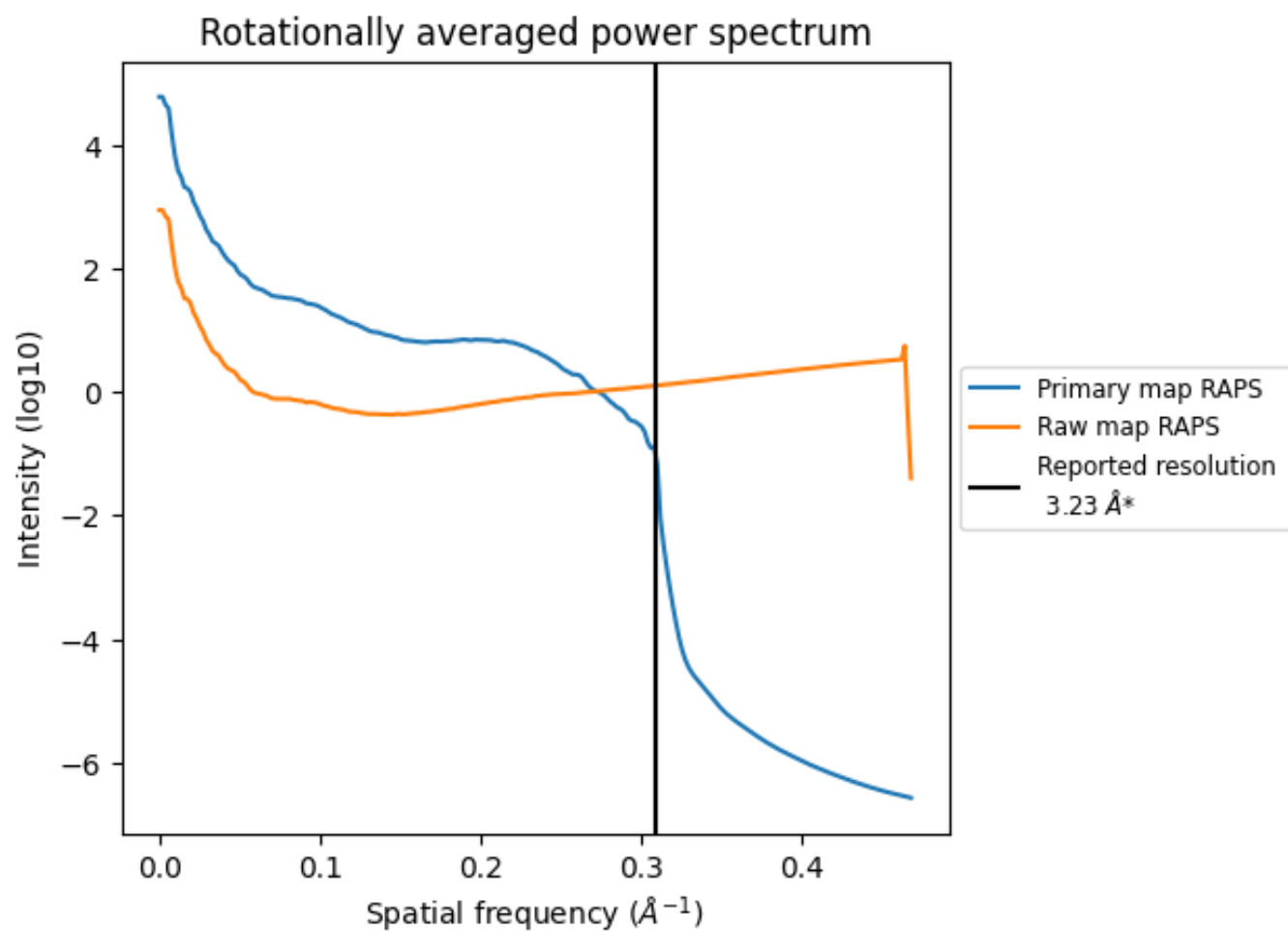
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1199 nm<sup>3</sup>; this corresponds to an approximate mass of 1083 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 ⓘ

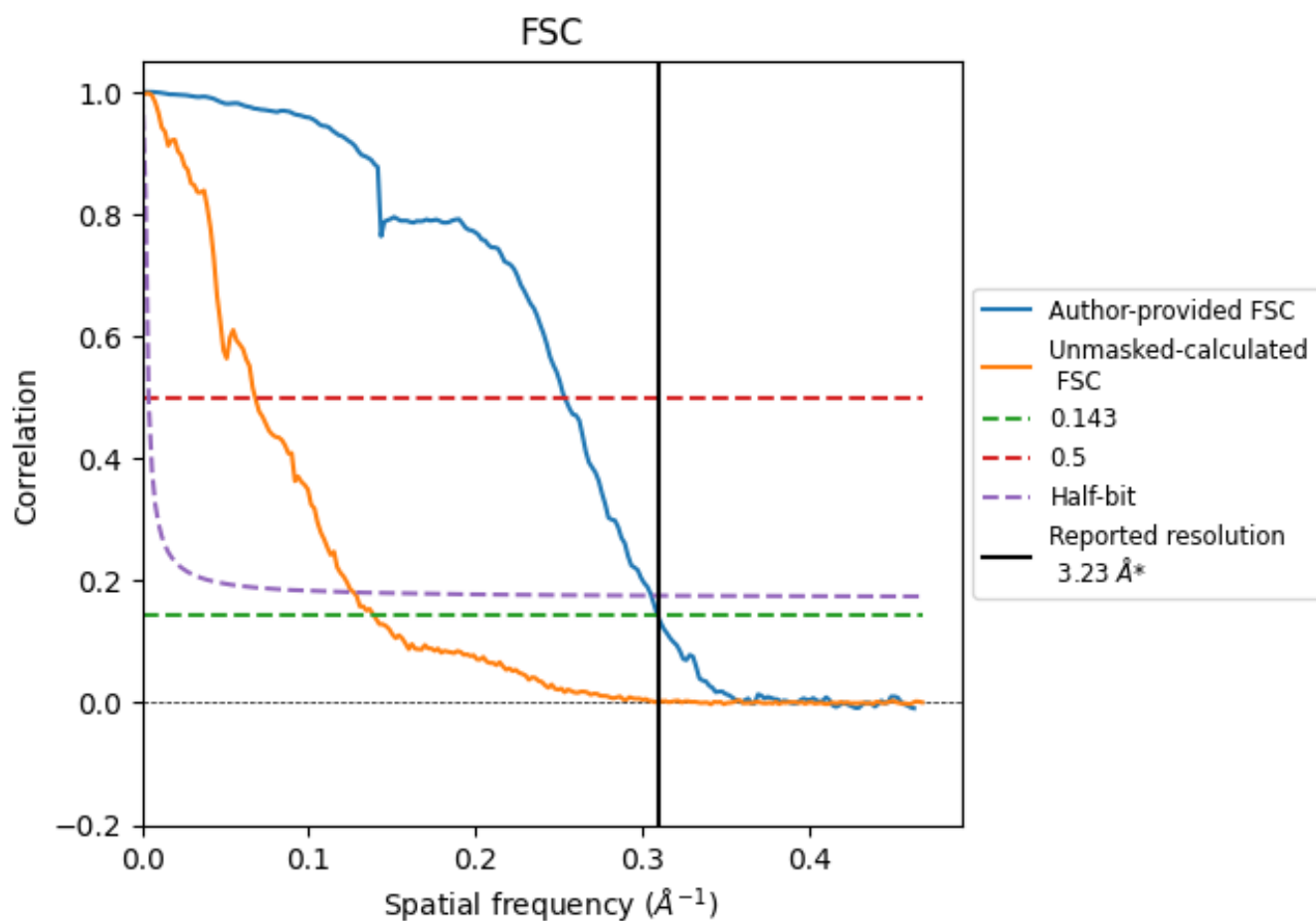


\*Reported resolution corresponds to spatial frequency of 0.310  $\text{\AA}^{-1}$

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



## 8.2 Resolution estimates [i](#)

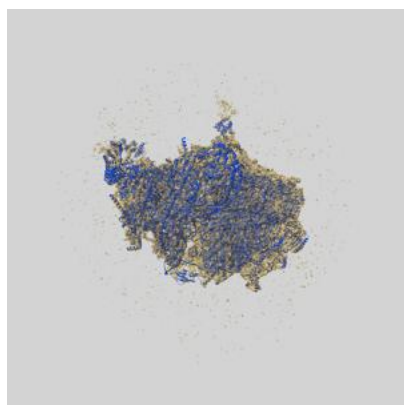
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.23	3.94	3.27
Unmasked-calculated*	7.19	14.75	7.88

\*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 7.19 differs from the reported value 3.23 by more than 10 %

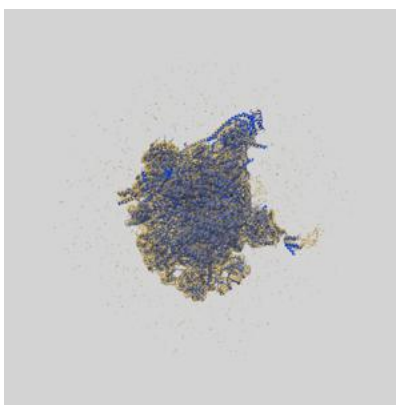
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71815 and PDB model 9PRX. Per-residue inclusion information can be found in section 3 on page 27.

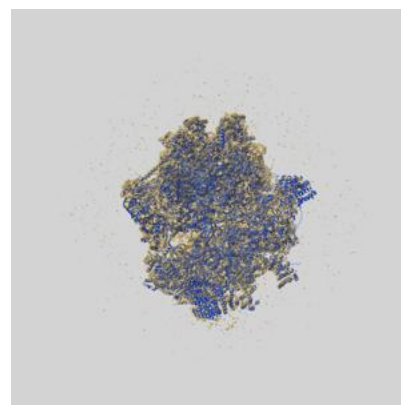
### 9.1 Map-model overlay [i](#)



X



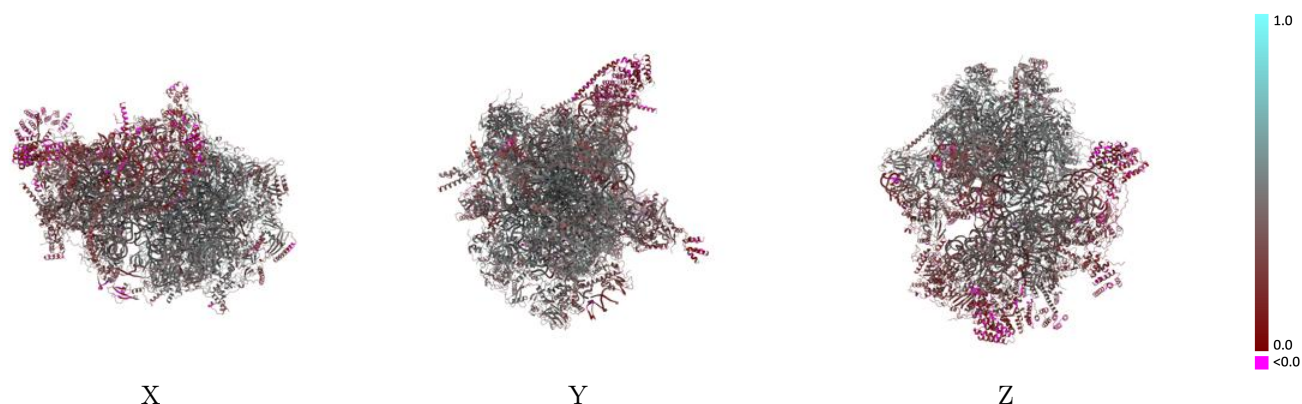
Y



Z

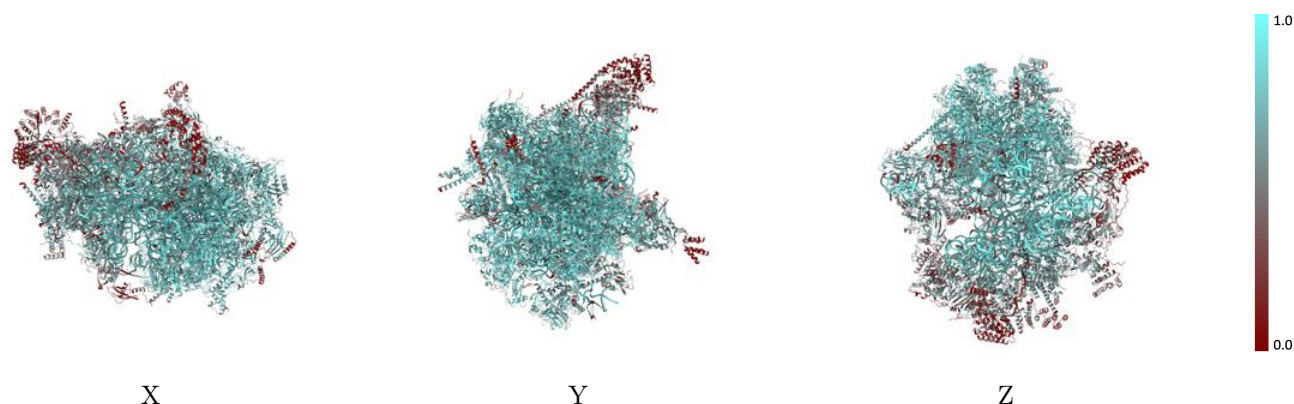
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



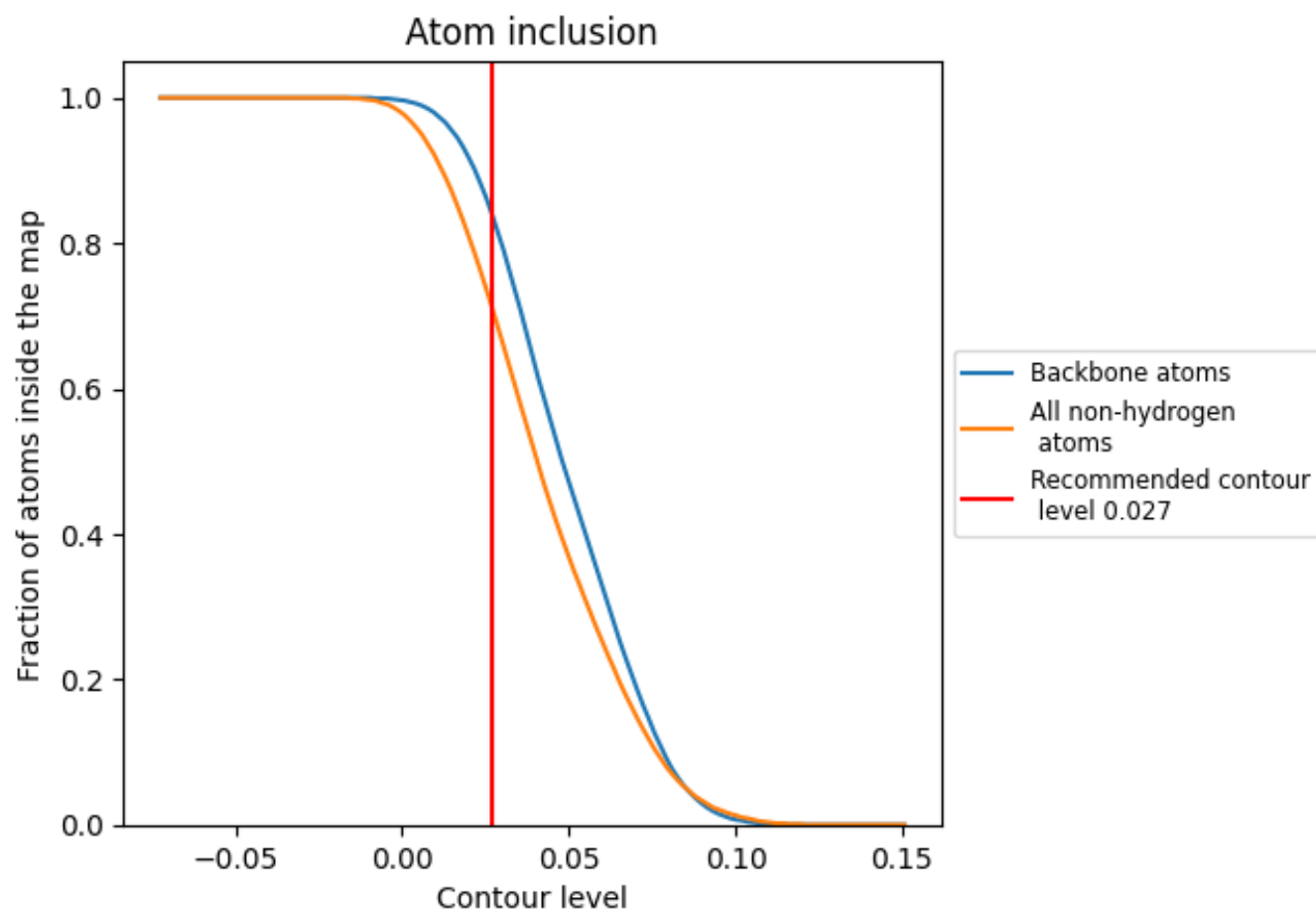
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 71% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.3880
0	 0.7570	 0.4620
1	 0.7120	 0.4400
2	 0.8480	 0.5080
3	 0.8360	 0.5120
4	 0.7920	 0.4850
5	 0.7680	 0.4540
6	 0.7310	 0.4120
7	 0.6960	 0.4120
8	 0.5290	 0.3020
9	 0.7570	 0.4450
A	 0.9130	 0.4530
A0	 0.3670	 0.2020
A1	 0.4750	 0.2740
A2	 0.5460	 0.3410
A3	 0.7030	 0.4180
A4	 0.2860	 0.1640
AA	 0.8970	 0.4080
AB	 0.6480	 0.3720
AC	 0.5920	 0.3910
AD	 0.5700	 0.3530
AE	 0.6360	 0.4220
AF	 0.5960	 0.3540
AG	 0.5600	 0.3130
AH	 0.5080	 0.3180
AI	 0.6280	 0.3970
AJ	 0.6280	 0.4020
AK	 0.6740	 0.3740
AL	 0.6150	 0.3710
AM	 0.4790	 0.2350
AN	 0.6200	 0.3860
AO	 0.4880	 0.2710
AP	 0.6600	 0.4030
AQ	 0.6850	 0.4080
AR	 0.3900	 0.2060































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Chain	Atom inclusion	Q-score
AS	 0.5260	 0.3040
AT	 0.5940	 0.3360
AU	 0.5080	 0.2540
AV	 0.2040	 0.1460
AW	 0.5720	 0.3690
AX	 0.4930	 0.2600
AY	 0.4320	 0.2500
AZ	 0.5230	 0.3030
Aw	 0.7180	 0.2210
Ax	 0.7440	 0.3370
Az	 0.3790	 0.2400
B	 0.7710	 0.3000
D	 0.8120	 0.4930
E	 0.7960	 0.4810
F	 0.7970	 0.4850
H	 0.4200	 0.2740
I	 0.5880	 0.3410
J	 0.4940	 0.2580
K	 0.8040	 0.4800
L	 0.7540	 0.4860
M	 0.7900	 0.4750
N	 0.7810	 0.4770
O	 0.7930	 0.4760
OX	 0.3480	 0.2520
P	 0.7500	 0.4450
Q	 0.7000	 0.4430
R	 0.8040	 0.4820
S	 0.7580	 0.4820
T	 0.8040	 0.4950
U	 0.6900	 0.4360
V	 0.7210	 0.4280
W	 0.7950	 0.4930
X	 0.7570	 0.4530
Y	 0.7790	 0.4540
Z	 0.7750	 0.4830
a	 0.6730	 0.4130
b	 0.7920	 0.4810
c	 0.7360	 0.4400
d	 0.5770	 0.3780
e	 0.4790	 0.2580
f	 0.6020	 0.3530
g	 0.7830	 0.4710

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*Continued from previous page...*

Chain	Atom inclusion	Q-score
h	 0.7220	 0.4150
i	 0.8290	 0.4960
j	 0.7220	 0.4300
k	 0.6030	 0.3680
l	 0.5370	 0.3120
m	 0.4890	 0.2830
n	 0.2790	 0.3060
o	 0.8290	 0.4840
p	 0.6260	 0.3820
q	 0.5700	 0.3090
r	 0.7790	 0.4600
s	 0.7630	 0.4540
t	 0.2460	 0.1860
u	 0.1370	 0.1490