Full wwPDB EM Validation Report

Apr 5, 2026 – 02:44 PM UTC

PDB ID	:	9PGM / pdb_00009pgm
EMDB ID	:	EMD-71635
Title	:	In situ structure of the human mitoribosome in the P-E state from TACO1-knockout cells
Authors	:	Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on	:	2025-07-08
Resolution	:	3.18 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

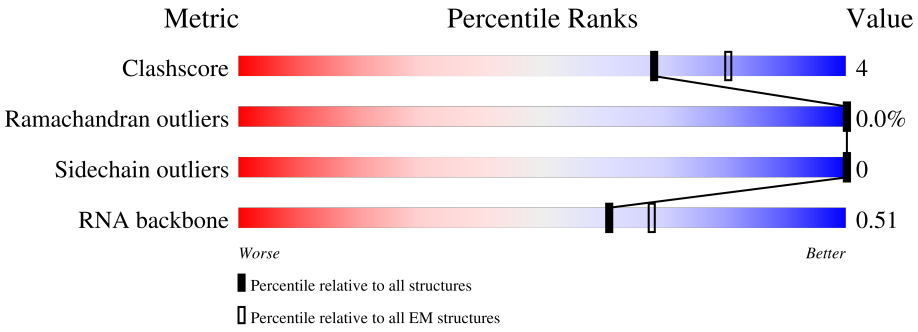
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

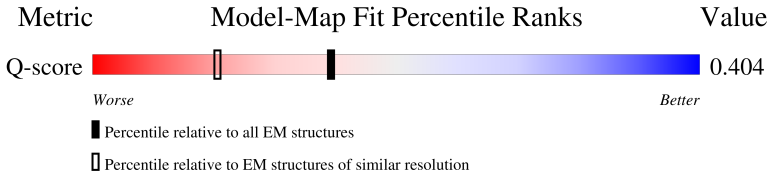
1 Overall quality at a glance

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

The reported resolution of this entry is 3.18 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	14470 (2.68 - 3.68)

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

Mol	Chain	Length	Quality of chain
1	0	188	57% 41%
2	1	65	5% 69% 17% 14%
3	2	92	50% 50%

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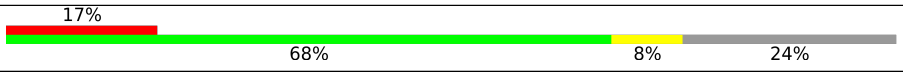
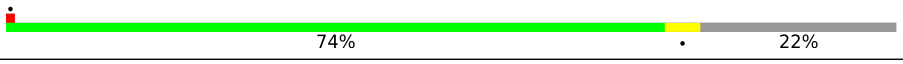
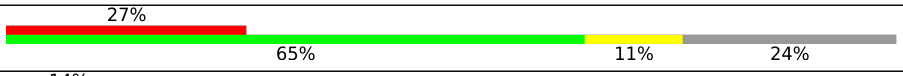
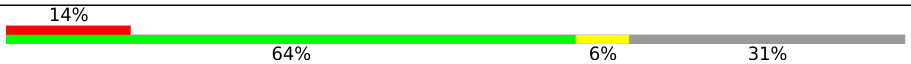
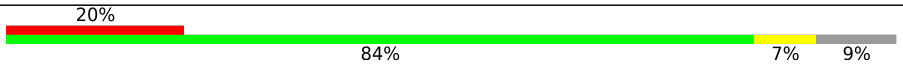
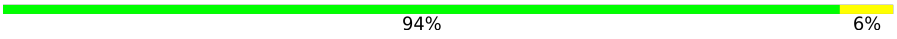
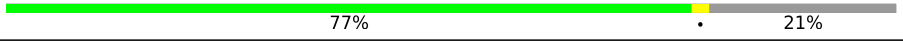
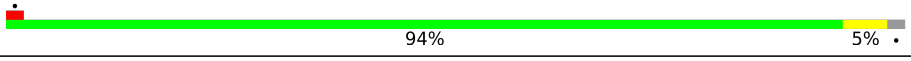
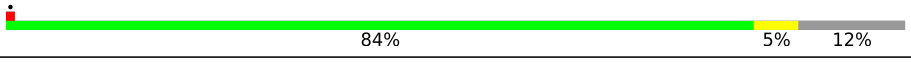
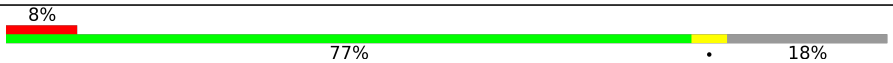
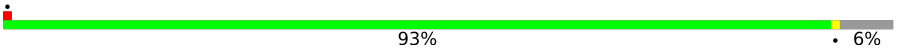
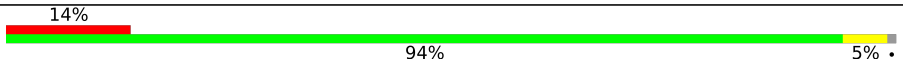
Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1561	
12	D	305	
13	E	348	
14	F	311	
15	H	267	
16	I	261	
17	J	192	
18	K	178	
19	L	145	
20	M	296	
21	N	251	
22	O	175	
23	P	180	
24	Q	292	
25	R	149	
26	S	205	
27	T	206	
28	U	153	

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Mol	Chain	Length	Quality of chain
29	W	148	78% 22%
30	X	256	91% 5% 5%
31	Y	250	72% 28%
32	Z	161	75% 24%
33	z	325	66% 61% 16% 22%
34	V	216	89% 6% 5%
35	b	215	68% 30%
36	d	306	17% 73% 11% 15%
37	e	279	18% 77% 9% 15%
38	g	166	78% 19%
39	h	158	69% 30%
40	i	128	75% 24%
41	j	123	5% 76% 24%
42	k	112	8% 85% 6% 9%
43	l	138	14% 56% 41%
44	m	128	27% 64% 8% 28%
45	n	43	56% 100%
46	o	102	90% 8%
47	q	222	17% 69% 10% 20%
48	r	196	75% 8% 17%
49	t	198	15% 21% 77%
49	u	198	11% 13% 84%
50	c	332	83% 14%
51	f	212	10% 66% 8% 26%
52	p	206	11% 67% 29%

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Mol	Chain	Length	Quality of chain
53	s	439	82% 6% 12%
54	AB	296	5% 74% 24%
55	AC	167	9% 68% 11% 21%
56	AD	430	12% 74% 6% 20%
57	AE	125	6% 86% 12%
58	AF	242	9% 78% 8% 14%
59	AG	396	13% 77% 6% 17%
60	AH	201	14% 60% 9% 30%
61	AJ	138	9% 72% 6% 22%
62	AK	128	7% 65% 14% 21%
63	AL	257	9% 65% 32%
64	AM	137	23% 72% 15% 13%
65	AN	130	8% 78% 7% 15%
66	AO	258	21% 68% 7% 25%
67	AP	142	63% 5% 32%
68	AR	360	35% 74% 8% 18%
69	AS	190	15% 67% 29%
70	AT	173	9% 88% 9%
71	AU	205	16% 81% 14%
72	AV	414	59% 71% 17% 13%
73	AW	187	5% 45% 8% 47%
74	AZ	106	17% 85% 9% 6%
75	A0	217	43% 82% 17%
76	A1	323	21% 79% 7% 14%
77	A3	199	33% 65%

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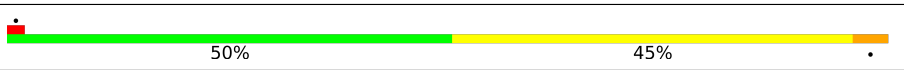
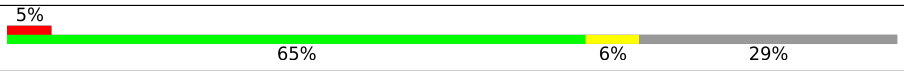
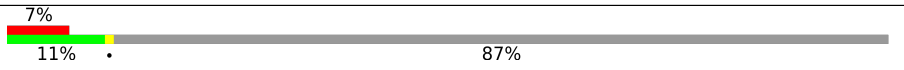
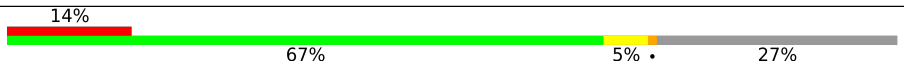
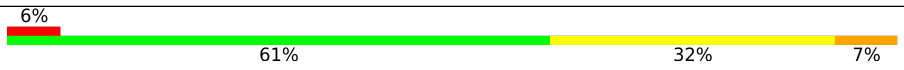
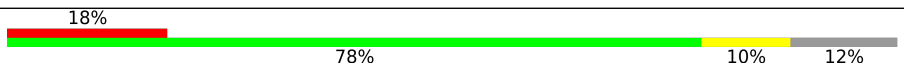
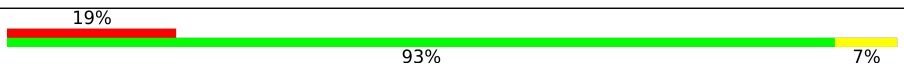
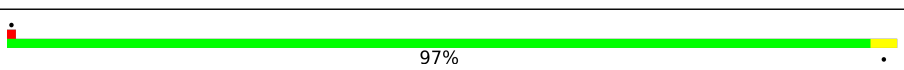
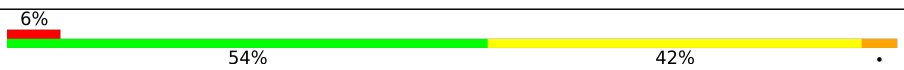
Mol	Chain	Length	Quality of chain
78	Az	34	
79	AY	395	
80	AA	954	
81	AI	194	
82	OX	435	
83	a	142	
84	Ax	71	
85	Ay	76	
86	A4	689	
87	AX	398	
88	A2	118	
89	AQ	87	
90	B	72	

2 Entry composition

There are 101 unique types of molecules in this entry. The entry contains 179960 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 12 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	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	179	ACE	-	acetylation	UNP H2QWN0
K	310	TYR	ASP	conflict	UNP H2QWN0

- Molecule 19 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 29 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL1m.

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

- 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	113	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 E/E-tRNA.

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

- 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	119	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	88	ACE	-	acetylation	UNP P82921
AQ	137	ARG	CYS	variant	UNP P82921

- Molecule 90 is a RNA chain called mitochondrial tRNAVal.

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

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

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

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

Mol	Chain	Residues	Atoms		AltConf
92	6	1	Total	K	0
			1	1	
92	A	29	Total	K	0
			29	29	
92	D	1	Total	K	0
			1	1	
92	M	2	Total	K	0
			2	2	
92	N	1	Total	K	0
			1	1	

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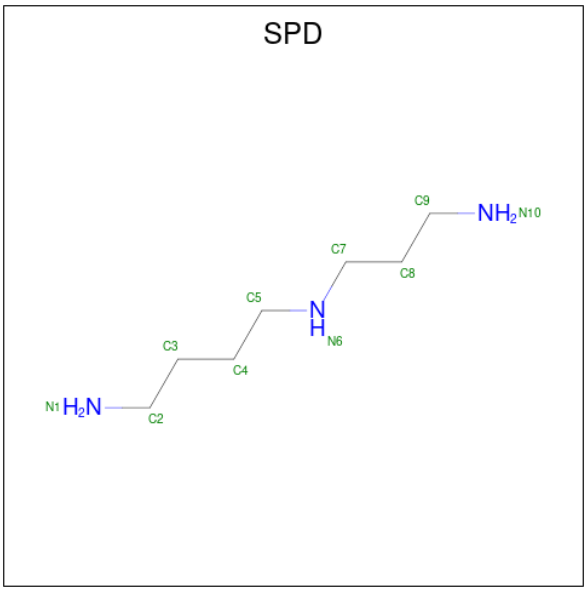
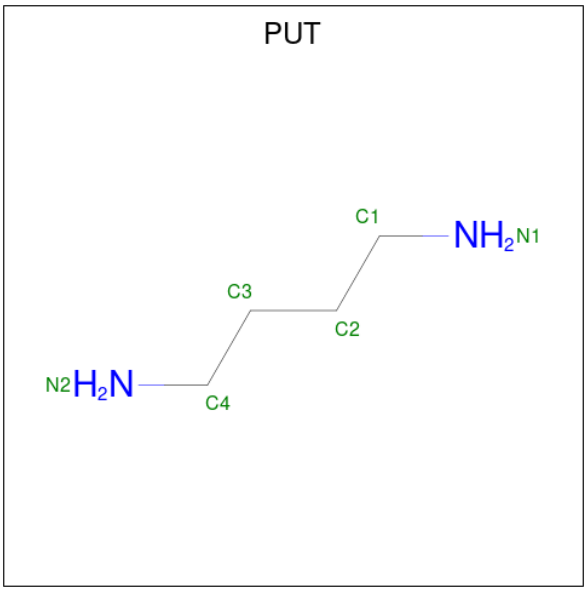
Mol	Chain	Residues	Atoms	AltConf
92	W	1	Total K 1 1	0
92	o	1	Total K 1 1	0
92	AA	18	Total K 18 18	0

- 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 10 7 3	0
93	A	1	Total C N 10 7 3	0
93	A	1	Total C N 10 7 3	0
93	A	1	Total C N 10 7 3	0
93	A	1	Total C N 10 7 3	0
93	AG	1	Total C N 10 7 3	0
93	AA	1	Total C N 10 7 3	0

- Molecule 94 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).

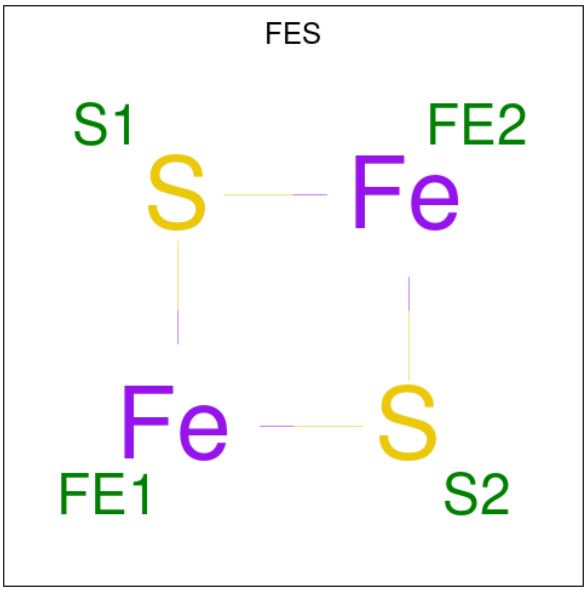


Mol	Chain	Residues	Atoms	AltConf
94	A	1	Total C N 6 4 2	0

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

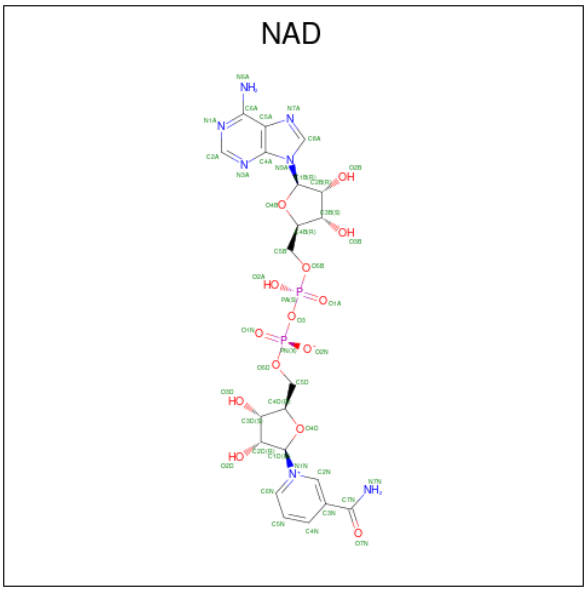
Mol	Chain	Residues	Atoms	AltConf
95	A	137	Total Mg 137 137	0
95	D	2	Total Mg 2 2	0
95	E	1	Total Mg 1 1	0
95	g	1	Total Mg 1 1	0
95	AB	1	Total Mg 1 1	0
95	AK	1	Total Mg 1 1	0
95	A3	1	Total Mg 1 1	0
95	AA	59	Total Mg 59 59	0
95	AX	1	Total Mg 1 1	0

- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



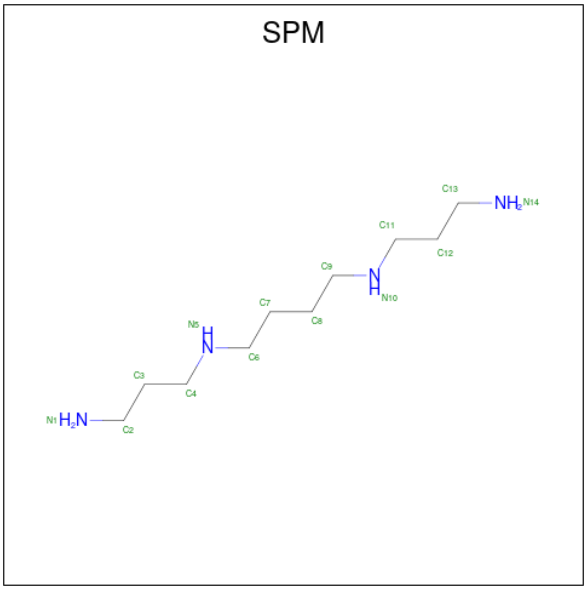
Mol	Chain	Residues	Atoms			AltConf
96	r	1	Total 4	Fe 2	S 2	0
96	AP	1	Total 4	Fe 2	S 2	0
96	AT	1	Total 4	Fe 2	S 2	0

- 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).



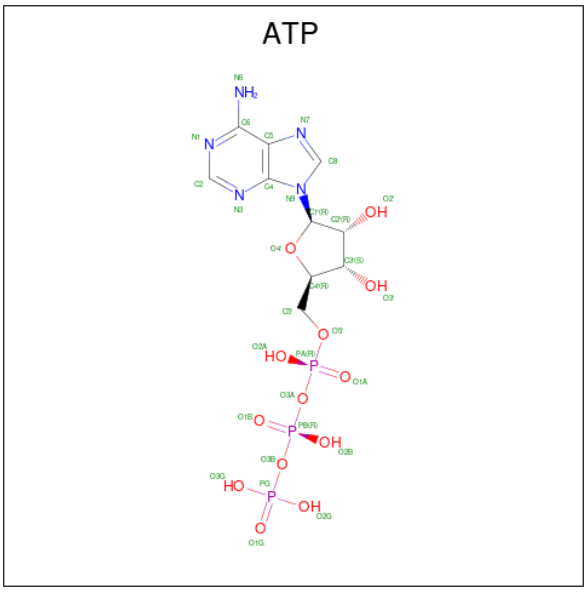
Mol	Chain	Residues	Atoms					AltConf
97	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



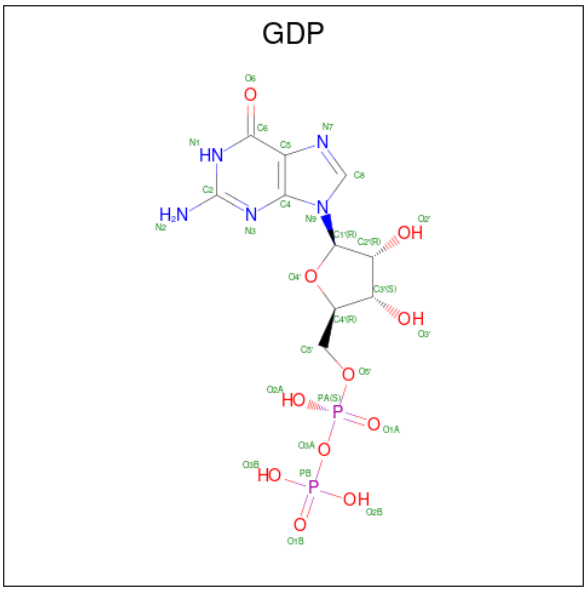
Mol	Chain	Residues	Atoms			AltConf
98	AA	1	Total	C	N	0
			14	10	4	
98	AA	1	Total	C	N	0
			14	10	4	

- 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).



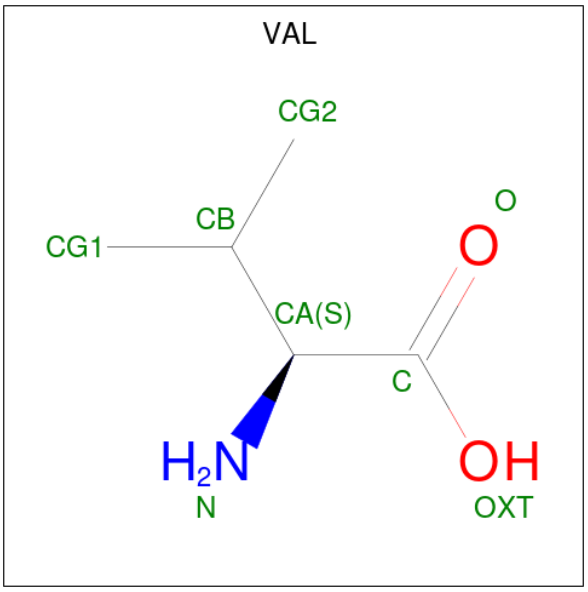
Mol	Chain	Residues	Atoms					AltConf
99	AX	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 100 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 101 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



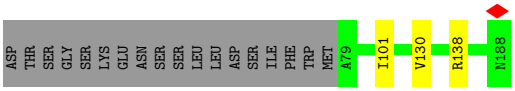
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
101	B	1	7	5	1	1	0

3 Residue-property plots (i)

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

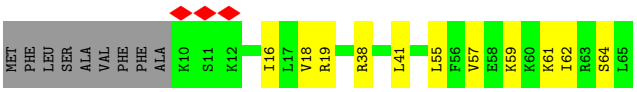
• Molecule 1: 39S ribosomal protein L32, mitochondrial

Chain 0:



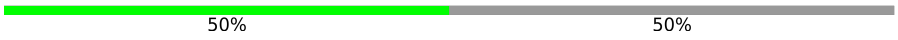
• Molecule 2: 39S ribosomal protein L33, mitochondrial

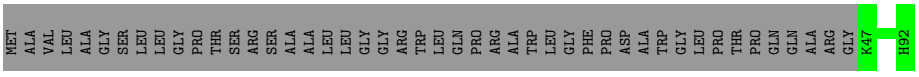
Chain 1:



• Molecule 3: 39S ribosomal protein L34, mitochondrial

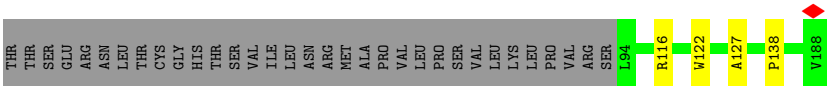
Chain 2:





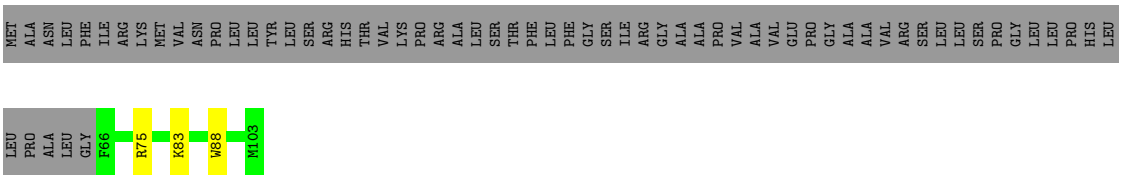
• Molecule 4: 39S ribosomal protein L35, mitochondrial

Chain 3:



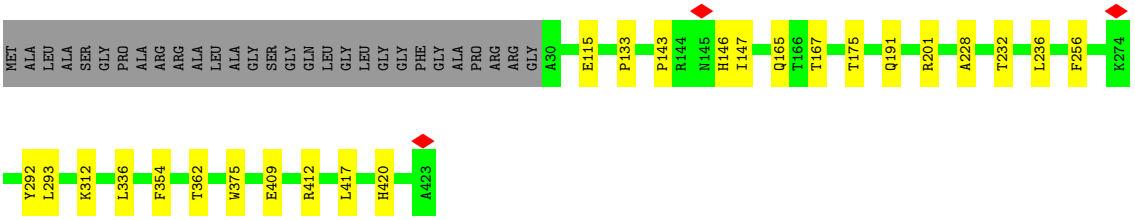
• Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:



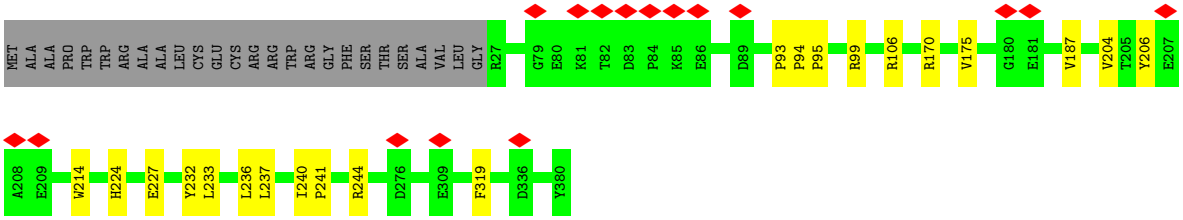
• Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:



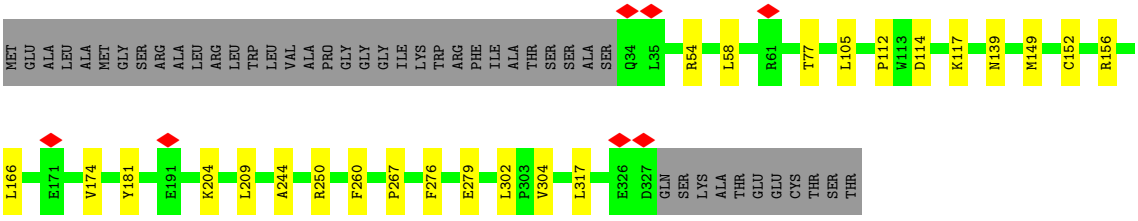
• Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:



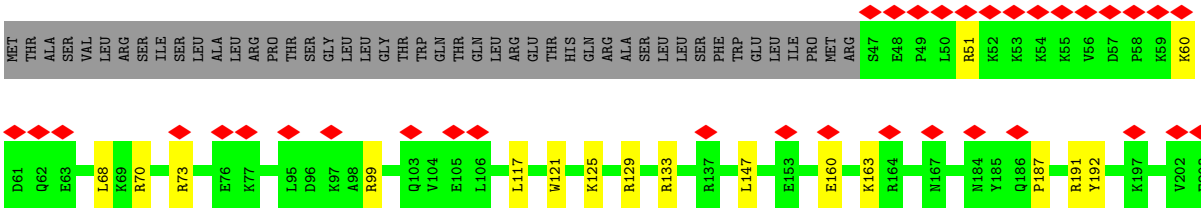
• Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:



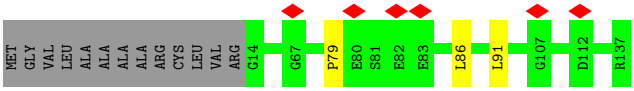
• Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:



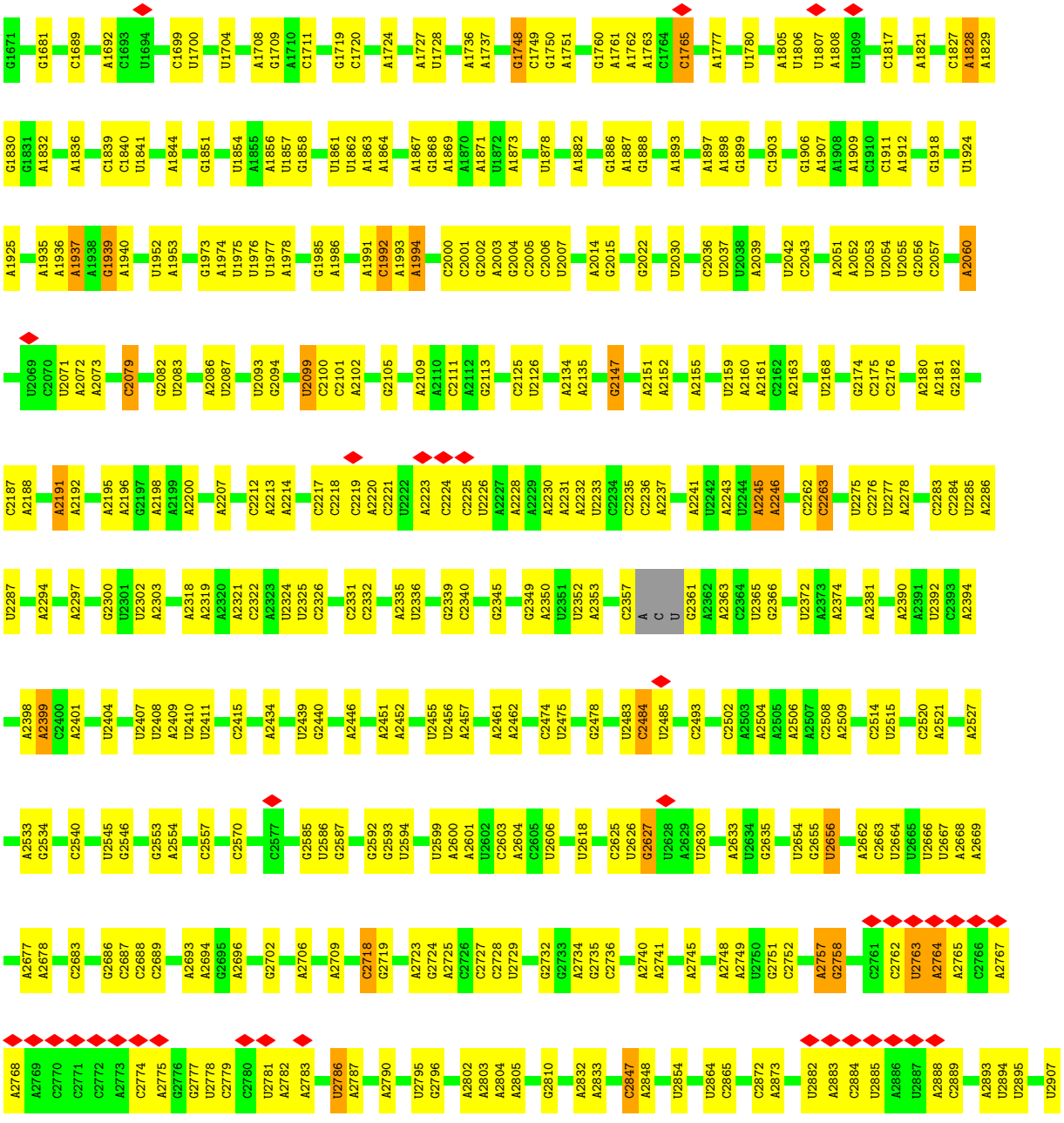
• Molecule 10: 39S ribosomal protein L41, mitochondrial

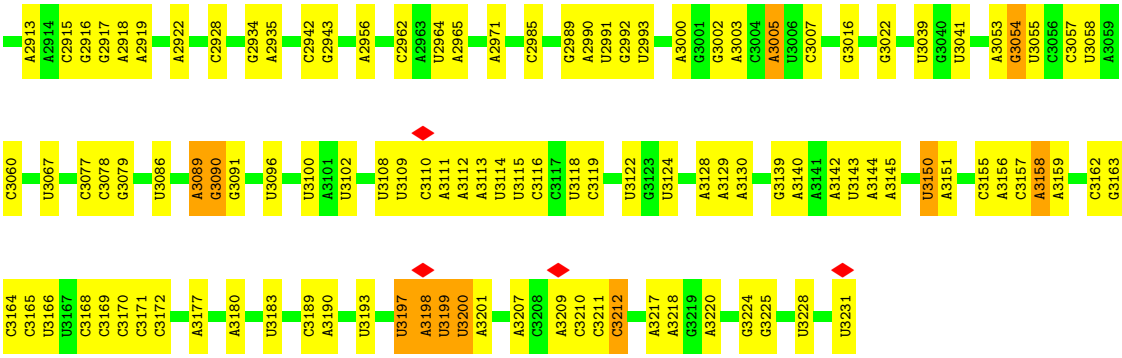
Chain 9:



• Molecule 11: 16S mitochondrial rRNA

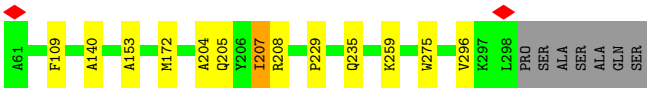
Chain A:





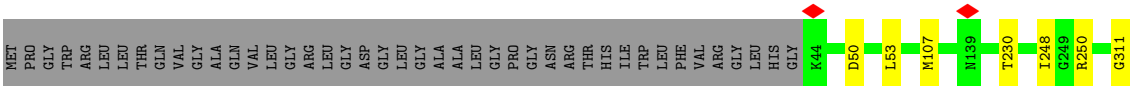
• Molecule 12: 39S ribosomal protein L2, mitochondrial

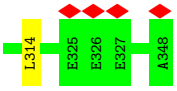
Chain D:



• Molecule 13: 39S ribosomal protein L3, mitochondrial

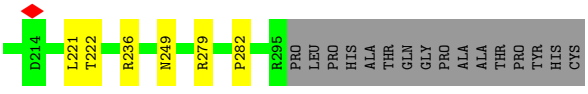
Chain E:





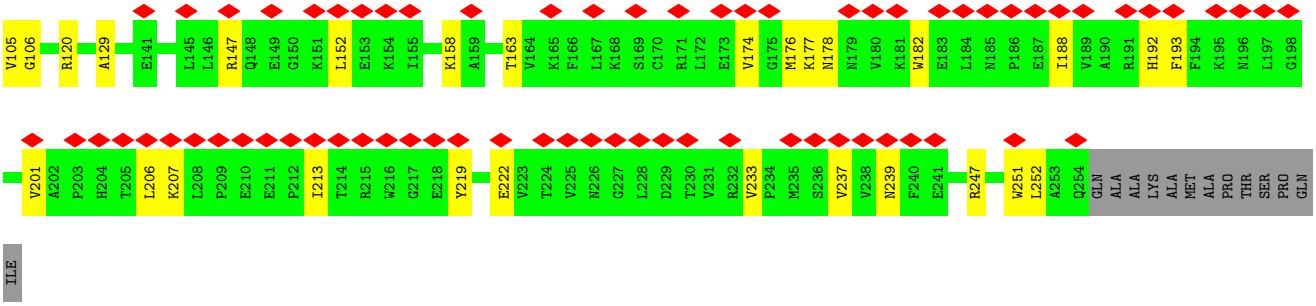
• Molecule 14: 39S ribosomal protein L4, mitochondrial

Chain F:



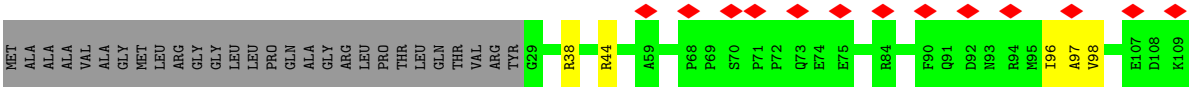
• Molecule 15: 39S ribosomal protein L9, mitochondrial

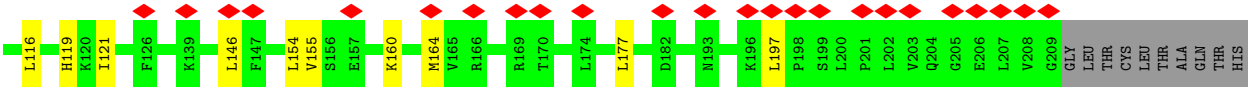
Chain H:



• Molecule 16: 39S ribosomal protein L10, mitochondrial

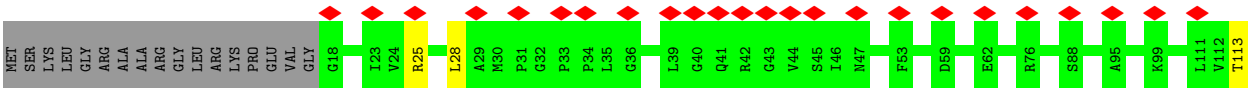
Chain I:

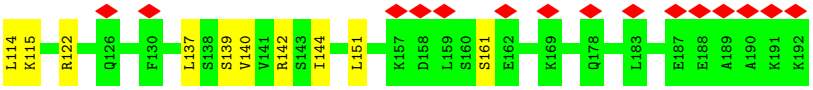




• Molecule 17: 39S ribosomal protein L11, mitochondrial

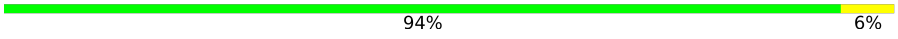
Chain J:





• Molecule 18: Large ribosomal subunit protein uL13m

Chain K:

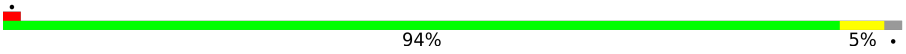


• Molecule 19: 39S ribosomal protein L14, mitochondrial

Chain L:

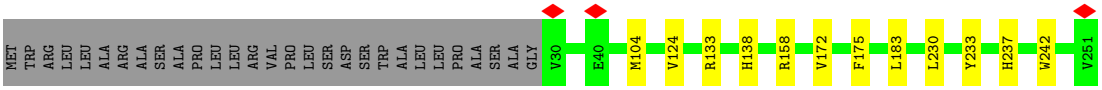
• Molecule 20: 39S ribosomal protein L15, mitochondrial

Chain M:



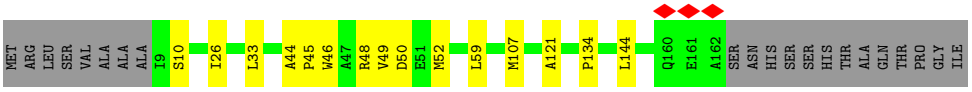
• Molecule 21: 39S ribosomal protein L16, mitochondrial

Chain N:



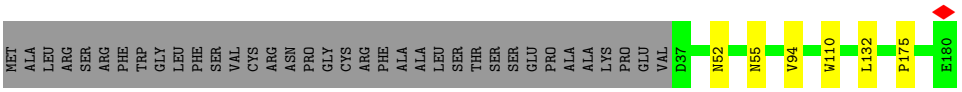
• Molecule 22: 39S ribosomal protein L17, mitochondrial

Chain O:



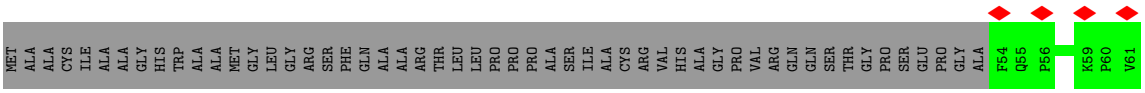
• Molecule 23: 39S ribosomal protein L18, mitochondrial

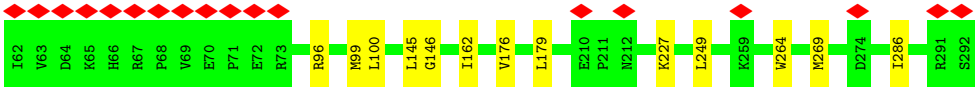
Chain P:



• Molecule 24: 39S ribosomal protein L19, mitochondrial

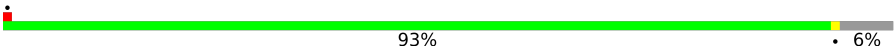
Chain Q:

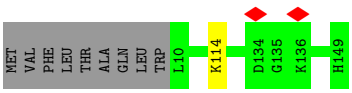




• Molecule 25: 39S ribosomal protein L20, mitochondrial

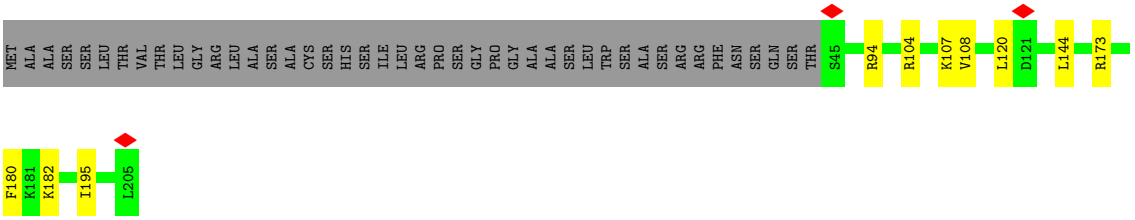
Chain R:



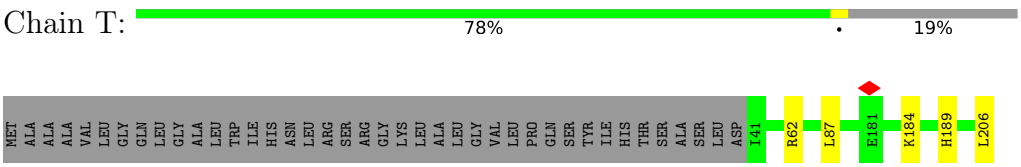


• Molecule 26: 39S ribosomal protein L21, mitochondrial

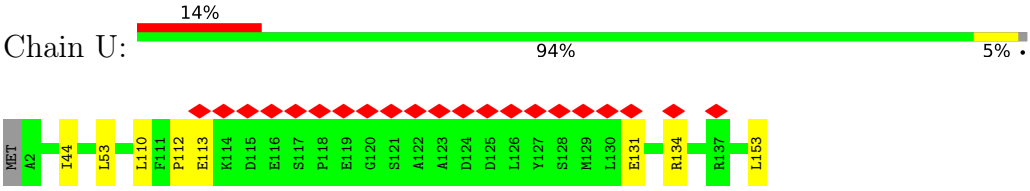
Chain S:



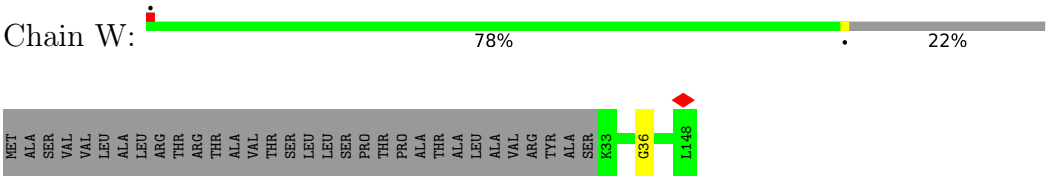
• Molecule 27: 39S ribosomal protein L22, mitochondrial



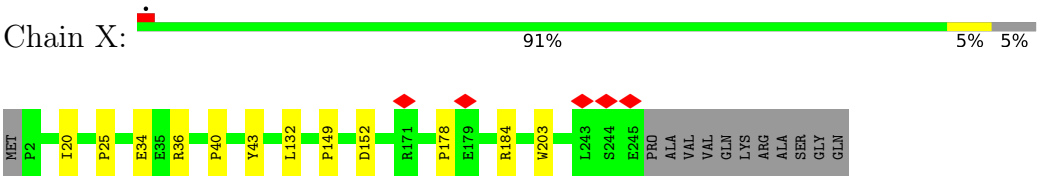
• Molecule 28: 39S ribosomal protein L23, mitochondrial



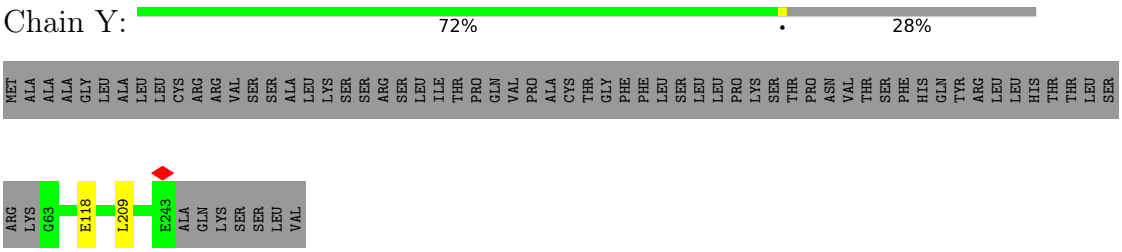
• Molecule 29: 39S ribosomal protein L27, mitochondrial



• Molecule 30: 39S ribosomal protein L28, mitochondrial

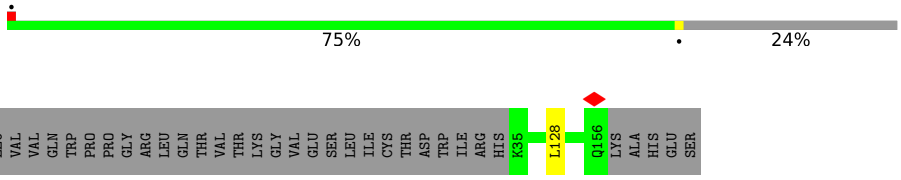


• Molecule 31: 39S ribosomal protein L47, mitochondrial



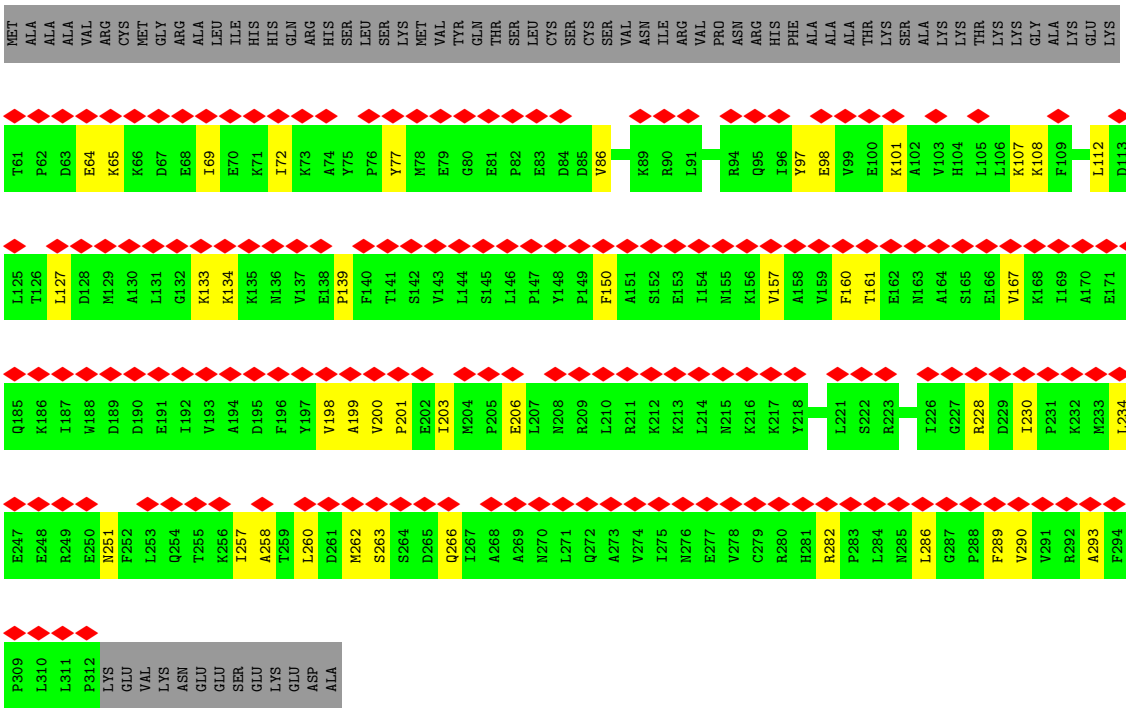
• Molecule 32: 39S ribosomal protein L30, mitochondrial

Chain Z:



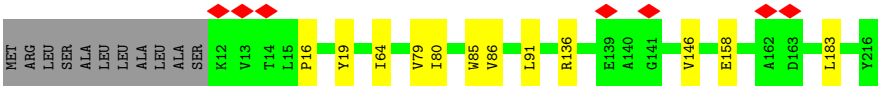
• Molecule 33: Large ribosomal subunit protein uL1m

Chain z:



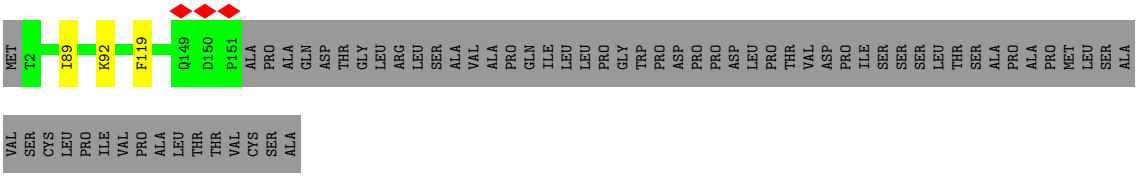
• Molecule 34: 39S ribosomal protein L24, mitochondrial

Chain V:



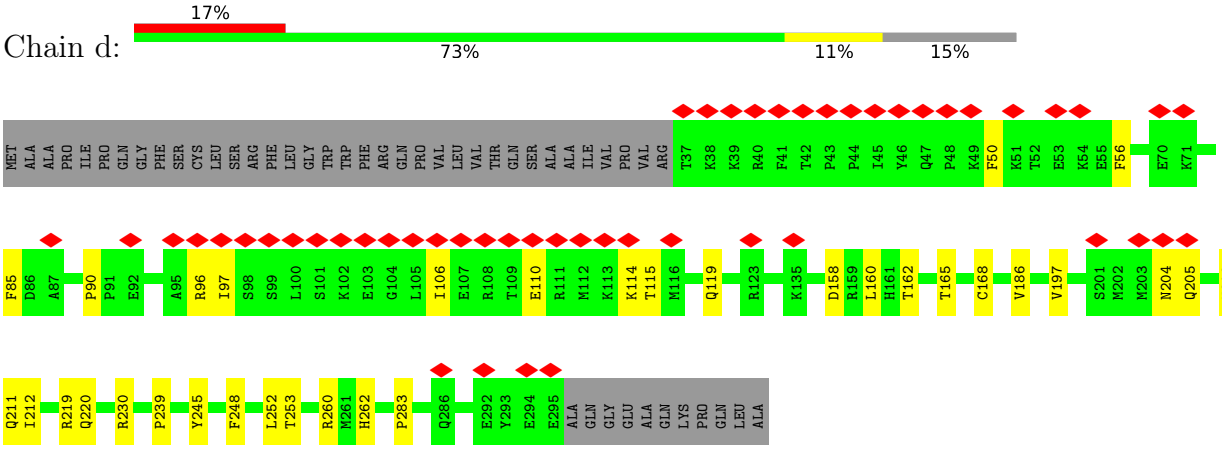
• Molecule 35: 39S ribosomal protein L43, mitochondrial

Chain b:



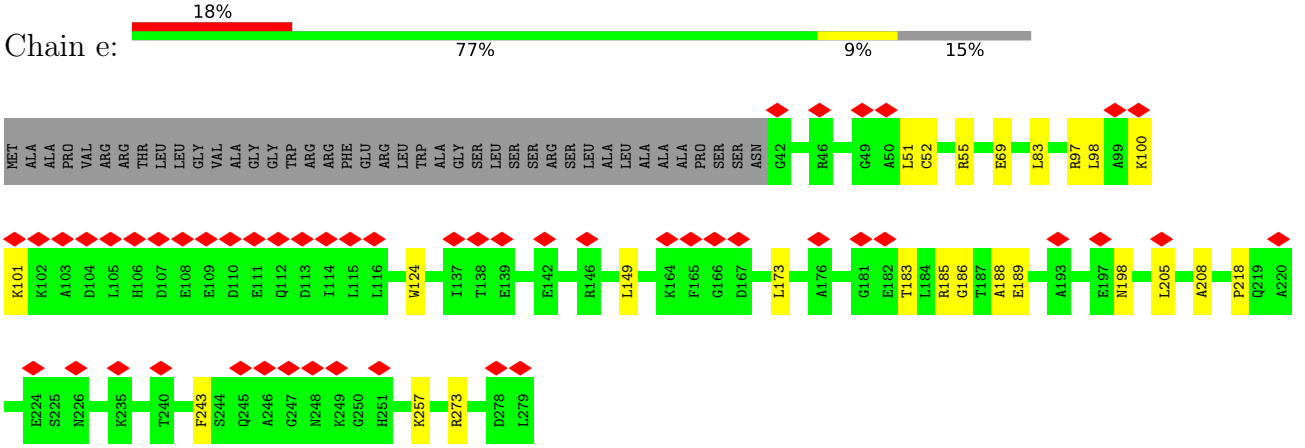
• Molecule 36: 39S ribosomal protein L45, mitochondrial

Chain d:



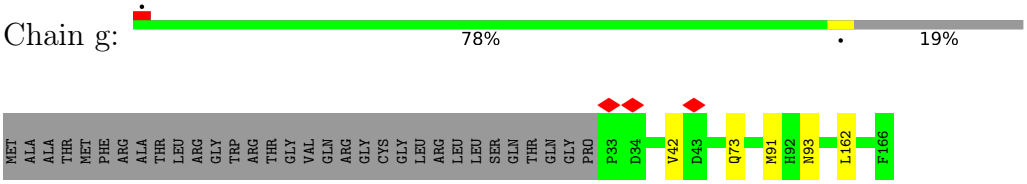
• Molecule 37: 39S ribosomal protein L46, mitochondrial

Chain e:



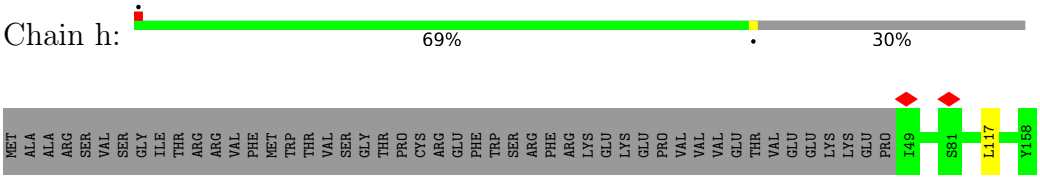
• Molecule 38: 39S ribosomal protein L49, mitochondrial

Chain g:



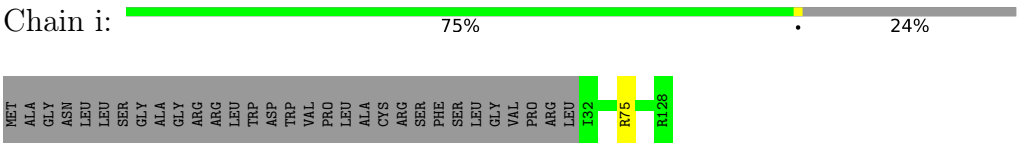
• Molecule 39: 39S ribosomal protein L50, mitochondrial

Chain h:



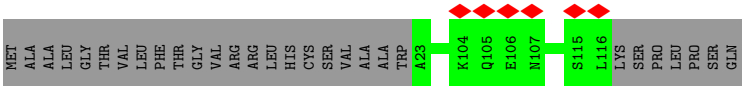
• Molecule 40: 39S ribosomal protein L51, mitochondrial

Chain i:



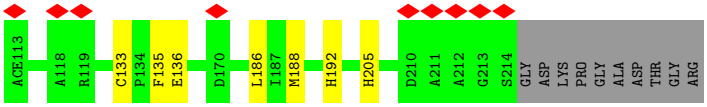
• Molecule 41: 39S ribosomal protein L52, mitochondrial

Chain j:



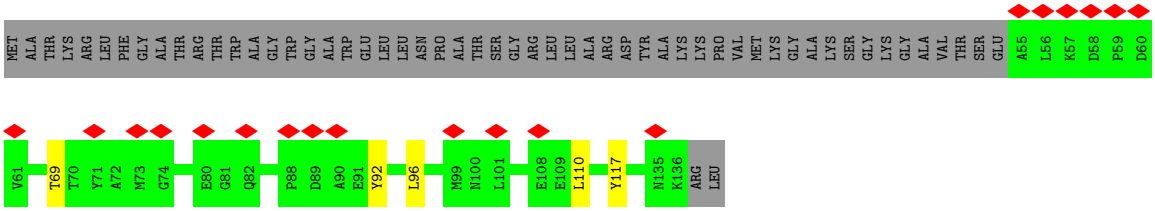
• Molecule 42: Large ribosomal subunit protein mL53

Chain k:



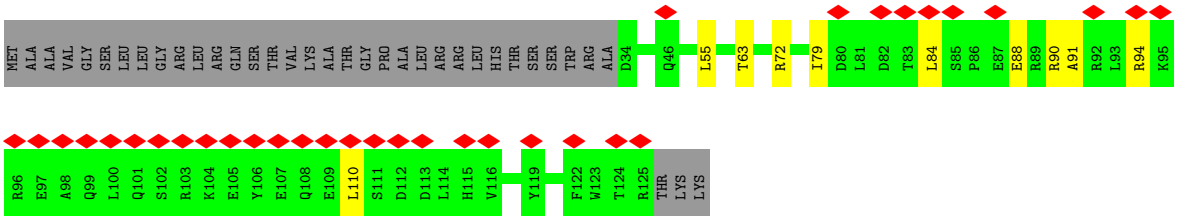
• Molecule 43: 39S ribosomal protein L54, mitochondrial

Chain l:



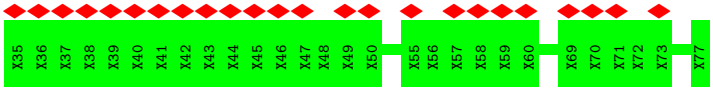
• Molecule 44: 39S ribosomal protein L55, mitochondrial

Chain m:



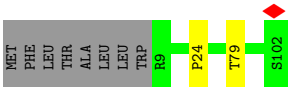
• Molecule 45: Nascent polypeptide

Chain n:



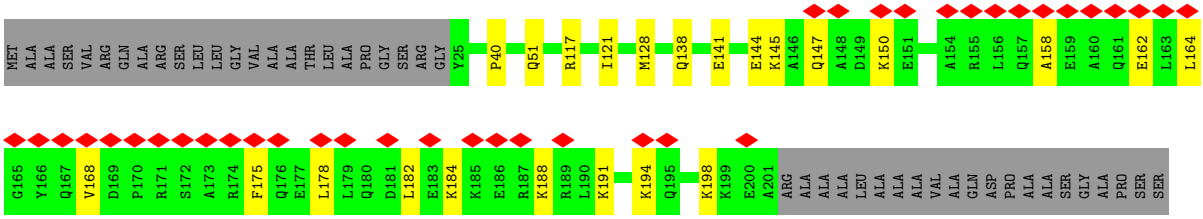
• Molecule 46: Ribosomal protein 63, mitochondrial

Chain o:



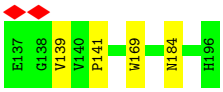
• Molecule 47: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



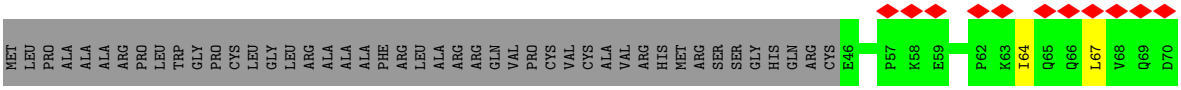
• Molecule 48: 39S ribosomal protein S18a, mitochondrial

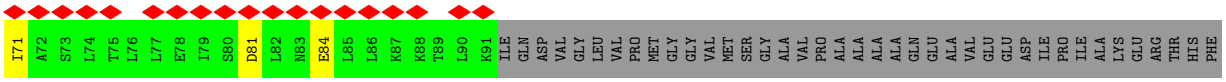
Chain r:

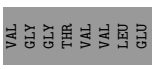


• Molecule 49: 39S ribosomal protein L12, mitochondrial

Chain t:

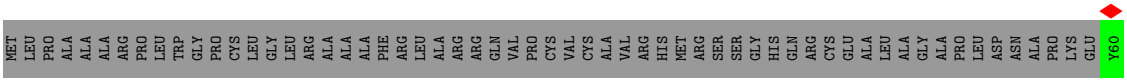


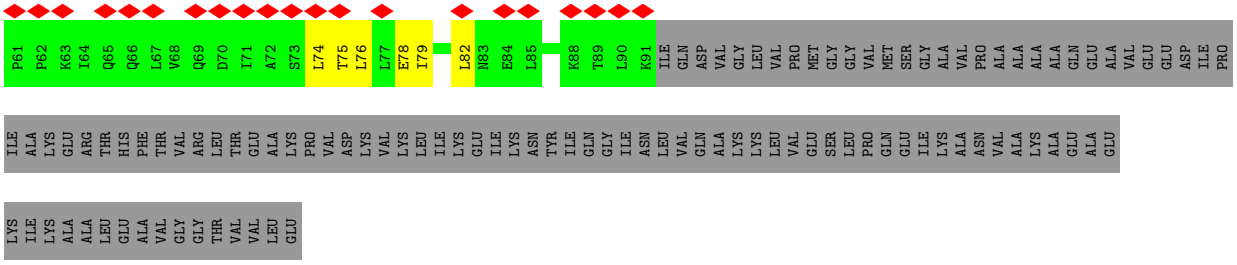




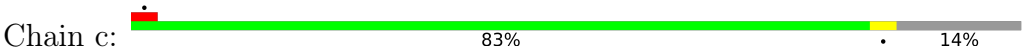
• Molecule 49: 39S ribosomal protein L12, mitochondrial

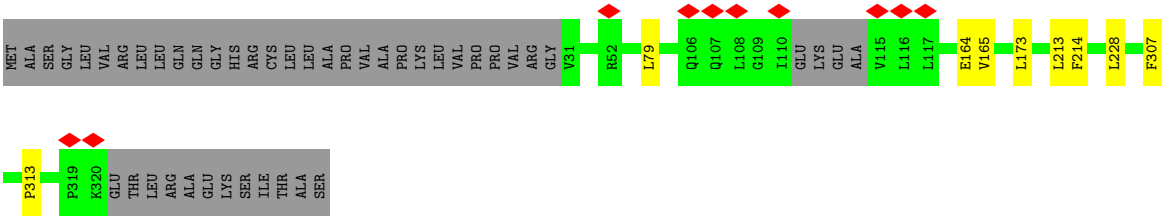
Chain u:



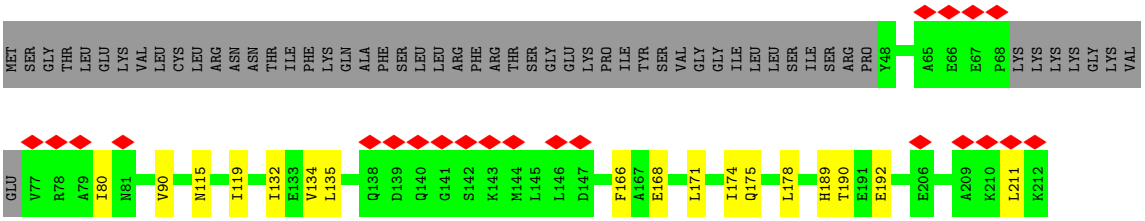


• Molecule 50: 39S ribosomal protein L44, mitochondrial

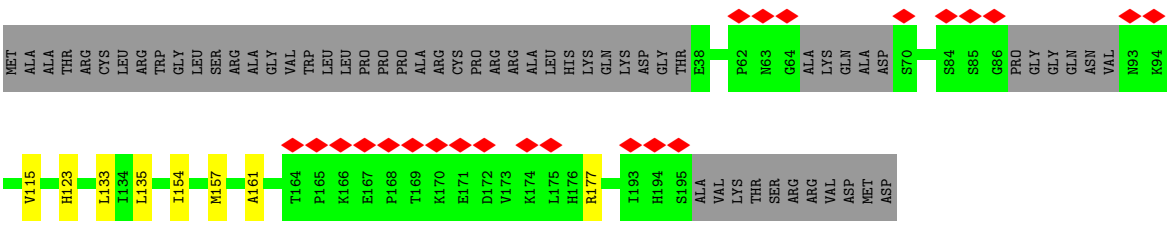




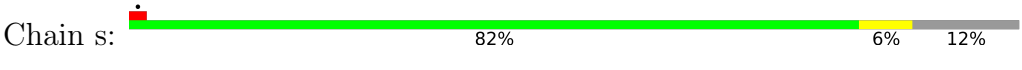
• Molecule 51: 39S ribosomal protein L48, mitochondrial

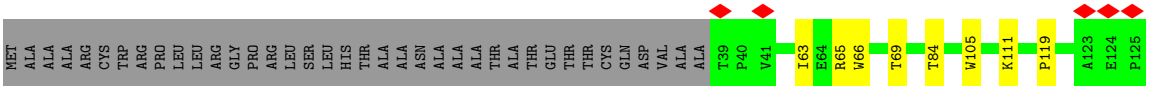


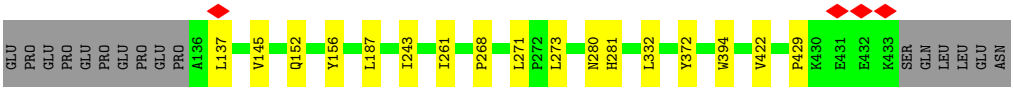
• Molecule 52: Peptidyl-tRNA hydrolase ICT1, mitochondrial



• Molecule 53: 39S ribosomal protein S30, mitochondrial

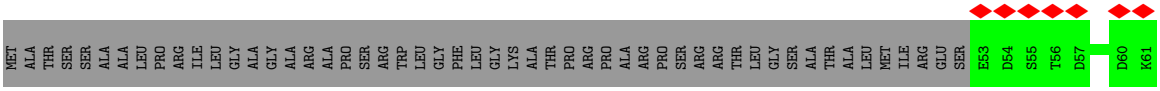


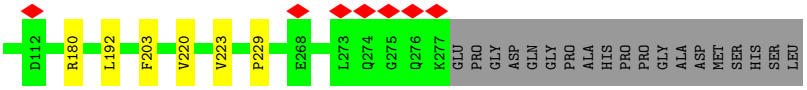




• Molecule 54: 28S ribosomal protein S2, mitochondrial

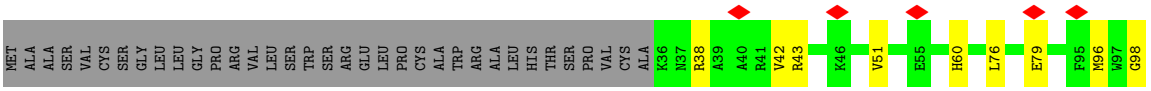
Chain AB:

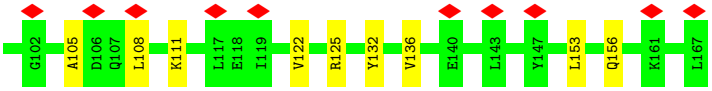




• Molecule 55: 28S ribosomal protein S24, mitochondrial

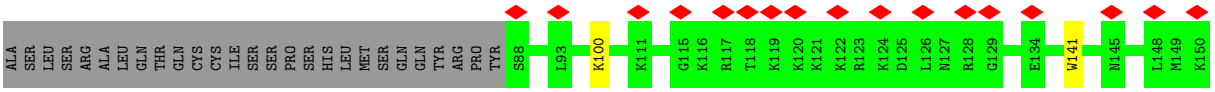
Chain AC:

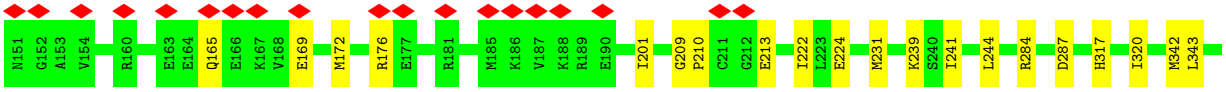


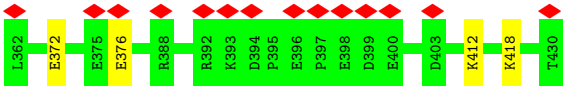


• Molecule 56: 28S ribosomal protein S5, mitochondrial

Chain AD:





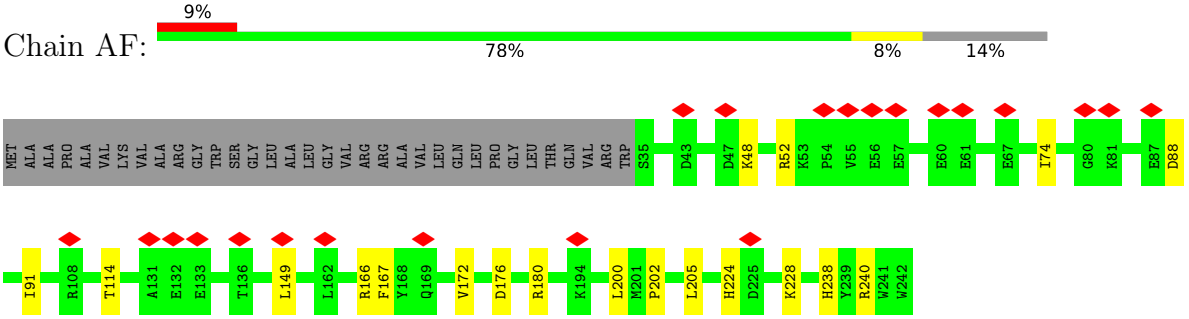


• Molecule 57: 28S ribosomal protein S6, mitochondrial

Chain AE:

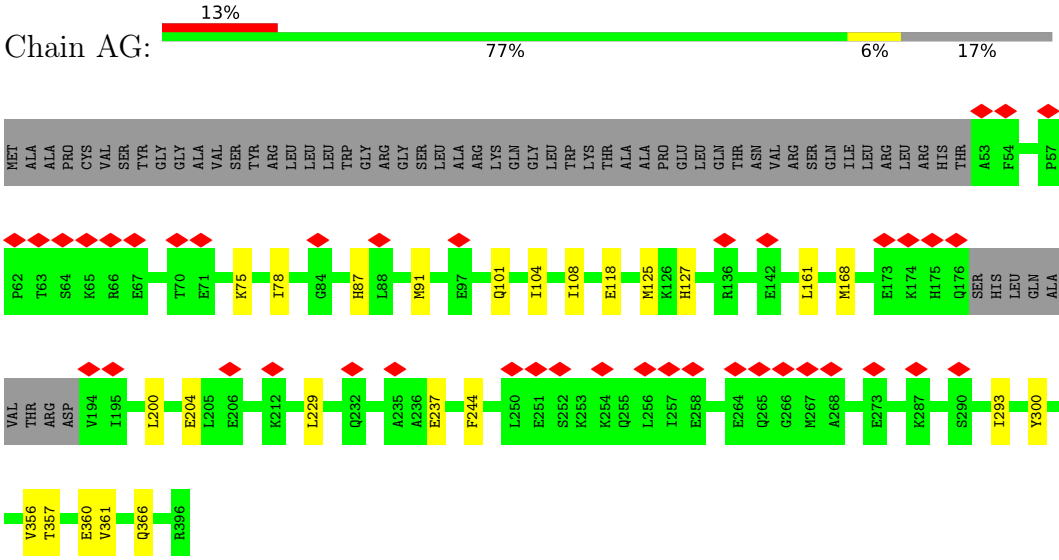
• Molecule 58: 28S ribosomal protein S7, mitochondrial

Chain AF:



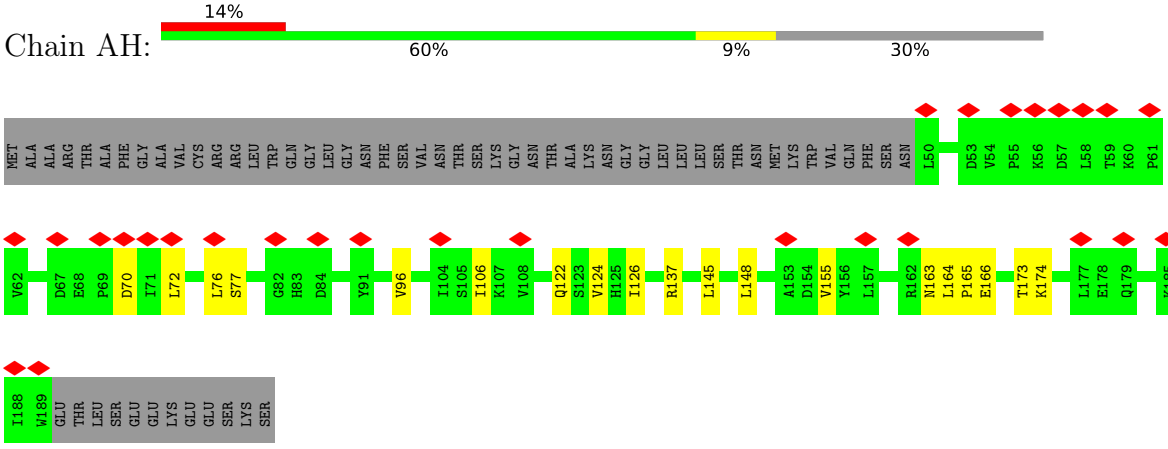
• Molecule 59: 28S ribosomal protein S9, mitochondrial

Chain AG:



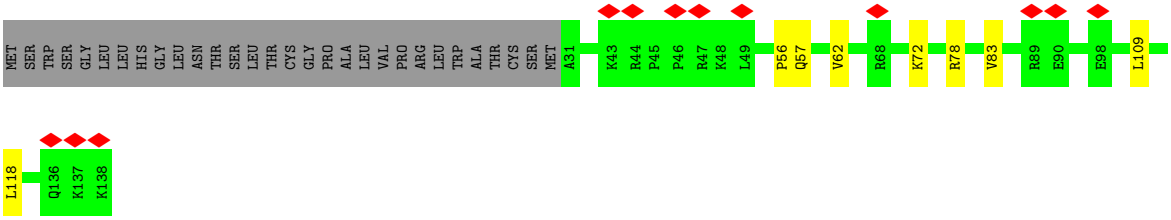
• Molecule 60: 28S ribosomal protein S10, mitochondrial

Chain AH:

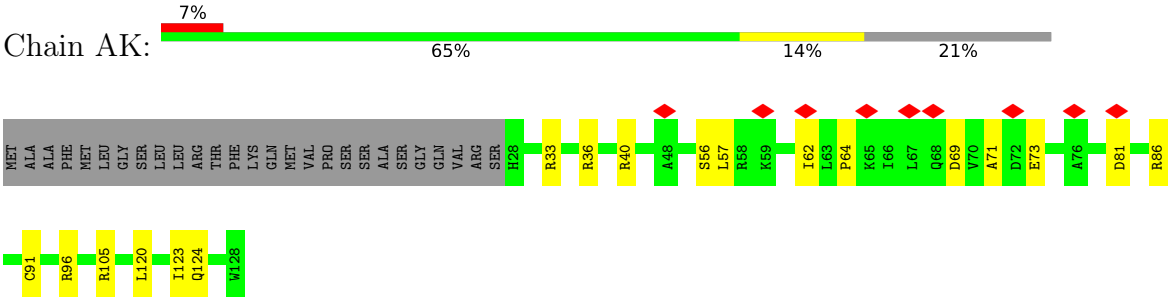


• Molecule 61: 28S ribosomal protein S12, mitochondrial

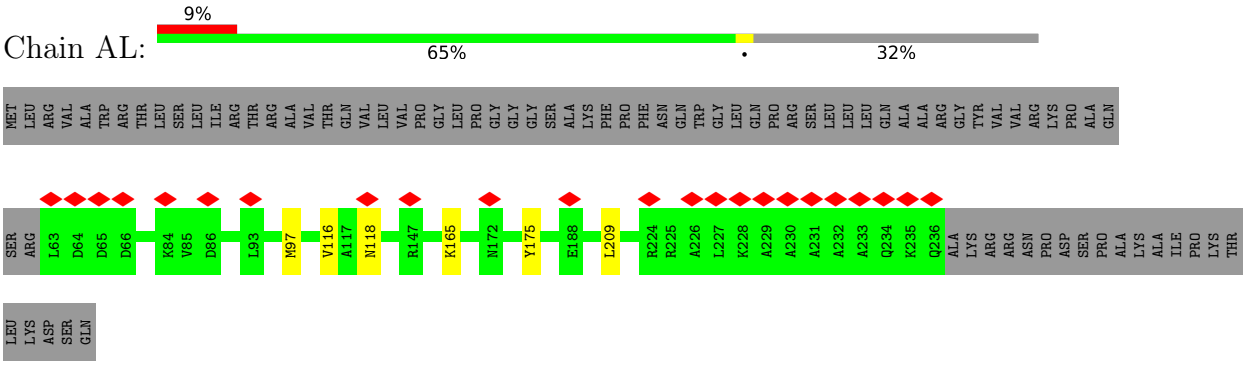
Chain AJ:



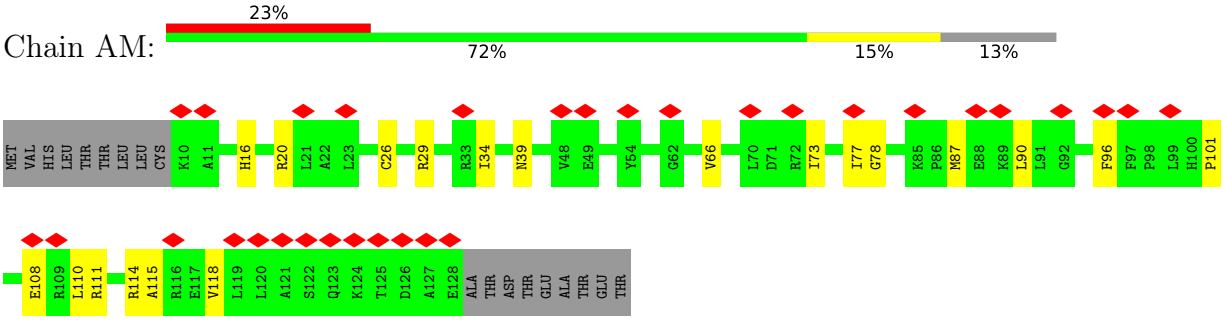
• Molecule 62: 28S ribosomal protein S14, mitochondrial



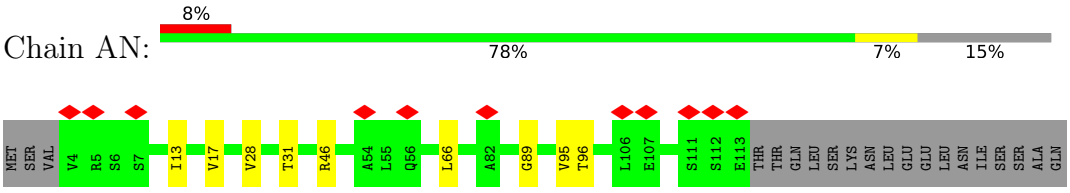
• Molecule 63: 28S ribosomal protein S15, mitochondrial



• Molecule 64: 28S ribosomal protein S16, mitochondrial

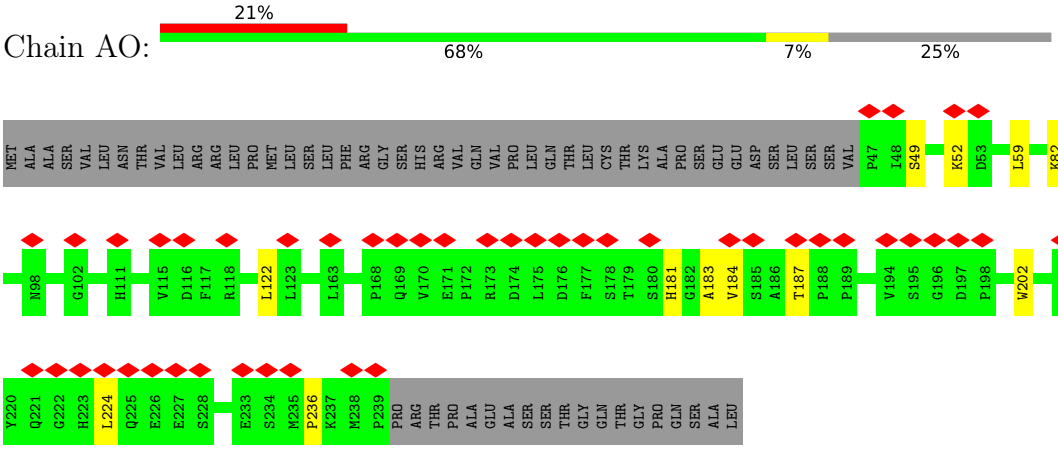


• Molecule 65: 28S ribosomal protein S17, mitochondrial



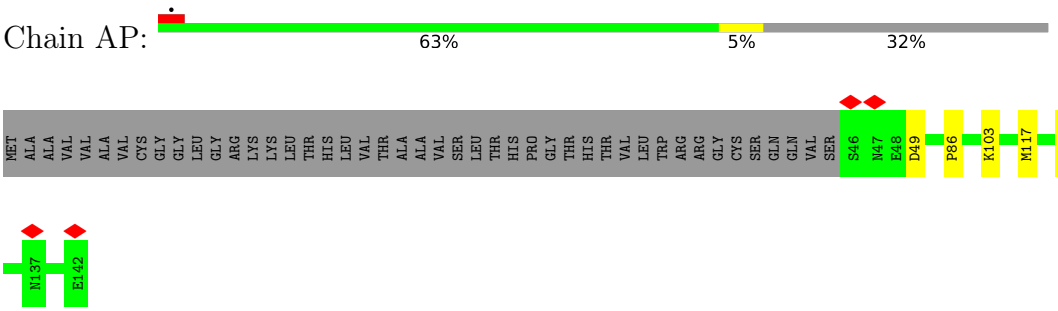
• Molecule 66: 28S ribosomal protein S18b, mitochondrial

Chain AO:



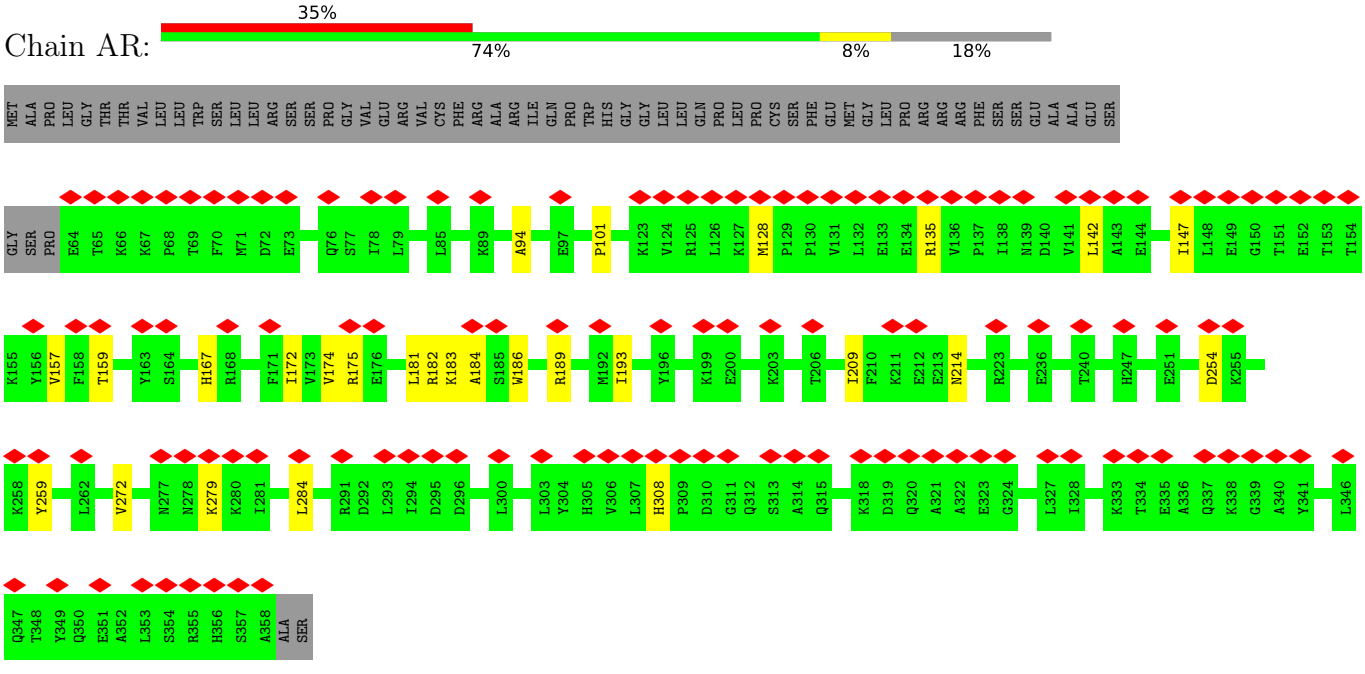
• Molecule 67: 28S ribosomal protein S18c, mitochondrial

Chain AP:



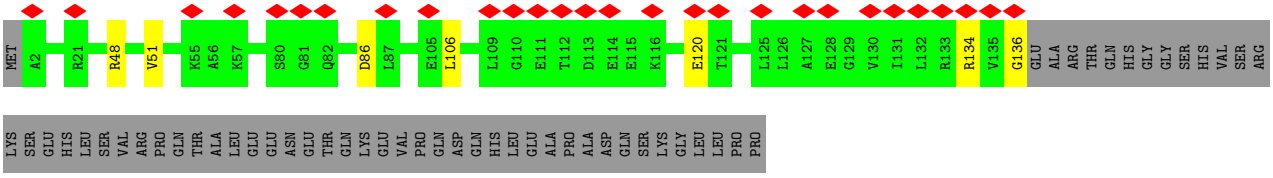
• Molecule 68: 28S ribosomal protein S22, mitochondrial

Chain AR:

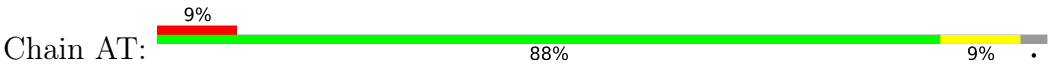


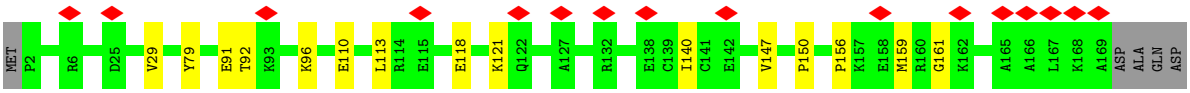
• Molecule 69: 28S ribosomal protein S23, mitochondrial

Chain AS:

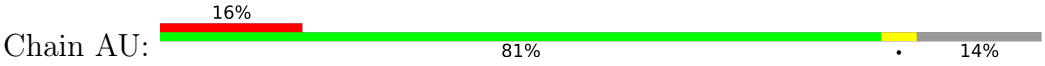


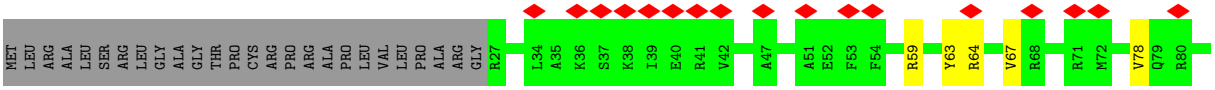
• Molecule 70: 28S ribosomal protein S25, mitochondrial

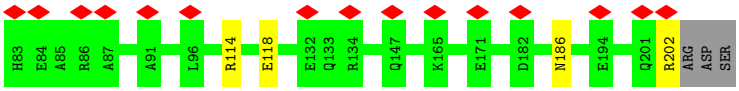




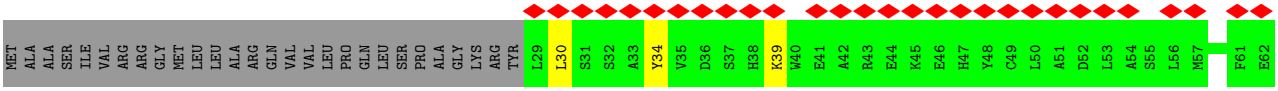
• Molecule 71: 28S ribosomal protein S26, mitochondrial

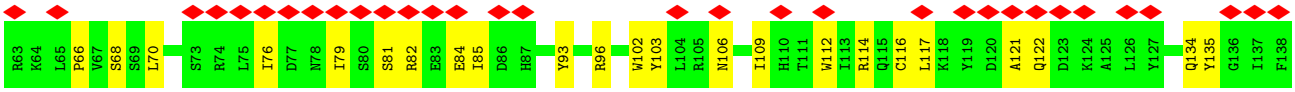


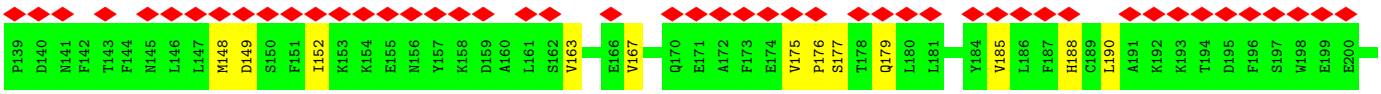


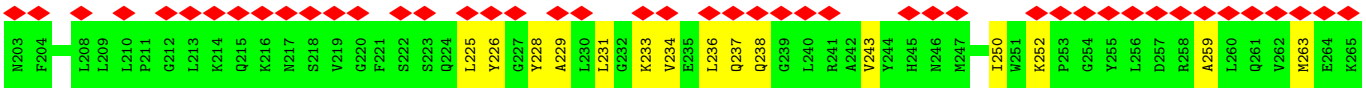


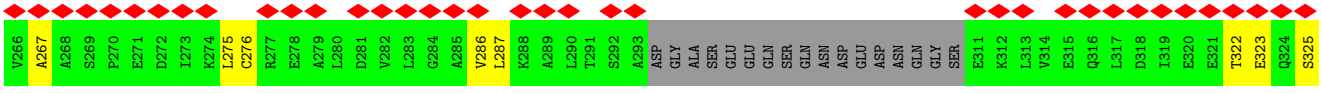
• Molecule 72: 28S ribosomal protein S27, mitochondrial

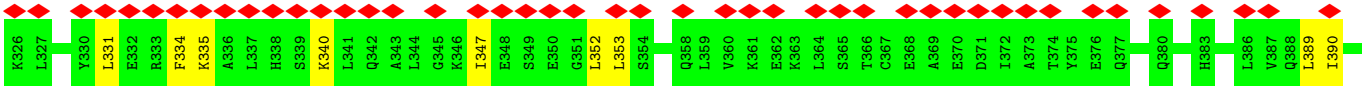


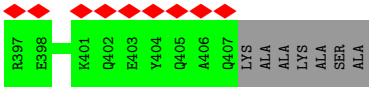






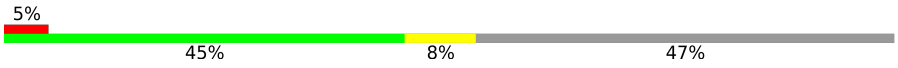


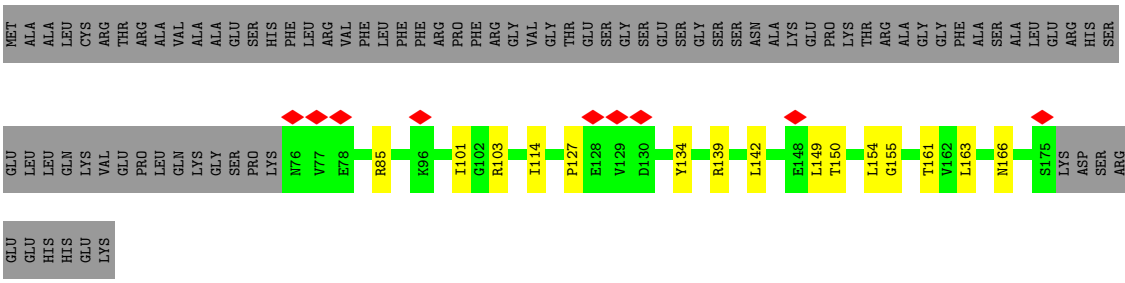




• Molecule 73: 28S ribosomal protein S28, mitochondrial

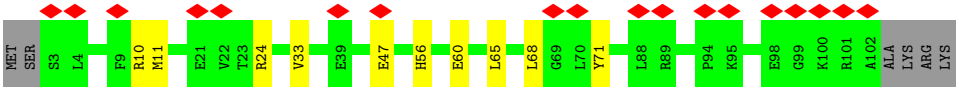
Chain AW:





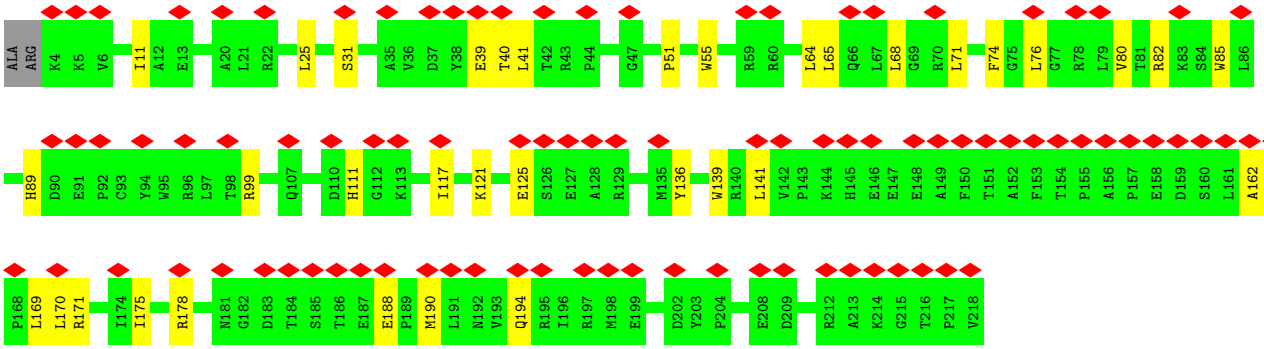
• Molecule 74: 28S ribosomal protein S33, mitochondrial

Chain AZ:



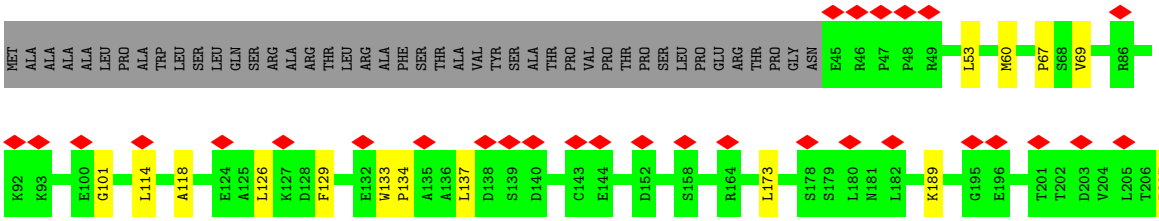
• Molecule 75: Small ribosomal subunit protein mS34

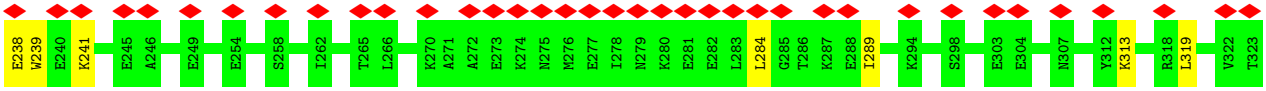
Chain A0:



• Molecule 76: 28S ribosomal protein S35, mitochondrial

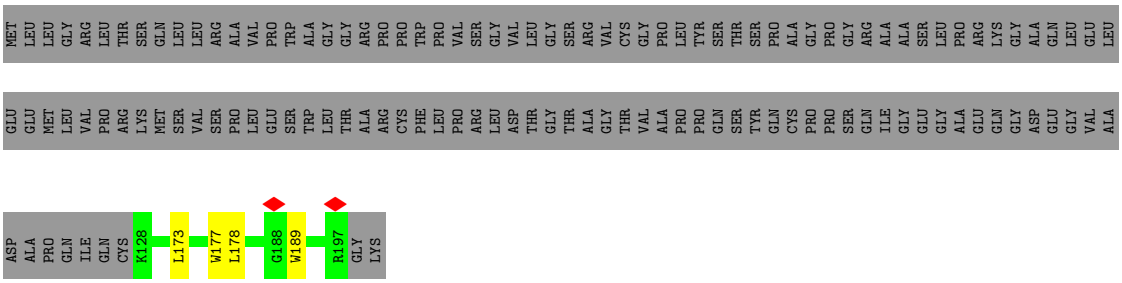
Chain A1:





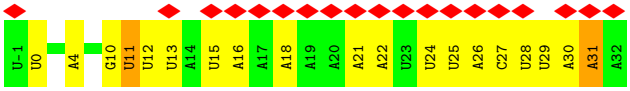
• Molecule 77: Aurora kinase A-interacting protein

Chain A3:



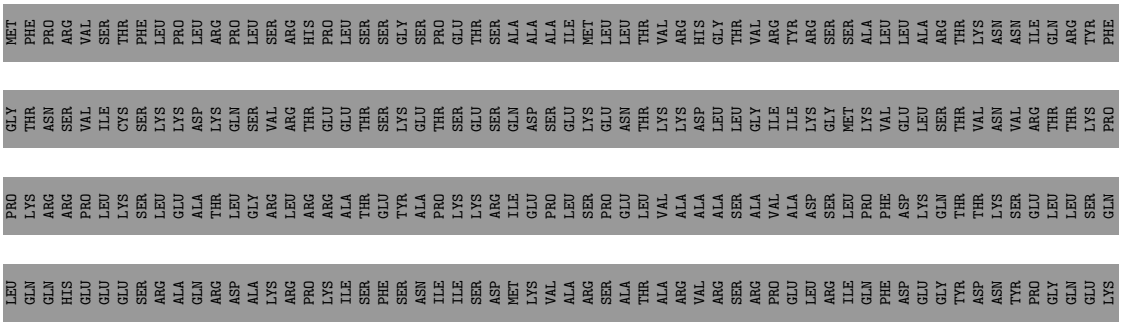
• Molecule 78: mRNA

Chain Az:



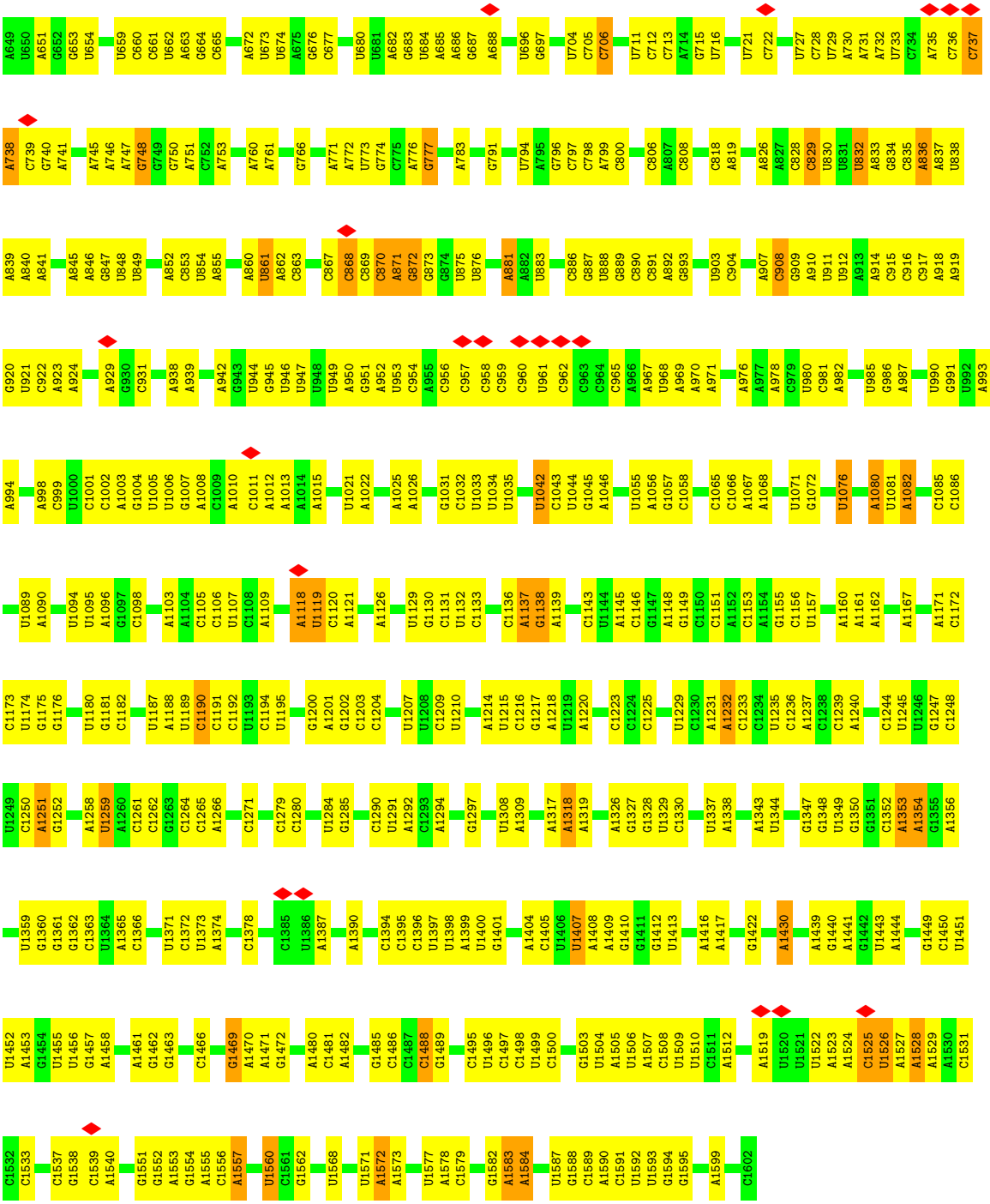
• Molecule 79: 28S ribosomal protein S31, mitochondrial

Chain AY:



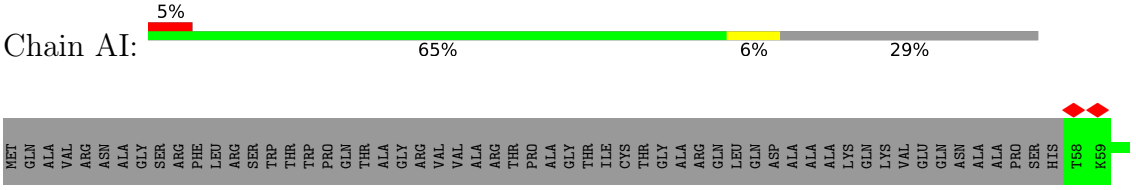
• Molecule 80: 12S mitochondrial rRNA

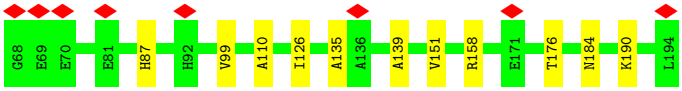
Chain AA:



• Molecule 81: 28S ribosomal protein S11, mitochondrial

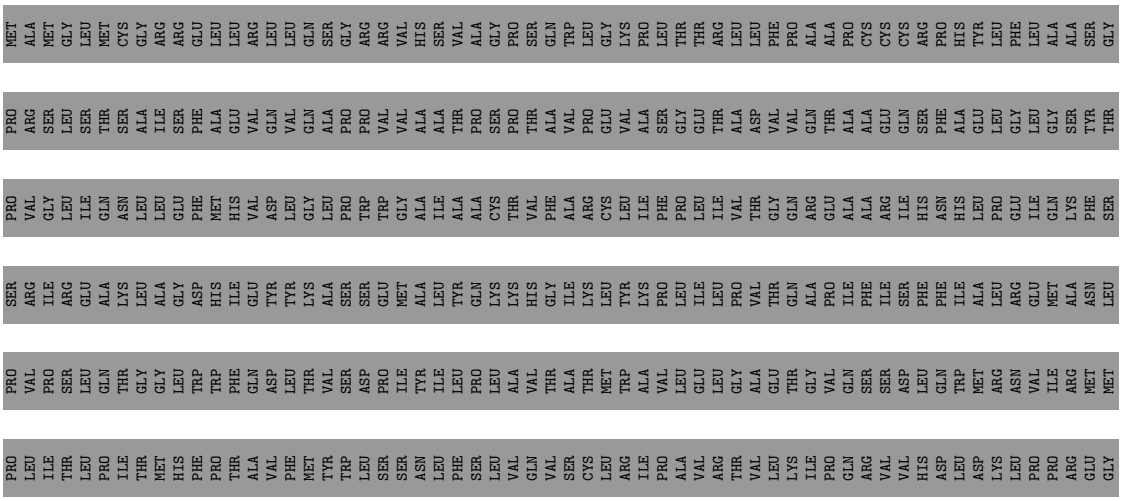
Chain AI:

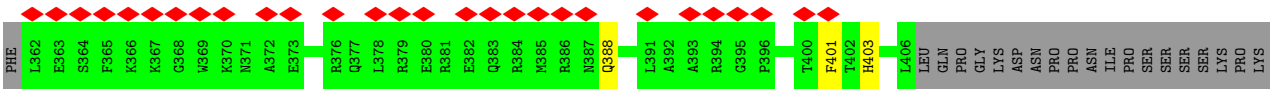


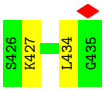


• Molecule 82: Mitochondrial inner membrane protein OXA1L

Chain OX:

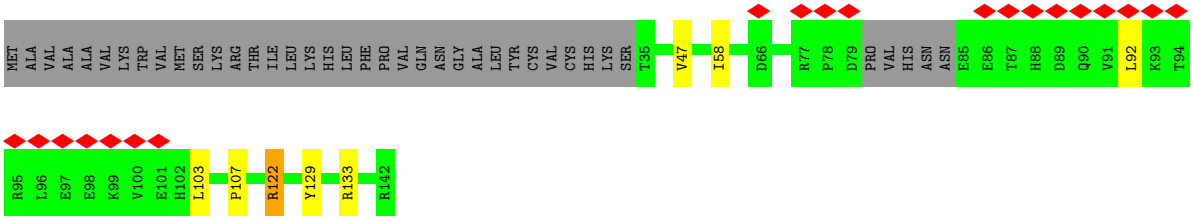






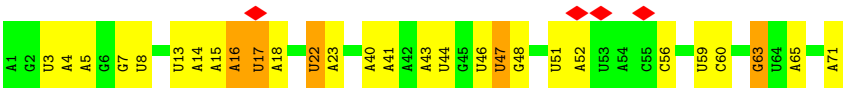
• Molecule 83: 39S ribosomal protein L42, mitochondrial

Chain a:



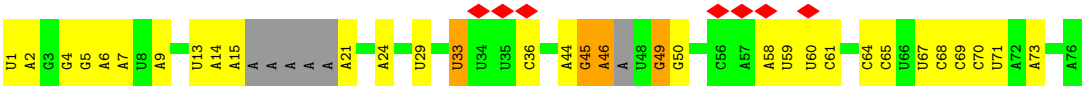
• Molecule 84: P/P-tRNA

Chain Ax:



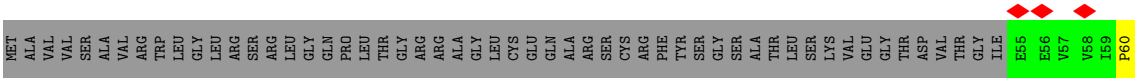
• Molecule 85: E/E-tRNA

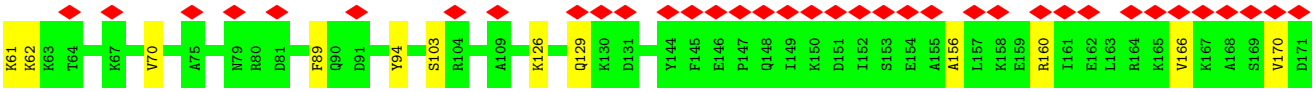
Chain Ay:

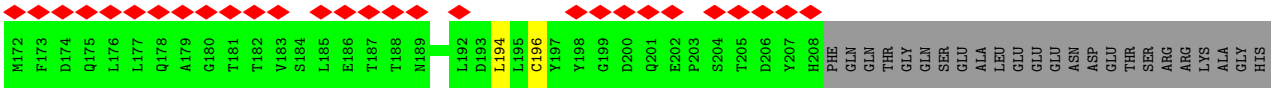


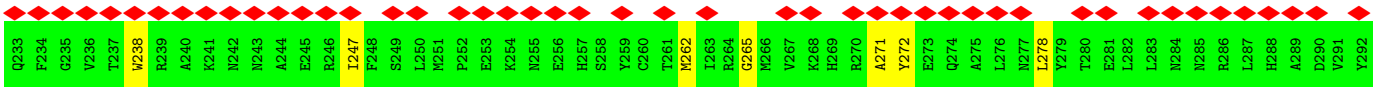
• Molecule 86: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

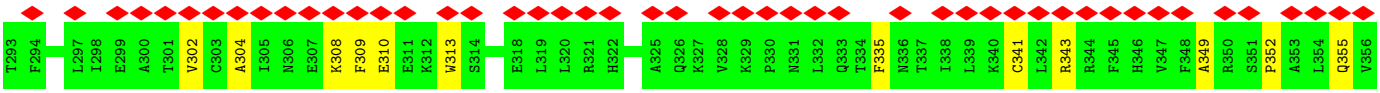
Chain A4:

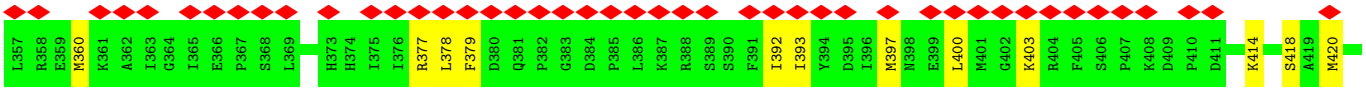


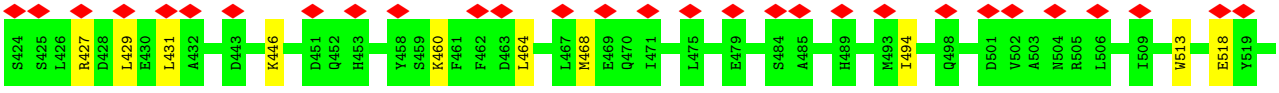


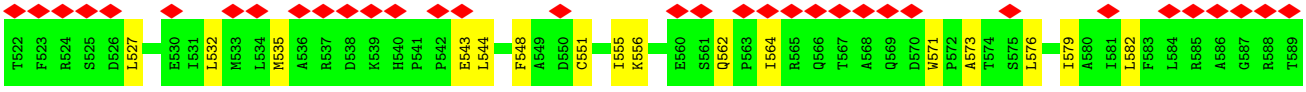


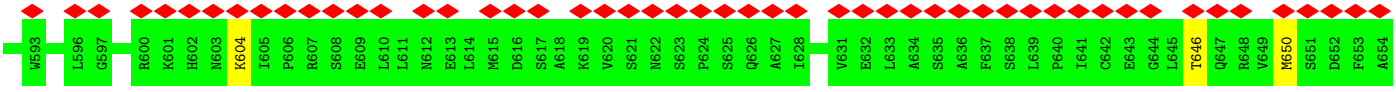


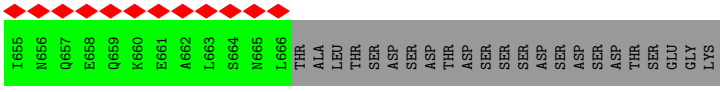






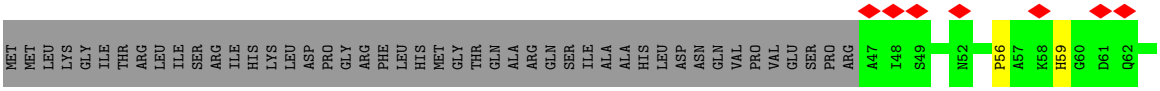


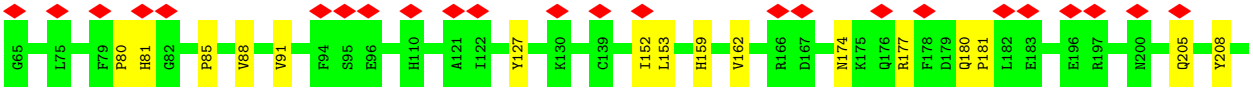


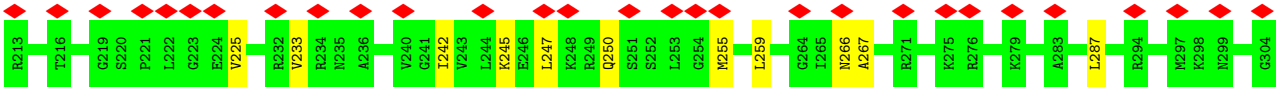


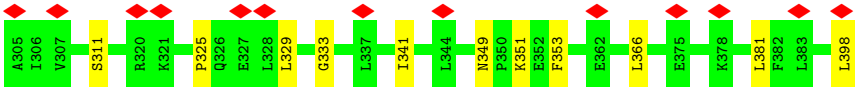
• Molecule 87: 28S ribosomal protein S29, mitochondrial

Chain AX:

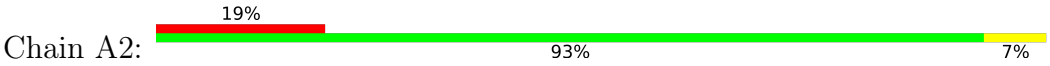


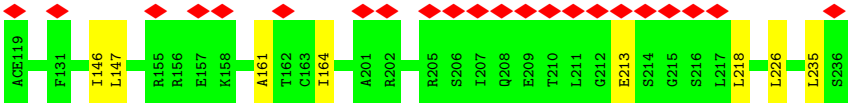




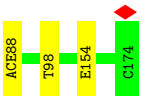


• Molecule 88: Small ribosomal subunit protein mS37

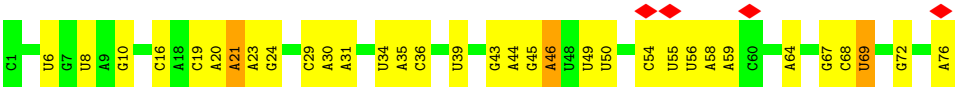




• Molecule 89: Small ribosomal subunit protein bS21m



• Molecule 90: mitochondrial tRNAVal



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20794	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 ($e^-/Å^2$)	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	0.162	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.24	0/913	0.27	0/1224
2	1	0.23	0/469	0.31	0/621
3	2	0.30	0/383	0.30	0/507
4	3	0.29	0/853	0.29	0/1136
5	4	0.28	0/350	0.28	0/461
6	5	0.24	0/3305	0.30	0/4502
7	6	0.21	0/3043	0.28	0/4140
8	7	0.21	0/2447	0.29	0/3310
9	8	0.18	0/1354	0.34	0/1819
10	9	0.23	0/1025	0.28	0/1379
11	A	0.30	0/36876	0.32	0/57402
12	D	0.26	0/1896	0.29	0/2549
13	E	0.26	0/2475	0.32	0/3355
14	F	0.28	0/2090	0.31	0/2842
15	H	0.18	0/1698	0.31	0/2292
16	I	0.19	0/1478	0.34	0/1999
17	J	0.17	0/1348	0.32	0/1813
18	K	0.28	0/1497	0.30	0/2031
19	L	0.25	0/905	0.29	0/1218
20	M	0.27	0/2381	0.31	0/3212
21	N	0.25	0/1833	0.28	0/2468
22	O	0.25	0/1283	0.29	0/1727
23	P	0.23	0/1199	0.27	0/1623
24	Q	0.23	0/2039	0.27	0/2750
25	R	0.28	0/1175	0.29	0/1572
26	S	0.28	0/1320	0.31	0/1789
27	T	0.28	0/1403	0.30	0/1886
28	U	0.25	0/1279	0.36	0/1730
29	W	0.27	0/926	0.29	0/1244
30	X	0.24	0/2099	0.26	0/2837
31	Y	0.26	0/1593	0.27	0/2136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Z	0.27	0/1021	0.28	0/1378
33	z	0.14	0/2067	0.36	0/2793
34	V	0.22	0/1721	0.27	0/2333
35	b	0.27	0/1218	0.31	0/1649
36	d	0.20	0/2181	0.36	0/2949
37	e	0.16	0/1970	0.34	0/2658
38	g	0.25	0/1151	0.28	0/1569
39	h	0.20	0/918	0.27	0/1249
40	i	0.29	0/850	0.30	0/1135
41	j	0.24	0/760	0.26	0/1023
42	k	0.17	0/783	0.25	0/1057
43	l	0.16	0/707	0.30	0/960
44	m	0.17	0/805	0.33	0/1081
46	o	0.29	0/819	0.32	0/1097
47	q	0.19	0/1529	0.29	0/2055
48	r	0.24	0/1362	0.30	0/1846
49	t	0.13	0/358	0.29	0/486
49	u	0.18	0/259	0.39	0/350
50	c	0.24	0/2347	0.27	0/3171
51	f	0.20	0/1273	0.36	0/1716
52	p	0.19	0/1223	0.27	0/1641
53	s	0.25	0/3231	0.31	0/4389
54	AB	0.18	0/1871	0.27	0/2531
55	AC	0.18	0/1113	0.29	0/1505
56	AD	0.17	0/2783	0.27	0/3724
57	AE	0.20	0/989	0.29	0/1335
58	AF	0.16	0/1767	0.26	0/2373
59	AG	0.16	0/2746	0.27	0/3681
60	AH	0.18	0/1178	0.31	0/1598
61	AJ	0.19	0/855	0.27	0/1148
62	AK	0.18	0/880	0.28	0/1182
63	AL	0.18	0/1477	0.23	0/1974
64	AM	0.17	0/963	0.32	0/1295
65	AN	0.17	0/886	0.29	0/1199
66	AO	0.16	0/1648	0.31	0/2243
67	AP	0.20	0/798	0.27	0/1070
68	AR	0.13	0/2456	0.28	0/3317
69	AS	0.15	0/1138	0.25	0/1533
70	AT	0.16	0/1402	0.32	0/1883
71	AU	0.15	0/1510	0.27	0/2025
72	AV	0.16	0/3030	0.36	0/4093
73	AW	0.17	0/801	0.29	0/1079
74	AZ	0.16	0/857	0.30	0/1141

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	A0	0.14	0/1834	0.29	0/2484
76	A1	0.15	0/2313	0.28	0/3129
77	A3	0.22	0/636	0.32	0/839
78	Az	0.17	0/804	0.36	0/1248
79	AY	0.17	0/1040	0.27	0/1402
80	AA	0.23	0/22537	0.30	0/35085
81	AI	0.19	0/1039	0.29	0/1400
82	OX	0.18	0/478	0.43	0/639
83	a	0.25	0/891	0.38	0/1208
84	Ax	0.21	0/1673	0.36	0/2602
85	Ay	0.16	0/1655	0.28	0/2567
86	A4	0.15	0/4877	0.34	0/6598
87	AX	0.16	0/2921	0.33	0/3954
88	A2	0.18	0/947	0.31	0/1266
89	AQ	0.21	0/754	0.25	0/1003
90	B	0.20	0/1626	0.28	0/2523
All	All	0.23	0/188661	0.31	0/268035

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
83	a	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
83	a	122	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	898	0	916	3	0
2	1	464	0	511	6	0
3	2	377	0	406	0	0
4	3	832	0	883	3	0
5	4	342	0	361	2	0
6	5	3210	0	3206	14	0
7	6	2948	0	2841	12	0
8	7	2390	0	2397	15	0
9	8	1327	0	1368	16	0
10	9	997	0	987	2	0
11	A	33070	0	16793	195	0
12	D	1859	0	1920	9	0
13	E	2406	0	2415	5	0
14	F	2031	0	2065	9	0
15	H	1661	0	1734	21	0
16	I	1446	0	1532	10	0
17	J	1330	0	1407	10	0
18	K	1455	0	1452	7	0
19	L	890	0	941	2	0
20	M	2327	0	2393	10	0
21	N	1786	0	1817	9	0
22	O	1259	0	1294	11	0
23	P	1173	0	1165	4	0
24	Q	1990	0	2031	9	0
25	R	1154	0	1214	1	0
26	S	1293	0	1365	8	0
27	T	1369	0	1410	7	0
28	U	1248	0	1228	5	0
29	W	904	0	935	1	0
30	X	2044	0	2060	7	0
31	Y	1556	0	1597	2	0
32	Z	996	0	1044	1	0
33	z	2027	0	2076	34	0
34	V	1676	0	1687	9	0
35	b	1193	0	1191	3	0
36	d	2124	0	2125	24	0
37	e	1931	0	1916	16	0
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	0	0
42	k	774	0	784	5	0
43	l	688	0	673	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	m	791	0	796	7	0
45	n	215	0	50	0	0
46	o	798	0	804	2	0
47	q	1495	0	1492	16	0
48	r	1322	0	1348	11	0
49	t	354	0	377	4	0
49	u	257	0	283	5	0
50	c	2299	0	2320	7	0
51	f	1252	0	1269	12	0
52	p	1205	0	1223	5	0
53	s	3148	0	3131	14	0
54	AB	1828	0	1815	4	0
55	AC	1083	0	1088	14	0
56	AD	2731	0	2804	16	0
57	AE	972	0	1000	10	0
58	AF	1725	0	1769	13	0
59	AG	2688	0	2687	14	0
60	AH	1152	0	1183	16	0
61	AJ	839	0	887	5	0
62	AK	862	0	885	13	0
63	AL	1453	0	1540	7	0
64	AM	942	0	965	16	0
65	AN	868	0	928	5	0
66	AO	1592	0	1557	12	0
67	AP	781	0	806	5	0
68	AR	2409	0	2428	18	0
69	AS	1111	0	1115	5	0
70	AT	1371	0	1393	11	0
71	AU	1488	0	1499	6	0
72	AV	2969	0	2961	48	0
73	AW	789	0	802	12	0
74	AZ	839	0	858	9	0
75	A0	1787	0	1796	25	0
76	A1	2265	0	2294	19	0
77	A3	625	0	698	4	0
78	Az	719	0	360	5	0
79	AY	1010	0	957	7	0
80	AA	20260	0	10286	333	0
81	AI	1019	0	1059	7	0
82	OX	468	0	464	6	0
83	a	865	0	829	6	0
84	Ax	1498	0	766	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	Ay	1483	0	754	18	0
86	A4	4768	0	4766	54	0
87	AX	2849	0	2844	27	0
88	A2	935	0	971	6	0
89	AQ	744	0	758	3	0
90	B	1524	0	779	12	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	18	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	50	0	95	1	0
93	AA	10	0	19	0	0
93	AG	10	0	19	0	0
94	A	6	0	12	0	0
95	A	137	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	AK	1	0	0	0	0
95	AX	1	0	0	0	0
95	D	2	0	0	0	0
95	E	1	0	0	0	0
95	g	1	0	0	0	0
96	AP	4	0	0	1	0
96	AT	4	0	0	0	0
96	r	4	0	0	1	0
97	AA	44	0	26	1	0
98	AA	28	0	52	0	0
99	AX	31	0	12	0	0
100	AX	28	0	12	2	0
101	B	7	0	8	1	0
All	All	179960	0	152420	1221	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1221) 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)
37:e:183:THR:HG23	37:e:186:GLY:H	1.46	0.81
80:AA:1562:G:H1’	80:AA:1583:MA6:H2	1.64	0.79
86:A4:556:LYS:HE3	86:A4:579:ILE:HD13	1.65	0.77
75:A0:99:ARG:HD3	80:AA:1526:U:H2’	1.67	0.74
36:d:208:VAL:HG22	36:d:253:THR:HG23	1.69	0.74
61:AJ:72:LYS:HG3	80:AA:1557:A:H5”	1.70	0.72
14:F:103:GLN:HE22	14:F:249:ASN:HD22	1.38	0.71
80:AA:1440:G:H2’	80:AA:1441:A:C8	2.26	0.70
72:AV:70:LEU:HD22	72:AV:389:LEU:HG	1.73	0.70
80:AA:839:A:H2’	80:AA:840:A:H8	1.56	0.69
79:AY:338:LEU:HD11	79:AY:351:MET:HB3	1.74	0.69
54:AB:180:ARG:HH21	56:AD:210:PRO:HB2	1.58	0.69
33:z:161:THR:HB	33:z:167:VAL:HG22	1.73	0.69
64:AM:20:ARG:HB2	80:AA:839:A:H5”	1.74	0.69
37:e:205:LEU:HB3	51:f:168:GLU:HB2	1.75	0.69
86:A4:400:LEU:HA	86:A4:403:LYS:HD3	1.74	0.69
36:d:90:PRO:HB3	36:d:245:TYR:HE2	1.56	0.68
55:AC:125:ARG:HH11	86:A4:94:TYR:HB2	1.58	0.68
9:8:187:PRO:HG2	44:m:79:ILE:HD11	1.75	0.67
11:A:2545:U:H5”	11:A:2546:G:H5’	1.76	0.67
76:A1:126:LEU:HD11	86:A4:70:VAL:HG13	1.76	0.67
34:V:79:VAL:HG12	34:V:86:VAL:HG12	1.74	0.67
33:z:127:LEU:HD22	33:z:290:VAL:HG13	1.75	0.67
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.75	0.66
62:AK:33:ARG:HG2	62:AK:36:ARG:HH22	1.59	0.66
80:AA:1528:A:H2’	80:AA:1529:A:H8	1.61	0.66
86:A4:397:MET:HG3	86:A4:431:LEU:HD11	1.78	0.65
86:A4:532:LEU:HD11	86:A4:555:ILE:HG21	1.79	0.65
64:AM:29:ARG:HE	70:AT:147:VAL:HB	1.62	0.65
60:AH:76:LEU:HB2	60:AH:145:LEU:HB2	1.78	0.65
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.79	0.65
80:AA:1265:C:H2’	80:AA:1266:A:H8	1.62	0.65
79:AY:290:ASN:HA	86:A4:446:LYS:HD3	1.79	0.65
11:A:2352:U:H3	11:A:2361:G:H1	1.45	0.64
80:AA:1201:A:H2’	80:AA:1202:G:H8	1.62	0.64
11:A:2778:U:H5”	33:z:115:THR:HG22	1.78	0.64
68:AR:157:VAL:HG22	68:AR:174:VAL:HG22	1.78	0.64
56:AD:244:LEU:HD22	56:AD:343:LEU:HD23	1.80	0.64
67:AP:49:ASP:HA	73:AW:85:ARG:HH11	1.62	0.64
80:AA:740:G:H2’	80:AA:741:A:C8	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:77:THR:HG23	36:d:283:PRO:HA	1.79	0.63
86:A4:429:LEU:HA	86:A4:464:LEU:HD21	1.80	0.63
11:A:2392:U:H2'	11:A:2394:A:H62	1.62	0.63
80:AA:1317:A:H3'	80:AA:1318:A:H8	1.62	0.63
15:H:106:GLY:HA2	15:H:158:LYS:HB2	1.80	0.63
9:8:192:TYR:HB3	51:f:132:ILE:HD11	1.80	0.63
80:AA:740:G:H2'	80:AA:741:A:H8	1.64	0.62
33:z:181:THR:HA	33:z:184:ILE:HD12	1.80	0.62
11:A:2082:G:H2'	11:A:2083:U:O4'	1.99	0.62
72:AV:66:PRO:HD3	80:AA:1529:A:H1'	1.81	0.62
80:AA:1398:U:H2'	80:AA:1399:A:H8	1.63	0.62
80:AA:1006:U:H2'	80:AA:1007:G:H8	1.65	0.62
87:AX:153:LEU:HD21	87:AX:247:LEU:HD13	1.82	0.61
80:AA:1308:U:H2'	80:AA:1309:A:H8	1.65	0.61
80:AA:1347:G:H2'	80:AA:1348:G:H8	1.65	0.61
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.83	0.61
30:X:20:ILE:HG22	82:OX:434:LEU:HD23	1.80	0.61
80:AA:871:A:H4'	80:AA:872:G:H5'	1.83	0.61
6:5:409:GLU:HG3	6:5:412:ARG:HH21	1.66	0.60
80:AA:867:C:H2'	80:AA:870:C:H42	1.65	0.60
87:AX:174:ASN:HB3	87:AX:177:ARG:HG3	1.84	0.60
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.83	0.60
58:AF:224:HIS:HB3	58:AF:228:LYS:HZ1	1.66	0.60
80:AA:1089:U:H2'	80:AA:1090:A:H8	1.64	0.60
80:AA:1132:U:H2'	80:AA:1133:C:C6	2.37	0.60
80:AA:839:A:H2'	80:AA:840:A:C8	2.37	0.59
11:A:1994:A:H61	11:A:2736:C:H4'	1.67	0.59
84:Ax:40:A:H2'	84:Ax:41:A:C8	2.37	0.59
2:1:19:ARG:HB2	2:1:62:ILE:HD11	1.85	0.59
61:AJ:57:GLN:HB3	61:AJ:109:LEU:HD11	1.84	0.59
80:AA:1201:A:H2'	80:AA:1202:G:C8	2.36	0.59
80:AA:1239:C:H2'	80:AA:1240:A:C8	2.38	0.59
9:8:160:GLU:HA	9:8:163:LYS:HE3	1.83	0.59
80:AA:773:U:H2'	80:AA:774:G:H8	1.65	0.59
80:AA:836:A:H2'	80:AA:837:A:H8	1.68	0.59
88:A2:213:GLU:HB3	88:A2:218:LEU:HG	1.84	0.59
78:Az:28:U:H1'	86:A4:414:LYS:HG2	1.85	0.58
80:AA:663:A:H2'	80:AA:664:G:C8	2.38	0.58
64:AM:29:ARG:HH22	70:AT:140:ILE:HG23	1.69	0.58
72:AV:267:ALA:HB2	72:AV:340:LYS:HZ3	1.68	0.58
80:AA:868:C:H2'	80:AA:869:C:H6	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:s:271:LEU:HD23	53:s:273:LEU:HD13	1.84	0.58
80:AA:1239:C:H2'	80:AA:1240:A:H8	1.68	0.58
80:AA:1042:U:H2'	80:AA:1043:C:C6	2.39	0.58
80:AA:1131:C:H2'	80:AA:1132:U:C6	2.39	0.58
87:AX:242:ILE:HD11	100:AX:503:GDP:C5	2.38	0.58
30:X:178:PRO:HA	30:X:184:ARG:HH12	1.68	0.58
60:AH:155:VAL:HG13	76:A1:126:LEU:HD12	1.86	0.58
80:AA:918:A:H4'	80:AA:920:G:H4'	1.86	0.58
11:A:2409:A:H2'	11:A:2410:U:C6	2.39	0.58
14:F:221:LEU:HG	14:F:222:THR:HG23	1.86	0.58
62:AK:56:SER:HB2	74:AZ:33:VAL:HG13	1.85	0.58
9:8:147:LEU:HD21	37:e:208:ALA:HB1	1.86	0.57
60:AH:70:ASP:HA	86:A4:62:LYS:HE3	1.84	0.57
9:8:68:LEU:HD21	51:f:211:LEU:HB2	1.86	0.57
86:A4:343:ARG:HA	86:A4:378:LEU:HD13	1.85	0.57
71:AU:186:ASN:HD21	71:AU:202:ARG:HH11	1.50	0.57
80:AA:1180:U:H2'	80:AA:1181:G:H8	1.69	0.57
12:D:172:MET:HE1	57:AE:86:ILE:HG12	1.87	0.57
63:AL:165:LYS:HE3	80:AA:947:U:H5"	1.86	0.57
33:z:160:PHE:HD2	33:z:199:ALA:HB2	1.68	0.57
76:A1:134:PRO:HG3	86:A4:60:PRO:HD3	1.86	0.57
86:A4:302:VAL:HG21	86:A4:341:CYS:HB3	1.85	0.57
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.85	0.57
30:X:34:GLU:OE2	30:X:36:ARG:HB2	2.04	0.57
47:q:164:LEU:HB3	47:q:168:VAL:HG21	1.87	0.57
11:A:1952:U:H2'	11:A:1953:A:C8	2.39	0.56
27:T:62:ARG:HE	36:d:230:ARG:HD2	1.70	0.56
90:B:29:C:H2'	90:B:30:A:H8	1.70	0.56
52:p:133:LEU:HD21	52:p:157:MET:HE1	1.87	0.56
11:A:2764:A:C6	15:H:252:LEU:HD11	2.40	0.56
80:AA:1373:U:H2'	80:AA:1374:A:C8	2.40	0.56
80:AA:1589:C:H2'	80:AA:1590:A:C8	2.40	0.56
16:I:116:LEU:HG	16:I:121:ILE:HB	1.86	0.56
53:s:84:THR:HB	53:s:280:ASN:HB2	1.86	0.56
80:AA:1025:A:H2'	80:AA:1026:A:C8	2.39	0.56
11:A:1862:U:H2'	11:A:1863:A:H8	1.70	0.56
37:e:55:ARG:HD3	37:e:149:LEU:HD22	1.87	0.56
11:A:1857:U:H2'	11:A:1858:G:C8	2.41	0.56
15:H:98:LEU:HD11	15:H:105:VAL:HG23	1.87	0.56
36:d:115:THR:O	36:d:119:GLN:HG2	2.06	0.56
36:d:219:ARG:HD3	36:d:239:PRO:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:AV:117:LEU:HA	72:AV:122:GLN:HE22	1.71	0.56
80:AA:1400:U:H2'	80:AA:1401:G:C8	2.41	0.56
11:A:1761:A:H2'	11:A:1762:A:C8	2.41	0.56
76:A1:67:PRO:HG3	76:A1:118:ALA:HB2	1.88	0.56
80:AA:1007:G:H2'	80:AA:1008:A:H8	1.70	0.56
68:AR:209:ILE:HD12	68:AR:214:ASN:HB3	1.89	0.55
80:AA:1258:A:H4'	80:AA:1259:U:H3'	1.87	0.55
11:A:3150:U:H2'	11:A:3151:A:H8	1.72	0.55
80:AA:1003:A:H2'	80:AA:1004:G:H8	1.71	0.55
11:A:3198:A:H5"	11:A:3199:U:H6	1.70	0.55
11:A:2408:U:H2'	11:A:2409:A:H8	1.71	0.55
11:A:3143:U:H2'	11:A:3144:A:H8	1.70	0.55
50:c:228:LEU:HB2	50:c:307:PHE:CD2	2.41	0.55
86:A4:571:TRP:HE3	86:A4:576:LEU:HD21	1.72	0.55
11:A:2093:U:H2'	11:A:2094:G:C8	2.42	0.55
58:AF:166:ARG:NH2	80:AA:994:A:H1'	2.22	0.55
60:AH:96:VAL:HA	60:AH:106:ILE:HD13	1.88	0.55
80:AA:1440:G:H2'	80:AA:1441:A:H8	1.71	0.55
11:A:2740:A:H2'	11:A:2741:A:C8	2.42	0.55
15:H:207:LYS:HB3	15:H:222:GLU:HB3	1.89	0.55
17:J:140:VAL:O	17:J:144:ILE:HG12	2.06	0.55
87:AX:80:PRO:HG2	87:AX:81:HIS:HD2	1.72	0.55
87:AX:329:LEU:HB3	87:AX:333:GLY:HA3	1.88	0.55
11:A:3128:A:H2'	11:A:3129:A:C8	2.42	0.55
37:e:98:LEU:HG	37:e:101:LYS:HE3	1.87	0.55
54:AB:192:LEU:HD11	54:AB:220:VAL:HG23	1.89	0.55
80:AA:739:C:H2'	80:AA:740:G:O4'	2.07	0.55
80:AA:773:U:H2'	80:AA:774:G:C8	2.40	0.55
87:AX:159:HIS:HE1	87:AX:311:SER:HB3	1.71	0.55
80:AA:705:C:H3'	80:AA:706:C:H6	1.72	0.55
53:s:63:ILE:HA	53:s:66:TRP:CD1	2.42	0.55
8:7:204:LYS:HE3	83:a:92:LEU:HD13	1.90	0.54
11:A:2727:C:H2'	11:A:2728:C:C6	2.42	0.54
24:Q:100:LEU:HD21	24:Q:286:ILE:HG12	1.88	0.54
51:f:171:LEU:HD13	51:f:174:ILE:HD11	1.89	0.54
80:AA:1439:A:H2'	80:AA:1440:G:H8	1.71	0.54
11:A:2006:C:H2'	11:A:2007:U:C6	2.43	0.54
11:A:2099:U:H2'	11:A:2100:C:C6	2.42	0.54
34:V:158:GLU:HG2	82:OX:388:GLN:HE22	1.73	0.54
55:AC:136:VAL:HG22	55:AC:153:LEU:HD22	1.88	0.54
80:AA:1452:U:H2'	80:AA:1453:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:166:LEU:HB3	8:7:181:TYR:HE2	1.72	0.54
80:AA:1007:G:H2'	80:AA:1008:A:C8	2.42	0.54
33:z:108:LYS:O	33:z:112:LEU:HB2	2.07	0.54
80:AA:1439:A:H2'	80:AA:1440:G:C8	2.43	0.54
87:AX:181:PRO:HB2	87:AX:233:VAL:HG22	1.90	0.54
72:AV:322:THR:HG23	72:AV:325:SER:H	1.72	0.54
80:AA:1006:U:H2'	80:AA:1007:G:C8	2.43	0.54
80:AA:1042:U:H2'	80:AA:1043:C:H6	1.73	0.54
72:AV:231:LEU:HD12	72:AV:243:VAL:HG13	1.90	0.54
80:AA:672:A:H2'	80:AA:673:U:C6	2.43	0.54
80:AA:799:A:H2'	80:AA:800:C:C6	2.42	0.54
80:AA:1578:A:H2'	80:AA:1579:C:C6	2.43	0.54
11:A:2086:A:H2'	11:A:2087:U:C6	2.43	0.54
33:z:198:VAL:HB	33:z:230:ILE:HG23	1.90	0.54
36:d:197:VAL:HG22	36:d:212:ILE:HG23	1.89	0.54
80:AA:951:G:H2'	80:AA:952:A:H8	1.72	0.54
80:AA:1408:A:H2'	80:AA:1409:A:H8	1.72	0.54
9:8:99:ARG:HG2	37:e:83:LEU:HB3	1.90	0.53
11:A:1936:A:H4'	11:A:1937:A:N7	2.23	0.53
60:AH:77:SER:HB2	60:AH:173:THR:HB	1.90	0.53
72:AV:81:SER:HB3	72:AV:84:GLU:HG3	1.90	0.53
85:Ay:33:U:H2'	85:Ay:36:C:H41	1.74	0.53
51:f:175:GLN:HA	51:f:178:LEU:HD23	1.90	0.53
72:AV:103:TYR:CZ	80:AA:1524:A:H4'	2.43	0.53
86:A4:513:TRP:CD1	86:A4:551:CYS:HG	2.26	0.53
87:AX:152:ILE:HG12	87:AX:259:LEU:HD23	1.90	0.53
6:5:143:PRO:HA	6:5:146:HIS:HD1	1.73	0.53
76:A1:134:PRO:HB2	76:A1:137:LEU:HD23	1.90	0.53
80:AA:1587:U:H2'	80:AA:1588:G:H8	1.73	0.53
86:A4:196:CYS:HB3	86:A4:265:GLY:HA3	1.91	0.53
72:AV:70:LEU:HD21	72:AV:390:ILE:HD13	1.88	0.53
74:AZ:11:MET:HE1	76:A1:189:LYS:HG3	1.90	0.53
85:Ay:6:A:H2'	85:Ay:7:A:C8	2.43	0.53
11:A:1952:U:H2'	11:A:1953:A:H8	1.73	0.53
18:K:238:MET:HE2	18:K:311:ILE:HD11	1.91	0.53
11:A:1911:C:H2'	11:A:1912:A:H8	1.73	0.53
48:r:136:PRO:HG2	48:r:139:VAL:HG21	1.91	0.53
2:1:18:VAL:HG12	2:1:61:LYS:HA	1.91	0.53
60:AH:122:GLN:HG3	80:AA:1265:C:H4'	1.91	0.53
68:AR:182:ARG:HH12	68:AR:184:ALA:HA	1.74	0.53
80:AA:1190:C:H2'	80:AA:1191:C:H6	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:165:GLN:NE2	6:5:175:THR:HG22	2.24	0.53
33:z:184:ILE:HD13	33:z:206:GLU:HB2	1.91	0.53
43:l:110:LEU:HB3	43:l:117:TYR:HB2	1.90	0.53
52:p:135:LEU:HD22	52:p:154:ILE:HG13	1.91	0.53
64:AM:66:VAL:HG11	64:AM:90:LEU:HD11	1.91	0.53
65:AN:95:VAL:HG23	65:AN:96:THR:HG23	1.89	0.53
73:AW:154:LEU:HB3	88:A2:147:LEU:HG	1.91	0.53
80:AA:673:U:H2'	80:AA:674:U:C6	2.44	0.53
7:6:206:TYR:HH	7:6:214:TRP:CD1	2.27	0.53
56:AD:376:GLU:HB2	68:AR:94:ALA:H	1.73	0.53
80:AA:1129:U:H2'	80:AA:1130:G:H8	1.73	0.53
80:AA:1504:U:H2'	80:AA:1505:A:C8	2.44	0.53
72:AV:229:ALA:HB1	72:AV:286:VAL:HG11	1.91	0.53
80:AA:1365:A:H2'	80:AA:1366:C:C6	2.44	0.53
84:Ax:3:U:H2'	84:Ax:4:A:H8	1.74	0.53
11:A:1851:G:H2'	11:A:2693:A:N7	2.24	0.52
11:A:2318:A:H2'	11:A:2319:A:C8	2.44	0.52
53:s:145:VAL:HG21	53:s:187:LEU:HD11	1.90	0.52
59:AG:108:ILE:HG13	59:AG:125:MET:HB2	1.91	0.52
72:AV:76:ILE:HD12	72:AV:112:TRP:HD1	1.73	0.52
80:AA:705:C:H3'	80:AA:706:C:C6	2.44	0.52
80:AA:797:C:H2'	80:AA:798:C:H6	1.74	0.52
80:AA:916:C:H2'	80:AA:917:C:C6	2.44	0.52
80:AA:1002:C:H2'	80:AA:1003:A:C8	2.44	0.52
5:4:75:ARG:HH22	11:A:2964:U:H3'	1.74	0.52
15:H:201:VAL:HG11	15:H:206:LEU:HG	1.91	0.52
80:AA:833:A:H2'	80:AA:834:G:H8	1.74	0.52
80:AA:1552:G:H2'	80:AA:1553:A:H8	1.75	0.52
90:B:30:A:H2'	90:B:31:A:H8	1.74	0.52
11:A:2212:C:H2'	11:A:2213:A:C8	2.44	0.52
11:A:2777:G:H4'	15:H:177:LYS:HG2	1.90	0.52
72:AV:103:TYR:HA	80:AA:1525:C:H5	1.75	0.52
11:A:1829:A:H2'	11:A:1830:G:H8	1.75	0.52
11:A:2727:C:H2'	11:A:2728:C:H6	1.74	0.52
80:AA:682:A:H2'	80:AA:683:G:H8	1.75	0.52
80:AA:1349:U:H2'	80:AA:1350:G:C8	2.45	0.52
6:5:201:ARG:HB3	6:5:232:THR:HG22	1.90	0.52
69:AS:51:VAL:HG13	88:A2:235:LEU:HD11	1.91	0.52
80:AA:1488:5MC:H2'	80:AA:1489:G:C8	2.44	0.52
80:AA:949:U:O2	97:AA:1701:NAD:H6N	2.09	0.52
15:H:201:VAL:HA	33:z:86:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:f:90:VAL:HG13	51:f:189:HIS:HB3	1.91	0.52
80:AA:833:A:H2'	80:AA:834:G:C8	2.45	0.52
86:A4:494:ILE:HD11	86:A4:527:LEU:HA	1.90	0.52
11:A:2212:C:H2'	11:A:2213:A:H8	1.75	0.52
53:s:152:GLN:HA	53:s:156:TYR:HB2	1.91	0.52
57:AE:96:HIS:HB3	57:AE:99:THR:HG23	1.91	0.52
80:AA:1470:A:H2'	80:AA:1471:A:H8	1.75	0.52
11:A:1868:G:H2'	20:M:40:PRO:HG3	1.92	0.51
16:I:98:VAL:HG12	16:I:177:LEU:HD12	1.92	0.51
69:AS:134:ARG:HG2	69:AS:136:GLY:H	1.75	0.51
80:AA:1161:A:H2'	80:AA:1162:A:H8	1.75	0.51
86:A4:89:PHE:HZ	86:A4:103:SER:HB2	1.75	0.51
11:A:2151:A:H2'	11:A:2152:A:C8	2.46	0.51
72:AV:114:ARG:HA	72:AV:117:LEU:HD12	1.93	0.51
11:A:2055:U:H2'	11:A:2056:G:H8	1.75	0.51
62:AK:81:ASP:HA	62:AK:86:ARG:HD3	1.92	0.51
72:AV:233:LYS:HD3	72:AV:286:VAL:HG23	1.92	0.51
80:AA:872:G:H2'	80:AA:873:G:C8	2.45	0.51
80:AA:1232:A:H2	80:AA:1404:A:H5'	1.75	0.51
86:A4:335:PHE:CG	86:A4:360:MET:HE2	2.46	0.51
11:A:2134:A:H62	11:A:2135:A:H62	1.58	0.51
80:AA:1002:C:H2'	80:AA:1003:A:H8	1.75	0.51
80:AA:1231:A:H1'	80:AA:1236:C:H41	1.75	0.51
87:AX:159:HIS:HA	87:AX:162:VAL:HG12	1.93	0.51
11:A:2677:A:H2'	11:A:2678:A:C8	2.46	0.51
9:8:51:ARG:HH12	80:AA:1560:U:H5"	1.74	0.51
20:M:261:ASP:HB3	20:M:264:GLN:HB2	1.92	0.51
71:AU:64:ARG:HA	71:AU:67:VAL:HG12	1.92	0.51
80:AA:990:U:H2'	80:AA:991:G:O4'	2.10	0.51
80:AA:1034:U:H2'	80:AA:1035:U:C6	2.46	0.51
58:AF:172:VAL:HG12	58:AF:240:ARG:HD3	1.91	0.51
80:AA:1066:C:H2'	80:AA:1067:A:H8	1.76	0.51
80:AA:1136:C:H2'	80:AA:1137:A:C8	2.46	0.51
11:A:2439:U:H2'	11:A:2440:G:H8	1.76	0.51
11:A:2718:C:H2'	11:A:2991:U:H4'	1.93	0.51
80:AA:980:U:H2'	80:AA:981:C:H6	1.75	0.51
88:A2:161:ALA:HB1	88:A2:164:ILE:HD11	1.93	0.51
72:AV:163:VAL:O	72:AV:167:VAL:HG23	2.11	0.51
75:A0:51:PRO:HG3	80:AA:705:C:H5'	1.93	0.51
80:AA:1066:C:H2'	80:AA:1067:A:C8	2.46	0.51
11:A:2101:C:H2'	11:A:2102:A:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3089:A:H3'	11:A:3090:G:C5'	2.41	0.51
34:V:146:VAL:HG21	82:OX:401:PHE:HE1	1.75	0.51
80:AA:661:C:H2'	80:AA:662:U:C6	2.46	0.51
11:A:1906:G:H2'	11:A:2014:A:H61	1.76	0.50
36:d:197:VAL:HG13	36:d:212:ILE:HG12	1.93	0.50
64:AM:96:PHE:HD1	75:A0:169:LEU:HD22	1.76	0.50
79:AY:351:MET:HE3	79:AY:380:PHE:HE2	1.75	0.50
80:AA:1055:U:H2'	80:AA:1056:A:O4'	2.12	0.50
72:AV:30:LEU:HD23	72:AV:149:ASP:HB2	1.92	0.50
80:AA:818:C:H2'	80:AA:819:A:H8	1.77	0.50
80:AA:868:C:H2'	80:AA:869:C:C6	2.47	0.50
86:A4:548:PHE:HB3	86:A4:582:LEU:HD22	1.94	0.50
12:D:205:GLN:HA	12:D:208:ARG:HH21	1.76	0.50
33:z:282:ARG:HH21	33:z:289:PHE:HA	1.75	0.50
75:A0:25:LEU:HD21	80:AA:1531:C:H2'	1.94	0.50
80:AA:1407:U:H2'	80:AA:1408:A:H8	1.76	0.50
11:A:2702:G:H5'	18:K:292:LYS:HE2	1.94	0.50
21:N:124:VAL:HG12	21:N:158:ARG:HE	1.76	0.50
61:AJ:62:VAL:HA	61:AJ:83:VAL:HG12	1.93	0.50
80:AA:1359:U:H2'	80:AA:1360:G:H8	1.77	0.50
80:AA:1552:G:H2'	80:AA:1553:A:C8	2.46	0.50
11:A:2174:G:H4'	17:J:151:LEU:HD23	1.93	0.50
11:A:3114:U:H2'	11:A:3115:U:C6	2.46	0.50
63:AL:209:LEU:HD12	77:A3:189:TRP:CE2	2.46	0.50
84:Ax:3:U:H2'	84:Ax:4:A:C8	2.46	0.50
11:A:1911:C:H2'	11:A:1912:A:C8	2.47	0.50
11:A:2457:A:H3'	22:O:10:SER:HB2	1.94	0.50
11:A:3143:U:H2'	11:A:3144:A:C8	2.46	0.50
34:V:136:ARG:NH2	82:OX:403:HIS:HB2	2.27	0.50
43:l:92:TYR:HB3	43:l:96:LEU:HD13	1.94	0.50
80:AA:1089:U:H2'	80:AA:1090:A:C8	2.46	0.50
7:6:224:HIS:CE1	7:6:227:GLU:H	2.29	0.50
11:A:1862:U:H2'	11:A:1863:A:C8	2.47	0.50
72:AV:102:TRP:HA	75:A0:74:PHE:HE2	1.76	0.50
86:A4:272:TYR:HB2	86:A4:304:ALA:HB2	1.93	0.50
2:1:38:ARG:HH12	2:1:41:LEU:HD11	1.77	0.50
61:AJ:78:ARG:HG3	61:AJ:118:LEU:HD21	1.93	0.50
63:AL:209:LEU:HD13	77:A3:173:LEU:HD12	1.94	0.50
75:A0:64:LEU:HD12	75:A0:139:TRP:CD2	2.47	0.50
50:c:228:LEU:HB2	50:c:307:PHE:HD2	1.75	0.50
66:AO:82:LYS:HB3	80:AA:881:A:N6	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:AT:150:PRO:HB2	80:AA:684:U:H4'	1.93	0.50
87:AX:266:ASN:HA	87:AX:329:LEU:HD23	1.93	0.50
1:0:138:ARG:HB3	11:A:2321:A:C8	2.46	0.49
11:A:2275:U:H2'	11:A:2276:C:H6	1.76	0.49
80:AA:1207:U:H5"	80:AA:1218:A:H61	1.76	0.49
80:AA:1578:A:H2'	80:AA:1579:C:H6	1.77	0.49
87:AX:85:PRO:HA	87:AX:88:VAL:HG12	1.93	0.49
87:AX:250:GLN:HB3	87:AX:255:MET:SD	2.52	0.49
11:A:2748:A:H2'	11:A:2749:A:C8	2.47	0.49
46:o:24:PRO:HG2	48:r:169:TRP:HB2	1.94	0.49
72:AV:175:VAL:HG12	72:AV:177:SER:H	1.77	0.49
80:AA:661:C:H2'	80:AA:662:U:H6	1.78	0.49
80:AA:872:G:H2'	80:AA:873:G:H8	1.77	0.49
80:AA:1161:A:H2'	80:AA:1162:A:C8	2.47	0.49
80:AA:1452:U:H2'	80:AA:1453:A:C8	2.47	0.49
11:A:1977:U:H2'	11:A:1978:A:H8	1.76	0.49
11:A:2748:A:H2'	11:A:2749:A:H8	1.77	0.49
34:V:64:ILE:HD11	34:V:91:LEU:HB3	1.95	0.49
37:e:183:THR:HG23	37:e:186:GLY:N	2.20	0.49
60:AH:155:VAL:HG21	76:A1:129:PHE:HB2	1.94	0.49
75:A0:39:GLU:HG2	75:A0:40:THR:HG23	1.94	0.49
80:AA:736:C:H2'	80:AA:737:C:H5	1.77	0.49
90:B:68:C:H2'	90:B:69:U:C6	2.47	0.49
8:7:54:ARG:HH12	8:7:58:LEU:HD11	1.77	0.49
27:T:206:LEU:HA	35:b:119:PHE:HE2	1.77	0.49
30:X:149:PRO:HD2	30:X:152:ASP:HB2	1.94	0.49
72:AV:79:ILE:HD13	72:AV:85:ILE:HD12	1.93	0.49
76:A1:53:LEU:HD12	86:A4:518:GLU:HG2	1.93	0.49
80:AA:944:U:H2'	80:AA:945:G:H8	1.78	0.49
86:A4:392:ILE:HG13	86:A4:393:ILE:N	2.27	0.49
11:A:2942:C:H2'	11:A:2943:G:H8	1.77	0.49
33:z:200:VAL:HG12	33:z:228:ARG:HA	1.94	0.49
53:s:105:TRP:HZ3	53:s:268:PRO:HA	1.78	0.49
55:AC:42:VAL:HG11	55:AC:51:VAL:HG11	1.95	0.49
80:AA:922:C:H2'	80:AA:923:A:C8	2.48	0.49
80:AA:1347:G:H2'	80:AA:1348:G:C8	2.46	0.49
33:z:139:PRO:HG2	33:z:245:VAL:HG23	1.94	0.49
86:A4:646:THR:O	86:A4:650:MET:HG2	2.12	0.49
48:r:99:MET:HE1	48:r:115:ILE:HG22	1.94	0.49
60:AH:163:ASN:HB3	76:A1:114:LEU:HD11	1.93	0.49
66:AO:82:LYS:HB3	80:AA:881:A:H62	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:B:23:A:H2'	90:B:24:G:C8	2.48	0.49
12:D:109:PHE:HB3	12:D:204:ALA:HB3	1.95	0.49
33:z:180:GLY:HA2	33:z:203:ILE:HD12	1.95	0.49
72:AV:68:SER:N	80:AA:1523:A:H5"	2.27	0.49
80:AA:832:U:H2'	80:AA:833:A:H8	1.76	0.49
80:AA:956:C:H2'	80:AA:957:C:O4'	2.12	0.49
11:A:2060:A:C8	11:A:2079:C:C4	3.01	0.49
11:A:3224:G:H2'	11:A:3225:G:H8	1.78	0.49
80:AA:970:A:H2'	80:AA:971:A:C8	2.48	0.49
80:AA:1012:A:H2'	80:AA:1013:A:C8	2.48	0.49
80:AA:1065:C:H2'	80:AA:1066:C:O4'	2.12	0.49
80:AA:1308:U:H2'	80:AA:1309:A:C8	2.48	0.49
80:AA:1523:A:H2'	80:AA:1524:A:C8	2.47	0.49
85:Ay:1:U:H2'	85:Ay:2:A:C8	2.48	0.49
8:7:276:PHE:HB2	8:7:304:VAL:HG22	1.95	0.49
11:A:2056:G:H2'	11:A:2057:C:H6	1.78	0.49
44:m:90:ARG:HE	44:m:94:ARG:HG3	1.77	0.49
56:AD:201:ILE:HB	56:AD:222:ILE:HD12	1.94	0.49
56:AD:412:LYS:HG2	56:AD:418:LYS:HB2	1.95	0.49
80:AA:1156:C:H2'	80:AA:1157:U:C6	2.48	0.49
11:A:2514:C:H2'	11:A:2515:U:H6	1.78	0.48
11:A:3193:U:H5"	48:r:141:PRO:HB3	1.95	0.48
33:z:119:GLN:HB2	33:z:260:LEU:HD12	1.95	0.48
72:AV:225:LEU:HD13	72:AV:275:LEU:HD21	1.95	0.48
80:AA:1408:A:H2'	80:AA:1409:A:C8	2.48	0.48
80:AA:1469:G:H2'	80:AA:1470:A:H8	1.78	0.48
81:AI:151:VAL:HG21	81:AI:158:ARG:HG3	1.95	0.48
84:Ax:47:U:H2'	84:Ax:48:G:C8	2.48	0.48
85:Ay:21:A:H61	85:Ay:46:A:H2'	1.78	0.48
87:AX:180:GLN:HE22	87:AX:287:LEU:HD12	1.78	0.48
11:A:2275:U:H2'	11:A:2276:C:C6	2.48	0.48
47:q:40:PRO:HG2	47:q:51:GLN:HB3	1.95	0.48
80:AA:838:U:H2'	80:AA:839:A:H8	1.78	0.48
80:AA:1132:U:H2'	80:AA:1133:C:H6	1.77	0.48
80:AA:1328:G:H2'	80:AA:1329:U:C6	2.48	0.48
80:AA:1407:U:H2'	80:AA:1408:A:C8	2.48	0.48
87:AX:225:VAL:HG21	87:AX:242:ILE:HG21	1.95	0.48
13:E:107:MET:HE3	24:Q:145:LEU:HD12	1.95	0.48
28:U:153:LEU:HD21	36:d:220:GLN:HB2	1.93	0.48
34:V:16:PRO:HD2	34:V:19:TYR:HB2	1.96	0.48
37:e:97:ARG:HA	37:e:100:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:k:188:MET:HG2	48:r:49:ILE:HD13	1.95	0.48
54:AB:223:VAL:HG11	54:AB:229:PRO:HB3	1.94	0.48
80:AA:867:C:H2'	80:AA:870:C:N4	2.28	0.48
80:AA:908:C:H2'	80:AA:909:G:C8	2.48	0.48
80:AA:1119:U:H2'	80:AA:1120:C:O4'	2.14	0.48
83:a:122:ARG:HH11	83:a:122:ARG:HG2	1.78	0.48
11:A:3171:C:H5'	11:A:3197:U:H3	1.78	0.48
36:d:96:ARG:HG2	36:d:97:ILE:H	1.79	0.48
62:AK:36:ARG:HE	62:AK:40:ARG:HH22	1.60	0.48
80:AA:1441:A:H2	80:AA:1449:G:H22	1.60	0.48
80:AA:1506:U:H2'	80:AA:1507:A:H8	1.79	0.48
11:A:3078:C:H2'	11:A:3079:G:H8	1.77	0.48
15:H:193:PHE:HZ	15:H:233:VAL:HG21	1.79	0.48
18:K:202:LYS:HG2	18:K:203:MET:HG2	1.95	0.48
44:m:55:LEU:HD23	44:m:63:THR:HG21	1.94	0.48
75:A0:163:SER:HB3	75:A0:190:MET:HB3	1.96	0.48
11:A:3211:C:H4'	11:A:3212:C:H5	1.78	0.48
14:F:123:GLY:HA3	14:F:142:ARG:HG2	1.96	0.48
19:L:32:ILE:HD11	19:L:103:ASN:HB3	1.95	0.48
55:AC:38:ARG:HD2	55:AC:43:ARG:NH2	2.27	0.48
58:AF:166:ARG:HD2	85:Ay:36:C:H42	1.79	0.48
80:AA:847:G:H2'	80:AA:848:U:C6	2.49	0.48
80:AA:1033:U:H2'	80:AA:1034:U:C6	2.48	0.48
80:AA:1455:U:H2'	80:AA:1456:U:C6	2.49	0.48
64:AM:115:ALA:HA	64:AM:118:VAL:HG12	1.96	0.48
68:AR:142:LEU:HD21	68:AR:183:LYS:HE3	1.96	0.48
80:AA:1156:C:H2'	80:AA:1157:U:H6	1.79	0.48
80:AA:1194:C:H2'	80:AA:1195:U:C6	2.49	0.48
80:AA:1504:U:H2'	80:AA:1505:A:H8	1.78	0.48
11:A:2245:A:H4'	11:A:2246:A:OP1	2.13	0.48
47:q:138:GLN:O	47:q:141:GLU:HG3	2.13	0.48
57:AE:92:ASN:HB2	67:AP:117:MET:HE3	1.95	0.48
59:AG:87:HIS:O	59:AG:91:MET:HG2	2.14	0.48
70:AT:110:GLU:HA	70:AT:113:LEU:HD12	1.96	0.48
72:AV:149:ASP:HA	72:AV:152:ILE:HG22	1.96	0.48
75:A0:89:HIS:ND1	75:A0:121:LYS:HD3	2.29	0.48
80:AA:727:U:H2'	80:AA:728:C:O4'	2.14	0.48
9:8:129:ARG:HE	9:8:133:ARG:HH21	1.62	0.48
11:A:2764:A:C4	15:H:252:LEU:HD21	2.48	0.48
20:M:281:LYS:HG2	38:g:42:VAL:HG22	1.96	0.48
35:b:89:ILE:HA	35:b:92:LYS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:A0:82:ARG:HB2	75:A0:85:TRP:CD2	2.48	0.48
80:AA:875:U:H2'	80:AA:876:U:C6	2.49	0.48
80:AA:920:G:H2'	80:AA:921:U:C6	2.49	0.48
80:AA:958:C:H4'	80:AA:959:C:O4'	2.13	0.48
80:AA:970:A:H2'	80:AA:971:A:H8	1.77	0.48
80:AA:980:U:H2'	80:AA:981:C:C6	2.48	0.48
11:A:1935:A:C2	11:A:1936:A:H1'	2.49	0.48
11:A:2191:A:H4'	17:J:142:ARG:HG2	1.95	0.48
11:A:3144:A:H2'	11:A:3145:A:H8	1.79	0.48
80:AA:871:A:H1'	80:AA:872:G:C8	2.49	0.48
80:AA:1416:A:H2'	80:AA:1417:A:C8	2.49	0.48
11:A:2277:U:H2'	11:A:2278:A:H8	1.78	0.47
17:J:161:SER:HA	43:l:69:THR:HG21	1.95	0.47
66:AO:59:LEU:HD11	66:AO:122:LEU:HD12	1.94	0.47
80:AA:1173:C:H2'	80:AA:1174:U:C6	2.49	0.47
87:AX:366:LEU:HD22	87:AX:398:LEU:HD22	1.96	0.47
11:A:1765:C:H5'	40:i:75:ARG:HH22	1.80	0.47
11:A:1839:C:H2'	11:A:1840:C:C6	2.49	0.47
11:A:2774:C:H2'	11:A:2775:A:C5	2.49	0.47
26:S:144:LEU:HB2	83:a:58:ILE:HB	1.95	0.47
59:AG:168:MET:HE3	59:AG:237:GLU:HG3	1.97	0.47
74:AZ:10:ARG:HH12	76:A1:239:TRP:CD1	2.33	0.47
81:AI:99:VAL:HG11	81:AI:139:ALA:HB2	1.96	0.47
11:A:2728:C:H2'	11:A:2729:U:H6	1.78	0.47
11:A:3165:C:H2'	11:A:3166:U:C6	2.48	0.47
34:V:146:VAL:HG21	82:OX:401:PHE:CE1	2.49	0.47
68:AR:135:ARG:CZ	68:AR:186:TRP:HB3	2.44	0.47
80:AA:854:U:H2'	80:AA:855:A:C8	2.50	0.47
80:AA:976:A:H5"	89:AQ:88:ACE:H1	1.96	0.47
86:A4:397:MET:HA	86:A4:400:LEU:HG	1.96	0.47
7:6:237:LEU:HB2	7:6:240:ILE:HD11	1.97	0.47
11:A:2483:U:H2'	11:A:2484:C:O4'	2.15	0.47
11:A:2779:C:H5'	33:z:116:SER:HB3	1.96	0.47
51:f:119:ILE:HD11	51:f:166:PHE:HE2	1.78	0.47
58:AF:200:LEU:HB3	58:AF:202:PRO:HD2	1.97	0.47
80:AA:730:A:H3'	80:AA:731:A:H8	1.79	0.47
80:AA:838:U:H2'	80:AA:839:A:C8	2.49	0.47
80:AA:1043:C:H2'	80:AA:1044:U:C6	2.49	0.47
67:AP:120:MET:HG2	67:AP:121:PRO:O	2.15	0.47
72:AV:176:PRO:HA	72:AV:179:GLN:CD	2.40	0.47
76:A1:313:LYS:HG3	87:AX:341:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:659:U:H2'	80:AA:660:C:H6	1.79	0.47
80:AA:1025:A:H2'	80:AA:1026:A:H8	1.79	0.47
80:AA:1094:U:H2'	80:AA:1095:U:H6	1.79	0.47
80:AA:1191:C:H2'	80:AA:1192:C:C6	2.49	0.47
80:AA:1353:A:H5'	80:AA:1354:A:H5'	1.97	0.47
84:Ax:15:A:O2'	84:Ax:16:A:H5'	2.15	0.47
70:AT:91:GLU:HG2	70:AT:92:THR:HG23	1.96	0.47
80:AA:914:A:H2'	80:AA:915:C:C6	2.50	0.47
80:AA:1209:C:H2'	80:AA:1210:U:H6	1.80	0.47
80:AA:1555:A:H2'	80:AA:1556:C:O4'	2.14	0.47
11:A:1829:A:H2'	11:A:1830:G:C8	2.50	0.47
11:A:2533:A:H2'	11:A:2534:G:H8	1.78	0.47
63:AL:175:TYR:HB2	65:AN:89:GLY:HA3	1.97	0.47
72:AV:236:LEU:HD21	72:AV:323:GLU:HB3	1.97	0.47
80:AA:1190:C:H2'	80:AA:1191:C:C6	2.49	0.47
80:AA:1450:C:H2'	80:AA:1451:U:C6	2.49	0.47
80:AA:1495:C:H2'	80:AA:1496:U:C6	2.50	0.47
11:A:3163:G:H2'	11:A:3164:C:H6	1.79	0.47
22:O:26:ILE:HG13	24:Q:264:TRP:CD1	2.50	0.47
55:AC:105:ALA:HB3	55:AC:122:VAL:HG12	1.96	0.47
75:A0:71:LEU:HD11	75:A0:141:LEU:HD11	1.97	0.47
80:AA:1032:C:H2'	80:AA:1033:U:H6	1.80	0.47
11:A:2795:U:H2'	11:A:2796:G:H8	1.80	0.47
11:A:2803:A:H2'	11:A:2804:A:O4'	2.15	0.47
49:t:64:ILE:HD11	49:u:82:LEU:HB2	1.97	0.47
53:s:111:LYS:HG2	53:s:261:ILE:HD13	1.97	0.47
53:s:137:LEU:HD21	53:s:422:VAL:HG11	1.95	0.47
58:AF:88:ASP:HB3	58:AF:91:ILE:HB	1.96	0.47
68:AR:172:ILE:HD12	68:AR:189:ARG:HG2	1.97	0.47
70:AT:118:GLU:HA	70:AT:121:LYS:HD3	1.97	0.47
75:A0:82:ARG:HB2	75:A0:85:TRP:CG	2.49	0.47
80:AA:738:A:H3'	80:AA:739:C:H6	1.79	0.47
80:AA:985:U:H2'	80:AA:986:G:C8	2.50	0.47
15:H:178:ASN:HD22	15:H:239:ASN:HD21	1.63	0.47
33:z:201:PRO:HD2	33:z:228:ARG:HG3	1.97	0.47
47:q:188:LYS:O	47:q:191:LYS:HG2	2.14	0.47
58:AF:238:HIS:HE1	81:AI:126:ILE:HG22	1.80	0.47
80:AA:1181:G:H2'	80:AA:1182:C:C6	2.50	0.47
80:AA:1372:C:H2'	80:AA:1373:U:C6	2.50	0.47
80:AA:1409:A:H2'	80:AA:1410:G:H8	1.80	0.47
86:A4:646:THR:HG23	86:A4:650:MET:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:115:GLU:HG3	6:5:256:PHE:CD2	2.51	0.46
11:A:1861:U:H2'	11:A:1862:U:C6	2.50	0.46
11:A:2410:U:H2'	11:A:2411:U:C6	2.49	0.46
59:AG:293:ILE:HB	59:AG:300:TYR:HB3	1.97	0.46
80:AA:832:U:H2'	80:AA:833:A:C8	2.50	0.46
80:AA:1131:C:H2'	80:AA:1132:U:H6	1.79	0.46
80:AA:1455:U:H2'	80:AA:1456:U:H6	1.80	0.46
11:A:1863:A:H2'	11:A:1864:A:H8	1.79	0.46
11:A:2688:C:H2'	11:A:2689:C:C6	2.50	0.46
15:H:98:LEU:HD23	15:H:129:ALA:HB2	1.96	0.46
21:N:138:HIS:CE1	29:W:36:GLY:HA2	2.50	0.46
22:O:46:TRP:CD1	22:O:121:ALA:HB2	2.51	0.46
62:AK:91:CYS:HB3	62:AK:96:ARG:H	1.80	0.46
80:AA:738:A:H3'	80:AA:739:C:C6	2.50	0.46
80:AA:1233:C:H41	80:AA:1444:A:H62	1.63	0.46
85:Ay:1:U:H2'	85:Ay:2:A:H8	1.80	0.46
2:1:55:LEU:H	47:q:128:MET:HE2	1.80	0.46
11:A:3078:C:H2'	11:A:3079:G:C8	2.50	0.46
17:J:25:ARG:HB2	17:J:28:LEU:HB2	1.96	0.46
18:K:272:GLN:O	18:K:276:ARG:HG2	2.15	0.46
72:AV:228:TYR:HB3	72:AV:259:ALA:HB2	1.97	0.46
74:AZ:65:LEU:HA	74:AZ:68:LEU:HD12	1.96	0.46
15:H:174:VAL:HG23	15:H:237:VAL:HA	1.98	0.46
33:z:69:ILE:HA	33:z:72:ILE:HG12	1.95	0.46
80:AA:798:C:H2'	80:AA:799:A:C8	2.50	0.46
80:AA:1148:A:H2'	80:AA:1149:G:C8	2.50	0.46
85:Ay:67:U:H2'	85:Ay:68:C:C6	2.50	0.46
86:A4:89:PHE:CZ	86:A4:103:SER:HB2	2.50	0.46
33:z:98:GLU:HB3	33:z:101:LYS:HB2	1.97	0.46
37:e:124:TRP:CD2	44:m:72:ARG:HG2	2.51	0.46
70:AT:156:PRO:HD2	70:AT:159:MET:HE3	1.97	0.46
80:AA:1554:G:H2'	80:AA:1555:A:C8	2.50	0.46
83:a:103:LEU:HD12	83:a:107:PRO:HB2	1.97	0.46
11:A:1863:A:H2'	11:A:1864:A:C8	2.50	0.46
36:d:158:ASP:O	36:d:162:THR:HG23	2.14	0.46
36:d:186:VAL:HG21	36:d:239:PRO:HB3	1.98	0.46
75:A0:11:ILE:HB	80:AA:806:C:C2	2.50	0.46
80:AA:797:C:H2'	80:AA:798:C:C6	2.49	0.46
80:AA:1399:A:H2'	80:AA:1400:U:C6	2.51	0.46
1:0:130:VAL:HG21	22:O:134:PRO:HD3	1.98	0.46
11:A:3002:G:H2'	11:A:3003:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
93:A:3301:SPD:H52	12:D:275:TRP:CE2	2.51	0.46
38:g:73:GLN:HB3	38:g:162:LEU:HD11	1.98	0.46
42:k:186:LEU:HD13	42:k:205:HIS:CD2	2.51	0.46
44:m:84:LEU:HD12	44:m:88:GLU:HG3	1.96	0.46
47:q:184:LYS:O	47:q:188:LYS:HG2	2.15	0.46
52:p:115:VAL:HG13	52:p:161:ALA:HB3	1.98	0.46
62:AK:62:ILE:HG21	79:AY:349:HIS:HB3	1.97	0.46
80:AA:861:U:H2'	80:AA:862:A:H8	1.81	0.46
6:5:293:LEU:HD13	6:5:312:LYS:HE2	1.97	0.46
10:9:79:PRO:HD2	34:V:183:LEU:HD21	1.98	0.46
11:A:3198:A:H5'	11:A:3199:U:H5"	1.97	0.46
57:AE:26:ILE:HG22	57:AE:30:MET:HE2	1.98	0.46
67:AP:86:PRO:HA	67:AP:125:LYS:HB2	1.97	0.46
69:AS:106:LEU:HD13	69:AS:120:GLU:HG3	1.98	0.46
22:O:44:ALA:HB3	22:O:49:VAL:HG23	1.98	0.46
36:d:204:ASN:O	36:d:205:GLN:HG2	2.16	0.46
51:f:80:ILE:HG23	51:f:90:VAL:HG12	1.97	0.46
58:AF:74:ILE:HD13	59:AG:366:GLN:HA	1.97	0.46
59:AG:78:ILE:HG12	59:AG:127:HIS:CE1	2.51	0.46
60:AH:164:LEU:HD12	60:AH:165:PRO:HD2	1.97	0.46
75:A0:68:LEU:HD21	75:A0:80:VAL:HG21	1.97	0.46
78:Az:10:G:H5'	78:Az:11:U:OP2	2.16	0.46
11:A:1899:G:H21	20:M:35:LYS:HE3	1.81	0.46
15:H:120:ARG:HD3	30:X:132:LEU:HD13	1.98	0.46
75:A0:136:TYR:CZ	80:AA:705:C:H2'	2.51	0.46
80:AA:735:A:H2'	80:AA:736:C:O4'	2.16	0.46
80:AA:911:U:H2'	80:AA:912:U:C6	2.51	0.46
80:AA:965:C:C4	80:AA:1022:A:H4'	2.52	0.46
80:AA:1033:U:H2'	80:AA:1034:U:H6	1.81	0.46
51:f:190:THR:HG23	51:f:192:GLU:HG3	1.99	0.45
56:AD:172:MET:HE2	56:AD:176:ARG:HH22	1.80	0.45
64:AM:78:GLY:HA3	71:AU:78:VAL:HG21	1.97	0.45
72:AV:263:MET:HE1	72:AV:334:PHE:HD1	1.81	0.45
73:AW:155:GLY:HA3	88:A2:146:ILE:HG23	1.96	0.45
80:AA:732:A:H2'	80:AA:733:U:C6	2.51	0.45
80:AA:1171:A:H2'	80:AA:1172:C:O4'	2.16	0.45
80:AA:1572:A:H2'	80:AA:1573:A:C8	2.51	0.45
85:Ay:69:C:H2'	85:Ay:70:C:C6	2.51	0.45
9:8:117:LEU:HD11	37:e:69:GLU:HB3	1.97	0.45
11:A:1762:A:H2'	11:A:1763:A:C8	2.51	0.45
11:A:3139:G:H2'	11:A:3140:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3198:A:H5”	11:A:3199:U:C6	2.50	0.45
56:AD:372:GLU:HG3	68:AR:101:PRO:HB2	1.98	0.45
64:AM:73:ILE:O	64:AM:77:ILE:HG12	2.17	0.45
66:AO:217:ARG:HG2	66:AO:224:LEU:HD13	1.98	0.45
80:AA:951:G:H2’	80:AA:952:A:C8	2.50	0.45
80:AA:1495:C:H2’	80:AA:1496:U:H6	1.82	0.45
86:A4:166:VAL:HG12	86:A4:194:LEU:HG	1.99	0.45
11:A:1897:A:H2’	11:A:1898:A:H8	1.82	0.45
26:S:108:VAL:HB	26:S:195:ILE:HG13	1.98	0.45
38:g:91:MET:HB2	38:g:93:ASN:HD22	1.80	0.45
60:AH:124:VAL:HG13	80:AA:1264:C:H1’	1.98	0.45
64:AM:26:CYS:HB2	70:AT:150:PRO:HG2	1.99	0.45
65:AN:13:ILE:HG13	65:AN:66:LEU:HB2	1.99	0.45
80:AA:696:U:H2’	80:AA:697:G:C8	2.50	0.45
80:AA:1068:A:H5”	81:AI:190:LYS:HD3	1.99	0.45
84:Ax:8:U:O4	84:Ax:14:A:N7	2.49	0.45
86:A4:308:LYS:HE3	86:A4:310:GLU:HB2	1.99	0.45
37:e:52:CYS:HA	37:e:173:LEU:HD21	1.99	0.45
54:AB:203:PHE:HE1	73:AW:163:LEU:HD11	1.80	0.45
57:AE:108:ILE:HG13	96:AP:201:FES:S1	2.56	0.45
64:AM:34:ILE:HG12	64:AM:87:MET:HE1	1.97	0.45
75:A0:171:ARG:HE	75:A0:188:GLU:HG2	1.81	0.45
11:A:2668:A:H2’	11:A:2669:A:C8	2.52	0.45
28:U:110:LEU:HD12	31:Y:118:GLU:HG2	1.98	0.45
57:AE:6:LEU:HD21	57:AE:8:LEU:HD13	1.99	0.45
60:AH:76:LEU:HD23	60:AH:174:LYS:HA	1.99	0.45
64:AM:114:ARG:NH2	66:AO:236:PRO:HD2	2.31	0.45
90:B:49:U:H2’	90:B:50:U:C6	2.50	0.45
11:A:2217:C:H2’	11:A:2218:C:O4’	2.17	0.45
24:Q:96:ARG:HA	24:Q:99:MET:HE3	1.98	0.45
33:z:293:ALA:HB3	33:z:305:LEU:HB2	1.99	0.45
60:AH:72:LEU:HD12	76:A1:133:TRP:CZ3	2.51	0.45
68:AR:167:HIS:HB3	68:AR:193:ILE:HD13	1.98	0.45
80:AA:798:C:H2’	80:AA:799:A:H8	1.82	0.45
80:AA:1203:C:H2’	80:AA:1204:C:H6	1.82	0.45
80:AA:1503:G:H2’	80:AA:1504:U:C6	2.51	0.45
84:Ax:5:A:H2	84:Ax:63:G:H22	1.65	0.45
11:A:3077:C:H2’	11:A:3078:C:H6	1.81	0.45
12:D:207:ILE:HG12	12:D:229:PRO:HD3	1.99	0.45
14:F:138:HIS:CD2	14:F:146:TRP:HE1	2.34	0.45
37:e:51:LEU:HD13	37:e:188:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AF:167:PHE:HB2	85:Ay:33:U:H4'	1.98	0.45
61:AJ:56:PRO:HB3	80:AA:924:A:N3	2.32	0.45
80:AA:875:U:H2'	80:AA:876:U:H6	1.81	0.45
80:AA:1485:G:H2'	80:AA:1486:B8T:O4'	2.16	0.45
8:7:156:ARG:HH12	8:7:260:PHE:HB2	1.82	0.45
8:7:244:ALA:HB1	8:7:250:ARG:HE	1.82	0.45
11:A:1828:A:H4'	11:A:1829:A:C8	2.51	0.45
11:A:1897:A:H2'	11:A:1898:A:C8	2.52	0.45
11:A:3115:U:H2'	11:A:3116:C:C6	2.52	0.45
53:s:332:LEU:HD13	53:s:372:TYR:HB2	1.98	0.45
80:AA:981:C:H2'	80:AA:982:A:H8	1.81	0.45
80:AA:1175:G:H2'	80:AA:1176:G:H8	1.81	0.45
80:AA:1203:C:H2'	80:AA:1204:C:C6	2.52	0.45
86:A4:379:PHE:CE2	86:A4:392:ILE:HG21	2.52	0.45
11:A:3199:U:H4'	11:A:3200:U:O5'	2.17	0.45
16:I:97:ALA:HB3	16:I:154:LEU:HB2	1.99	0.45
57:AE:35:ILE:HD12	63:AL:97:MET:HE2	1.98	0.45
62:AK:69:ASP:O	62:AK:73:GLU:HG2	2.17	0.45
62:AK:120:LEU:HB3	62:AK:123:ILE:HG13	1.99	0.45
65:AN:17:VAL:HG22	65:AN:28:VAL:HG22	1.99	0.45
80:AA:673:U:H2'	80:AA:674:U:H6	1.81	0.45
80:AA:684:U:H2'	80:AA:685:A:H8	1.82	0.45
80:AA:1200:G:C2	80:AA:1201:A:C8	3.04	0.45
90:B:43:G:H2'	90:B:44:A:C8	2.51	0.45
11:A:3150:U:C2	11:A:3151:A:C8	3.05	0.45
34:V:80:ILE:HB	34:V:85:TRP:HB2	1.99	0.45
47:q:191:LYS:HA	47:q:194:LYS:HG2	1.98	0.45
55:AC:156:GLN:HE22	76:A1:101:GLY:H	1.65	0.45
76:A1:60:MET:HE3	76:A1:69:VAL:HG21	1.99	0.45
80:AA:682:A:H2'	80:AA:683:G:C8	2.52	0.45
80:AA:946:U:H2'	80:AA:947:U:C6	2.52	0.45
11:A:2757:A:H2'	11:A:2758:G:O4'	2.17	0.44
14:F:200:PRO:HD3	14:F:236:ARG:NH2	2.32	0.44
37:e:218:PRO:HD2	101:B:101:VAL:HG22	2.00	0.44
48:r:79:HIS:HB3	48:r:184:ASN:HA	1.98	0.44
74:AZ:24:ARG:HD3	79:AY:349:HIS:CD2	2.51	0.44
80:AA:676:G:H2'	80:AA:677:C:C6	2.52	0.44
80:AA:1244:C:H2'	80:AA:1245:U:C6	2.51	0.44
80:AA:1258:A:H62	80:AA:1329:U:H2'	1.82	0.44
80:AA:1430:A:N1	80:AA:1458:A:H5"	2.32	0.44
80:AA:1488:5MC:H2'	80:AA:1489:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1497:C:H2'	80:AA:1498:C:H6	1.82	0.44
85:Ay:49:G:H2'	85:Ay:50:G:H8	1.82	0.44
7:6:224:HIS:HA	7:6:232:TYR:CZ	2.52	0.44
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.99	0.44
11:A:1750:G:H2'	11:A:1751:A:C8	2.53	0.44
11:A:2302:U:H2'	11:A:2303:A:C8	2.52	0.44
11:A:2553:G:H2'	11:A:2554:A:C8	2.52	0.44
49:t:64:ILE:HD12	49:u:78:GLU:HG3	1.99	0.44
80:AA:659:U:H2'	80:AA:660:C:C6	2.52	0.44
80:AA:891:C:H2'	80:AA:892:A:O4'	2.17	0.44
80:AA:950:A:H2'	80:AA:951:G:C8	2.52	0.44
87:AX:349:ASN:HD21	87:AX:351:LYS:HB3	1.81	0.44
11:A:1719:G:H2'	11:A:1720:C:H6	1.82	0.44
11:A:2553:G:H2'	11:A:2554:A:H8	1.82	0.44
14:F:65:TRP:CD1	39:h:117:LEU:HD11	2.52	0.44
23:P:52:ASN:HB3	23:P:55:ASN:HB2	1.98	0.44
47:q:158:ALA:O	47:q:162:GLU:HG2	2.17	0.44
72:AV:190:LEU:HD11	72:AV:226:TYR:CE2	2.53	0.44
80:AA:1005:U:H4'	81:AI:87:HIS:CE1	2.52	0.44
80:AA:1044:U:H2'	80:AA:1045:G:O4'	2.17	0.44
80:AA:1590:A:H2'	80:AA:1591:C:H6	1.82	0.44
11:A:1936:A:H4'	11:A:1937:A:C8	2.52	0.44
11:A:3129:A:H2'	11:A:3130:A:C8	2.53	0.44
55:AC:76:LEU:HB2	55:AC:79:GLU:HG3	2.00	0.44
57:AE:3:ARG:HD3	57:AE:69:TYR:CZ	2.52	0.44
57:AE:32:ARG:HB3	57:AE:74:ALA:HB1	1.98	0.44
65:AN:31:THR:HG22	65:AN:46:ARG:HB3	1.99	0.44
72:AV:96:ARG:HG2	72:AV:134:GLN:C	2.42	0.44
73:AW:154:LEU:HB2	89:AQ:154:GLU:HG3	1.99	0.44
78:Az:30:A:H2'	78:Az:31:A:C4	2.52	0.44
80:AA:873:G:H1'	80:AA:921:U:H1'	2.00	0.44
6:5:167:THR:HG21	53:s:281:HIS:CE1	2.52	0.44
11:A:2474:C:H2'	11:A:2475:U:O4'	2.18	0.44
53:s:105:TRP:CG	53:s:271:LEU:HD13	2.52	0.44
59:AG:101:GLN:HA	59:AG:104:ILE:HD12	1.98	0.44
70:AT:161:GLY:HA3	80:AA:855:A:O3'	2.17	0.44
80:AA:1021:U:H4'	80:AA:1022:A:H5'	2.00	0.44
80:AA:1191:C:H2'	80:AA:1192:C:H6	1.83	0.44
85:Ay:68:C:H2'	85:Ay:69:C:H6	1.83	0.44
86:A4:352:PRO:O	86:A4:355:GLN:HG3	2.18	0.44
86:A4:427:ARG:HB3	86:A4:468:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:147:ILE:HG12	6:5:191:GLN:CD	2.43	0.44
11:A:2408:U:H2'	11:A:2409:A:C8	2.52	0.44
11:A:2751:G:H2'	11:A:2752:C:C6	2.52	0.44
11:A:2894:U:H5"	11:A:2895:U:O4'	2.18	0.44
16:I:146:LEU:HD11	42:k:135:PHE:CZ	2.52	0.44
36:d:168:CYS:HB2	36:d:262:HIS:O	2.18	0.44
49:u:74:LEU:HD23	49:u:79:ILE:HG12	1.99	0.44
57:AE:5:GLU:HB3	57:AE:96:HIS:CD2	2.53	0.44
72:AV:275:LEU:O	72:AV:347:ILE:HA	2.18	0.44
73:AW:114:ILE:HG21	73:AW:142:LEU:HD11	2.00	0.44
80:AA:1080:A:H1'	80:AA:1082:A:N7	2.33	0.44
80:AA:1348:G:H2'	80:AA:1349:U:C6	2.53	0.44
80:AA:1395:C:H2'	80:AA:1396:C:H6	1.83	0.44
86:A4:468:MET:HE3	86:A4:468:MET:HB3	1.92	0.44
7:6:95:PRO:HD3	7:6:170:ARG:HD3	2.00	0.44
9:8:121:TRP:CZ2	9:8:125:LYS:HD2	2.53	0.44
11:A:2187:C:H2'	11:A:2188:A:C8	2.53	0.44
11:A:2324:U:H2'	11:A:2325:U:C6	2.53	0.44
11:A:3155:C:H2'	11:A:3156:A:C8	2.53	0.44
47:q:141:GLU:HA	47:q:144:GLU:HG3	1.99	0.44
55:AC:98:GLY:HA3	74:AZ:71:TYR:CE1	2.52	0.44
56:AD:224:GLU:HB2	56:AD:342:MET:HG2	1.99	0.44
60:AH:145:LEU:HB3	60:AH:148:LEU:HD11	2.00	0.44
70:AT:96:LYS:HD2	70:AT:96:LYS:HA	1.83	0.44
72:AV:82:ARG:O	72:AV:85:ILE:HG22	2.17	0.44
72:AV:233:LYS:HB2	72:AV:286:VAL:HG21	2.00	0.44
75:A0:167:PRO:HG2	75:A0:170:LEU:HB2	2.00	0.44
80:AA:1214:A:N3	80:AA:1239:C:H1'	2.32	0.44
80:AA:1505:A:H2'	80:AA:1506:U:H6	1.83	0.44
9:8:60:LYS:HD2	9:8:60:LYS:HA	1.82	0.44
47:q:168:VAL:HG12	47:q:175:PHE:HB2	1.99	0.44
77:A3:177:TRP:CD1	77:A3:178:LEU:HD12	2.53	0.44
78:Az:29:U:H2'	78:Az:30:A:C4	2.53	0.44
86:A4:238:TRP:HB3	86:A4:271:ALA:HB2	1.99	0.44
86:A4:573:ALA:HB2	86:A4:604:LYS:HD3	2.00	0.44
4:3:127:ALA:HA	20:M:79:PRO:HD3	2.00	0.44
7:6:106:ARG:HG2	23:P:110:TRP:CE2	2.52	0.44
8:7:149:MET:HG2	8:7:209:LEU:HD23	2.00	0.44
58:AF:176:ASP:O	58:AF:180:ARG:HG3	2.17	0.44
64:AM:108:GLU:HG2	68:AR:147:ILE:HD11	1.99	0.44
68:AR:279:LYS:HE2	68:AR:308:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:AT:29:VAL:HB	70:AT:79:TYR:HB2	1.99	0.44
80:AA:712:C:H2'	80:AA:713:C:O4'	2.17	0.44
86:A4:61:LYS:HA	86:A4:61:LYS:HD3	1.76	0.44
87:AX:159:HIS:CD2	87:AX:267:ALA:HB2	2.53	0.44
15:H:163:THR:HG21	33:z:86:VAL:HG23	2.00	0.43
30:X:40:PRO:HB3	30:X:43:TYR:CZ	2.53	0.43
47:q:147:GLN:O	47:q:150:LYS:HG3	2.18	0.43
56:AD:100:LYS:HG2	80:AA:1262:C:H4'	2.00	0.43
56:AD:209:GLY:HA3	56:AD:213:GLU:HB2	2.00	0.43
62:AK:57:LEU:HD23	62:AK:71:ALA:HB2	2.00	0.43
63:AL:209:LEU:HD22	77:A3:173:LEU:HD12	1.98	0.43
73:AW:103:ARG:HE	73:AW:139:ARG:HH21	1.65	0.43
73:AW:149:LEU:HD11	73:AW:166:ASN:HB2	1.98	0.43
80:AA:687:G:H3'	80:AA:829:C:H41	1.83	0.43
80:AA:1396:C:H2'	80:AA:1397:U:C6	2.53	0.43
80:AA:1498:C:H2'	80:AA:1499:U:H6	1.83	0.43
80:AA:1577:U:H2'	80:AA:1578:A:C8	2.53	0.43
80:AA:1577:U:H2'	80:AA:1578:A:H8	1.83	0.43
86:A4:156:ALA:O	86:A4:160:ARG:HG2	2.18	0.43
86:A4:262:MET:HB3	86:A4:278:LEU:HD21	2.00	0.43
86:A4:562:GLN:HB3	86:A4:564:ILE:HG22	2.00	0.43
2:1:57:VAL:HG23	2:1:59:LYS:HE3	2.00	0.43
11:A:2626:U:H4'	11:A:2627:G:C8	2.53	0.43
15:H:247:ARG:HG2	15:H:251:TRP:HE1	1.83	0.43
22:O:50:ASP:HB2	22:O:107:MET:HE1	2.00	0.43
23:P:175:PRO:HG3	52:p:177:ARG:HD2	2.00	0.43
47:q:164:LEU:HD13	47:q:168:VAL:HG11	2.00	0.43
49:u:75:THR:O	49:u:79:ILE:HG13	2.18	0.43
66:AO:202:TRP:HD1	71:AU:59:ARG:HG2	1.82	0.43
72:AV:234:VAL:HA	72:AV:238:GLN:HE22	1.83	0.43
72:AV:276:CYS:SG	72:AV:352:LEU:HD21	2.58	0.43
80:AA:728:C:H2'	80:AA:729:U:O4'	2.18	0.43
80:AA:1003:A:H2'	80:AA:1004:G:C8	2.52	0.43
80:AA:1395:C:H2'	80:AA:1396:C:C6	2.53	0.43
80:AA:1409:A:H2'	80:AA:1410:G:C8	2.53	0.43
84:Ax:16:A:H4'	84:Ax:17:U:H5"	2.00	0.43
85:Ay:70:C:H2'	85:Ay:71:U:C6	2.53	0.43
11:A:1737:A:H61	11:A:1760:G:H1'	1.83	0.43
11:A:2187:C:H2'	11:A:2188:A:H8	1.83	0.43
11:A:2802:A:H2'	11:A:2803:A:O4'	2.19	0.43
11:A:2804:A:H2'	11:A:2805:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AC:125:ARG:NH1	86:A4:94:TYR:HB2	2.31	0.43
59:AG:161:LEU:HD21	59:AG:244:PHE:CE1	2.53	0.43
72:AV:287:LEU:HD21	72:AV:331:LEU:HA	2.00	0.43
80:AA:771:A:H2'	80:AA:772:A:C8	2.54	0.43
80:AA:1118:A:H3'	80:AA:1119:U:H5"	2.00	0.43
80:AA:1209:C:H2'	80:AA:1210:U:C6	2.53	0.43
15:H:213:ILE:HG12	15:H:219:TYR:CZ	2.53	0.43
80:AA:672:A:H2'	80:AA:673:U:H6	1.83	0.43
80:AA:852:A:H3'	80:AA:853:C:H6	1.82	0.43
80:AA:886:C:H2'	80:AA:887:G:C8	2.53	0.43
80:AA:985:U:H2'	80:AA:986:G:H8	1.82	0.43
11:A:2101:C:H2'	11:A:2102:A:C8	2.51	0.43
11:A:2175:C:H2'	11:A:2176:C:H6	1.82	0.43
11:A:2687:C:H2'	11:A:2688:C:H6	1.83	0.43
11:A:2728:C:H2'	11:A:2729:U:C6	2.54	0.43
16:I:44:ARG:HH11	21:N:230:LEU:HD22	1.84	0.43
26:S:94:ARG:HA	50:c:313:PRO:HD3	2.01	0.43
47:q:178:LEU:O	47:q:182:LEU:HG	2.19	0.43
50:c:213:LEU:HD23	50:c:213:LEU:HA	1.90	0.43
59:AG:357:THR:HG23	59:AG:360:GLU:H	1.83	0.43
72:AV:106:ASN:HA	72:AV:109:ILE:HD12	1.99	0.43
84:Ax:8:U:H3	84:Ax:14:A:H62	1.66	0.43
11:A:2409:A:H2'	11:A:2410:U:H6	1.83	0.43
11:A:2778:U:O2'	33:z:116:SER:HB2	2.17	0.43
12:D:235:GLN:HE21	12:D:296:VAL:HG21	1.83	0.43
36:d:106:ILE:O	36:d:110:GLU:HG2	2.19	0.43
59:AG:75:LYS:HA	59:AG:78:ILE:HD12	2.00	0.43
80:AA:887:G:H2'	80:AA:888:U:O4'	2.18	0.43
83:a:129:TYR:CZ	83:a:133:ARG:HD2	2.53	0.43
11:A:2175:C:H2'	11:A:2176:C:C6	2.53	0.43
11:A:2339:G:H2'	11:A:2340:C:H6	1.83	0.43
33:z:123:LEU:HD23	33:z:257:ILE:HD11	1.99	0.43
63:AL:116:VAL:HG12	63:AL:118:ASN:H	1.84	0.43
71:AU:114:ARG:O	71:AU:118:GLU:HG2	2.19	0.43
80:AA:1496:U:H2'	80:AA:1497:C:C6	2.54	0.43
11:A:2461:A:H2'	11:A:2462:A:H8	1.84	0.43
16:I:119:HIS:HB3	16:I:160:LYS:HE2	2.01	0.43
20:M:189:LYS:HB3	20:M:192:PRO:HG2	2.01	0.43
26:S:120:LEU:HD23	26:S:120:LEU:HA	1.89	0.43
27:T:62:ARG:NE	36:d:230:ARG:HD2	2.34	0.43
33:z:263:SER:HB3	33:z:266:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:85:PHE:HZ	36:d:209:TYR:HB2	1.83	0.43
36:d:208:VAL:HG23	36:d:252:LEU:HB2	2.01	0.43
44:m:110:LEU:HD13	79:AY:344:GLN:HE22	1.84	0.43
73:AW:103:ARG:HE	73:AW:139:ARG:NH2	2.17	0.43
80:AA:1175:G:H2'	80:AA:1176:G:C8	2.53	0.43
82:OX:427:LYS:HD2	82:OX:427:LYS:HA	1.90	0.43
6:5:133:PRO:HG3	6:5:375:TRP:CD2	2.53	0.43
9:8:192:TYR:HE1	51:f:134:VAL:HG22	1.84	0.43
11:A:2192:A:H5"	17:J:142:ARG:HH21	1.84	0.43
11:A:3057:C:H2'	11:A:3058:U:O4'	2.19	0.43
11:A:3144:A:H2'	11:A:3145:A:C8	2.54	0.43
15:H:174:VAL:HG12	15:H:192:HIS:CB	2.49	0.43
24:Q:227:LYS:HD2	24:Q:249:LEU:HD21	2.01	0.43
36:d:160:LEU:HD12	36:d:160:LEU:HA	1.80	0.43
44:m:91:ALA:HA	44:m:94:ARG:HE	1.83	0.43
56:AD:141:TRP:HZ2	74:AZ:68:LEU:HB3	1.84	0.43
72:AV:237:GLN:HB3	72:AV:238:GLN:NE2	2.34	0.43
84:Ax:22:U:C2	84:Ax:23:A:C8	3.07	0.43
86:A4:397:MET:HE3	86:A4:397:MET:HB3	1.90	0.43
87:AX:88:VAL:HA	87:AX:91:VAL:HG22	2.00	0.43
11:A:2335:A:H2'	11:A:2336:U:H6	1.84	0.43
11:A:3142:A:H2'	11:A:3143:U:C6	2.54	0.43
12:D:140:ALA:HB2	12:D:153:ALA:HB2	2.00	0.43
33:z:157:VAL:HB	33:z:234:LEU:HD13	2.00	0.43
53:s:65:ARG:O	53:s:69:THR:HG23	2.19	0.43
75:A0:175:ILE:HG22	75:A0:178:ARG:NH1	2.34	0.43
80:AA:1590:A:H2'	80:AA:1591:C:C6	2.54	0.43
6:5:336:LEU:HD21	6:5:362:THR:HG23	2.00	0.42
7:6:241:PRO:HB2	7:6:244:ARG:HH21	1.83	0.42
11:A:2235:C:H2'	11:A:2236:C:O4'	2.19	0.42
21:N:233:TYR:HB3	21:N:237:HIS:CD2	2.54	0.42
66:AO:187:THR:HB	68:AR:183:LYS:NZ	2.34	0.42
80:AA:664:G:H2'	80:AA:665:C:C6	2.54	0.42
80:AA:746:A:H2'	80:AA:747:A:H8	1.84	0.42
80:AA:840:A:H2'	80:AA:841:A:H8	1.84	0.42
80:AA:845:A:H2'	80:AA:846:A:H8	1.83	0.42
80:AA:1216:C:C2	80:AA:1217:G:C8	3.07	0.42
80:AA:1506:U:H2'	80:AA:1507:A:C8	2.54	0.42
87:AX:245:LYS:HD2	100:AX:503:GDP:H5'	2.01	0.42
11:A:2533:A:H2'	11:A:2534:G:C8	2.54	0.42
11:A:3118:U:H2'	11:A:3119:C:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AR:254:ASP:HA	68:AR:259:TYR:CE1	2.55	0.42
72:AV:152:ILE:HD12	72:AV:185:VAL:HG22	2.00	0.42
80:AA:686:A:H2'	80:AA:687:G:H8	1.84	0.42
80:AA:1145:A:H2'	80:AA:1146:C:H6	1.85	0.42
86:A4:309:PHE:HB2	86:A4:313:TRP:HZ3	1.84	0.42
86:A4:349:ALA:HB3	86:A4:378:LEU:HD11	2.01	0.42
11:A:2005:C:H2'	11:A:2006:C:C6	2.53	0.42
13:E:248:ILE:HG13	13:E:250:ARG:H	1.84	0.42
22:O:33:LEU:HD21	22:O:59:LEU:HD22	2.01	0.42
26:S:173:ARG:HB2	26:S:182:LYS:HG3	2.01	0.42
72:AV:93:TYR:HB2	72:AV:135:TYR:CE1	2.54	0.42
73:AW:150:THR:HG22	73:AW:161:THR:HA	2.00	0.42
80:AA:686:A:H2'	80:AA:687:G:C8	2.54	0.42
90:B:21:A:H61	90:B:46:A:H2'	1.84	0.42
11:A:2734:A:H2'	11:A:2735:G:H8	1.85	0.42
11:A:2847:C:H2'	11:A:2848:A:O4'	2.19	0.42
16:I:197:LEU:HD22	49:u:76:LEU:HD12	2.00	0.42
18:K:300:MET:HE3	18:K:300:MET:HB3	1.90	0.42
23:P:94:VAL:HG23	23:P:132:LEU:HD21	2.01	0.42
33:z:150:PHE:CD1	33:z:258:ALA:HA	2.54	0.42
47:q:198:LYS:HD2	47:q:198:LYS:HA	1.88	0.42
50:c:164:GLU:HG2	50:c:165:VAL:N	2.35	0.42
66:AO:183:ALA:HA	68:AR:183:LYS:HE2	2.01	0.42
80:AA:952:A:H2'	80:AA:953:U:C6	2.53	0.42
80:AA:1362:G:H2'	80:AA:1363:C:C6	2.54	0.42
86:A4:343:ARG:CZ	86:A4:377:ARG:HB3	2.50	0.42
88:A2:226:LEU:HD23	88:A2:226:LEU:HA	1.84	0.42
11:A:2109:A:C6	11:A:2111:C:C2	3.07	0.42
11:A:2656:U:H4'	13:E:230:THR:OG1	2.19	0.42
14:F:279:ARG:HH12	14:F:282:PRO:HD3	1.83	0.42
15:H:147:ARG:HG2	15:H:152:LEU:HB3	2.02	0.42
25:R:114:LYS:HG2	83:a:47:VAL:HG21	2.01	0.42
33:z:133:LYS:HG3	33:z:134:LYS:H	1.84	0.42
47:q:145:LYS:HA	47:q:145:LYS:HD2	1.89	0.42
58:AF:48:LYS:O	58:AF:52:ARG:HG2	2.20	0.42
58:AF:114:THR:HG21	58:AF:205:LEU:HG	2.00	0.42
72:AV:188:HIS:CD2	72:AV:353:LEU:HG	2.55	0.42
80:AA:1076:5MU:H2'	80:AA:1076:5MU:O2	2.19	0.42
80:AA:1509:U:H2'	80:AA:1510:U:C6	2.53	0.42
86:A4:535:MET:HE1	86:A4:551:CYS:HB3	2.00	0.42
87:AX:353:PHE:CZ	87:AX:381:LEU:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:83:LYS:HE3	5:4:88:TRP:NE1	2.33	0.42
6:5:228:ALA:HB3	6:5:292:TYR:HB2	2.02	0.42
21:N:183:LEU:HD23	21:N:183:LEU:HA	1.89	0.42
49:t:81:ASP:O	49:t:84:GLU:HG3	2.20	0.42
53:s:243:ILE:HD12	53:s:429:PRO:HG3	2.00	0.42
56:AD:165:GLN:HE21	56:AD:169:GLU:HG3	1.84	0.42
56:AD:317:HIS:HB3	56:AD:320:ILE:HG13	2.02	0.42
75:A0:162:ALA:HA	75:A0:194:GLN:HG2	2.00	0.42
80:AA:747:A:H2'	80:AA:748:G:C8	2.54	0.42
80:AA:1071:U:H2'	80:AA:1072:G:H8	1.84	0.42
85:Ay:67:U:H2'	85:Ay:68:C:H6	1.84	0.42
87:AX:159:HIS:CE1	87:AX:311:SER:HB3	2.54	0.42
4:3:116:ARG:HB2	4:3:122:TRP:CZ3	2.54	0.42
6:5:354:PHE:HB3	6:5:417:LEU:HD11	2.01	0.42
7:6:233:LEU:HD21	7:6:236:LEU:HD22	2.01	0.42
11:A:1939:G:C8	12:D:259:LYS:HD2	2.54	0.42
11:A:1991:A:H5"	11:A:1992:C:OP1	2.19	0.42
11:A:2666:U:H2'	11:A:2667:U:O4'	2.20	0.42
11:A:2778:U:H4'	33:z:115:THR:HA	2.01	0.42
11:A:3198:A:H4'	11:A:3199:U:OP2	2.20	0.42
14:F:123:GLY:HA2	14:F:141:ILE:HG12	2.02	0.42
37:e:198:ASN:HB3	37:e:243:PHE:CE1	2.55	0.42
42:k:192:HIS:O	48:r:36:ARG:HD2	2.20	0.42
51:f:115:ASN:HD21	90:B:36:C:H4'	1.84	0.42
53:s:119:PRO:HG3	53:s:394:TRP:CE3	2.54	0.42
59:AG:356:VAL:HG23	59:AG:361:VAL:HG23	2.02	0.42
80:AA:1349:U:H2'	80:AA:1350:G:H8	1.84	0.42
80:AA:1398:U:H2'	80:AA:1399:A:C8	2.50	0.42
80:AA:1450:C:H2'	80:AA:1451:U:H6	1.85	0.42
80:AA:1528:A:H2'	80:AA:1529:A:C8	2.48	0.42
85:Ay:64:C:H2'	85:Ay:65:C:H6	1.85	0.42
11:A:2051:A:H2'	11:A:2052:A:H8	1.85	0.42
11:A:2763:U:O2	15:H:252:LEU:HD13	2.20	0.42
27:T:184:LYS:HD3	27:T:189:HIS:CE1	2.54	0.42
33:z:133:LYS:HE3	33:z:286:LEU:HD13	2.01	0.42
52:p:123:HIS:CE1	52:p:157:MET:HG2	2.54	0.42
62:AK:64:PRO:HG2	79:AY:387:LEU:HD13	2.01	0.42
76:A1:173:LEU:HD22	76:A1:207:ILE:HD12	2.02	0.42
78:Az:29:U:H1'	86:A4:343:ARG:HH12	1.84	0.42
80:AA:1071:U:H2'	80:AA:1072:G:C8	2.55	0.42
80:AA:1505:A:H2'	80:AA:1506:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2042:U:H2'	11:A:2043:C:C6	2.55	0.42
11:A:2286:A:H2'	11:A:2287:U:C6	2.55	0.42
11:A:3151:A:H4'	24:Q:146:GLY:O	2.20	0.42
17:J:113:THR:HG23	17:J:115:LYS:H	1.85	0.42
33:z:296:ARG:HB3	33:z:302:GLY:HA2	2.02	0.42
36:d:110:GLU:O	36:d:114:LYS:HG2	2.20	0.42
73:AW:127:PRO:HG2	73:AW:134:TYR:CZ	2.55	0.42
75:A0:65:LEU:HD23	75:A0:68:LEU:HB2	2.02	0.42
80:AA:715:G:H2'	80:AA:716:U:C6	2.54	0.42
86:A4:126:LYS:HA	86:A4:129:GLN:HG2	2.01	0.42
11:A:2398:A:H2'	11:A:2399:A:O4'	2.20	0.42
11:A:2804:A:H2'	11:A:2805:A:C8	2.55	0.42
13:E:50:ASP:HA	13:E:53:LEU:HG	2.01	0.42
18:K:183:SER:HB2	18:K:186:PRO:HD2	2.01	0.42
19:L:98:PRO:HA	24:Q:162:ILE:HG12	2.01	0.42
37:e:185:ARG:O	37:e:189:GLU:HG2	2.20	0.42
66:AO:91:ARG:HD2	66:AO:94:CYS:SG	2.60	0.42
72:AV:102:TRP:HE1	75:A0:76:LEU:HD11	1.85	0.42
80:AA:747:A:H2'	80:AA:748:G:H8	1.85	0.42
6:5:236:LEU:HD22	6:5:420:HIS:CE1	2.54	0.41
11:A:2109:A:H5'	21:N:133:ARG:HD3	2.02	0.41
11:A:2751:G:H2'	11:A:2752:C:H6	1.85	0.41
11:A:3170:C:H2'	11:A:3171:C:H6	1.85	0.41
15:H:176:MET:HE1	15:H:188:ILE:HD11	2.02	0.41
21:N:104:MET:HB3	21:N:104:MET:HE3	1.81	0.41
50:c:173:LEU:HA	50:c:173:LEU:HD23	1.85	0.41
66:AO:208:PRO:HG2	66:AO:213:LEU:HD21	2.02	0.41
80:AA:711:U:H5'	80:AA:712:C:C5	2.54	0.41
80:AA:908:C:H2'	80:AA:909:G:H8	1.84	0.41
80:AA:944:U:H2'	80:AA:945:G:C8	2.55	0.41
80:AA:968:U:H2'	80:AA:969:A:C8	2.55	0.41
80:AA:1174:U:H2'	80:AA:1175:G:C8	2.55	0.41
86:A4:170:VAL:HG23	86:A4:247:ILE:HD11	2.01	0.41
6:5:256:PHE:CD1	6:5:256:PHE:N	2.88	0.41
11:A:2455:U:H2'	11:A:2456:U:C6	2.55	0.41
27:T:206:LEU:HA	35:b:119:PHE:CE2	2.55	0.41
60:AH:137:ARG:HG3	62:AK:124:GLN:NE2	2.35	0.41
64:AM:111:ARG:HD2	64:AM:114:ARG:HH21	1.84	0.41
75:A0:117:ILE:HD11	75:A0:125:GLU:C	2.45	0.41
86:A4:543:GLU:HG2	86:A4:544:LEU:N	2.35	0.41
9:8:191:ARG:NE	51:f:135:LEU:HG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2231:A:C6	11:A:3005:A:C6	3.08	0.41
11:A:3054:G:H2'	11:A:3055:U:C6	2.55	0.41
22:O:59:LEU:HB2	24:Q:269:MET:HE1	2.01	0.41
55:AC:132:TYR:HD1	55:AC:132:TYR:HA	1.80	0.41
59:AG:229:LEU:HD23	59:AG:229:LEU:HA	1.88	0.41
69:AS:48:ARG:HH22	80:AA:1119:U:H5'	1.85	0.41
72:AV:116:CYS:HA	72:AV:121:ALA:HB3	2.01	0.41
75:A0:41:LEU:HG	75:A0:55:TRP:CG	2.55	0.41
76:A1:237:GLU:HB3	76:A1:238:GLU:H	1.76	0.41
80:AA:848:U:H2'	80:AA:849:U:C6	2.56	0.41
80:AA:1412:G:H2'	80:AA:1413:U:O4'	2.21	0.41
80:AA:1507:A:H2'	80:AA:1508:C:C6	2.55	0.41
90:B:68:C:O2'	90:B:69:U:H5'	2.20	0.41
9:8:70:ARG:NH1	84:Ax:46:U:H5'	2.35	0.41
11:A:2586:U:H2'	11:A:2587:G:H8	1.84	0.41
11:A:2663:C:H2'	11:A:2664:U:H6	1.85	0.41
11:A:3150:U:H2'	11:A:3151:A:C8	2.55	0.41
16:I:154:LEU:HD12	16:I:164:MET:HE3	2.02	0.41
55:AC:111:LYS:HD2	60:AH:166:GLU:HG3	2.02	0.41
64:AM:16:HIS:H	64:AM:39:ASN:HB2	1.85	0.41
80:AA:736:C:H2'	80:AA:737:C:C5	2.54	0.41
80:AA:1251:A:H2'	80:AA:1252:G:O4'	2.19	0.41
80:AA:1360:G:H2'	80:AA:1361:G:H8	1.85	0.41
80:AA:1372:C:H2'	80:AA:1373:U:H6	1.86	0.41
81:AI:176:THR:HB	89:AQ:98:THR:HG23	2.03	0.41
85:Ay:14:A:H2'	85:Ay:15:A:O4'	2.20	0.41
86:A4:335:PHE:CE2	86:A4:360:MET:HB2	2.54	0.41
87:AX:255:MET:HE3	87:AX:255:MET:HB3	1.94	0.41
7:6:93:PRO:HA	7:6:94:PRO:HD3	1.97	0.41
11:A:2053:U:OP2	46:o:79:THR:HG23	2.20	0.41
11:A:2147:G:OP2	26:S:104:ARG:HD3	2.20	0.41
20:M:13:LEU:HD23	20:M:13:LEU:HA	1.91	0.41
59:AG:200:LEU:HD12	59:AG:204:GLU:HB3	2.03	0.41
72:AV:30:LEU:HB2	72:AV:149:ASP:OD2	2.21	0.41
72:AV:331:LEU:O	72:AV:335:LYS:HG2	2.21	0.41
75:A0:31:SER:HA	75:A0:111:HIS:ND1	2.36	0.41
76:A1:319:LEU:HD23	76:A1:319:LEU:HA	1.92	0.41
80:AA:1148:A:H2'	80:AA:1149:G:H8	1.84	0.41
85:Ay:68:C:H2'	85:Ay:69:C:C6	2.55	0.41
7:6:99:ARG:HH22	90:B:20:A:H2'	1.84	0.41
9:8:129:ARG:HE	9:8:133:ARG:HE	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1924:U:H2'	11:A:1925:A:C8	2.55	0.41
22:O:45:PRO:HB2	22:O:48:ARG:HG3	2.03	0.41
28:U:131:GLU:O	28:U:134:ARG:HG3	2.21	0.41
30:X:25:PRO:HG2	30:X:203:TRP:CE2	2.55	0.41
50:c:79:LEU:HD13	50:c:214:PHE:HE2	1.84	0.41
56:AD:239:LYS:HZ3	56:AD:241:ILE:HD11	1.85	0.41
67:AP:103:LYS:HA	67:AP:103:LYS:HD3	1.81	0.41
80:AA:986:G:H2'	80:AA:987:A:C8	2.55	0.41
80:AA:998:A:H2'	80:AA:999:C:C6	2.55	0.41
81:AI:110:ALA:HB3	81:AI:135:ALA:HB2	2.02	0.41
1:0:101:ILE:HG21	27:T:87:LEU:HD22	2.02	0.41
11:A:2285:U:H2'	11:A:2286:A:H8	1.85	0.41
12:D:109:PHE:CE1	12:D:208:ARG:HD3	2.56	0.41
72:AV:30:LEU:HD12	72:AV:34:TYR:CG	2.56	0.41
72:AV:148:MET:HE2	72:AV:185:VAL:HG21	2.03	0.41
80:AA:1138:G:H2'	80:AA:1139:A:H8	1.86	0.41
80:AA:1231:A:H1'	80:AA:1236:C:N4	2.35	0.41
87:AX:127:TYR:CD2	87:AX:325:PRO:HD3	2.55	0.41
7:6:175:VAL:HG22	7:6:204:VAL:HG22	2.03	0.41
8:7:152:CYS:HB2	8:7:260:PHE:CD2	2.56	0.41
9:8:70:ARG:NH1	9:8:73:ARG:HH22	2.19	0.41
11:A:2004:G:H2'	11:A:2005:C:C6	2.55	0.41
11:A:2786:U:H2'	11:A:2787:A:C8	2.56	0.41
11:A:3163:G:H2'	11:A:3164:C:C6	2.55	0.41
20:M:34:LYS:HA	20:M:34:LYS:HD3	1.89	0.41
20:M:202:LYS:HB3	20:M:263:ARG:HD2	2.03	0.41
31:Y:209:LEU:HD23	31:Y:209:LEU:HA	1.93	0.41
48:r:96:HIS:CE1	48:r:134:ARG:HB2	2.55	0.41
59:AG:118:GLU:HG2	80:AA:1308:U:H4'	2.01	0.41
68:AR:272:VAL:HG22	68:AR:284:LEU:HD21	2.02	0.41
80:AA:730:A:C4	80:AA:731:A:C8	3.08	0.41
80:AA:862:A:H2'	80:AA:863:C:C6	2.56	0.41
80:AA:915:C:H2'	80:AA:916:C:C6	2.55	0.41
80:AA:1462:G:H2'	80:AA:1463:G:H8	1.85	0.41
90:B:34:U:H2'	90:B:35:A:O4'	2.21	0.41
11:A:1840:C:H2'	11:A:1841:U:C6	2.56	0.41
11:A:1975:U:H2'	11:A:1976:U:C6	2.56	0.41
11:A:2072:A:H2'	11:A:2073:A:C8	2.56	0.41
11:A:2365:U:H2'	11:A:2366:G:H8	1.85	0.41
11:A:2872:C:H2'	11:A:2873:A:O4'	2.20	0.41
13:E:311:GLY:HA2	13:E:314:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:96:ILE:HA	16:I:155:VAL:HG12	2.03	0.41
18:K:319:LEU:HD23	18:K:319:LEU:HA	1.95	0.41
36:d:90:PRO:HB3	36:d:245:TYR:CE2	2.43	0.41
42:k:133:CYS:HB2	42:k:136:GLU:HG2	2.02	0.41
62:AK:33:ARG:NE	80:AA:1236:C:H5"	2.35	0.41
75:A0:11:ILE:HD12	80:AA:806:C:C4	2.56	0.41
80:AA:914:A:H2'	80:AA:915:C:H6	1.85	0.41
80:AA:1085:C:H2'	80:AA:1086:C:C6	2.56	0.41
80:AA:1129:U:H2'	80:AA:1130:G:C8	2.54	0.41
80:AA:1471:A:H2'	80:AA:1472:G:C8	2.55	0.41
80:AA:1497:C:H2'	80:AA:1498:C:C6	2.56	0.41
80:AA:1499:U:H2'	80:AA:1500:C:C6	2.55	0.41
85:Ay:4:G:H2'	85:Ay:5:G:H8	1.85	0.41
86:A4:446:LYS:HB3	86:A4:446:LYS:HE3	1.85	0.41
8:7:302:LEU:HD23	22:O:144:LEU:HD23	2.02	0.41
11:A:2263:C:H5'	26:S:180:PHE:CE1	2.56	0.41
11:A:2585:G:H2'	11:A:2586:U:C6	2.56	0.41
15:H:176:MET:HG2	15:H:182:TRP:CE2	2.56	0.41
20:M:116:ILE:HD12	20:M:152:VAL:HB	2.02	0.41
22:O:52:MET:HE3	22:O:52:MET:HB3	1.87	0.41
33:z:77:TYR:HB2	33:z:97:TYR:OH	2.21	0.41
36:d:50:PHE:HB3	36:d:56:PHE:HB2	2.03	0.41
48:r:70:CYS:HB3	96:r:201:FES:S2	2.61	0.41
48:r:89:LEU:HD22	48:r:115:ILE:HG23	2.02	0.41
64:AM:110:LEU:O	64:AM:114:ARG:HG3	2.20	0.41
69:AS:86:ASP:HB2	73:AW:101:ILE:HD13	2.03	0.41
72:AV:39:LYS:HE2	72:AV:39:LYS:HB2	1.88	0.41
72:AV:250:ILE:HG23	72:AV:252:LYS:H	1.86	0.41
80:AA:1396:C:H2'	80:AA:1397:U:H6	1.86	0.41
80:AA:1592:U:H2'	80:AA:1593:U:C6	2.56	0.41
17:J:122:ARG:HD2	17:J:137:LEU:HD21	2.04	0.40
21:N:172:VAL:HA	21:N:175:PHE:CE2	2.56	0.40
24:Q:176:VAL:HG11	24:Q:179:LEU:HB2	2.03	0.40
26:S:107:LYS:HD3	27:T:206:LEU:HD11	2.03	0.40
33:z:107:LYS:HB3	33:z:107:LYS:HE3	1.93	0.40
37:e:257:LYS:HE2	37:e:273:ARG:HE	1.86	0.40
62:AK:105:ARG:HH21	74:AZ:47:GLU:HG2	1.85	0.40
80:AA:653:G:H2'	80:AA:654:U:O4'	2.21	0.40
80:AA:776:A:O3'	80:AA:777:G:H8	2.05	0.40
80:AA:1094:U:H2'	80:AA:1095:U:C6	2.56	0.40
80:AA:1279:C:H2'	80:AA:1280:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1461:A:H4'	80:AA:1462:G:C8	2.57	0.40
80:AA:1507:A:H2'	80:AA:1508:C:H6	1.85	0.40
87:AX:56:PRO:HA	87:AX:59:HIS:CE1	2.55	0.40
2:1:16:ILE:HG22	2:1:64:SER:HA	2.04	0.40
11:A:2455:U:H2'	11:A:2456:U:H6	1.85	0.40
11:A:2508:C:H2'	11:A:2509:A:C8	2.57	0.40
11:A:3158:A:H2'	11:A:3159:A:C8	2.56	0.40
17:J:114:LEU:HD22	43:l:96:LEU:HD23	2.03	0.40
28:U:44:ILE:HG21	28:U:53:LEU:HD22	2.02	0.40
32:Z:128:LEU:HD23	32:Z:128:LEU:HA	1.97	0.40
36:d:165:THR:HA	36:d:260:ARG:CZ	2.51	0.40
49:t:67:LEU:O	49:t:71:ILE:HG12	2.22	0.40
55:AC:43:ARG:HD3	55:AC:43:ARG:HA	1.95	0.40
56:AD:284:ARG:HB2	56:AD:287:ASP:HA	2.03	0.40
64:AM:101:PRO:HD3	71:AU:63:TYR:CG	2.56	0.40
76:A1:284:LEU:HA	76:A1:289:ILE:HG21	2.03	0.40
80:AA:663:A:H2'	80:AA:664:G:H8	1.85	0.40
80:AA:1057:G:H2'	80:AA:1058:C:H6	1.87	0.40
80:AA:1214:A:H2'	80:AA:1352:C:O2	2.20	0.40
80:AA:1337:U:H2'	80:AA:1338:A:H8	1.86	0.40
80:AA:1589:C:H2'	80:AA:1590:A:H8	1.85	0.40
86:A4:377:ARG:HD3	86:A4:377:ARG:HA	1.80	0.40
11:A:2662:A:H2'	11:A:2663:C:C6	2.56	0.40
11:A:2795:U:H2'	11:A:2796:G:C8	2.56	0.40
14:F:137:ARG:H	14:F:137:ARG:HG2	1.74	0.40
33:z:64:GLU:HG2	33:z:65:LYS:N	2.36	0.40
33:z:262:MET:H	33:z:262:MET:HG3	1.74	0.40
36:d:211:GLN:HA	36:d:248:PHE:O	2.21	0.40
47:q:117:ARG:O	47:q:121:ILE:HG12	2.22	0.40
48:r:87:LEU:HD23	48:r:87:LEU:HA	1.89	0.40
55:AC:60:HIS:ND1	80:AA:1319:A:H5"	2.37	0.40
66:AO:181:HIS:HB3	66:AO:184:VAL:HG22	2.02	0.40
68:AR:159:THR:HG23	68:AR:172:ILE:HG12	2.02	0.40
80:AA:745:A:C4	80:AA:746:A:C8	3.10	0.40
80:AA:1258:A:N6	80:AA:1329:U:H2'	2.36	0.40
80:AA:1360:G:H2'	80:AA:1361:G:C8	2.55	0.40
80:AA:1371:U:H2'	80:AA:1372:C:C6	2.56	0.40
80:AA:1394:C:H2'	80:AA:1395:C:C6	2.56	0.40
80:AA:1456:U:H2'	80:AA:1457:G:O4'	2.21	0.40
11:A:1748:G:O5'	11:A:1749:C:H5"	2.22	0.40
11:A:1939:G:O2'	11:A:1973:G:H4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2099:U:H2'	11:A:2100:C:H6	1.87	0.40
11:A:2192:A:H4'	17:J:139:SER:HB3	2.03	0.40
11:A:2325:U:H2'	11:A:2326:C:H6	1.86	0.40
11:A:2410:U:H2'	11:A:2411:U:H6	1.84	0.40
28:U:112:PRO:N	28:U:113:GLU:HA	2.36	0.40
58:AF:149:LEU:HD23	58:AF:149:LEU:HA	1.86	0.40
68:AR:175:ARG:NH1	68:AR:181:LEU:HB2	2.35	0.40
72:AV:263:MET:HE1	72:AV:334:PHE:CD1	2.57	0.40
74:AZ:56:HIS:O	74:AZ:60:GLU:HG3	2.22	0.40
80:AA:750:G:H2'	80:AA:751:A:C8	2.56	0.40
80:AA:1236:C:H4'	80:AA:1237:A:O4'	2.21	0.40
80:AA:1499:U:H2'	80:AA:1500:C:H6	1.86	0.40
80:AA:1508:C:H2'	80:AA:1509:U:H6	1.87	0.40
80:AA:1588:G:H2'	80:AA:1589:C:C6	2.57	0.40
84:Ax:59:U:H2'	84:Ax:60:C:C6	2.56	0.40
86:A4:377:ARG:NH2	86:A4:418:SER:HA	2.36	0.40
86:A4:420:MET:HB3	86:A4:460:LYS:HB2	2.03	0.40
87:AX:208:TYR:CE2	87:AX:242:ILE:HD12	2.55	0.40
8:7:105:LEU:HD12	8:7:105:LEU:HA	1.87	0.40
8:7:279:GLU:HB3	8:7:317:LEU:HD21	2.03	0.40
11:A:2056:G:H2'	11:A:2057:C:C6	2.56	0.40
16:I:38:ARG:HB3	21:N:242:TRP:CZ2	2.56	0.40
33:z:127:LEU:O	33:z:251:ASN:HB3	2.22	0.40
55:AC:96:MET:HB2	55:AC:108:LEU:HD11	2.03	0.40
56:AD:231:MET:HE2	80:AA:1480:A:H1'	2.03	0.40
60:AH:76:LEU:HD12	60:AH:148:LEU:HD22	2.03	0.40
66:AO:49:SER:H	66:AO:52:LYS:NZ	2.19	0.40
68:AR:128:MET:H	68:AR:128:MET:HG2	1.64	0.40
76:A1:241:LYS:HE2	76:A1:241:LYS:HB2	1.89	0.40
80:AA:861:U:H2'	80:AA:862:A:C8	2.57	0.40
85:Ay:24:A:N6	85:Ay:45:G:H22	2.20	0.40
87:AX:205:GLN:HG2	87:AX:250:GLN:HE21	1.85	0.40
90:B:6:U:H3	90:B:67:G:H1	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	108/188 (57%)	108 (100%)	0	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	382 (97%)	10 (3%)	0	100	100
7	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
8	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
9	8	155/206 (75%)	154 (99%)	1 (1%)	0	100	100
10	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
12	D	236/305 (77%)	229 (97%)	6 (2%)	1 (0%)	30	60
13	E	303/348 (87%)	296 (98%)	7 (2%)	0	100	100
14	F	250/311 (80%)	249 (100%)	1 (0%)	0	100	100
15	H	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
16	I	179/261 (69%)	176 (98%)	3 (2%)	0	100	100
17	J	173/192 (90%)	173 (100%)	0	0	100	100
18	K	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
19	L	113/145 (78%)	107 (95%)	6 (5%)	0	100	100
20	M	289/296 (98%)	280 (97%)	9 (3%)	0	100	100
21	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
22	O	152/175 (87%)	147 (97%)	5 (3%)	0	100	100
23	P	142/180 (79%)	139 (98%)	3 (2%)	0	100	100
24	Q	237/292 (81%)	230 (97%)	7 (3%)	0	100	100
25	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
26	S	159/205 (78%)	157 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	T	164/206 (80%)	161 (98%)	3 (2%)	0	100	100
28	U	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
29	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
30	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
31	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
32	Z	120/161 (74%)	116 (97%)	4 (3%)	0	100	100
33	z	250/325 (77%)	234 (94%)	16 (6%)	0	100	100
34	V	203/216 (94%)	201 (99%)	2 (1%)	0	100	100
35	b	148/215 (69%)	142 (96%)	6 (4%)	0	100	100
36	d	257/306 (84%)	240 (93%)	17 (7%)	0	100	100
37	e	236/279 (85%)	226 (96%)	10 (4%)	0	100	100
38	g	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
39	h	108/158 (68%)	104 (96%)	4 (4%)	0	100	100
40	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
41	j	92/123 (75%)	89 (97%)	3 (3%)	0	100	100
42	k	100/112 (89%)	97 (97%)	3 (3%)	0	100	100
43	l	80/138 (58%)	78 (98%)	2 (2%)	0	100	100
44	m	90/128 (70%)	85 (94%)	5 (6%)	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%)	158 (99%)	2 (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%)	279 (99%)	3 (1%)	0	100	100
51	f	153/212 (72%)	148 (97%)	5 (3%)	0	100	100
52	p	141/206 (68%)	137 (97%)	4 (3%)	0	100	100
53	s	381/439 (87%)	372 (98%)	9 (2%)	0	100	100
54	AB	223/296 (75%)	218 (98%)	5 (2%)	0	100	100
55	AC	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
56	AD	341/430 (79%)	333 (98%)	8 (2%)	0	100	100
57	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	AF	206/242 (85%)	202 (98%)	4 (2%)	0	100	100
59	AG	323/396 (82%)	315 (98%)	8 (2%)	0	100	100
60	AH	138/201 (69%)	133 (96%)	4 (3%)	1 (1%)	18	50
61	AJ	106/138 (77%)	104 (98%)	2 (2%)	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%)	115 (98%)	2 (2%)	0	100	100
65	AN	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
66	AO	191/258 (74%)	185 (97%)	6 (3%)	0	100	100
67	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
68	AR	293/360 (81%)	286 (98%)	7 (2%)	0	100	100
69	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
70	AT	166/173 (96%)	163 (98%)	3 (2%)	0	100	100
71	AU	174/205 (85%)	174 (100%)	0	0	100	100
72	AV	358/414 (86%)	347 (97%)	11 (3%)	0	100	100
73	AW	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
74	AZ	98/106 (92%)	94 (96%)	4 (4%)	0	100	100
75	A0	213/217 (98%)	206 (97%)	7 (3%)	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%)	115 (98%)	2 (2%)	0	100	100
81	AI	135/194 (70%)	129 (96%)	5 (4%)	1 (1%)	18	50
82	OX	51/435 (12%)	47 (92%)	4 (8%)	0	100	100
83	a	99/142 (70%)	97 (98%)	2 (2%)	0	100	100
86	A4	584/689 (85%)	564 (97%)	20 (3%)	0	100	100
87	AX	350/398 (88%)	337 (96%)	13 (4%)	0	100	100
88	A2	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
89	AQ	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
All	All	14617/19127 (76%)	14261 (98%)	353 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	AH	126	ILE
81	AI	184	ASN
12	D	207	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	270/303 (89%)	270 (100%)	0	100	100
9	8	146/190 (77%)	146 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
12	D	192/245 (78%)	192 (100%)	0	100	100
13	E	260/290 (90%)	260 (100%)	0	100	100
14	F	219/262 (84%)	219 (100%)	0	100	100
15	H	182/228 (80%)	182 (100%)	0	100	100
16	I	165/232 (71%)	165 (100%)	0	100	100
17	J	138/150 (92%)	138 (100%)	0	100	100
18	K	155/155 (100%)	155 (100%)	0	100	100
19	L	98/124 (79%)	98 (100%)	0	100	100
20	M	246/249 (99%)	246 (100%)	0	100	100
21	N	189/211 (90%)	189 (100%)	0	100	100
22	O	134/150 (89%)	134 (100%)	0	100	100
23	P	126/155 (81%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Q	221/256 (86%)	221 (100%)	0	100	100
25	R	118/126 (94%)	118 (100%)	0	100	100
26	S	146/180 (81%)	146 (100%)	0	100	100
27	T	146/176 (83%)	146 (100%)	0	100	100
28	U	134/135 (99%)	134 (100%)	0	100	100
29	W	94/119 (79%)	94 (100%)	0	100	100
30	X	220/229 (96%)	220 (100%)	0	100	100
31	Y	163/223 (73%)	163 (100%)	0	100	100
32	Z	113/147 (77%)	113 (100%)	0	100	100
33	z	226/287 (79%)	226 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	13069/16529 (79%)	13069 (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 (106) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	31	ASN
4	3	178	GLN
4	3	185	ASN
6	5	94	HIS
6	5	191	GLN
6	5	214	ASN
7	6	373	HIS
8	7	165	ASN
8	7	246	GLN
8	7	284	HIS
9	8	103	GLN
9	8	186	GLN
12	D	168	HIS
12	D	182	HIS
12	D	235	GLN
14	F	103	GLN
15	H	196	ASN
15	H	239	ASN
17	J	84	GLN
18	K	218	GLN
18	K	272	GLN
19	L	48	ASN
19	L	103	ASN
20	M	71	GLN
20	M	130	GLN
21	N	210	GLN
24	Q	203	ASN
25	R	89	ASN
25	R	149	HIS
26	S	196	ASN
28	U	27	GLN
28	U	62	ASN
28	U	73	GLN
30	X	4	HIS
30	X	27	HIS

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Mol	Chain	Res	Type
32	Z	150	HIS
33	z	119	GLN
33	z	215	ASN
35	b	27	GLN
35	b	123	ASN
36	d	77	HIS
36	d	167	HIS
38	g	73	GLN
38	g	93	ASN
38	g	155	GLN
39	h	87	GLN
40	i	59	ASN
40	i	124	HIS
41	j	26	GLN
44	m	44	HIS
47	q	176	GLN
48	r	96	HIS
48	r	112	HIS
49	t	65	GLN
50	c	94	ASN
50	c	168	HIS
51	f	115	ASN
51	f	136	GLN
53	s	107	GLN
53	s	164	HIS
53	s	420	GLN
54	AB	201	ASN
56	AD	130	GLN
56	AD	155	GLN
56	AD	165	GLN
56	AD	302	HIS
57	AE	56	GLN
57	AE	92	ASN
58	AF	113	GLN
58	AF	238	HIS
59	AG	163	HIS
59	AG	288	HIS
61	AJ	57	GLN
62	AK	117	HIS
63	AL	77	GLN
63	AL	142	HIS
64	AM	28	ASN

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Mol	Chain	Res	Type
64	AM	75	HIS
65	AN	52	HIS
66	AO	65	GLN
66	AO	103	ASN
66	AO	169	GLN
68	AR	167	HIS
68	AR	288	GLN
68	AR	308	HIS
70	AT	85	GLN
72	AV	203	ASN
72	AV	224	GLN
72	AV	238	GLN
73	AW	106	HIS
74	AZ	56	HIS
75	A0	24	GLN
79	AY	344	GLN
81	AI	92	HIS
81	AI	96	GLN
81	AI	184	ASN
83	a	46	ASN
83	a	88	HIS
83	a	126	HIS
86	A4	201	GLN
86	A4	274	GLN
86	A4	491	GLN
86	A4	603	ASN
86	A4	656	ASN
87	AX	81	HIS
87	AX	180	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1561 (99%)	273 (17%)	4 (0%)
78	Az	33/34 (97%)	15 (45%)	0
80	AA	953/954 (99%)	155 (16%)	0
84	Ax	70/71 (98%)	15 (21%)	0
85	Ay	67/76 (88%)	13 (19%)	0
90	B	70/72 (97%)	16 (22%)	0
All	All	2749/2768 (99%)	487 (17%)	4 (0%)

All (487) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1681	G
11	A	1689	C
11	A	1692	A
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1708	A
11	A	1709	G
11	A	1711	C
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1736	A
11	A	1748	G
11	A	1765	C
11	A	1777	A
11	A	1780	U
11	A	1805	A
11	A	1806	U
11	A	1807	U
11	A	1808	A
11	A	1817	C
11	A	1821	A
11	A	1827	C
11	A	1828	A
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1854	U
11	A	1856	A
11	A	1867	A
11	A	1869	A
11	A	1871	A
11	A	1873	A
11	A	1878	U
11	A	1882	A
11	A	1886	G
11	A	1887	A
11	A	1888	G
11	A	1893	A
11	A	1903	C
11	A	1907	A
11	A	1909	A

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Mol	Chain	Res	Type
11	A	1918	G
11	A	1937	A
11	A	1939	G
11	A	1940	A
11	A	1974	A
11	A	1985	G
11	A	1986	A
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	2000	C
11	A	2001	C
11	A	2002	G
11	A	2003	A
11	A	2015	G
11	A	2022	G
11	A	2030	U
11	A	2036	C
11	A	2037	U
11	A	2039	A
11	A	2054	U
11	A	2060	A
11	A	2071	U
11	A	2079	C
11	A	2099	U
11	A	2105	G
11	A	2113	G
11	A	2125	C
11	A	2126	U
11	A	2147	G
11	A	2155	A
11	A	2159	U
11	A	2160	A
11	A	2161	A
11	A	2163	A
11	A	2168	U
11	A	2180	A
11	A	2181	A
11	A	2182	G
11	A	2191	A
11	A	2195	A
11	A	2196	A

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Mol	Chain	Res	Type
11	A	2198	A
11	A	2200	A
11	A	2207	A
11	A	2214	A
11	A	2219	C
11	A	2220	A
11	A	2221	C
11	A	2223	A
11	A	2224	C
11	A	2225	C
11	A	2226	U
11	A	2228	A
11	A	2230	A
11	A	2232	A
11	A	2233	U
11	A	2237	A
11	A	2241	A
11	A	2243	A
11	A	2245	A
11	A	2246	A
11	A	2262	C
11	A	2263	C
11	A	2283	C
11	A	2284	C
11	A	2294	A
11	A	2297	A
11	A	2300	G
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2345	G
11	A	2349	G
11	A	2350	A
11	A	2353	A
11	A	2357	C
11	A	2363	A
11	A	2372	U
11	A	2374	A
11	A	2381	A
11	A	2390	A
11	A	2399	A
11	A	2401	A

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Mol	Chain	Res	Type
11	A	2404	U
11	A	2407	U
11	A	2415	C
11	A	2434	A
11	A	2446	A
11	A	2451	A
11	A	2452	A
11	A	2478	G
11	A	2485	U
11	A	2493	C
11	A	2502	C
11	A	2504	A
11	A	2506	A
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2540	C
11	A	2557	C
11	A	2570	C
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2599	U
11	A	2600	A
11	A	2601	A
11	A	2603	C
11	A	2604	A
11	A	2606	U
11	A	2618	U
11	A	2625	C
11	A	2627	G
11	A	2630	U
11	A	2633	A
11	A	2635	G
11	A	2654	U
11	A	2655	G
11	A	2656	U
11	A	2683	C
11	A	2686	G
11	A	2694	A
11	A	2696	A
11	A	2706	A

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Mol	Chain	Res	Type
11	A	2709	A
11	A	2718	C
11	A	2719	G
11	A	2723	A
11	A	2724	G
11	A	2725	A
11	A	2732	G
11	A	2745	A
11	A	2757	A
11	A	2758	G
11	A	2762	C
11	A	2763	U
11	A	2764	A
11	A	2765	A
11	A	2767	A
11	A	2768	A
11	A	2781	U
11	A	2782	A
11	A	2783	A
11	A	2786	U
11	A	2790	A
11	A	2810	G
11	A	2832	A
11	A	2833	A
11	A	2847	C
11	A	2864	U
11	A	2865	C
11	A	2882	U
11	A	2883	A
11	A	2884	C
11	A	2885	U
11	A	2888	A
11	A	2889	C
11	A	2893	A
11	A	2907	U
11	A	2913	A
11	A	2915	C
11	A	2916	G
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A

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Mol	Chain	Res	Type
11	A	2928	C
11	A	2934	G
11	A	2935	A
11	A	2956	A
11	A	2962	C
11	A	2965	A
11	A	2971	A
11	A	2985	C
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2993	U
11	A	3000	A
11	A	3005	A
11	A	3007	C
11	A	3016	G
11	A	3022	G
11	A	3041	U
11	A	3053	A
11	A	3054	G
11	A	3060	C
11	A	3086	U
11	A	3089	A
11	A	3090	G
11	A	3091	G
11	A	3096	U
11	A	3100	U
11	A	3102	U
11	A	3108	U
11	A	3109	U
11	A	3110	C
11	A	3111	A
11	A	3112	A
11	A	3113	A
11	A	3122	U
11	A	3124	U
11	A	3150	U
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3168	C
11	A	3169	C

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Mol	Chain	Res	Type
11	A	3172	C
11	A	3177	A
11	A	3180	A
11	A	3183	U
11	A	3189	C
11	A	3190	A
11	A	3197	U
11	A	3198	A
11	A	3199	U
11	A	3200	U
11	A	3201	A
11	A	3207	A
11	A	3209	A
11	A	3210	C
11	A	3212	C
11	A	3217	A
11	A	3218	A
11	A	3220	A
11	A	3228	U
11	A	3231	U
78	Az	0	U
78	Az	4	A
78	Az	11	U
78	Az	12	U
78	Az	13	U
78	Az	15	U
78	Az	16	A
78	Az	18	A
78	Az	21	A
78	Az	22	A
78	Az	24	U
78	Az	25	U
78	Az	26	A
78	Az	27	C
78	Az	31	A
80	AA	651	A
80	AA	680	U
80	AA	688	A
80	AA	704	U
80	AA	706	C
80	AA	721	U
80	AA	722	C

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Mol	Chain	Res	Type
80	AA	737	C
80	AA	738	A
80	AA	748	G
80	AA	753	A
80	AA	760	A
80	AA	761	A
80	AA	766	G
80	AA	777	G
80	AA	783	A
80	AA	791	G
80	AA	794	U
80	AA	796	G
80	AA	808	C
80	AA	826	A
80	AA	828	C
80	AA	829	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	872	G
80	AA	881	A
80	AA	883	U
80	AA	889	G
80	AA	890	C
80	AA	893	G
80	AA	903	U
80	AA	904	C
80	AA	907	A
80	AA	908	C
80	AA	910	A
80	AA	919	A
80	AA	929	A
80	AA	931	C
80	AA	938	A
80	AA	939	A
80	AA	942	A

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Mol	Chain	Res	Type
80	AA	954	C
80	AA	960	C
80	AA	961	U
80	AA	962	C
80	AA	967	A
80	AA	978	A
80	AA	993	A
80	AA	1001	C
80	AA	1010	A
80	AA	1011	C
80	AA	1015	A
80	AA	1031	G
80	AA	1042	U
80	AA	1046	A
80	AA	1076	5MU
80	AA	1080	A
80	AA	1081	U
80	AA	1082	A
80	AA	1096	A
80	AA	1098	C
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	1143	C
80	AA	1151	C
80	AA	1153	C
80	AA	1155	G
80	AA	1160	A
80	AA	1167	A
80	AA	1187	U
80	AA	1188	A
80	AA	1189	U
80	AA	1190	C
80	AA	1215	U

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Mol	Chain	Res	Type
80	AA	1220	A
80	AA	1223	C
80	AA	1225	C
80	AA	1229	U
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	1259	U
80	AA	1261	C
80	AA	1271	C
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	1356	A
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	1443	U
80	AA	1466	C
80	AA	1469	G
80	AA	1481	C
80	AA	1482	A
80	AA	1512	A

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Mol	Chain	Res	Type
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	1551	G
80	AA	1557	A
80	AA	1560	U
80	AA	1568	U
80	AA	1571	U
80	AA	1572	A
80	AA	1582	G
80	AA	1584	MA6
80	AA	1594	G
80	AA	1595	G
80	AA	1599	A
84	Ax	7	G
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	51	U
84	Ax	52	A
84	Ax	56	C
84	Ax	63	G
84	Ax	65	A
84	Ax	71	A
85	Ay	9	A
85	Ay	13	U
85	Ay	29	U
85	Ay	33	U
85	Ay	44	A

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Mol	Chain	Res	Type
85	Ay	45	G
85	Ay	46	A
85	Ay	49	G
85	Ay	58	A
85	Ay	59	U
85	Ay	60	U
85	Ay	61	C
85	Ay	73	A
90	B	8	U
90	B	10	2MG
90	B	16	C
90	B	19	C
90	B	21	A
90	B	45	G
90	B	46	A
90	B	54	C
90	B	55	U
90	B	56	U
90	B	58	A
90	B	59	A
90	B	64	A
90	B	69	U
90	B	72	G
90	B	76	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2245	A
11	A	2484	C
11	A	3112	A
11	A	3199	U

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	$\#\|Z\| > 2$
80	MA6	AA	1584	80	23,26,27	0.33	0	33,38,41	0.72	1 (3%)
11	OMG	A	3040	11	23,26,27	0.35	0	32,38,41	0.41	0
11	PSU	A	3067	11	18,21,22	1.12	2 (11%)	21,30,33	0.84	1 (4%)
80	5MC	AA	1488	80	19,22,23	0.88	1 (5%)	26,32,35	0.51	0
11	1MA	A	2617	11	21,25,26	0.42	0	30,37,40	0.61	0
90	2MG	B	10	90	23,26,27	0.36	0	33,38,41	0.42	0
11	OMU	A	3039	11,92	19,22,23	0.30	0	25,31,34	0.67	1 (4%)
80	B8T	AA	1486	95,80	19,22,23	0.40	0	25,31,34	0.33	0
11	OMG	A	2815	11,92,84	23,26,27	0.36	0	32,38,41	0.42	0
80	MA6	AA	1583	80	23,26,27	0.34	0	33,38,41	0.74	1 (3%)
90	PSU	B	39	90	18,21,22	1.04	1 (5%)	21,30,33	0.70	0
80	5MU	AA	1076	80	19,22,23	0.40	0	27,32,35	0.70	0
90	1MA	B	9	90	21,25,26	0.40	0	30,37,40	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	MA6	AA	1584	80	-	1/11/29/30	0/3/3/3
11	OMG	A	3040	11	-	2/9/27/28	0/3/3/3
11	PSU	A	3067	11	-	0/7/25/26	0/2/2/2
80	5MC	AA	1488	80	-	0/7/25/26	0/2/2/2
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
90	2MG	B	10	90	-	0/9/27/28	0/3/3/3
11	OMU	A	3039	11,92	-	0/9/27/28	0/2/2/2
80	B8T	AA	1486	95,80	-	0/7/27/28	0/2/2/2
11	OMG	A	2815	11,92,84	-	0/9/27/28	0/3/3/3
80	MA6	AA	1583	80	-	0/11/29/30	0/3/3/3
90	PSU	B	39	90	-	0/7/25/26	0/2/2/2
80	5MU	AA	1076	80	-	5/7/25/26	0/2/2/2
90	1MA	B	9	90	-	0/7/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	B	39	PSU	C6-C5	3.53	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	AA	1488	5MC	C5-C4	-3.50	1.41	1.44
11	A	3067	PSU	C6-C5	3.44	1.39	1.35
11	A	3067	PSU	O4'-C1'	-2.59	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
80	AA	1584	MA6	C2-N1-C6	2.93	118.98	111.83
80	AA	1583	MA6	C2-N1-C6	2.92	118.96	111.83
11	A	3067	PSU	O4'-C1'-C2'	2.54	108.66	105.15
11	A	3039	OMU	C2'-C1'-N1	-2.48	109.53	114.24

There are no chirality outliers.

All (8) 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'
11	A	3040	OMG	O4'-C4'-C5'-O5'
11	A	3040	OMG	C3'-C4'-C5'-O5'
80	AA	1584	MA6	C4'-C5'-O5'-P
80	AA	1076	5MU	C4'-C5'-O5'-P
80	AA	1076	5MU	C2'-C1'-N1-C2
80	AA	1076	5MU	C2'-C1'-N1-C6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	AA	1488	5MC	2	0
80	AA	1486	B8T	1	0
80	AA	1583	MA6	1	0
80	AA	1076	5MU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
96	FES	AP	201	57,67	0,4,4	-	-	-		
100	GDP	AX	503	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	6 (13%)
101	VAL	B	101	90	4,6,7	0.78	0	6,7,9	0.99	1 (16%)
93	SPD	AG	401	-	9,9,9	0.16	0	8,8,8	0.24	0
96	FES	AT	201	70,64	0,4,4	-	-	-		
97	NAD	AA	1701	95	46,48,48	1.18	3 (6%)	64,73,73	0.84	3 (4%)
93	SPD	A	3470	-	9,9,9	0.16	0	8,8,8	0.23	0
93	SPD	A	3302	-	9,9,9	0.14	0	8,8,8	0.17	0
93	SPD	A	3472	-	9,9,9	0.16	0	8,8,8	0.19	0
96	FES	r	201	48,16	0,4,4	-	-	-		
94	PUT	A	3303	-	5,5,5	0.14	0	4,4,4	0.23	0
98	SPM	AA	1702	-	13,13,13	0.16	0	12,12,12	0.21	0
93	SPD	A	3471	-	9,9,9	0.15	0	8,8,8	0.25	0
98	SPM	AA	1780	-	13,13,13	0.15	0	12,12,12	0.31	0
99	ATP	AX	501	95	32,33,33	0.55	1 (3%)	48,52,52	0.36	0
93	SPD	A	3301	-	9,9,9	0.16	0	8,8,8	0.19	0
93	SPD	AA	1703	-	9,9,9	0.16	0	8,8,8	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	FES	AT	201	70,64	-	-	0/1/1/1
96	FES	AP	201	57,67	-	-	0/1/1/1
93	SPD	AG	401	-	-	0/7/7/7	-
97	NAD	AA	1701	95	-	2/30/62/62	0/5/5/5
100	GDP	AX	503	-	-	1/16/32/32	0/3/3/3
93	SPD	A	3470	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPD	A	3302	-	-	1/7/7/7	-
93	SPD	A	3472	-	-	1/7/7/7	-
98	SPM	AA	1702	-	-	0/11/11/11	-
94	PUT	A	3303	-	-	0/3/3/3	-
98	SPM	AA	1780	-	-	0/11/11/11	-
93	SPD	A	3471	-	-	1/7/7/7	-
99	ATP	AX	501	95	-	0/22/38/38	0/3/3/3
101	VAL	B	101	90	-	0/5/6/8	-
93	SPD	A	3301	-	-	0/7/7/7	-
93	SPD	AA	1703	-	-	0/7/7/7	-
96	FES	r	201	48,16	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AA	1701	NAD	PA-O3	4.70	1.64	1.59
100	AX	503	GDP	C5-C4	3.12	1.47	1.38
97	AA	1701	NAD	PN-O3	2.88	1.62	1.59
97	AA	1701	NAD	O4D-C1D	-2.58	1.37	1.40
100	AX	503	GDP	C6-N1	-2.57	1.34	1.38
99	AX	501	ATP	PB-O3B	-2.17	1.57	1.59
100	AX	503	GDP	C5-N7	-2.04	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
100	AX	503	GDP	C5-C4-N3	-6.15	118.60	128.39
100	AX	503	GDP	C2-N3-C4	5.01	120.93	112.30
100	AX	503	GDP	N9-C4-N3	4.67	135.29	125.95
100	AX	503	GDP	C6-C5-N7	3.21	136.12	130.29
97	AA	1701	NAD	O3-PA-O1A	-2.54	103.08	110.70
100	AX	503	GDP	C4-C5-N7	-2.51	106.70	110.67
100	AX	503	GDP	C3'-C2'-C1'	2.31	105.84	101.46
97	AA	1701	NAD	O2A-PA-O1A	2.30	123.13	112.44
101	B	101	VAL	O-C-CA	-2.28	118.92	124.77
97	AA	1701	NAD	O7N-C7N-N7N	2.02	125.54	122.62

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
100	AX	503	GDP	C5'-O5'-PA-O1A
93	A	3471	SPD	C2-C3-C4-C5
97	AA	1701	NAD	O4D-C4D-C5D-O5D
93	A	3302	SPD	N1-C2-C3-C4
93	A	3472	SPD	C8-C7-N6-C5
97	AA	1701	NAD	C3D-C4D-C5D-O5D

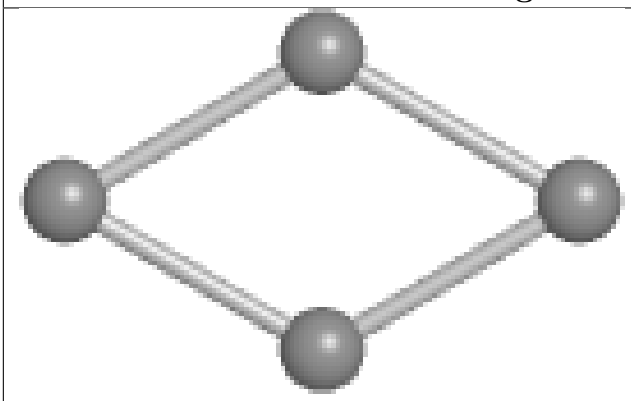
There are no ring outliers.

6 monomers are involved in 7 short contacts:

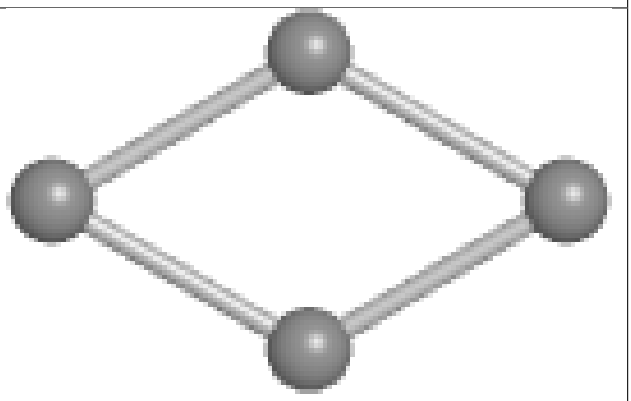
Mol	Chain	Res	Type	Clashes	Symm-Clashes
96	AP	201	FES	1	0
100	AX	503	GDP	2	0
101	B	101	VAL	1	0
97	AA	1701	NAD	1	0
96	r	201	FES	1	0
93	A	3301	SPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 FES AP 201



Bond lengths



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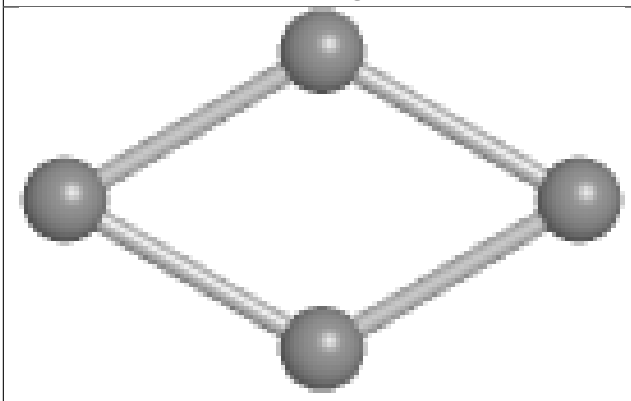
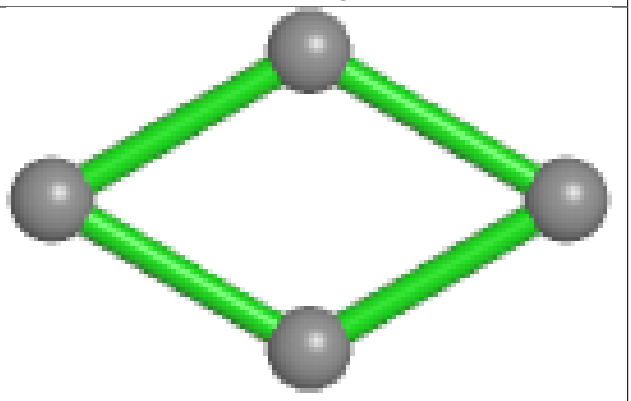
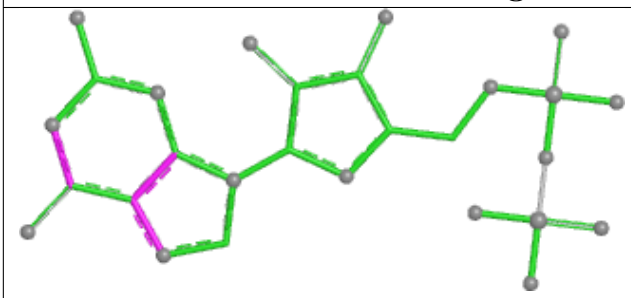


Torsions



Rings

Ligand GDP AX 503



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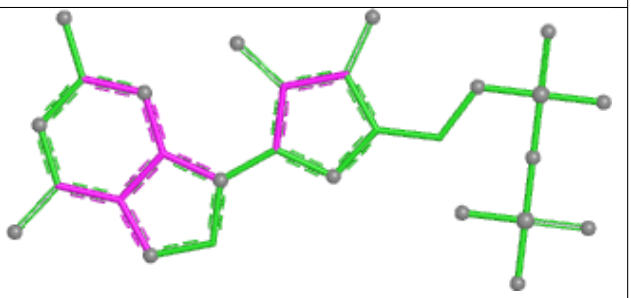

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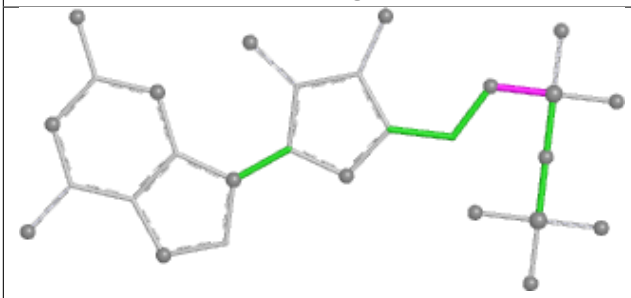

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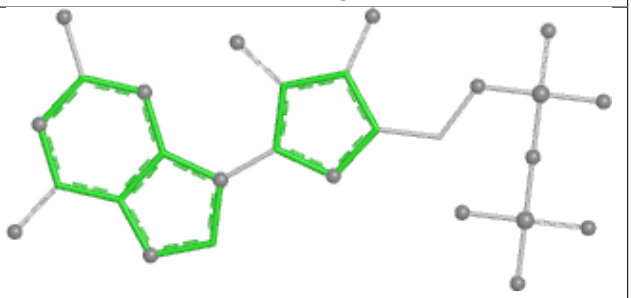
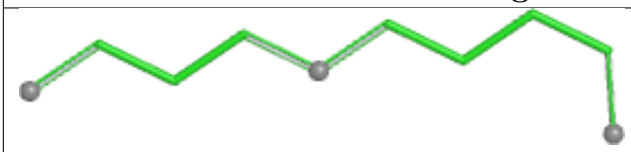


Rings

Ligand SPD AG 401



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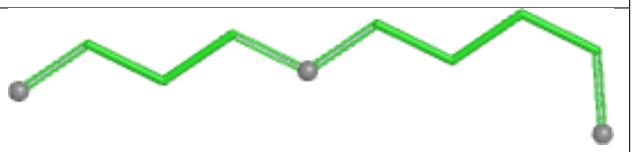

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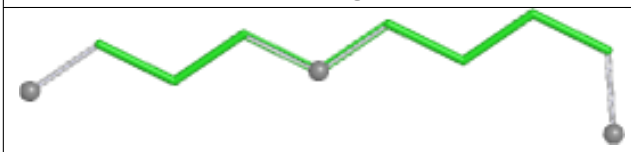

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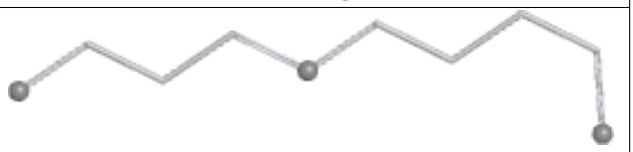
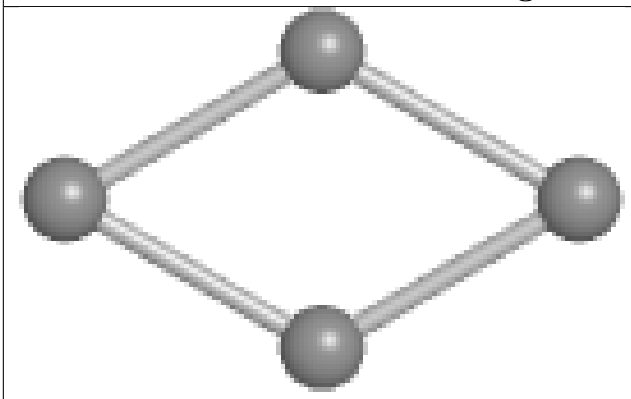


Rings

Ligand FES AT 201



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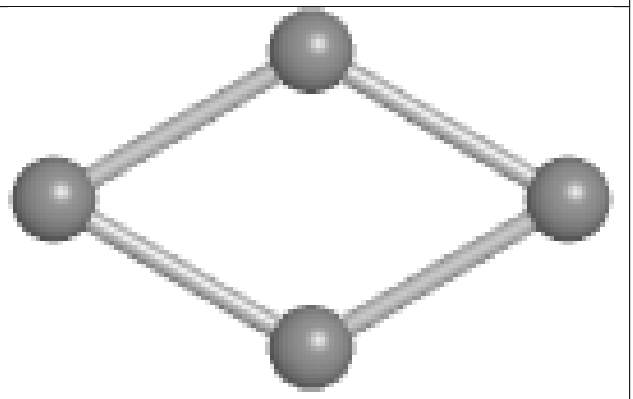

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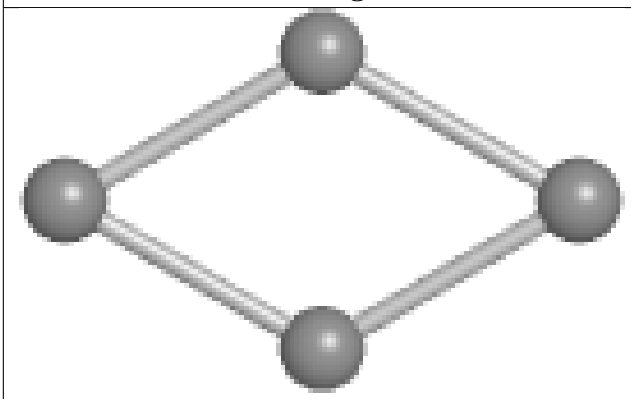

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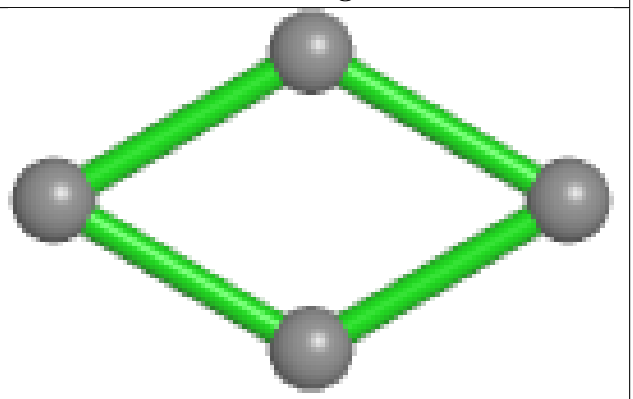
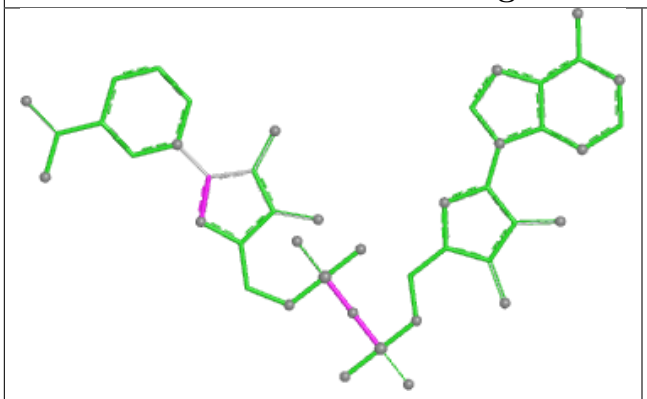


Rings

Ligand NAD AA 1701



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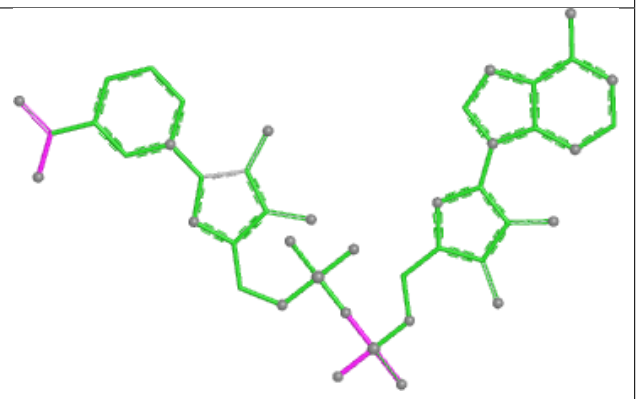

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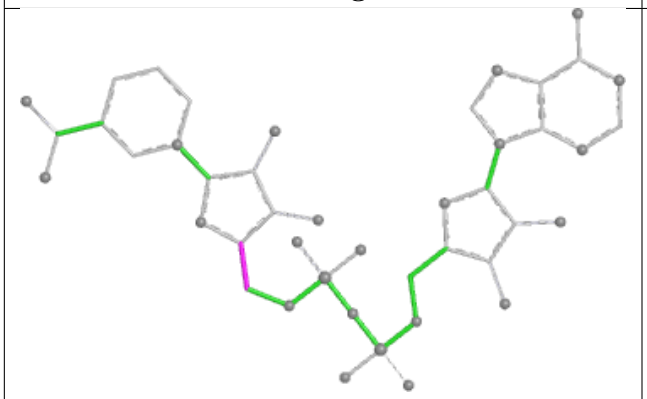

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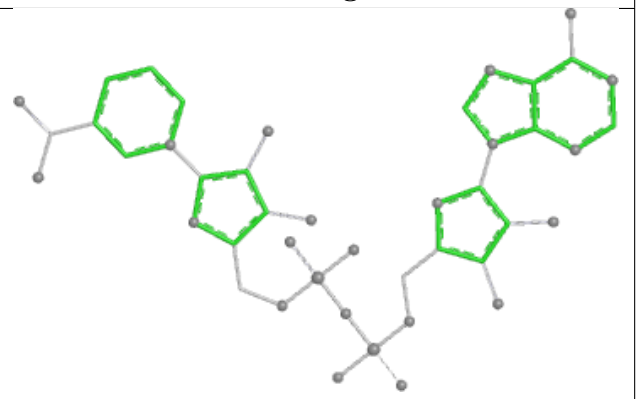
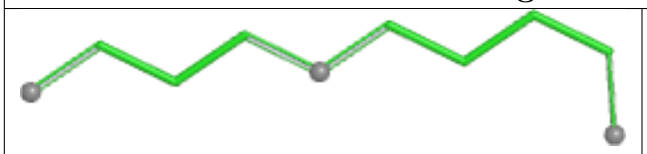


Rings

Ligand SPD A 3470



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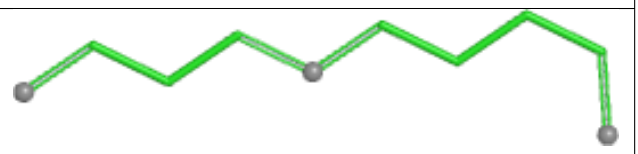

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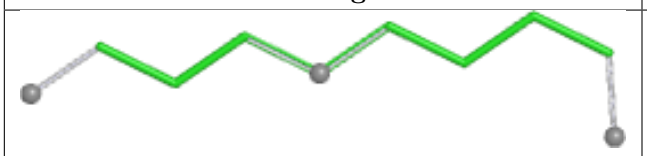

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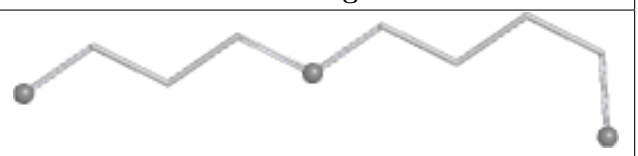
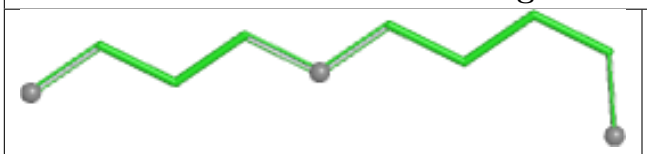


Rings

Ligand SPD A 3302



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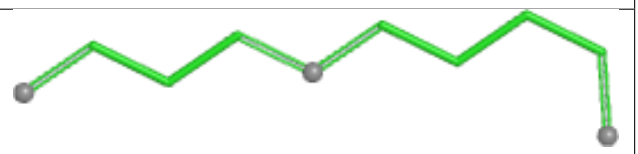

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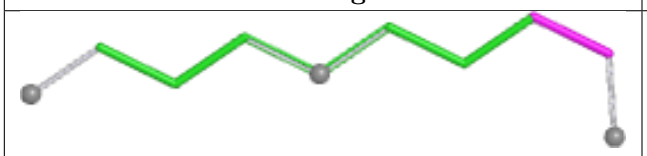

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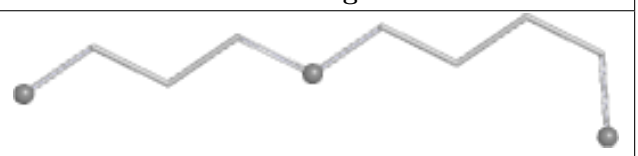
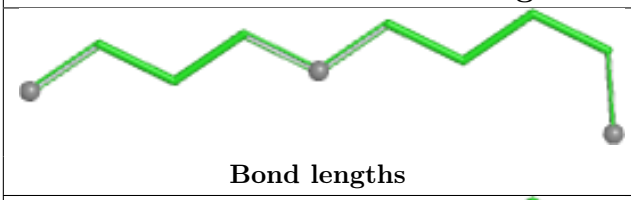


Rings

Ligand SPD A 3472



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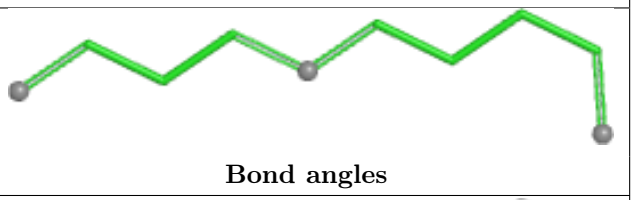

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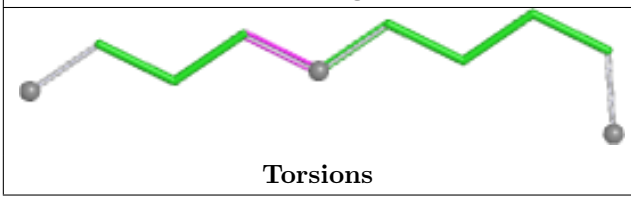

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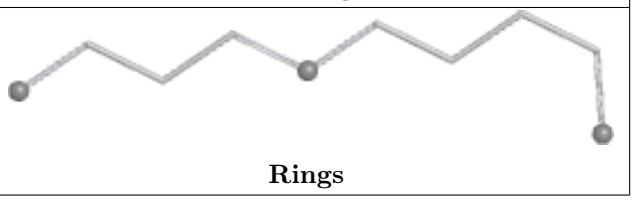
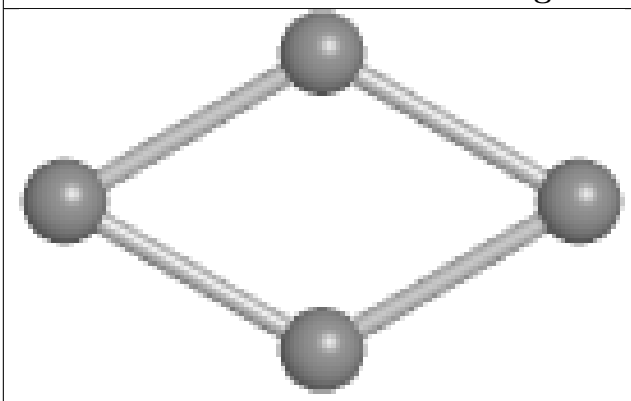


Rings

Ligand FES r 201



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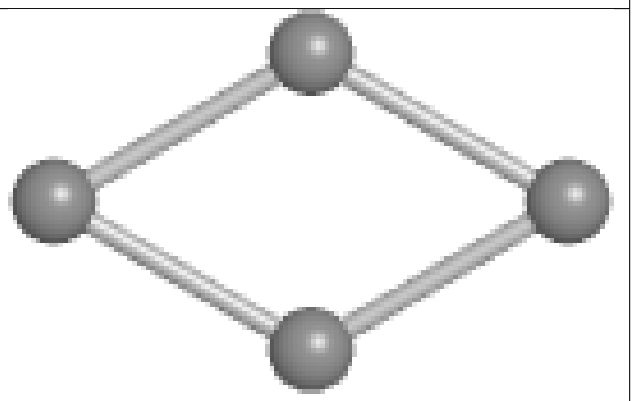
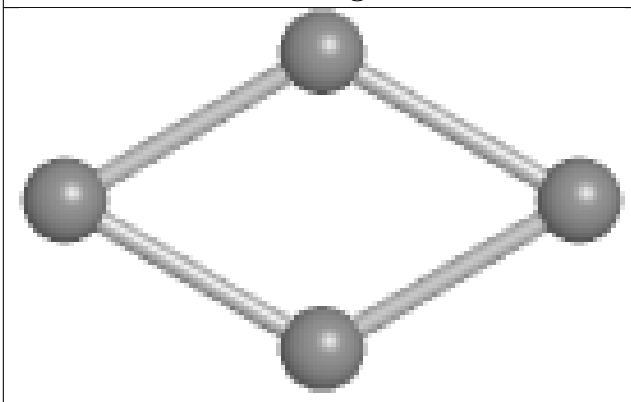


Bond angles



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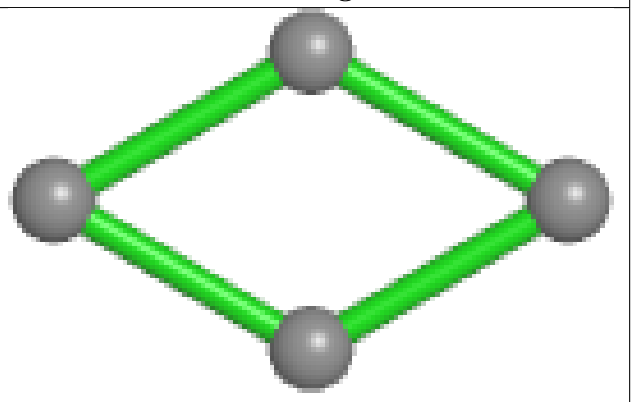
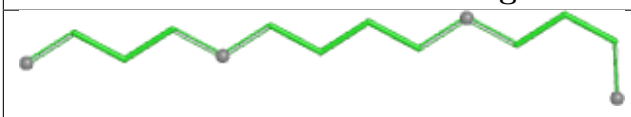


Rings

Ligand SPM AA 1702



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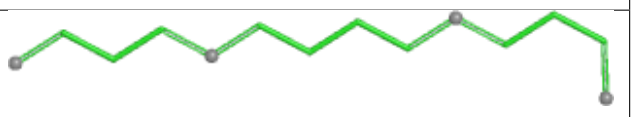

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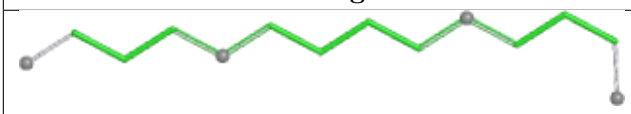

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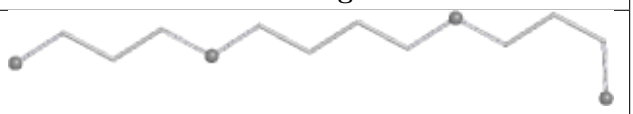
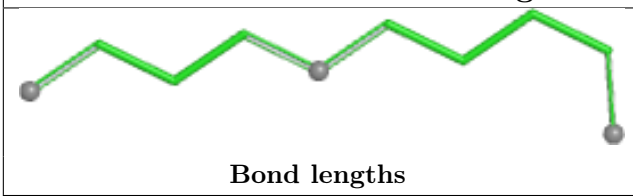


Rings

Ligand SPD A 3471



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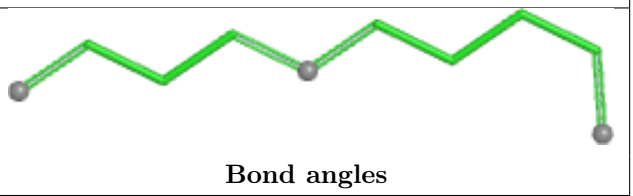

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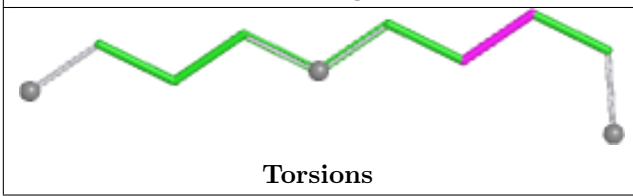

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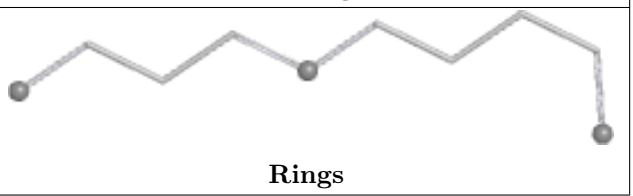
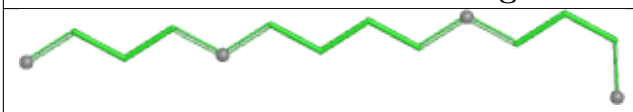


Rings

Ligand SPM AA 1780



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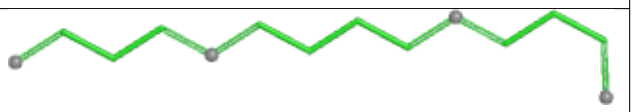
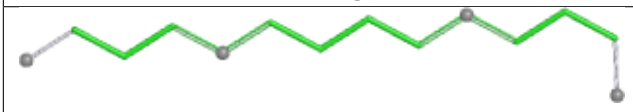


Bond angles



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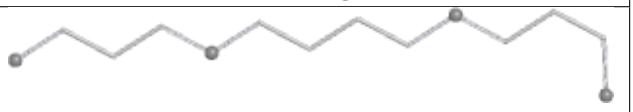
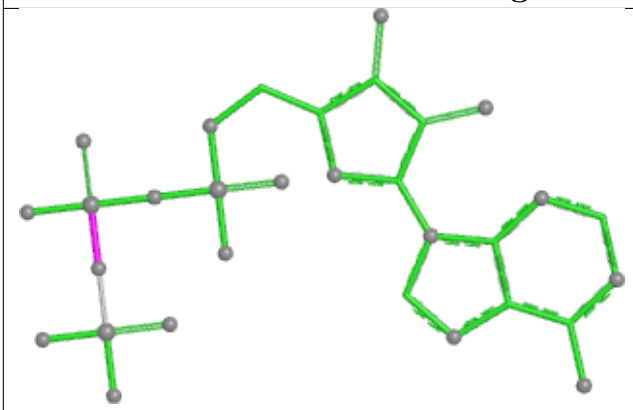


Rings

Ligand ATP AX 501



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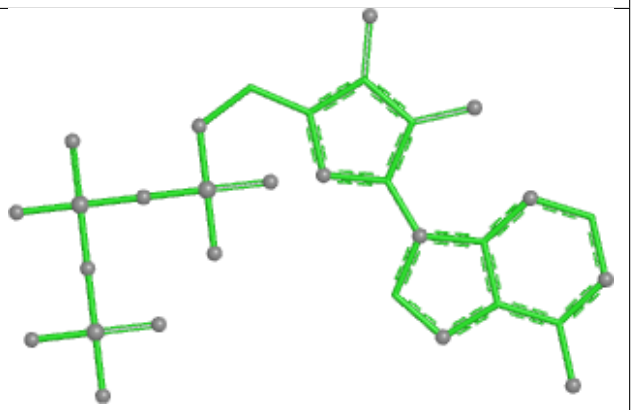
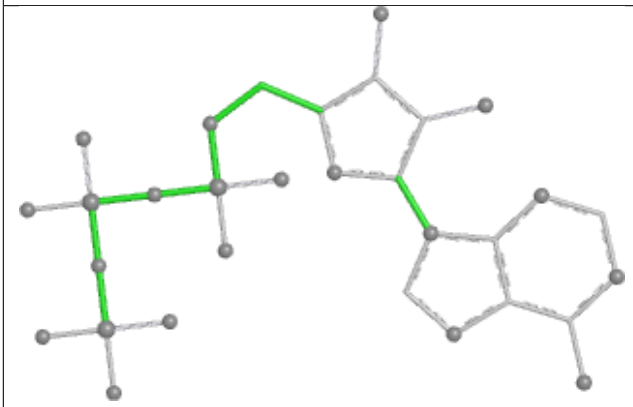


Bond angles



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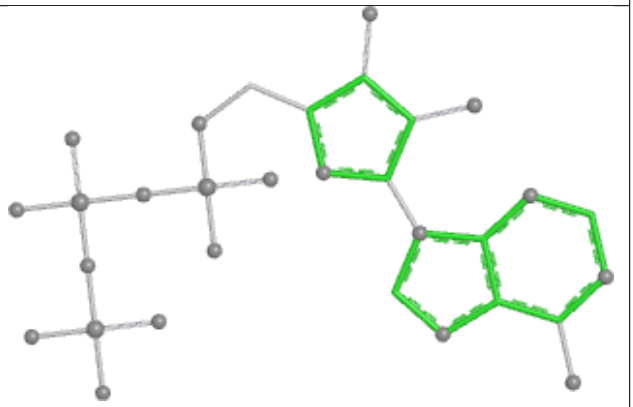
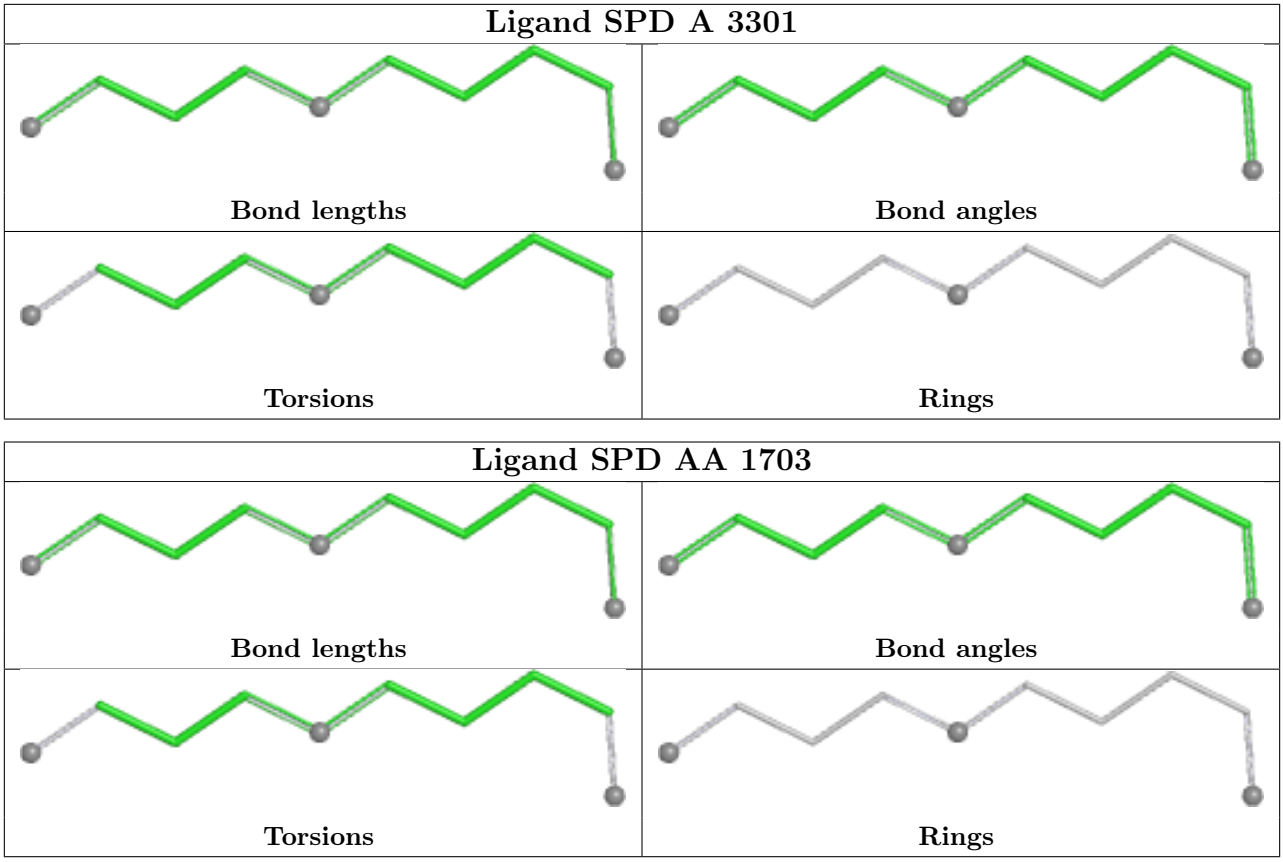


Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
90	B	1

All chain breaks are listed below:

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

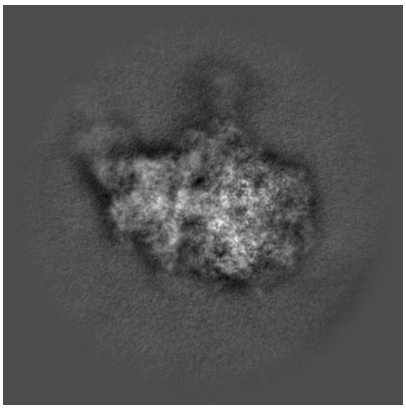
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-71635. These allow visual inspection of the internal detail of the map and identification of artifacts.

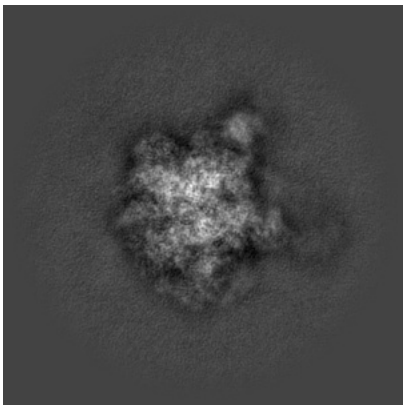
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

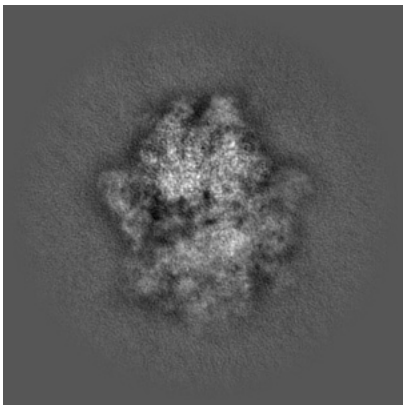
6.1.1 Primary map



X

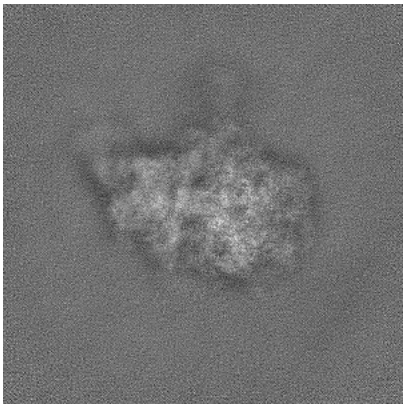


Y

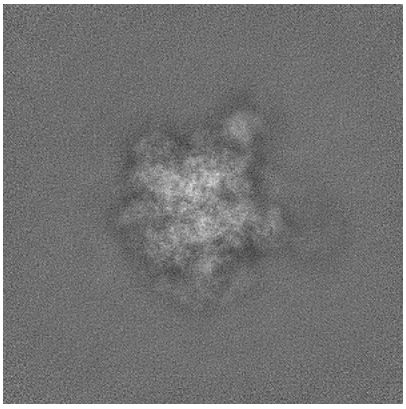


Z

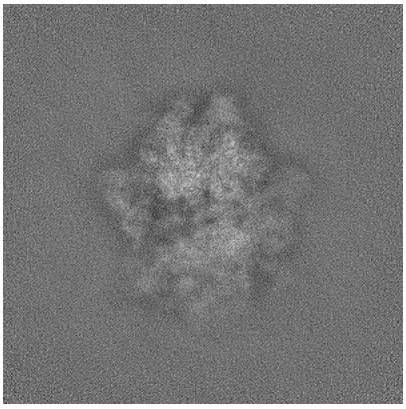
6.1.2 Raw map



X



Y

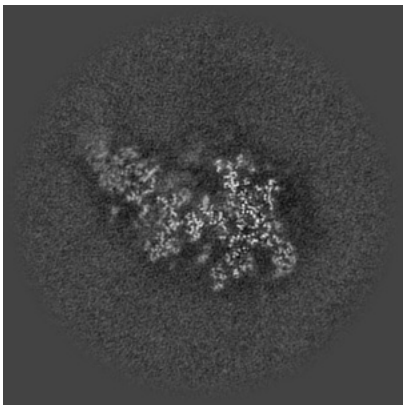


Z

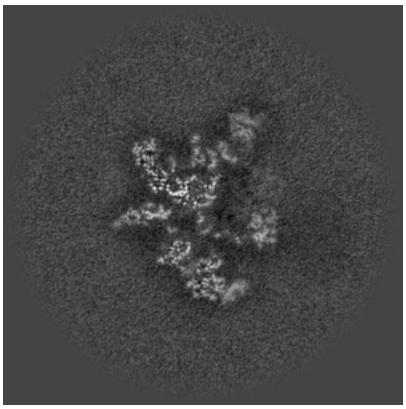
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

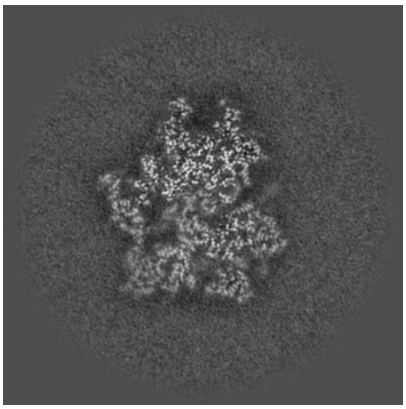
6.2.1 Primary map



X Index: 240

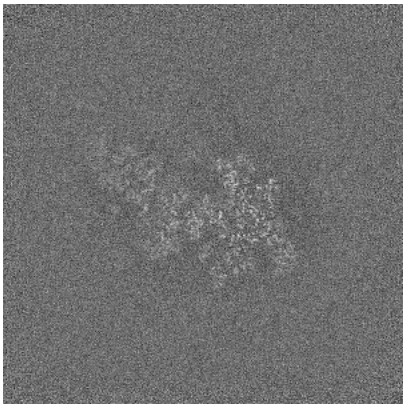


Y Index: 240

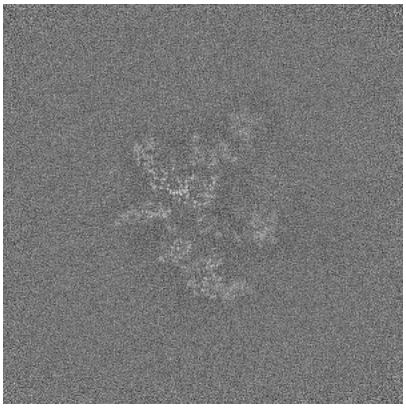


Z Index: 240

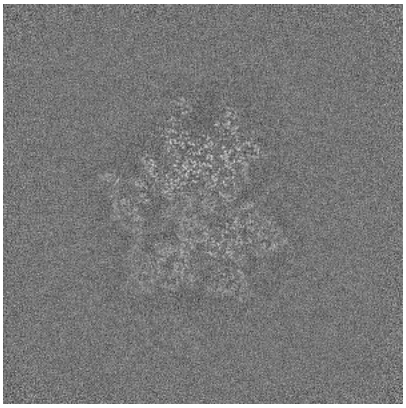
6.2.2 Raw map



X Index: 240



Y Index: 240

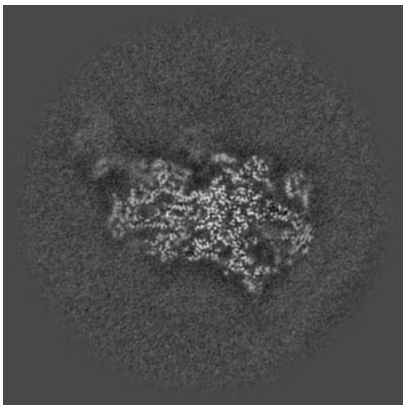


Z Index: 240

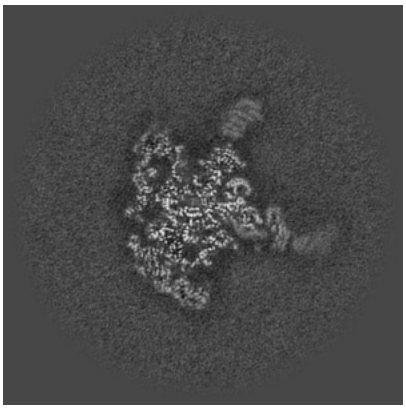
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

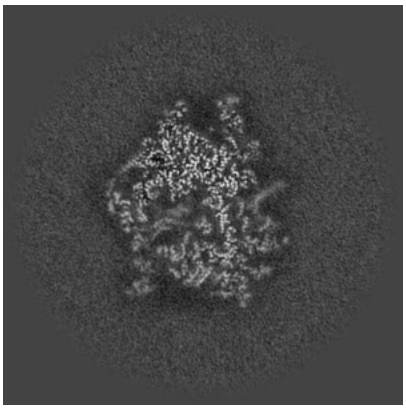
6.3.1 Primary map



X Index: 261

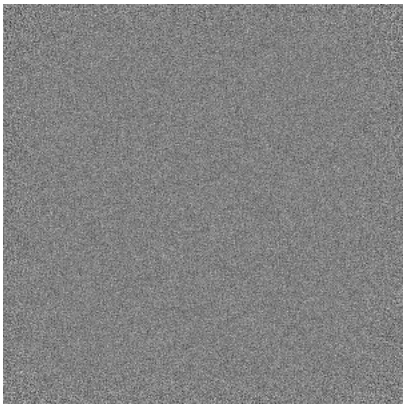


Y Index: 274

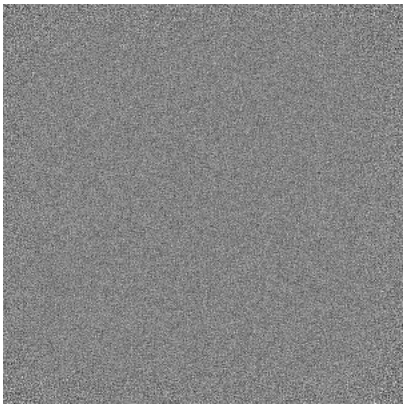


Z Index: 249

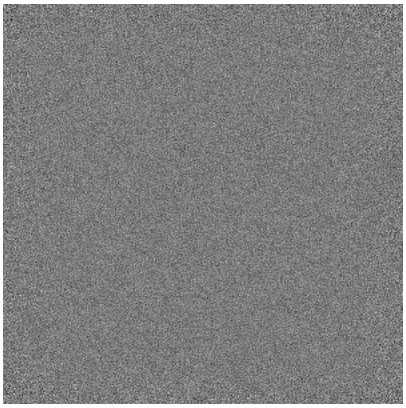
6.3.2 Raw map



X Index: 0



Y Index: 0

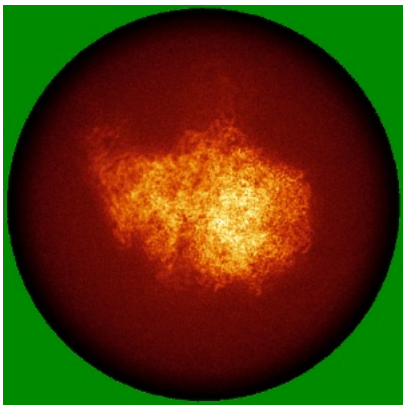


Z Index: 0

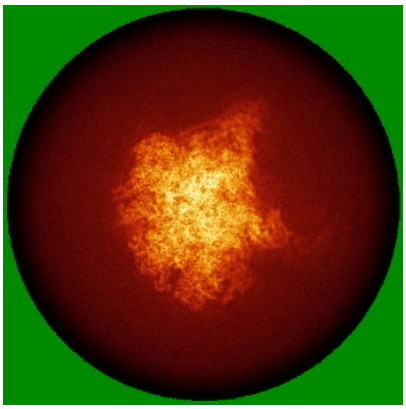
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

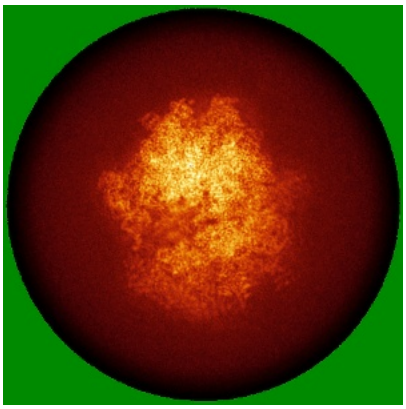
6.4.1 Primary map



X

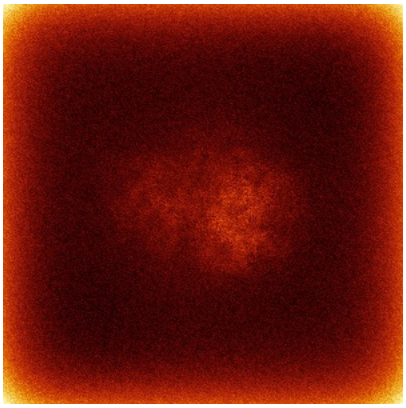


Y

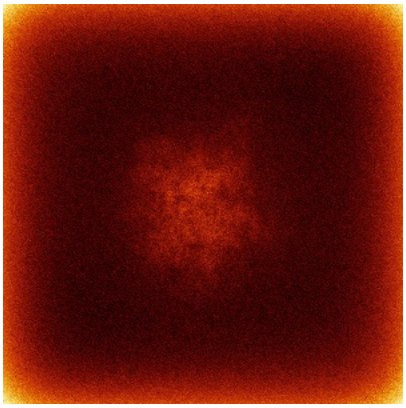


Z

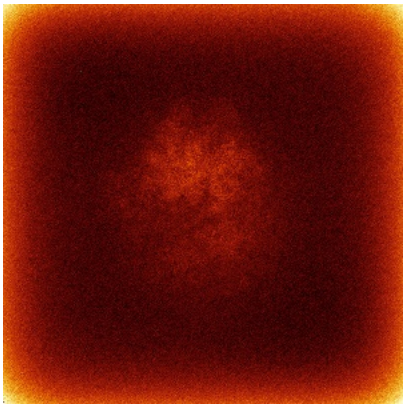
6.4.2 Raw map



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.

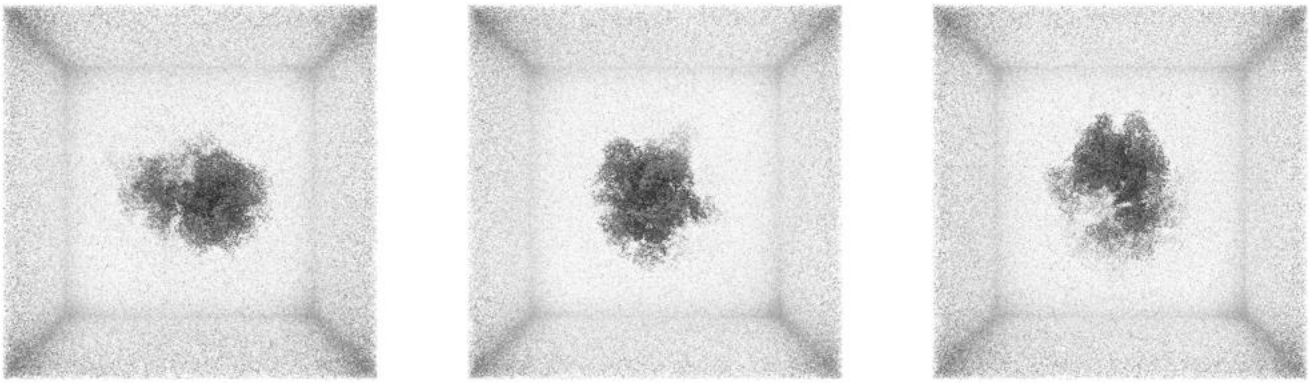
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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



X Y Z

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.

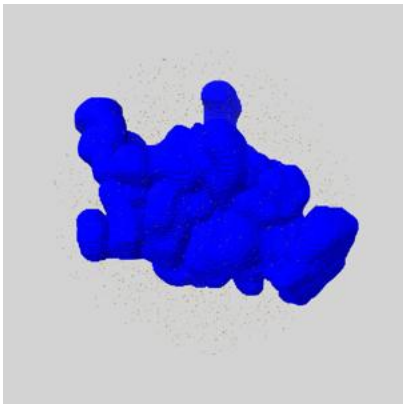
6.6 Mask visualisation

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

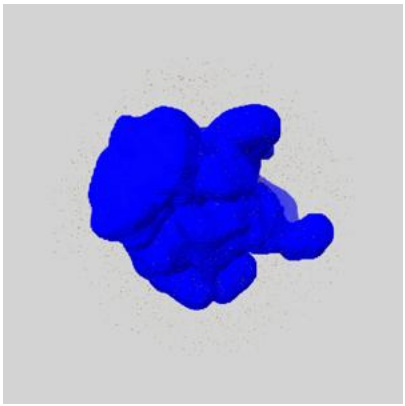
A mask typically either:

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

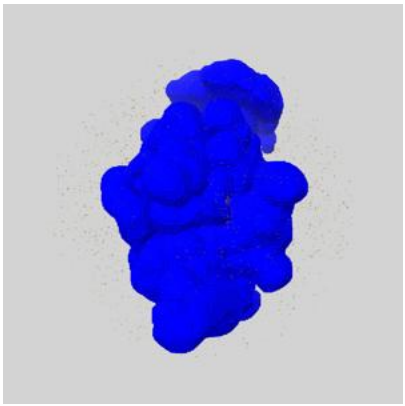
6.6.1 emd_71635_msk_1.map



X



Y

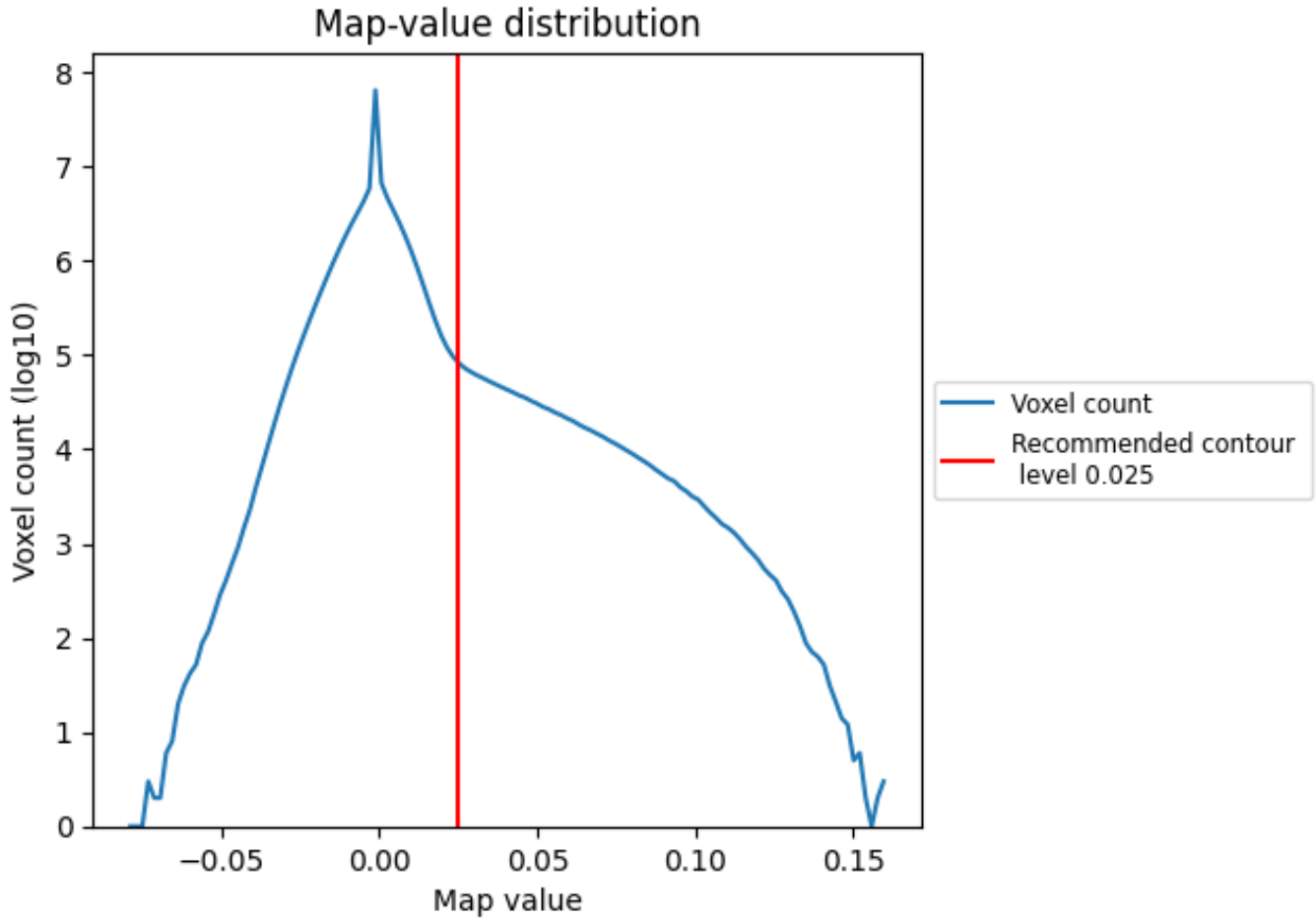


Z

7 Map analysis

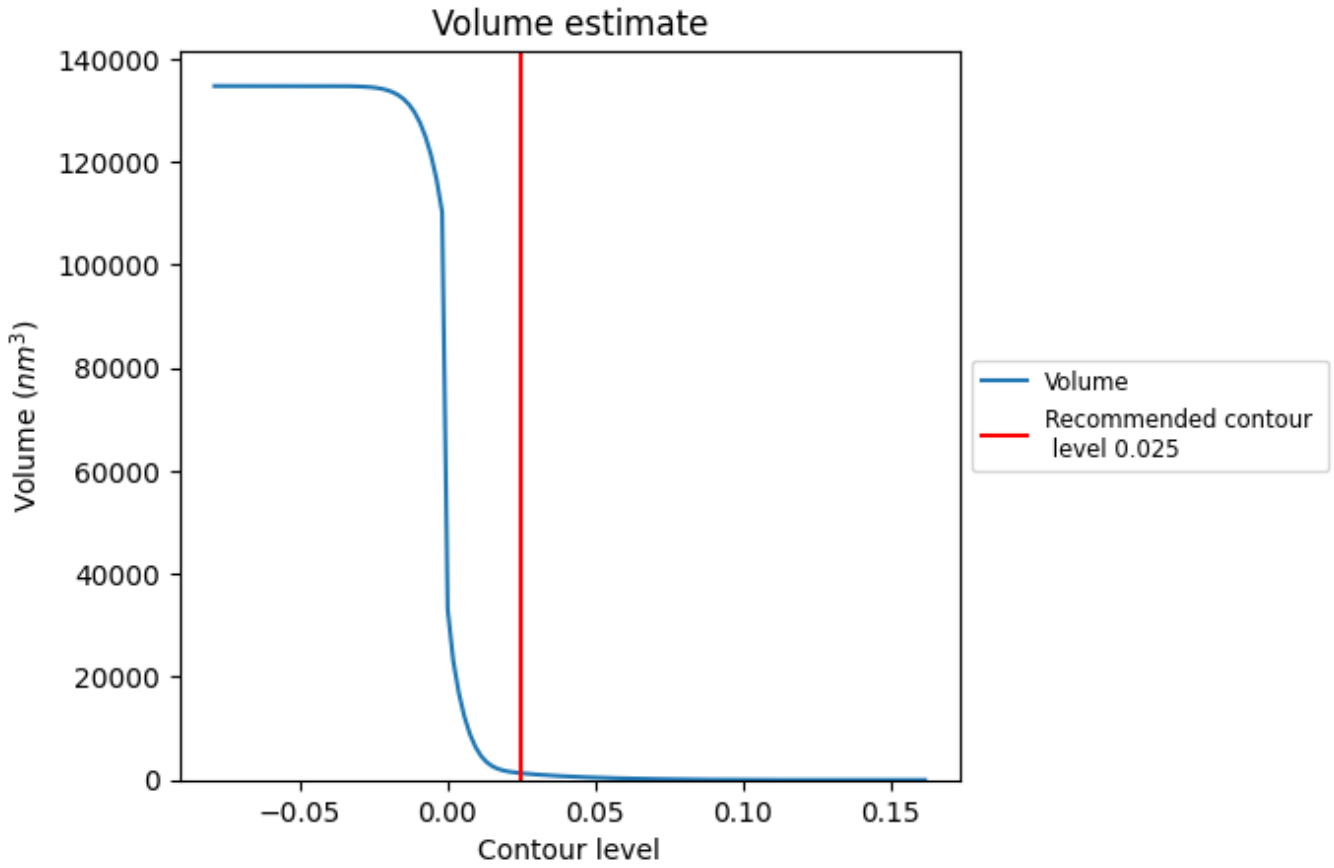
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

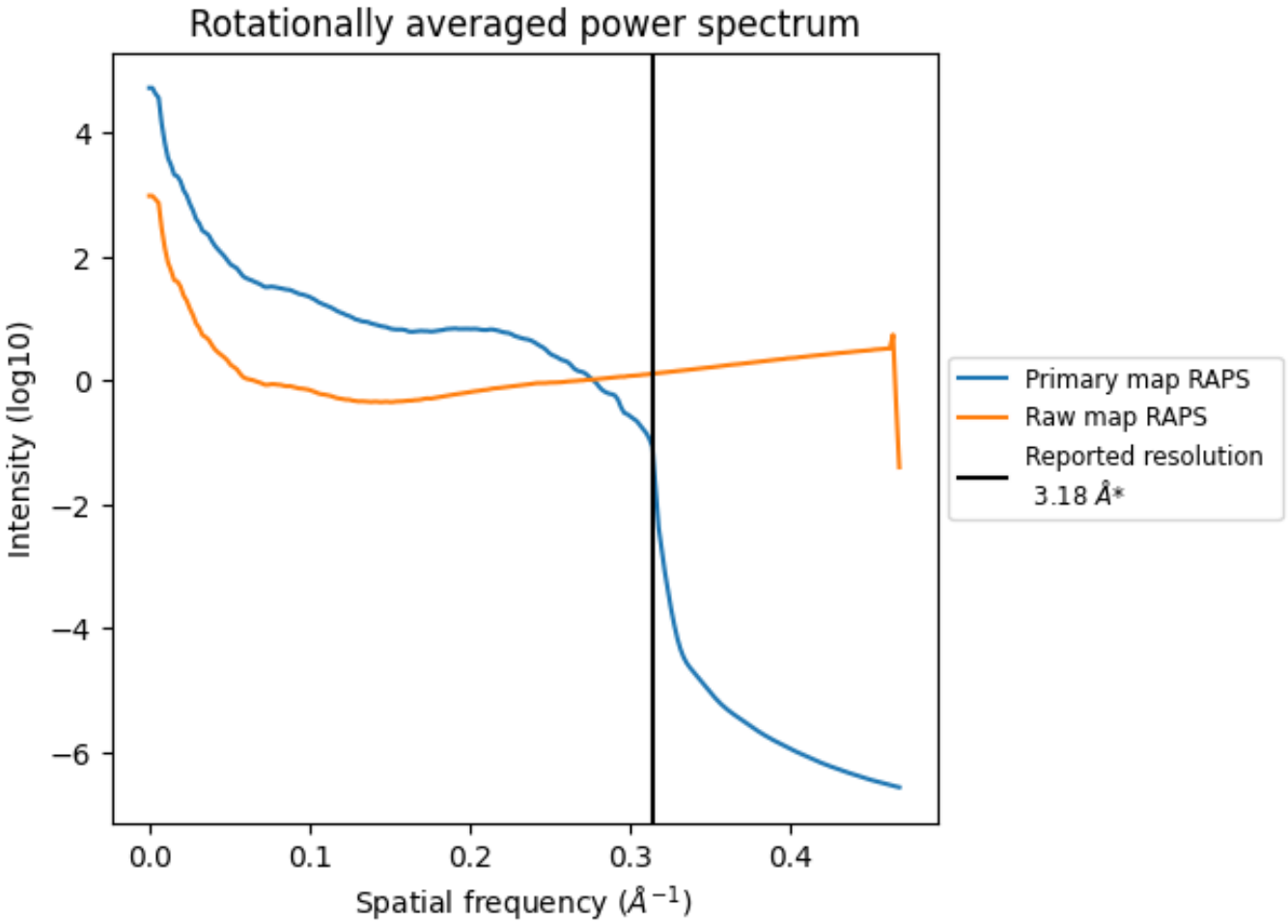
7.2 Volume estimate



The volume at the recommended contour level is 1306 nm^3; this corresponds to an approximate mass of 1180 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 (i)

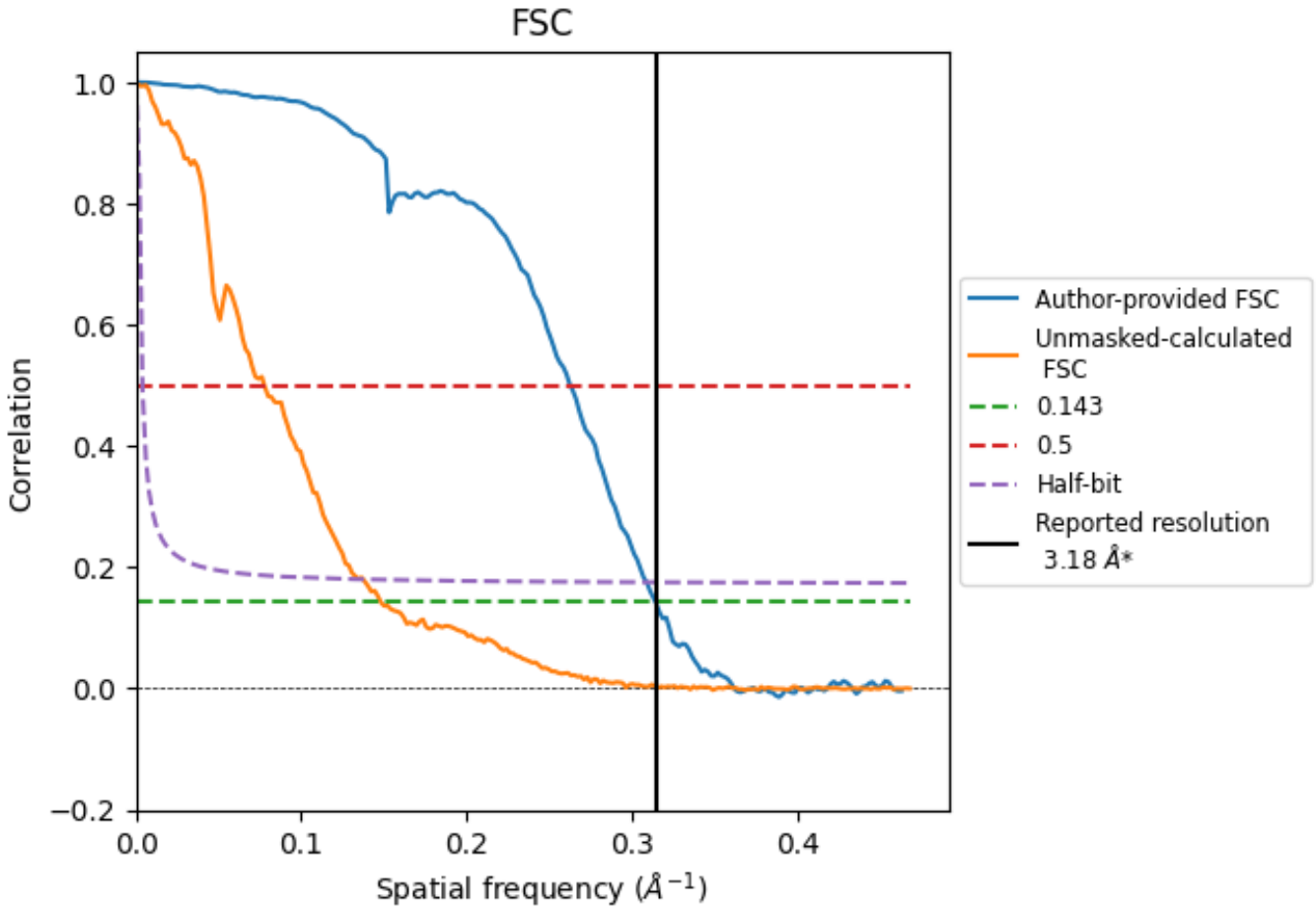


*Reported resolution corresponds to spatial frequency of 0.314 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.314 Å^{-1}

8.2 Resolution estimates (i)

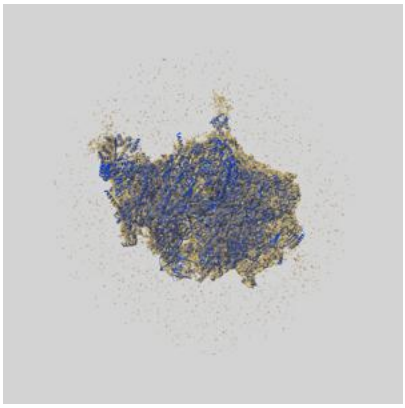
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.81	3.24
Unmasked-calculated*	6.76	12.87	7.28

*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 6.76 differs from the reported value 3.18 by more than 10 %

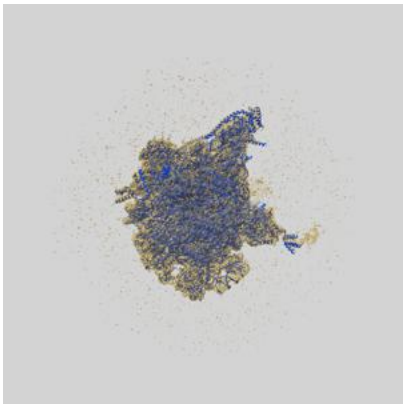
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-71635 and PDB model 9PGM. Per-residue inclusion information can be found in section 3 on page 27.

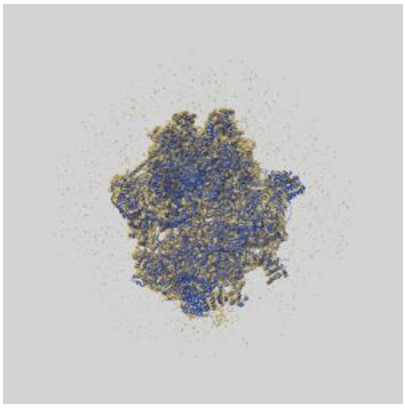
9.1 Map-model overlay



X



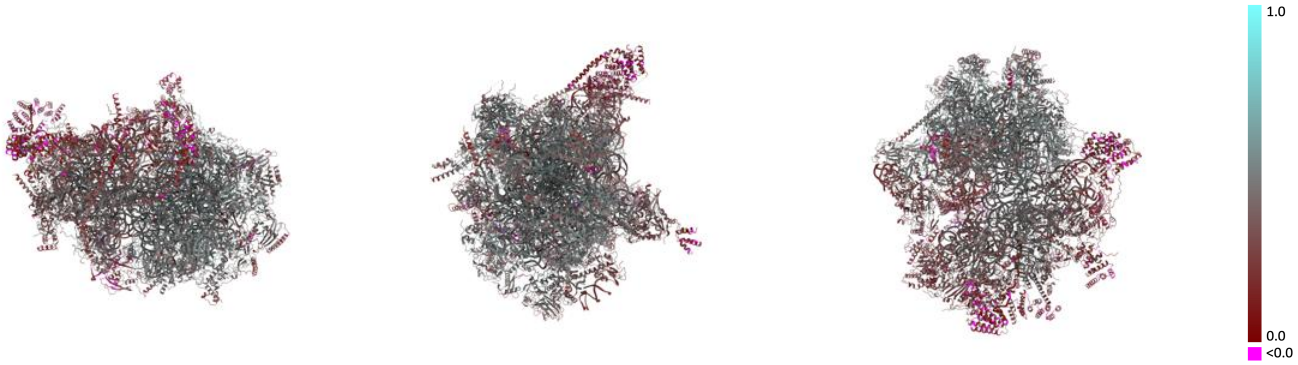
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

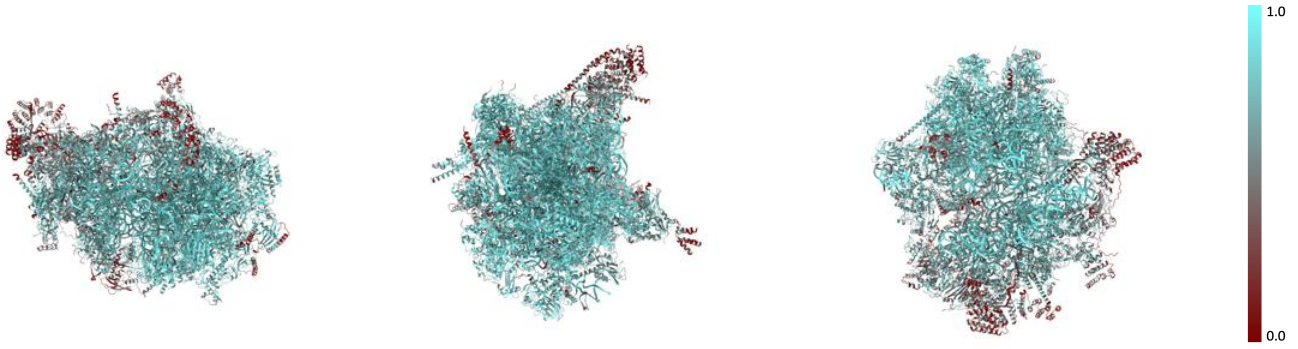
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

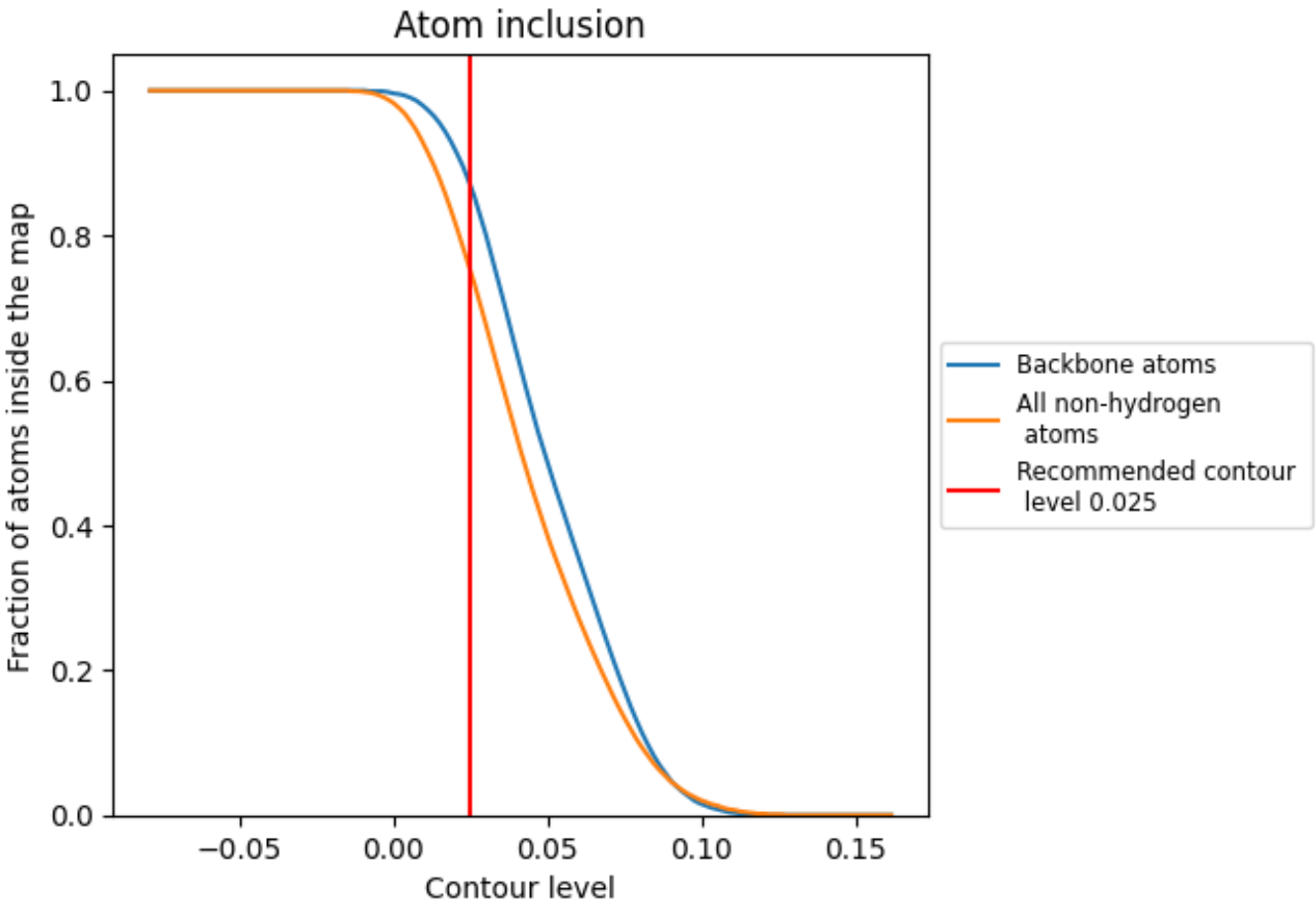
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 75% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7530	0.4040
0	0.7940	0.4780
1	0.7720	0.4720
2	0.9250	0.5250
3	0.8850	0.5250
4	0.8900	0.5090
5	0.8090	0.4700
6	0.7860	0.4360
7	0.7590	0.4350
8	0.5640	0.3070
9	0.7860	0.4550
A	0.9380	0.4700
A0	0.4530	0.2290
A1	0.5510	0.3060
A2	0.6140	0.3710
A3	0.7720	0.4470
A4	0.3500	0.1930
AA	0.9260	0.4210
AB	0.7140	0.4040
AC	0.6460	0.4100
AD	0.6310	0.3800
AE	0.6940	0.4310
AF	0.6280	0.3740
AG	0.6120	0.3510
AH	0.5750	0.3520
AI	0.7360	0.4280
AJ	0.6880	0.4300
AK	0.7120	0.3890
AL	0.6670	0.3950
AM	0.5700	0.2990
AN	0.6830	0.4080
AO	0.5480	0.2910
AP	0.7150	0.4240
AQ	0.7510	0.4310
AR	0.4600	0.2230

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Chain	Atom inclusion	Q-score
AS	0.6070	0.3420
AT	0.6730	0.3670
AU	0.5850	0.2900
AV	0.3060	0.1530
AW	0.6470	0.3820
AX	0.5640	0.2770
AY	0.5060	0.2610
AZ	0.6010	0.3190
Ax	0.8380	0.3480
Ay	0.6810	0.2250
Az	0.4230	0.2390
B	0.8370	0.3380
D	0.8510	0.5110
E	0.8230	0.4910
F	0.8460	0.5060
H	0.5120	0.3060
I	0.6220	0.3620
J	0.5660	0.2800
K	0.8450	0.4980
L	0.8180	0.5020
M	0.8310	0.4960
N	0.8280	0.4930
O	0.8320	0.4910
OX	0.4100	0.2810
P	0.8240	0.4670
Q	0.7370	0.4600
R	0.8320	0.4980
S	0.8200	0.4980
T	0.8520	0.5130
U	0.7340	0.4500
V	0.7820	0.4480
W	0.8430	0.5090
X	0.7990	0.4680
Y	0.8380	0.4830
Z	0.8370	0.5020
a	0.6770	0.4170
b	0.8290	0.5010
c	0.7820	0.4600
d	0.6410	0.4010
e	0.5790	0.2860
f	0.6470	0.3720
g	0.8220	0.4930

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Chain	Atom inclusion	Q-score
h	0.7770	0.4350
i	0.8710	0.5060
j	0.7730	0.4480
k	0.6800	0.3860
l	0.6070	0.3150
m	0.5260	0.2930
n	0.4470	0.3360
o	0.8730	0.5090
p	0.6550	0.3990
q	0.6180	0.3420
r	0.8290	0.4820
s	0.8050	0.4750
t	0.3030	0.1980
u	0.2580	0.1580
z	0.1470	0.1080