



## Full wwPDB EM Validation Report ⓘ

Apr 24, 2024 – 10:40 pm BST

PDB ID : 6ZS9  
EMDB ID : EMD-11390  
Title : Human mitochondrial ribosome in complex with ribosome recycling factor  
Authors : Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.  
Deposited on : 2020-07-15  
Resolution : 4.00 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

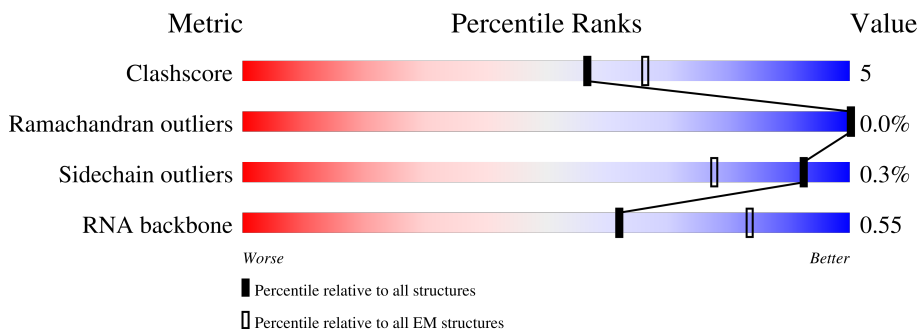
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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.






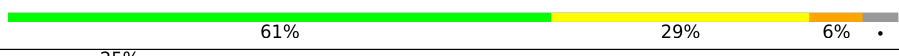
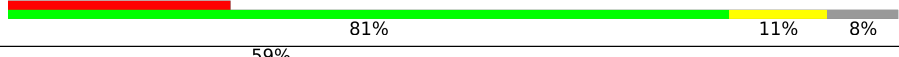



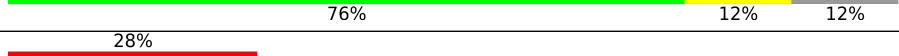
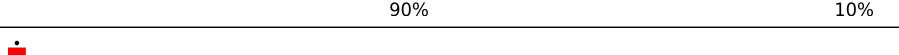
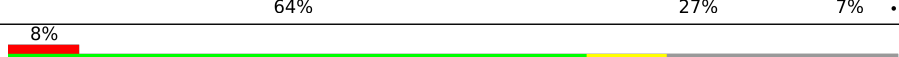
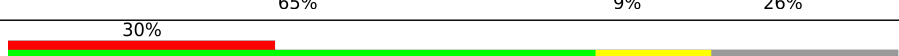

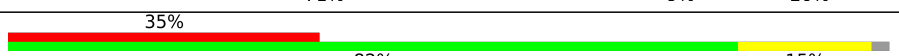

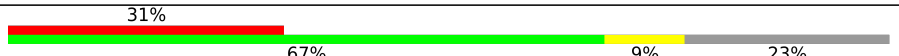
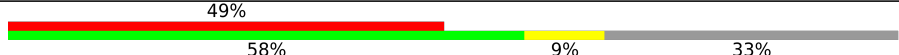




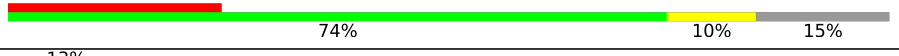

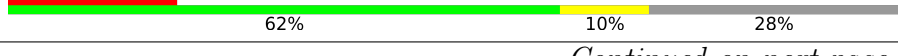

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	188	47% (green), 11% (yellow), 43% (grey)
2	1	65	74% (green), 8% (yellow), 18% (grey)
3	2	92	40% (green), 10% (yellow), 50% (grey)
4	3	188	40% (green), 10% (yellow), 49% (grey), 1% (red)
5	4	103	33% (green), 63% (grey), 1% (yellow)
6	5	423	81% (green), 11% (yellow), 7% (grey)
7	6	380	80% (green), 13% (yellow), 7% (grey), 1% (red)

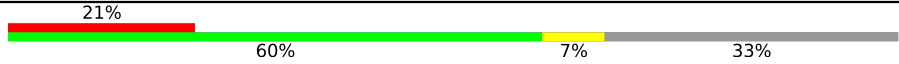
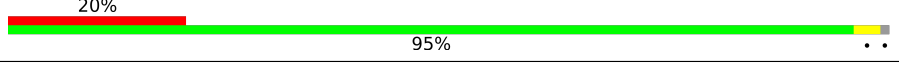
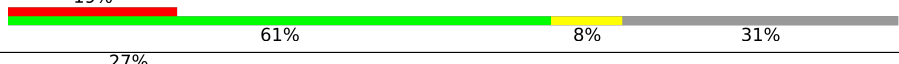



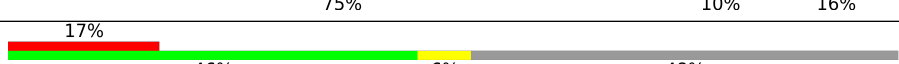
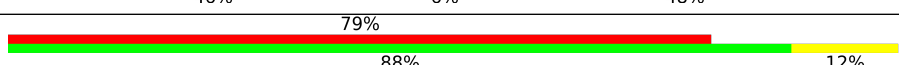

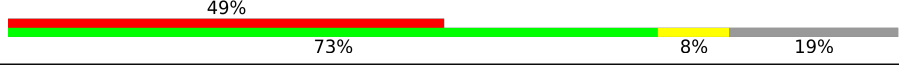

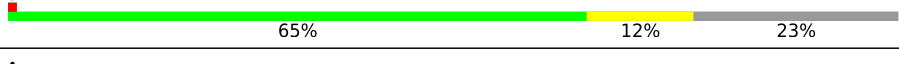
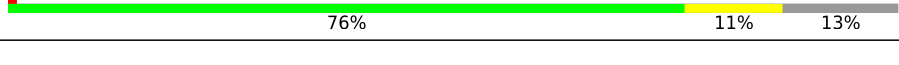

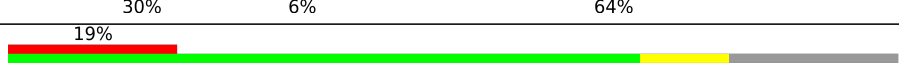

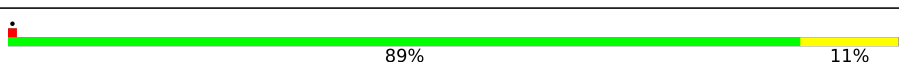








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Mol	Chain	Length	Quality of chain
8	7	338	
9	8	206	
10	9	137	
11	XA	1559	
12	A0	218	
13	A1	323	
14	A2	118	
15	A3	199	
16	A4	634	
17	A5	192	
18	AA	951	
19	AB	296	
20	AC	167	
21	AD	430	
22	AE	125	
23	AF	242	
24	AG	396	
25	AH	201	
26	AI	194	
27	AJ	138	
28	AK	128	
29	AL	257	
30	AM	137	
31	AN	130	
32	AO	258	

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Mol	Chain	Length	Quality of chain
33	AP	142	
34	AQ	86	
35	AR	360	
36	AS	190	
37	AT	173	
38	AU	205	
39	AV	414	
40	AW	187	
41	AX	348	
42	AY	395	
43	AZ	106	
44	XB	73	
45	XD	305	
46	XE	348	
47	XF	311	
48	XH	267	
49	XI	261	
50	XJ	192	
51	XK	178	
52	XL	145	
53	XM	296	
54	XN	251	
55	XO	175	
56	XP	179	
57	XQ	292	




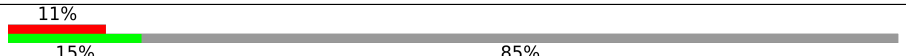
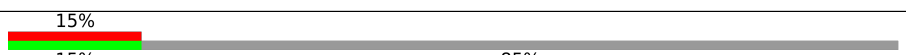
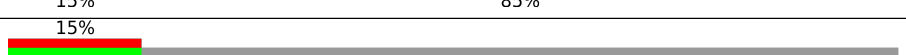
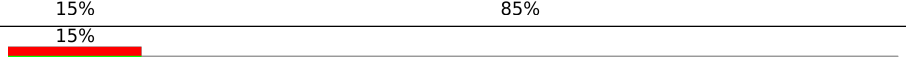


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Mol	Chain	Length	Quality of chain
58	XR	149	77% 17% 6%
59	XS	205	66% 12% 22%
60	XT	212	71% 7% 22%
61	XU	153	78% 14% 8%
62	XV	216	78% 15% 6%
63	XW	148	64% 11% 25%
64	XX	256	85% 10% 5%
65	XY	250	58% 13% 29%
66	XZ	161	69% 6% 25%
67	a	142	68% 32%
68	b	215	69% 31%
69	c	332	83% 17%
70	d	306	71% 29%
71	e	279	11% 76% 22%
72	f	212	8% 67% 33%
73	g	166	80% 20%
74	h	158	68% 32%
75	i	128	76% 24%
76	j	123	70% 30%
77	k	112	85% 15%
78	l	138	58% 42%
79	m	128	8% 47% 53%
80	o	102	92% 8%
81	p	206	62% 38%
82	q	198	19% 83% 17%

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Mol	Chain	Length	Quality of chain
83	r	196	 78% 22%
84	s	439	 84% 16%
85	t1	198	 17% 23% 77%
85	t2	198	 11% 15% 85%
85	t3	198	 15% 15% 85%
85	t4	198	 15% 15% 85%
85	t5	198	 15% 15% 85%
85	t6	198	 14% 14% 86%
86	A	8	 38% 25% 38%

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 313805 atoms, of which 144698 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	H	N	O			S
1	0	108	1782	545	902	172	157	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	1	53	919	281	480	84	72	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	2	46	782	233	406	83	59	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	3	95	1714	539	883	162	127	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	4	38	702	217	361	72	48	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	5	393	6405	2070	3201	559	564	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	6	354	5786	1881	2839	525	532	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	7	291	4738	1514	2373	401	432	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	8	135	2311	727	1171	202	209	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	9	124	1983	644	987	170	180	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
11	XA	1501	48058	14303	16183	5764	10307	1501	0	0

- Molecule 12 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	A0	201	3369	1065	1685	322	292	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	A1	275	4491	1414	2261	380	425	11	0	0

- Molecule 14 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.



Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	A2	116	1889	574	964	181	162	8	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	A3	69	1292	393	682	130	86	1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	A4	558	9067	2903	4546	764	826	28	0	0

- Molecule 17 is a protein called Ribosome-recycling factor, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	A5	192	3066	923	1577	267	291	8	0	0

- Molecule 18 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
18	AA	927	29687	8828	9997	3550	6385	927	0	0

- Molecule 19 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	AB	218	3545	1135	1769	322	309	10	0	0

- Molecule 20 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	AC	132	2170	699	1088	195	184	4	0	0

- Molecule 21 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	AD	343	5501	1706	2785	515	482	13	0	0

- Molecule 22 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	AE	122	1973	614	1001	177	177	4	0	0

- Molecule 23 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	AF	201	3384	1069	1716	305	283	11	0	0

- Molecule 24 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	AG	304	4997	1593	2492	444	454	14	0	0

- Molecule 25 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	AH	135	2241	712	1136	187	203	3	0	0

- Molecule 26 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	AI	136	2063	637	1052	192	178	4	0	0

- Molecule 27 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	AJ	108	1725	521	887	169	142	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	AK	101	1746	537	885	179	140	5	0	0

- Molecule 29 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	AL	164	2855	883	1473	257	235	7	0	0

- Molecule 30 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	AM	116	1871	582	951	182	150	6	0	0

- Molecule 31 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	AN	107	1754	549	908	153	141	3	0	0

- Molecule 32 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	AO	185	3018	970	1490	285	267	6	0	0

- Molecule 33 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
33	AP	95	1561	493	796	132	132	8	0	0

- Molecule 34 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
34	AQ	85	1483	455	749	149	123	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	conflict	UNP P82921

- Molecule 35 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	AR	250	4134	1314	2074	353	385	8	0	0

- Molecule 36 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	AS	133	2203	709	1103	196	194	1	0	0

- Molecule 37 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	AT	162	2673	850	1343	231	238	11	0	0

- Molecule 38 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	AU	173	2932	900	1471	294	263	4	0	0

- Molecule 39 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	AV	349	5729	1841	2862	478	536	12	0	0

- Molecule 40 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	AW	97	1551	486	785	137	139	4	0	0

- Molecule 41 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
41	AX	348	5616	1802	2802	491	510	11	0	0

- Molecule 42 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
42	AY	113	1868	621	912	157	176	2	0	0

- Molecule 43 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
43	AZ	86	1465	467	734	131	129	4	0	0

- Molecule 44 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
44	XB	59	1890	563	635	227	406	59	0	0

- Molecule 45 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
45	XD	236	3738	1145	1896	373	315	9	0	0

- Molecule 46 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
46	XE	304	4798	1539	2402	416	430	11	0	0

- Molecule 47 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
47	XF	250	4058	1294	2045	365	348	6	0	0

- Molecule 48 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	XH	95	Total	C	H	N	O	0	0
			1616	498	832	152	134		

- Molecule 49 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
49	XI	211	Total	C	H	N	O	S	0	0
			3474	1086	1783	303	291	11		

- Molecule 50 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
50	XJ	170	Total	C	H	N	O	S	0	0
			2658	825	1367	230	234	2		

- Molecule 51 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
51	XK	177	Total	C	H	N	O	S	0	0
			2899	934	1448	259	251	7		

- Molecule 52 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
52	XL	115	Total	C	H	N	O	S	0	0
			1830	559	941	171	154	5		

- Molecule 53 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
53	XM	287	Total	C	H	N	O	S	0	0
			4683	1472	2378	425	402	6		

- Molecule 54 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
54	XN	221	Total	C	H	N	O	S	0	0
			3586	1138	1808	325	305	10		

- Molecule 55 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
55	XO	152	2528	784	1283	239	215	7	0	0

- Molecule 56 is a protein called Mitochondrial ribosomal protein L18, isoform CRA\_b.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
56	XP	143	2326	729	1162	223	207	5	0	0

- Molecule 57 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
57	XQ	238	4000	1268	2022	352	349	9	0	0

- Molecule 58 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
58	XR	140	2367	732	1214	231	186	4	0	0

- Molecule 59 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
59	XS	160	2638	829	1354	226	225	4	0	0

- Molecule 60 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
60	XT	166	2778	875	1410	254	232	7	0	0

- Molecule 61 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
61	XU	141	2335	743	1164	222	203	3	0	0

- Molecule 62 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
62	XV	202	3304	1051	1656	294	295	8	0	0

- Molecule 63 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
63	XW	111	1769	558	898	164	146	3	0	0

- Molecule 64 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
64	XX	243	4089	1317	2054	351	362	5	0	0

- Molecule 65 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
65	XY	178	3109	981	1575	295	254	4	0	0

- Molecule 66 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
66	XZ	120	2008	626	1030	183	166	3	0	0

- Molecule 67 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
67	a	97	1590	512	777	145	151	5	0	0

- Molecule 68 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
68	b	148	2358	733	1180	229	213	3	0	0

- Molecule 69 is a protein called 39S ribosomal protein L44, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
69	c	275	4437	1415	2220	383	410	9	0	0

- Molecule 70 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
70	d	217	3510	1128	1747	306	316	13	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	62	PHE	GLU	conflict	UNP Q9BRJ2
d	63	ALA	PHE	conflict	UNP Q9BRJ2

- Molecule 71 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
71	e	217	3529	1124	1767	310	323	5	0	0

- Molecule 72 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
72	f	142	2291	731	1152	185	219	4	0	0

- Molecule 73 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
73	g	132	2183	710	1086	191	194	2	0	0

- Molecule 74 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
74	h	108	1749	560	867	154	165	3	0	0

- Molecule 75 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
75	i	97	1684	532	857	165	126	4	0	0

- Molecule 76 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
76	j	86	1367	426	678	134	127	2	0	0

- Molecule 77 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
77	k	95	1477	456	745	139	132	5	0	0

- Molecule 78 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
78	l	80	1327	427	654	118	125	3	0	0

- Molecule 79 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
79	m	60	1025	309	525	104	85	2	0	0

- Molecule 80 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
80	o	94	1601	501	804	165	128	3	0	0

- Molecule 81 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
81	p	127	2141	661	1083	201	192	4	0	0

- Molecule 82 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
82	q	164	2738	858	1359	267	249	5	0	0

- Molecule 83 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
83	r	152	2514	792	1267	239	208	8	0	0

- Molecule 84 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
84	s	370	6059	1946	3023	542	534	14	0	0

- Molecule 85 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
85	t1	46	733	228	379	56	70	2	0
85	t2	30	506	154	268	38	46	0	0
85	t3	30	506	154	268	38	46	0	0
85	t4	29	484	148	255	36	45	0	0
85	t5	29	484	148	255	36	45	0	0
85	t6	27	450	137	236	34	43	0	0

- Molecule 86 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
86	A	8	140	53	67	9	10	1	0	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	0	1	Total	Zn	0
			1	1	

*Continued on next page...*

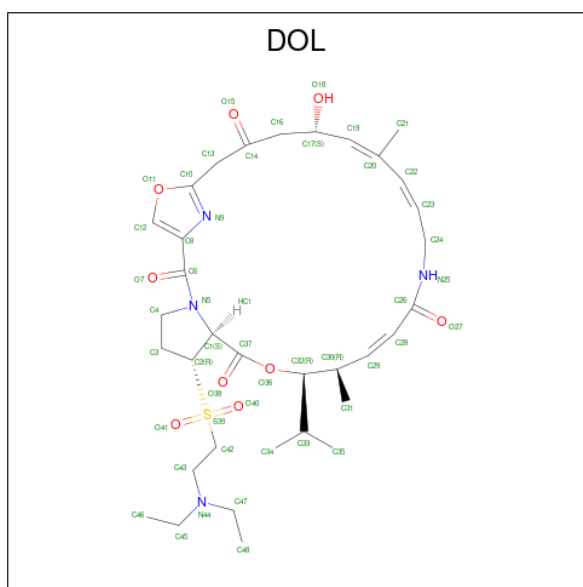
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Mol	Chain	Residues	Atoms		AltConf
87	4	1	Total 1	Zn 1	0
87	AB	1	Total 1	Zn 1	0
87	AO	1	Total 1	Zn 1	0
87	AP	1	Total 1	Zn 1	0
87	AT	1	Total 1	Zn 1	0
87	r	1	Total 1	Zn 1	0

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

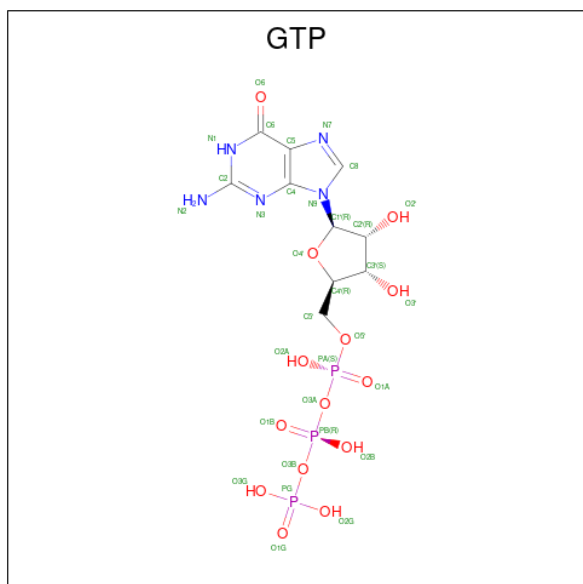
Mol	Chain	Residues	Atoms		AltConf
88	2	1	Total 1	Mg 1	0
88	9	1	Total 1	Mg 1	0
88	XA	140	Total 140	Mg 140	0
88	AA	45	Total 45	Mg 45	0
88	AH	1	Total 1	Mg 1	0
88	XD	1	Total 1	Mg 1	0
88	XI	1	Total 1	Mg 1	0
88	XM	2	Total 2	Mg 2	0
88	XW	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	o	1	Total 1	Mg 1	0

- Molecule 89 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C<sub>34</sub>H<sub>50</sub>N<sub>4</sub>O<sub>9</sub>S).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		S
89	XA	1	98	34	50	4	9	1	0

- Molecule 90 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



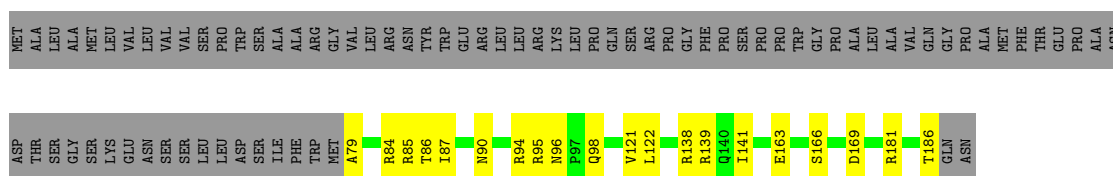
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
90	AX	1	42	10	10	5	14	3	0

### 3 Residue-property plots

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.

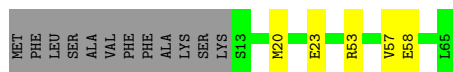
- Molecule 1: 39S ribosomal protein L32, mitochondrial

Chain 0: 




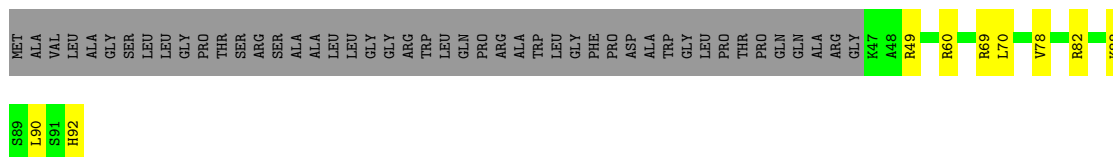
- Molecule 2: 39S ribosomal protein L33, mitochondrial

Chain 1: 




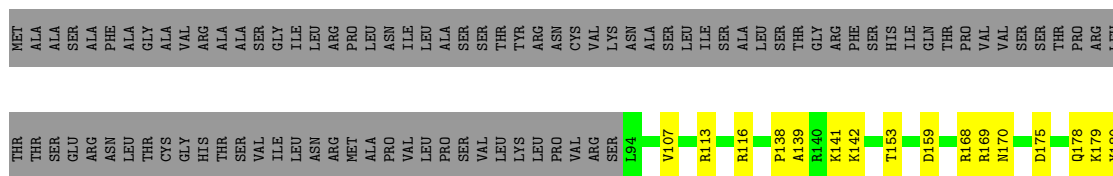
- Molecule 3: 39S ribosomal protein L34, mitochondrial

Chain 2: 



- Molecule 4: 39S ribosomal protein L35, mitochondrial

Chain 3: 





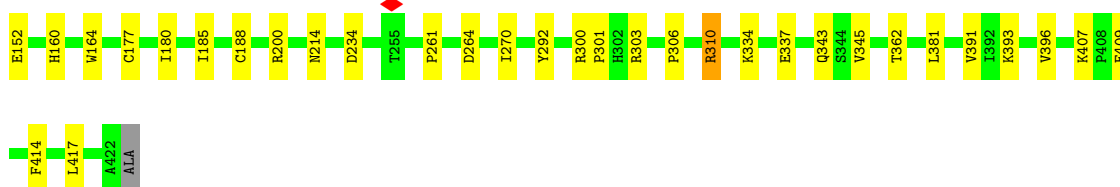
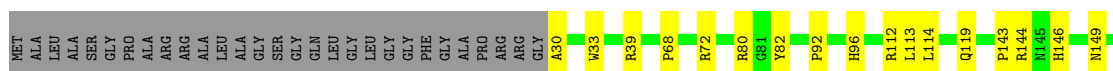
- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4: 33% 63%



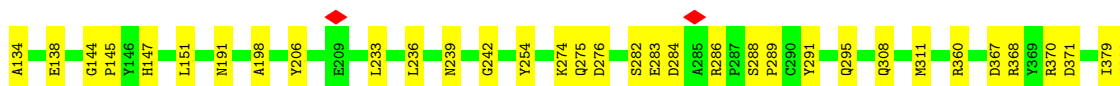
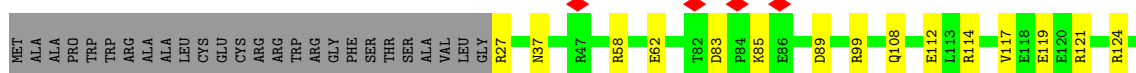
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5: 81% 11% 7%



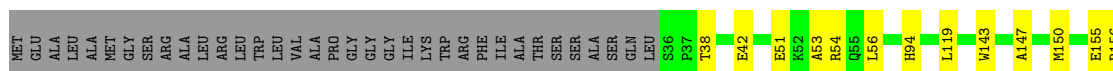
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6: 80% 13% 7%

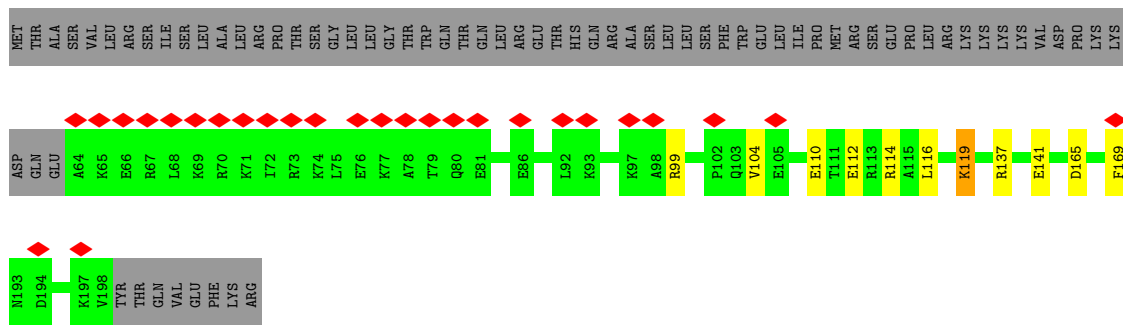


- Molecule 8: 39S ribosomal protein L39, mitochondrial

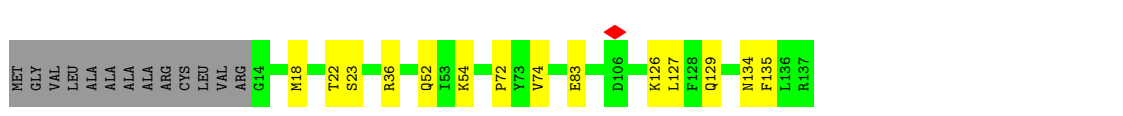
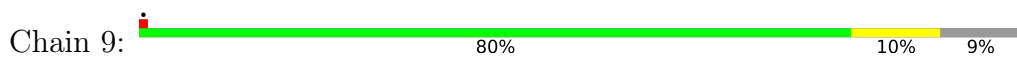
Chain 7: 75% 11% 14%



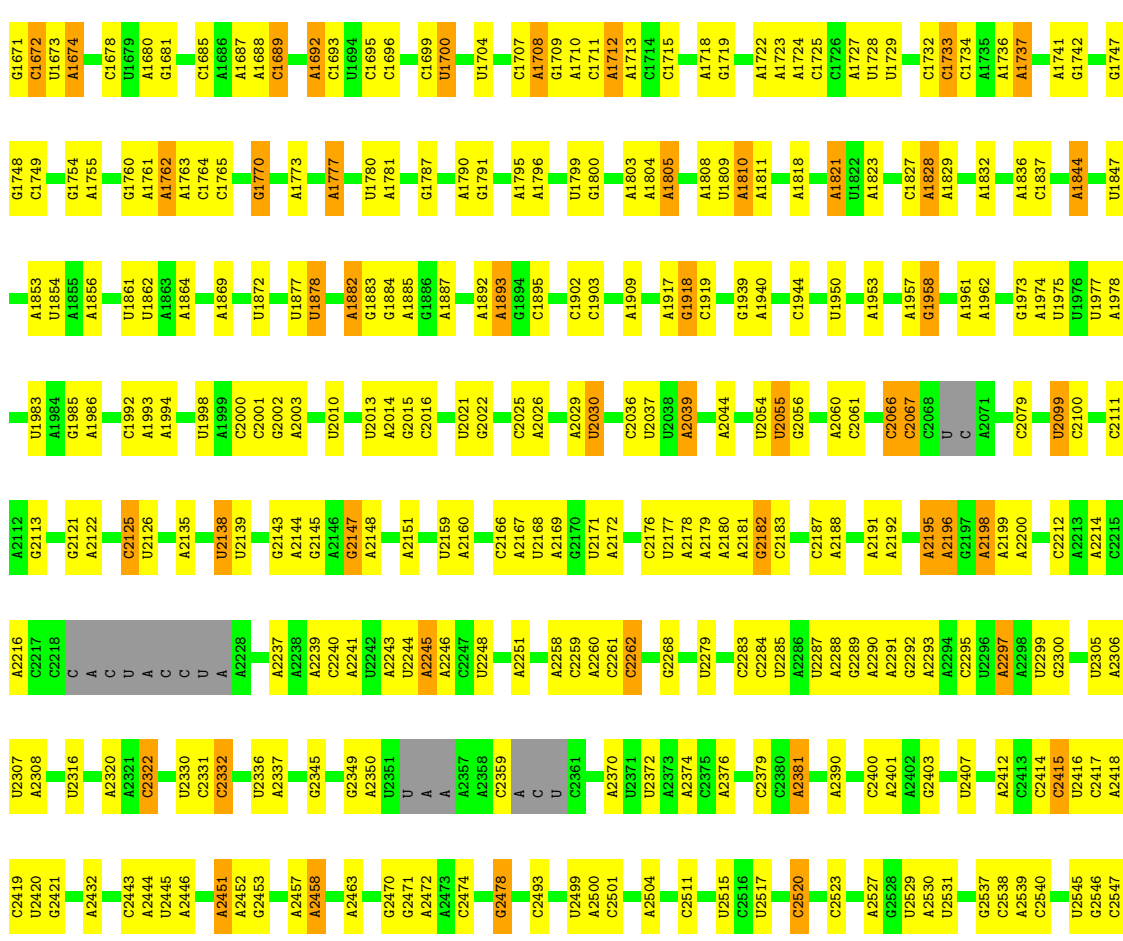
- Molecule 9: 39S ribosomal protein L40, mitochondrial



• Molecule 10: 39S ribosomal protein L41, mitochondrial

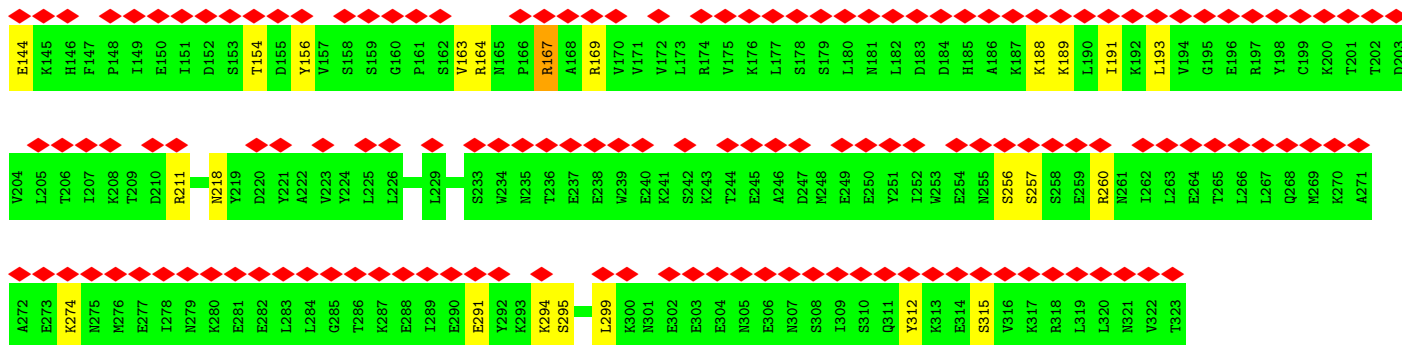


• Molecule 11: 16S rRNA

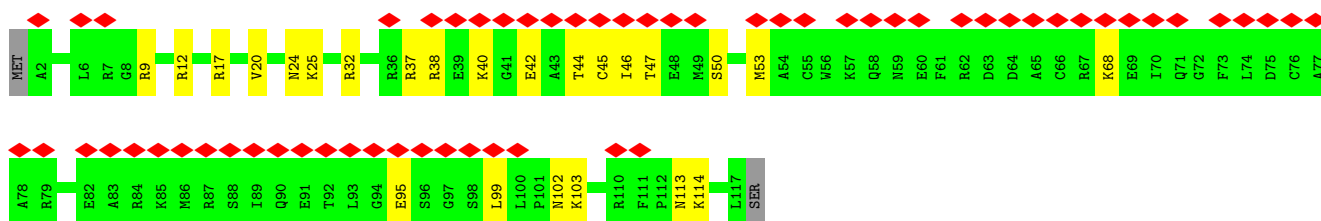




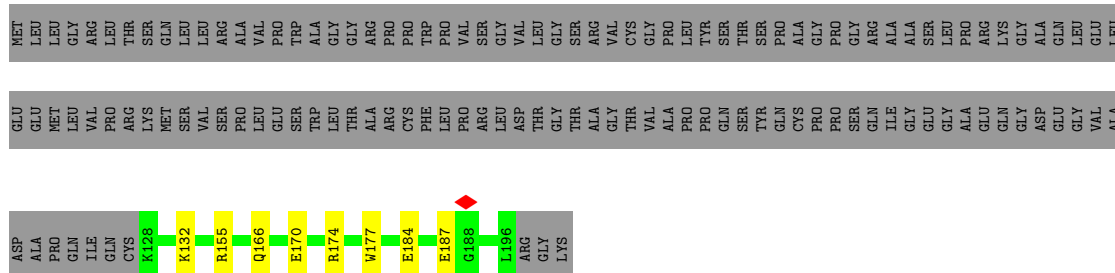




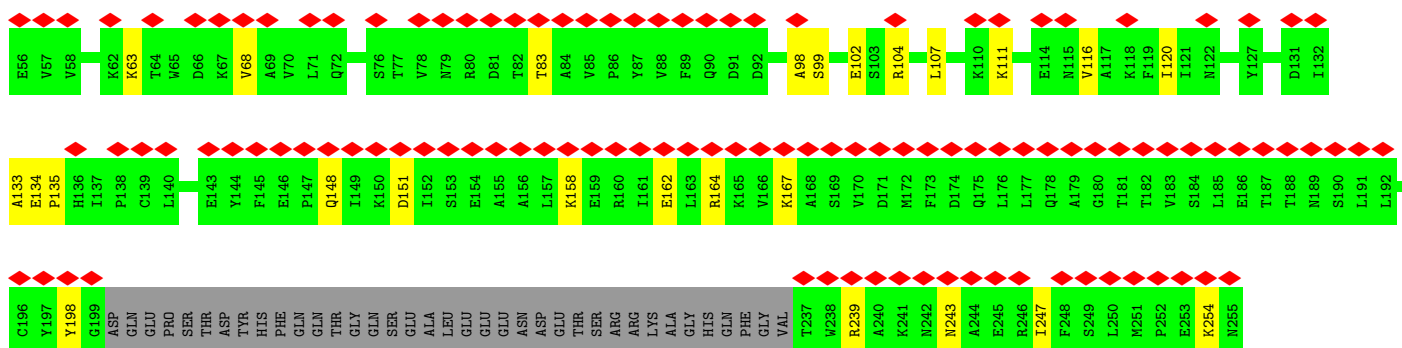
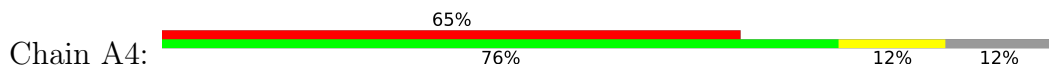
• Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

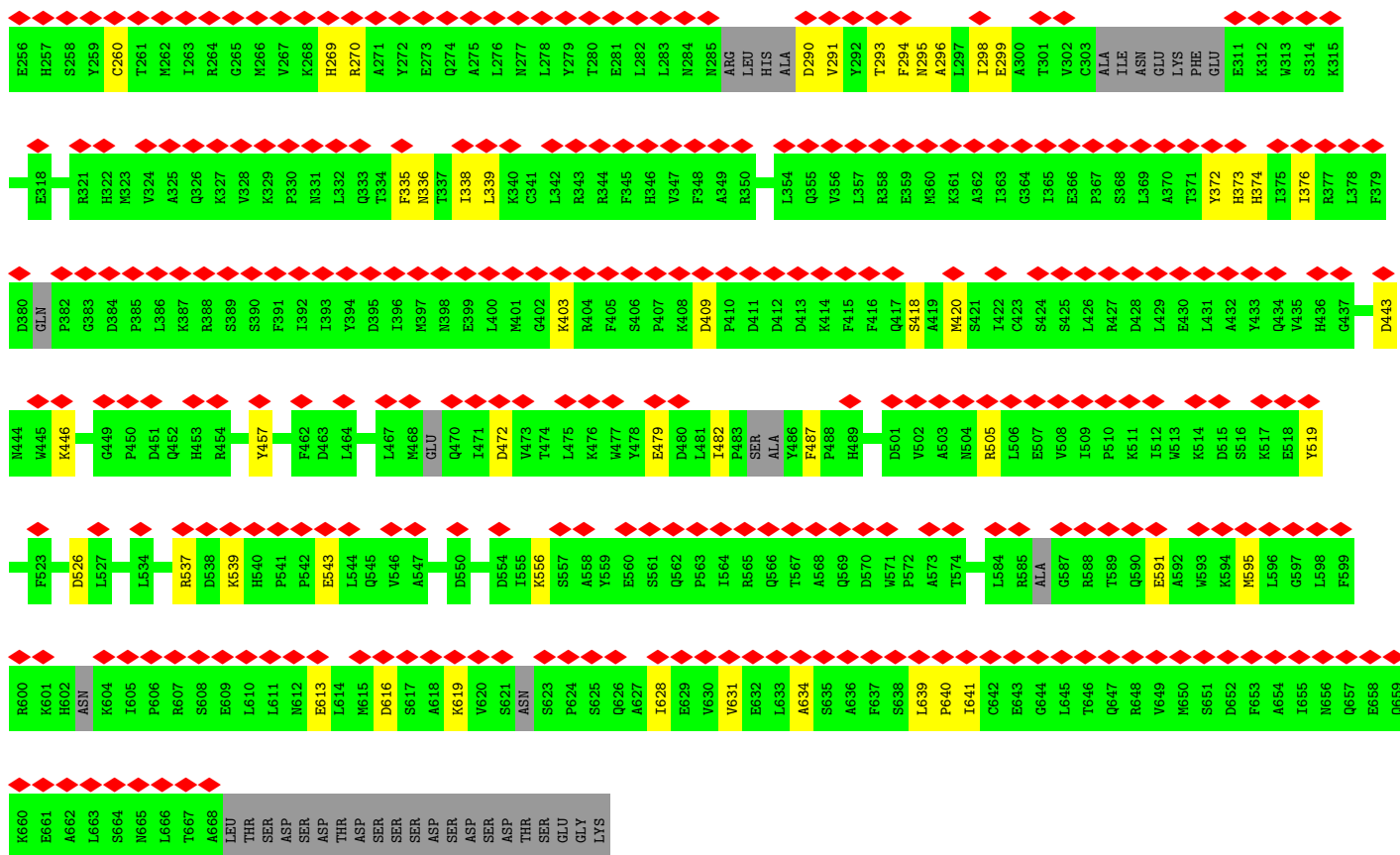


• Molecule 15: Aurora kinase A-interacting protein

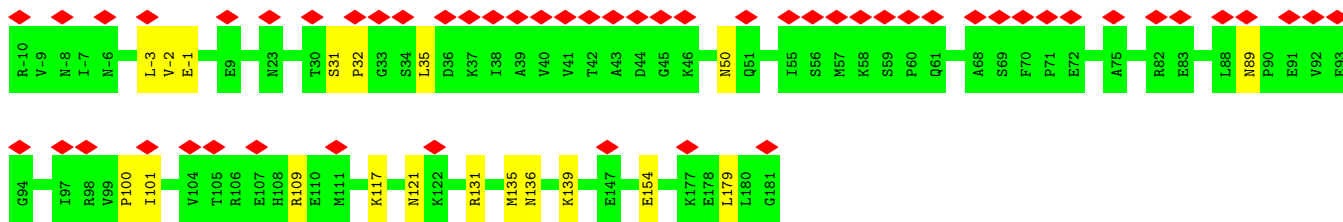
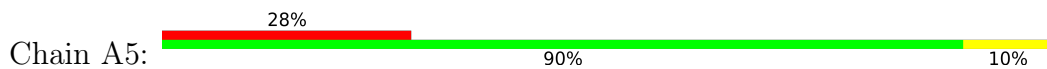


• Molecule 16: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

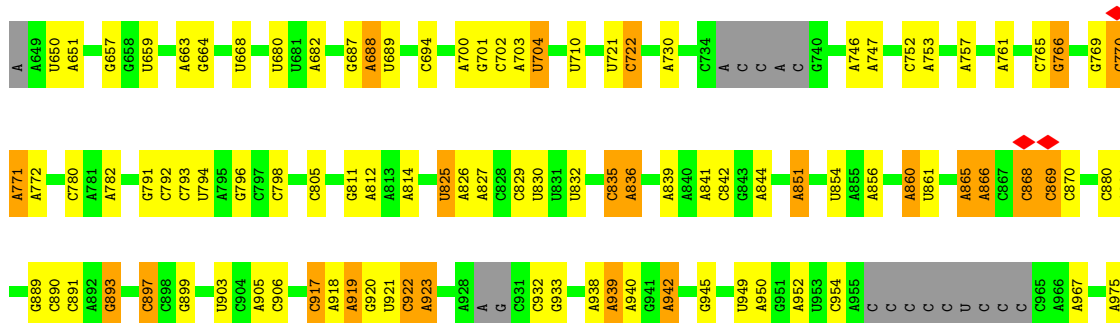


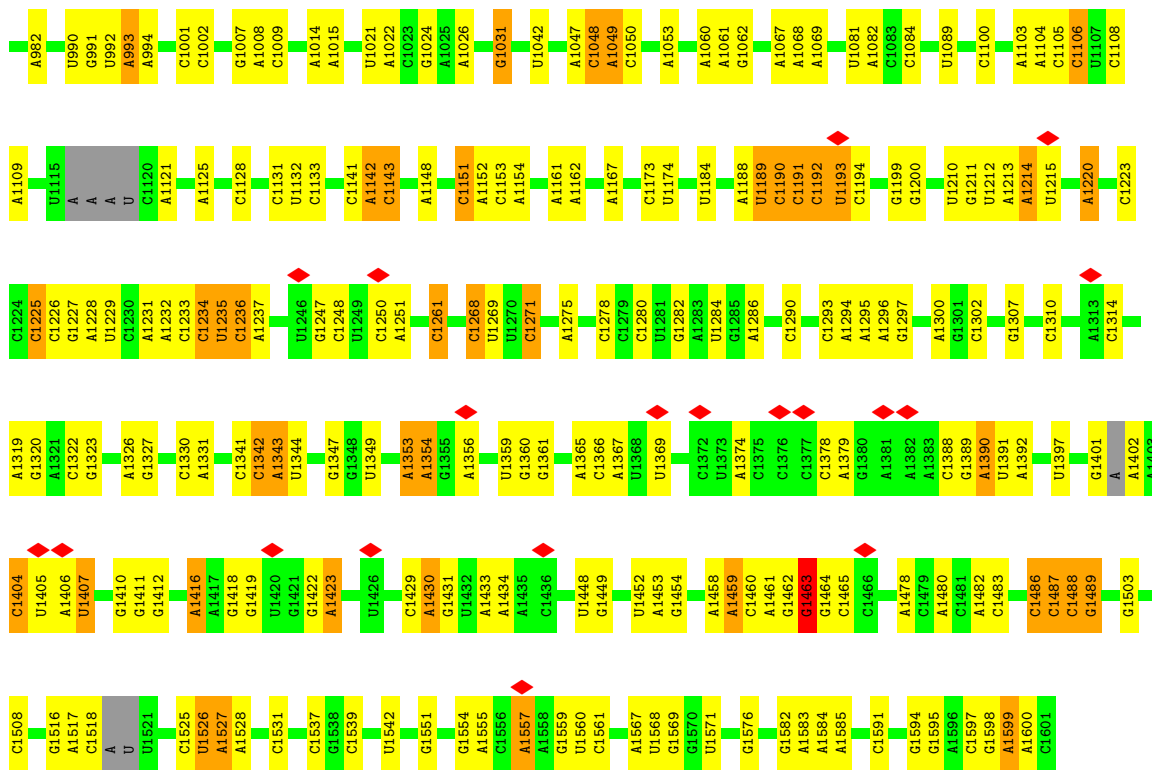


• Molecule 17: Ribosome-recycling factor, mitochondrial

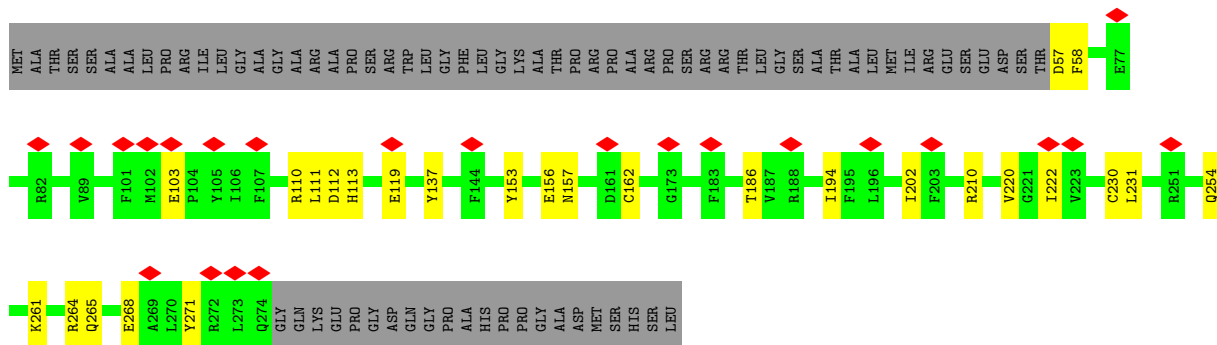


• Molecule 18: 12S rRNA

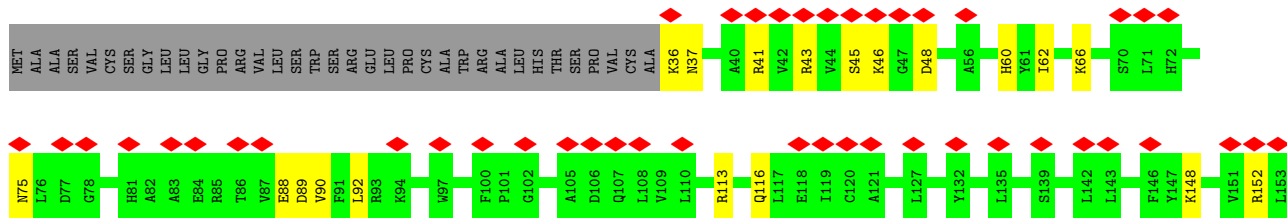




• Molecule 19: 28S ribosomal protein S2, mitochondrial

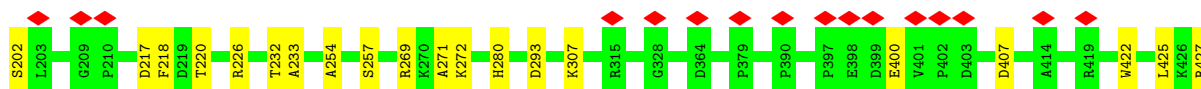
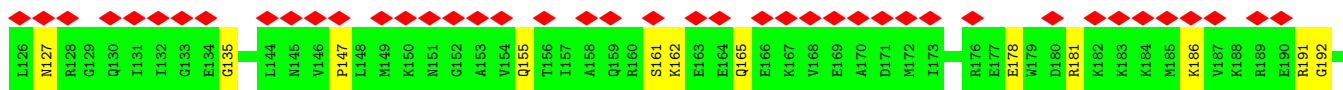
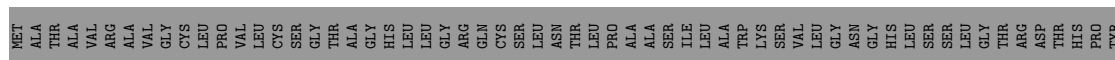
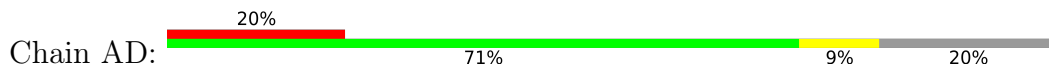


• Molecule 20: 28S ribosomal protein S24, mitochondrial

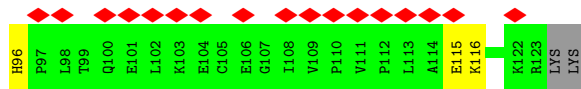
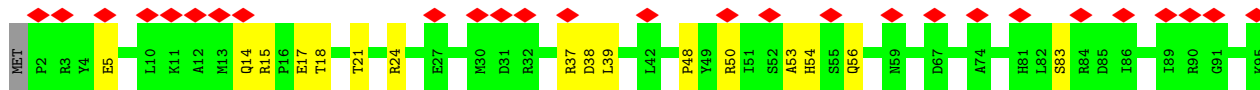
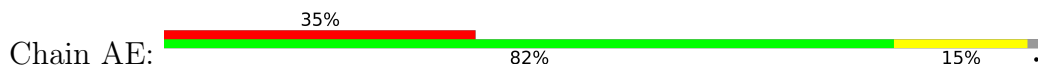




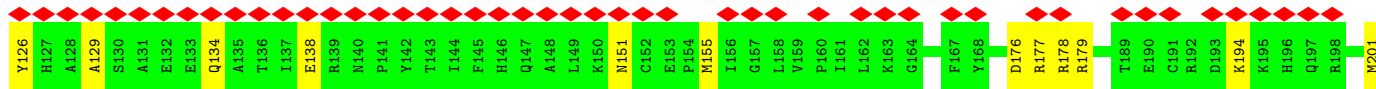
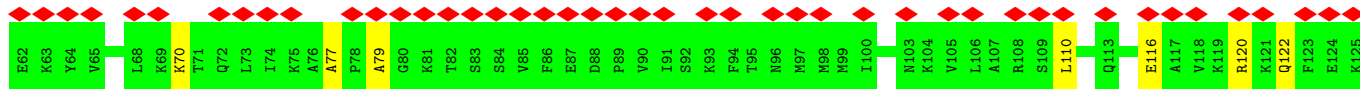
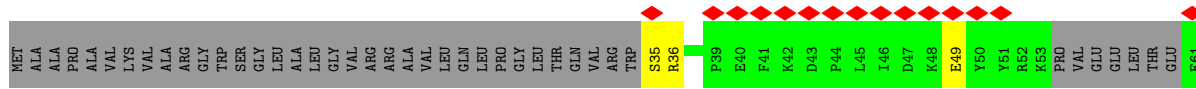
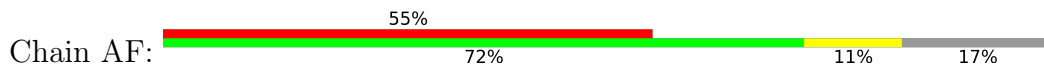
• Molecule 21: 28S ribosomal protein S5, mitochondrial

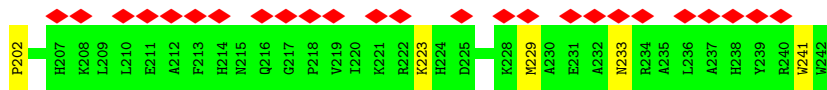


• Molecule 22: 28S ribosomal protein S6, mitochondrial

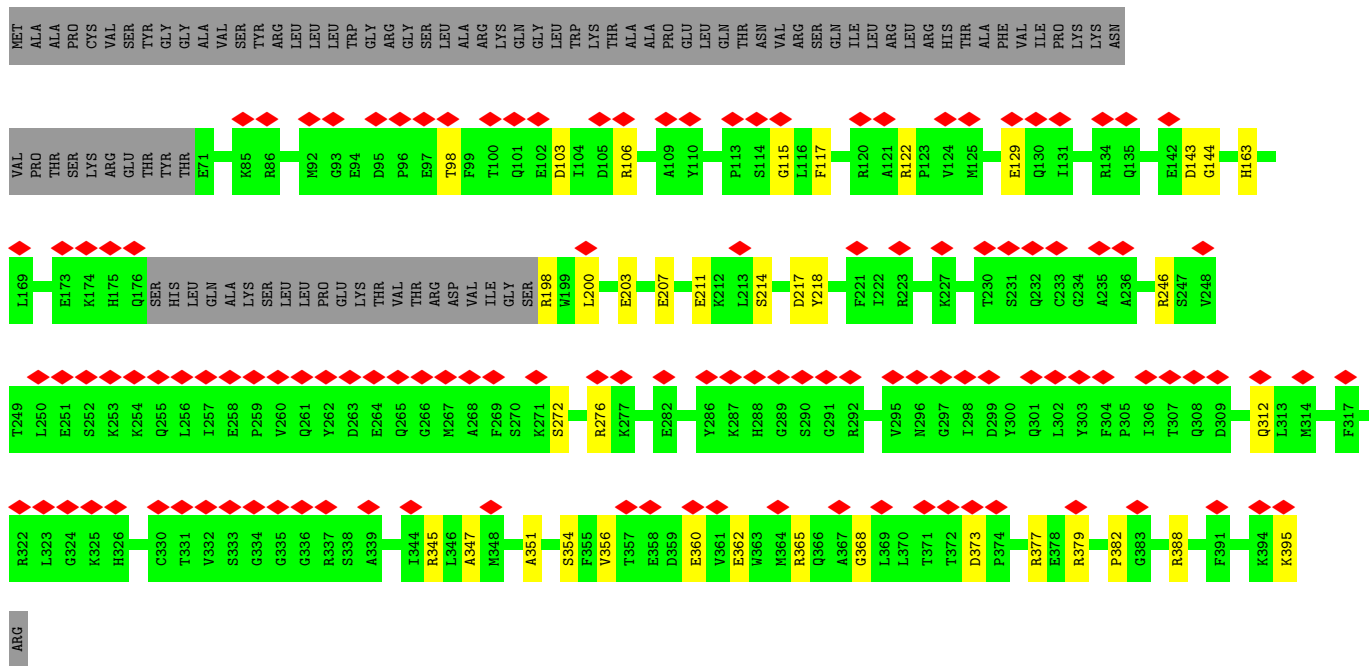


• Molecule 23: 28S ribosomal protein S7, mitochondrial

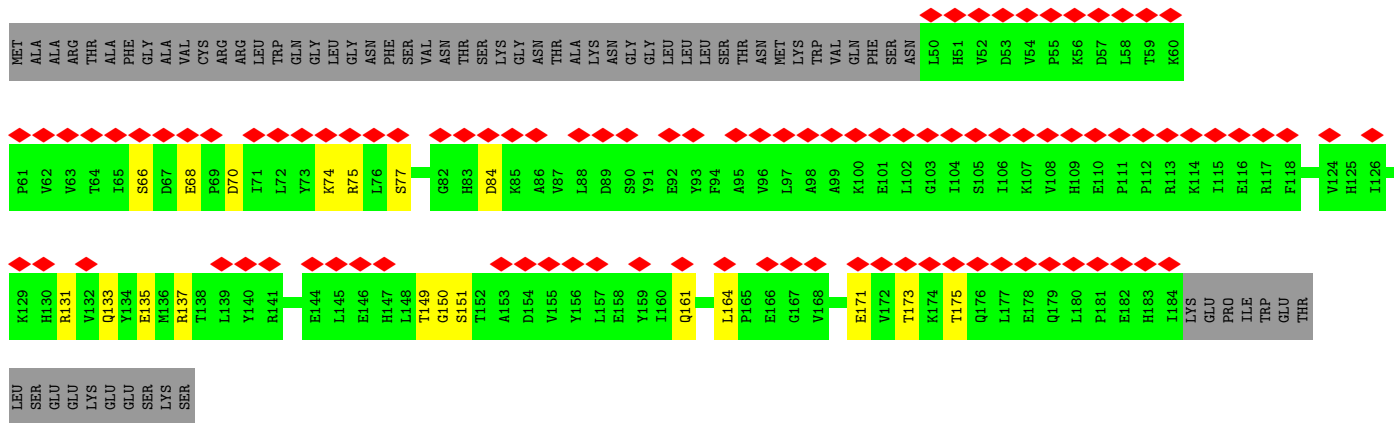




• Molecule 24: 28S ribosomal protein S9, mitochondrial

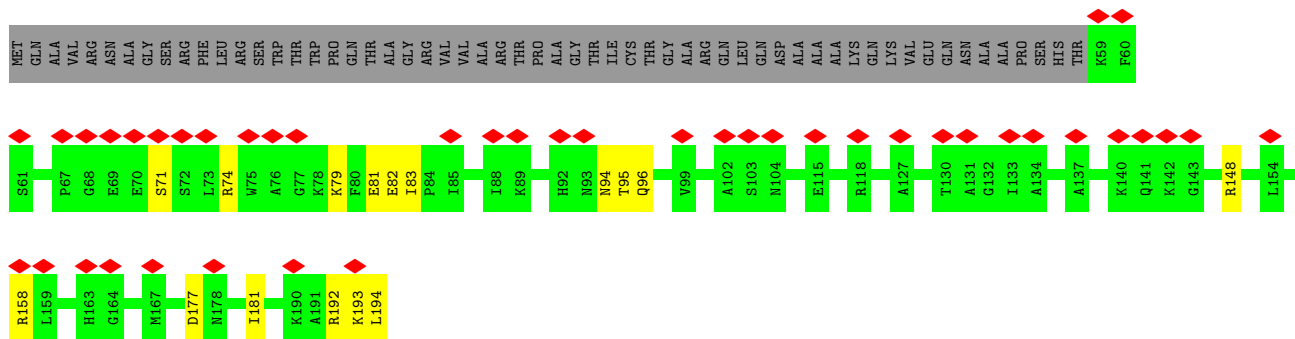


• Molecule 25: 28S ribosomal protein S10, mitochondrial

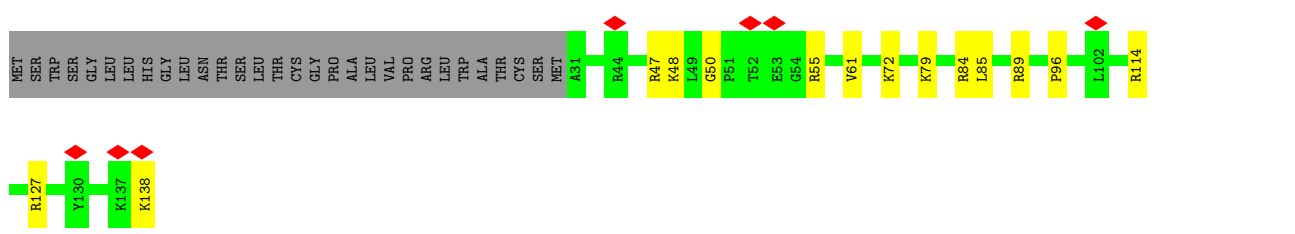


• Molecule 26: 28S ribosomal protein S11, mitochondrial

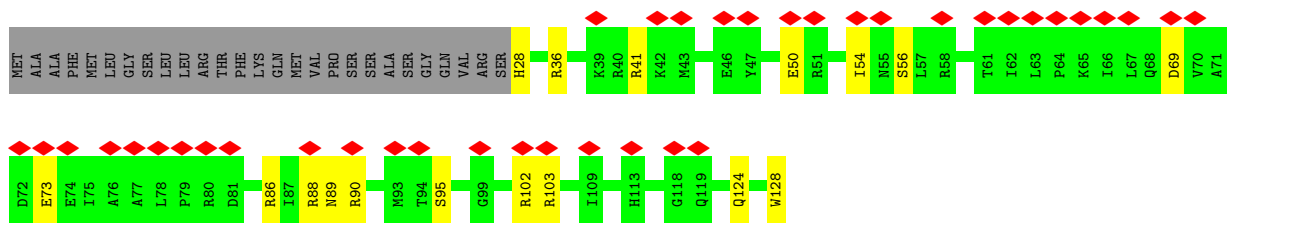




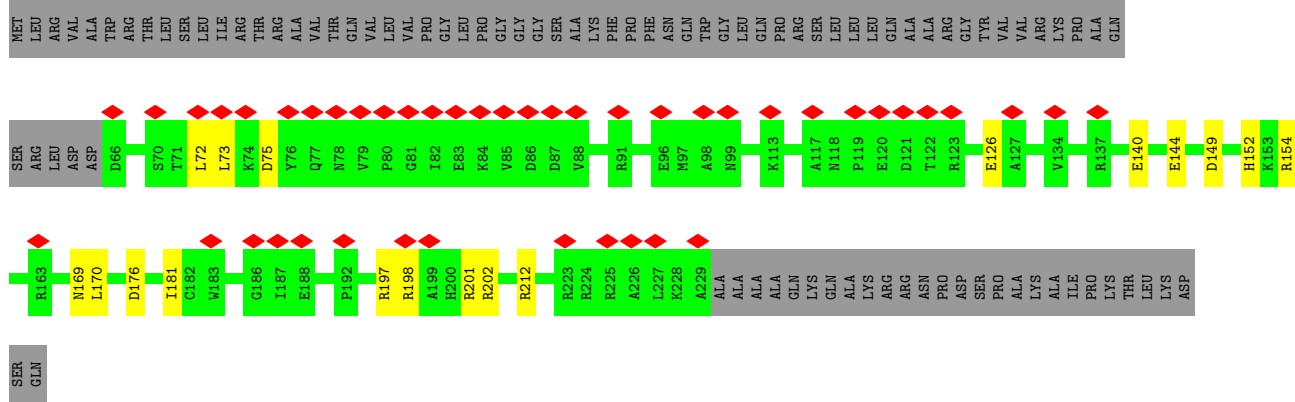
• Molecule 27: 28S ribosomal protein S12, mitochondrial



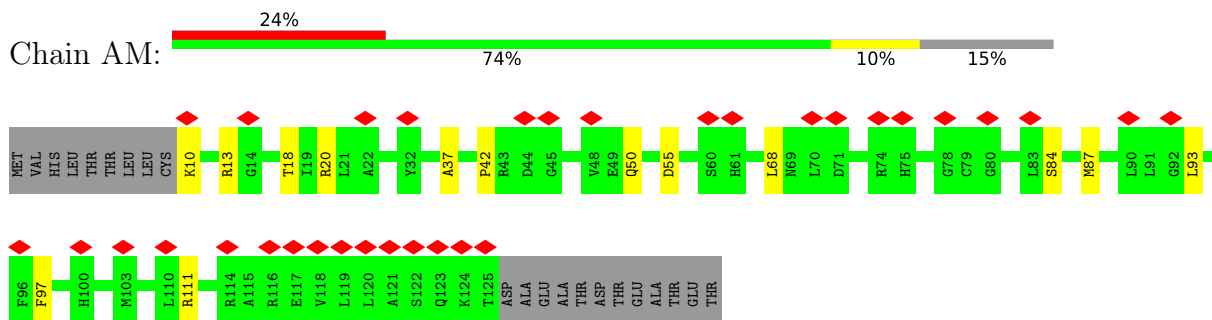
• Molecule 28: 28S ribosomal protein S14, mitochondrial



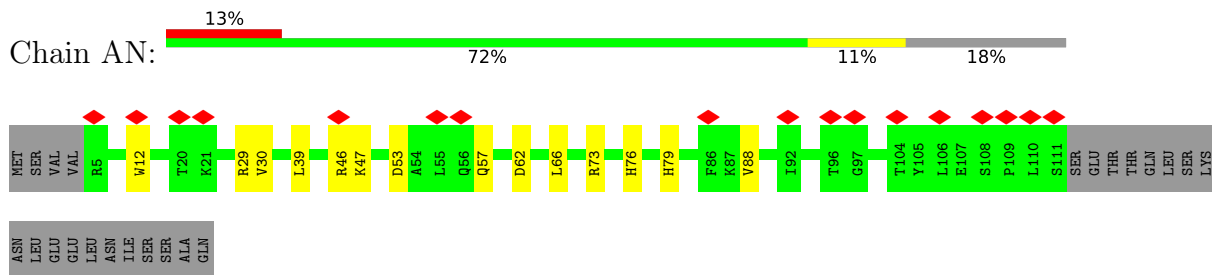
• Molecule 29: 28S ribosomal protein S15, mitochondrial



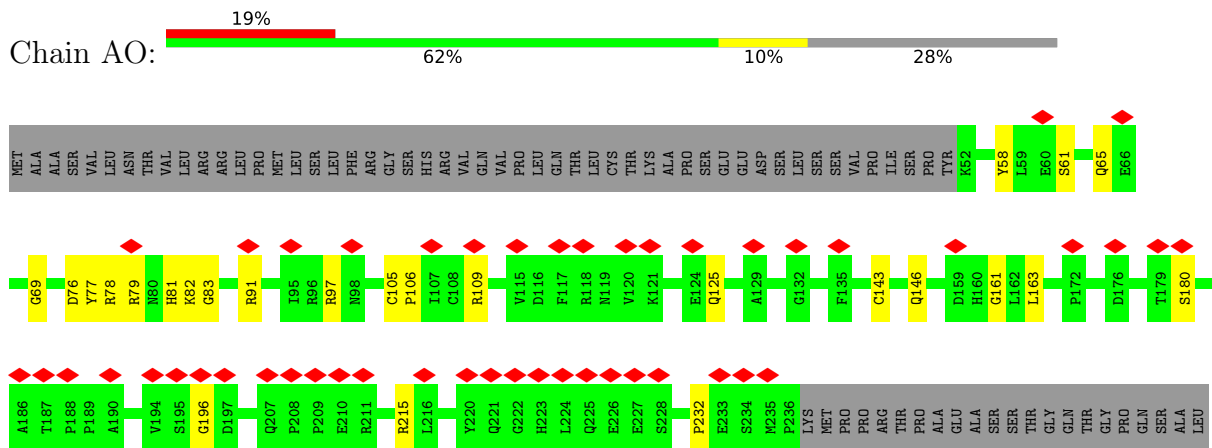
• Molecule 30: 28S ribosomal protein S16, mitochondrial



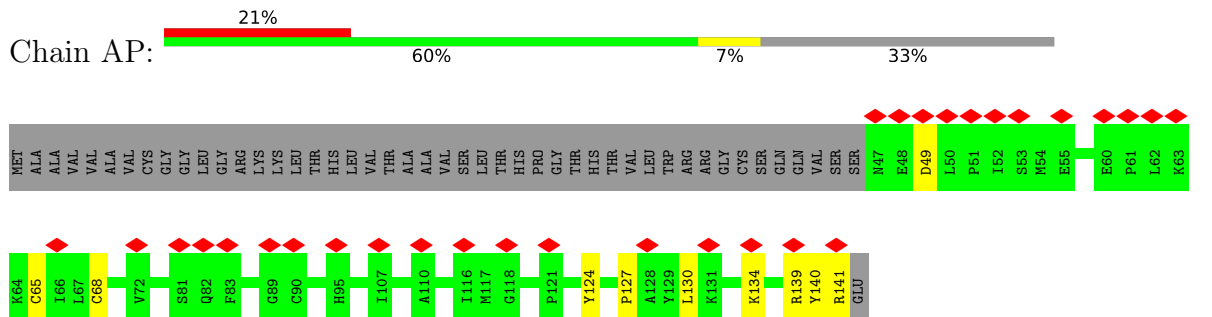
• Molecule 31: 28S ribosomal protein S17, mitochondrial



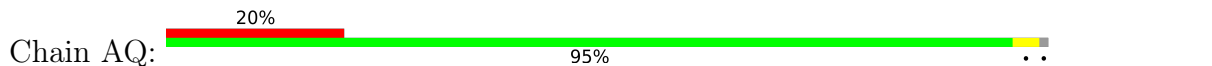
• Molecule 32: 28S ribosomal protein S18b, mitochondrial



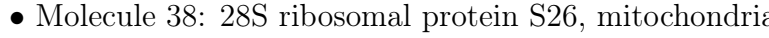
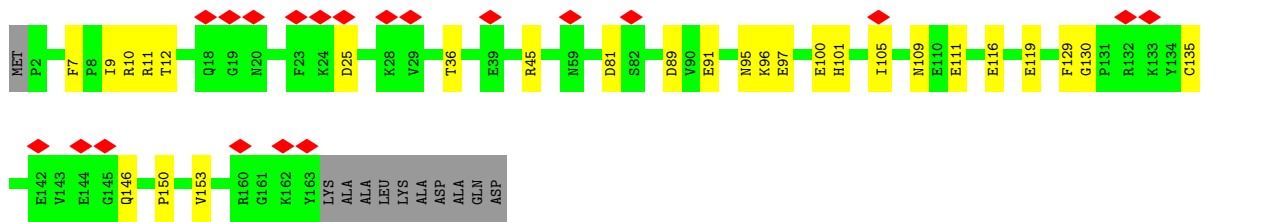
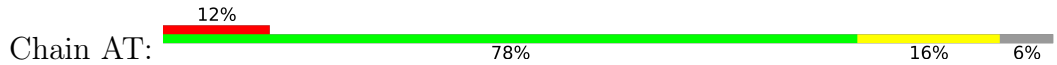
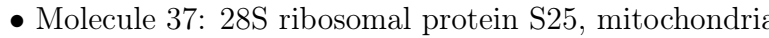
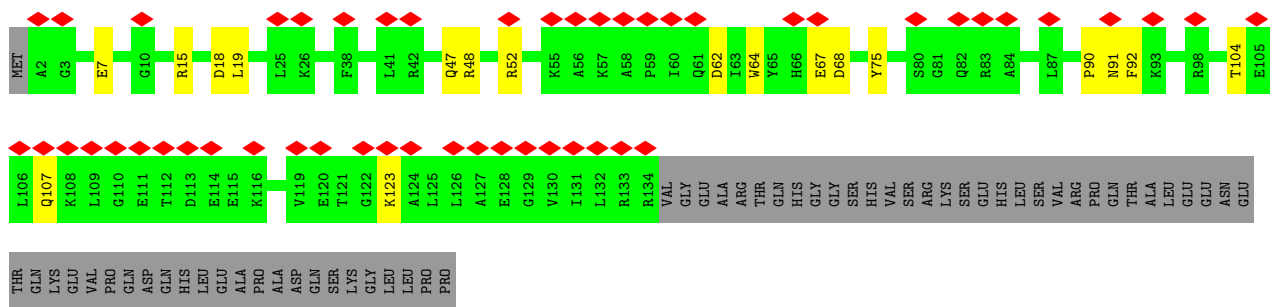
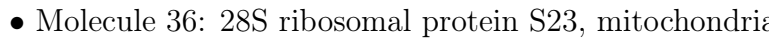
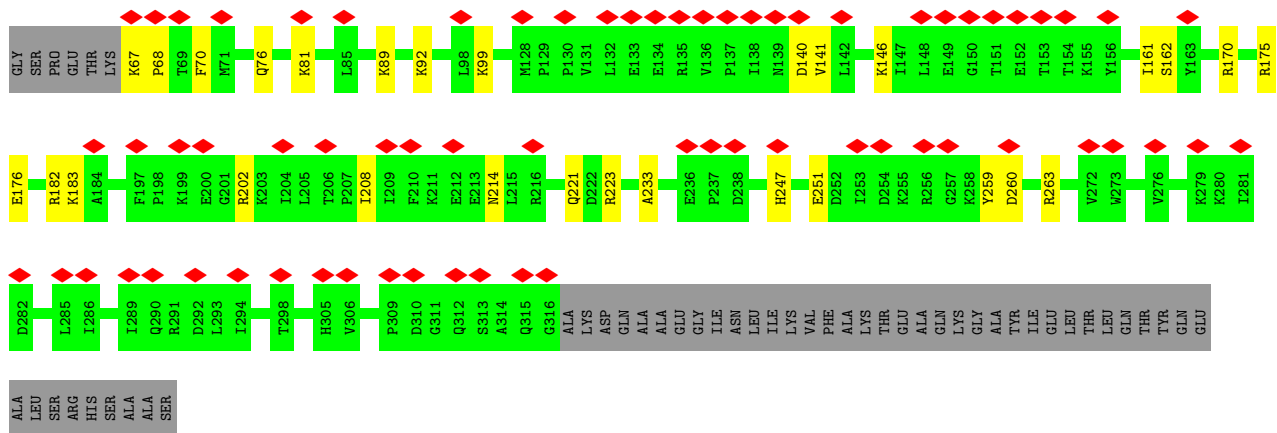
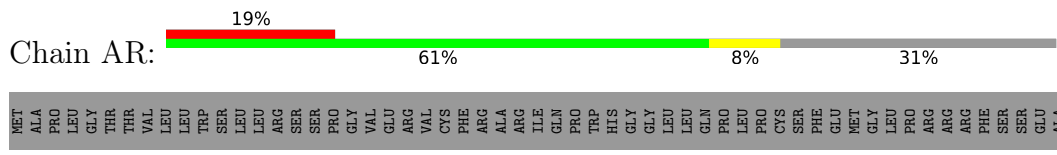
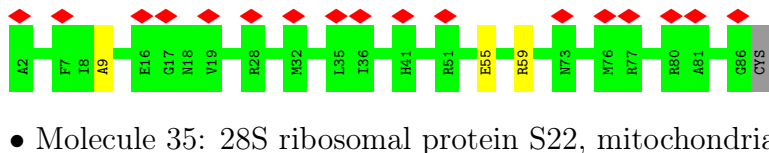
• Molecule 33: 28S ribosomal protein S18c, mitochondrial



• Molecule 34: 28S ribosomal protein S21, mitochondrial

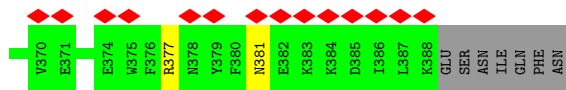




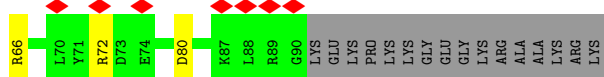
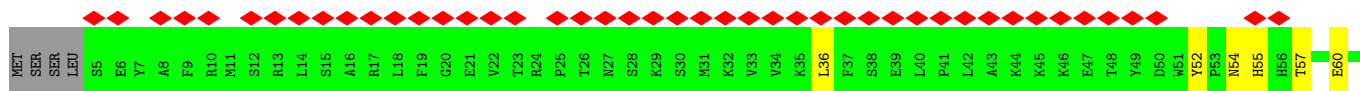
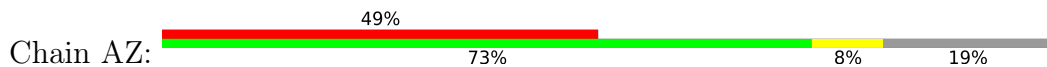








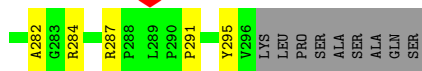
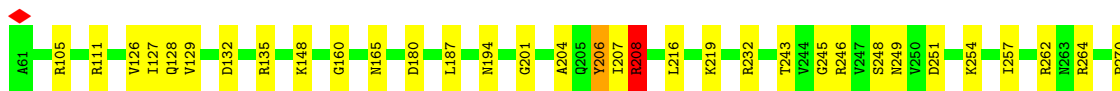
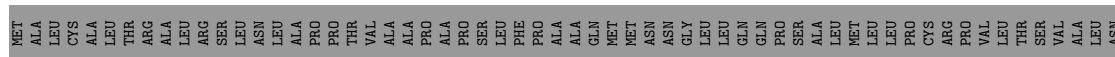
• Molecule 43: 28S ribosomal protein S33, mitochondrial



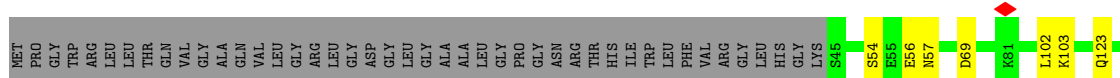
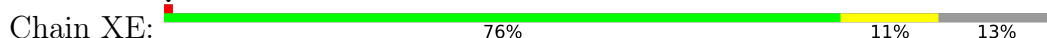
• Molecule 44: mt-tRNAVal



• Molecule 45: 39S ribosomal protein L2, mitochondrial



• Molecule 46: 39S ribosomal protein L3, mitochondrial




• Molecule 47: 39S ribosomal protein L4, mitochondrial





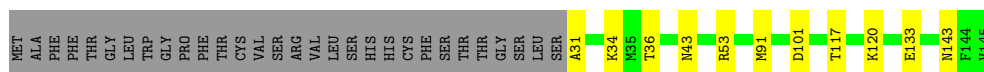
- Molecule 51: 39S ribosomal protein L13, mitochondrial

Chain XK:  89% 11%




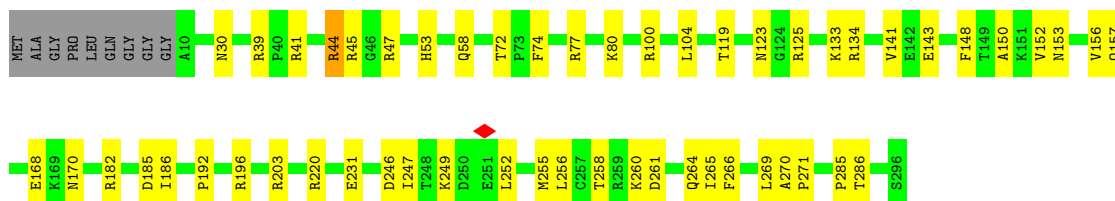
- Molecule 52: 39S ribosomal protein L14, mitochondrial

Chain XL:  72% 8% 21%




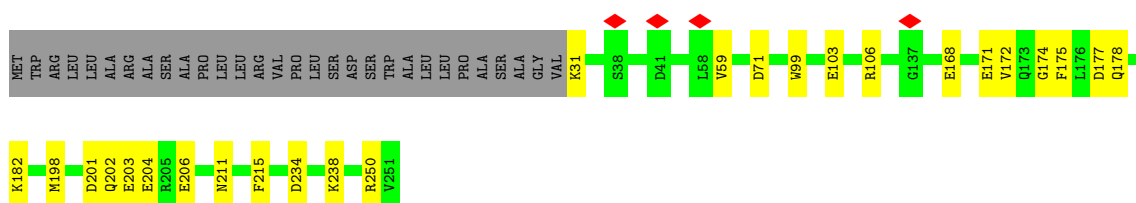
- Molecule 53: 39S ribosomal protein L15, mitochondrial

Chain XM:  79% 18%



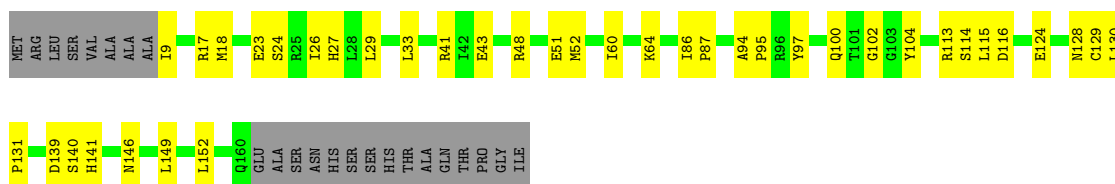
- Molecule 54: 39S ribosomal protein L16, mitochondrial

Chain XN:  78% 10% 12%



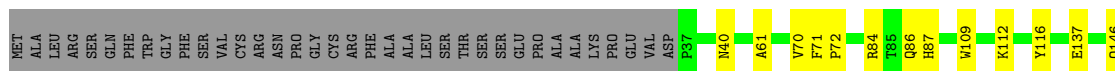
- Molecule 55: 39S ribosomal protein L17, mitochondrial

Chain XO:  65% 22% 13%

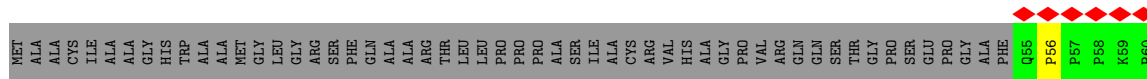


- Molecule 56: Mitochondrial ribosomal protein L18, isoform CRA\_b

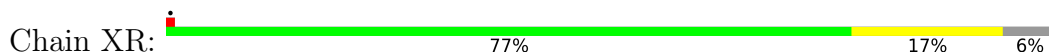
Chain XP:  72% 8% 20%



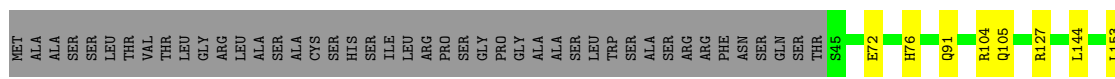
- Molecule 57: 39S ribosomal protein L19, mitochondrial



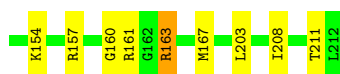
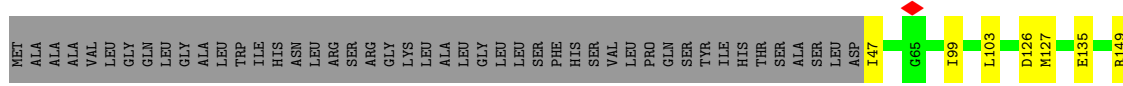
- Molecule 58: 39S ribosomal protein L20, mitochondrial




- Molecule 59: 39S ribosomal protein L21, mitochondrial

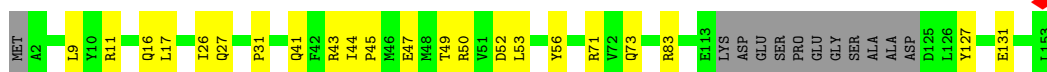


- Molecule 60: 39S ribosomal protein L22, mitochondrial




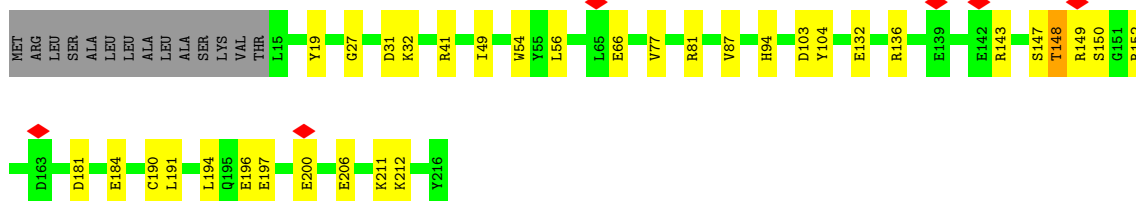
- Molecule 61: 39S ribosomal protein L23, mitochondrial

Chain XU:  78% 14% 8%



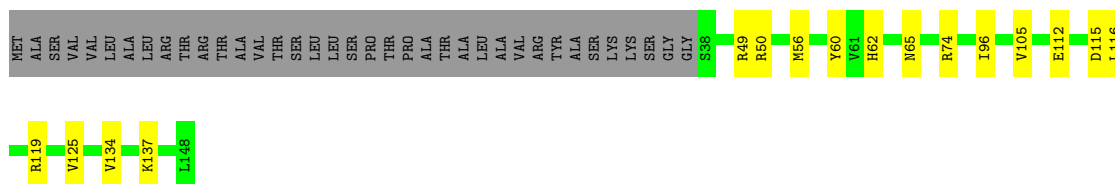
- Molecule 62: 39S ribosomal protein L24, mitochondrial

Chain XV:  78% 15% 6%




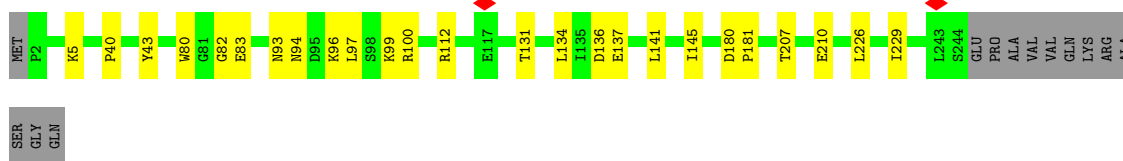
- Molecule 63: 39S ribosomal protein L27, mitochondrial

Chain XW:  64% 11% 25%



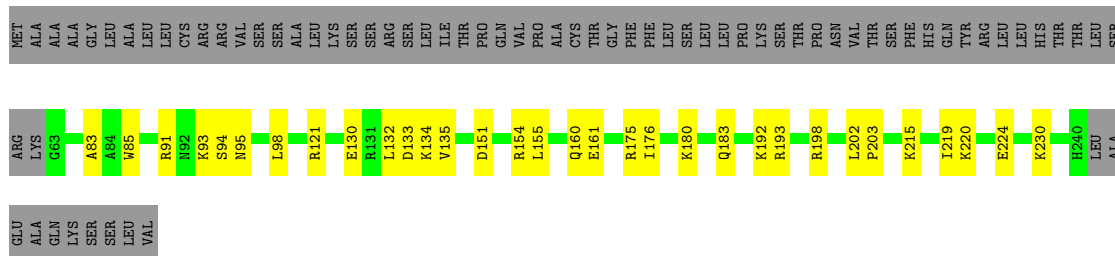
- Molecule 64: 39S ribosomal protein L28, mitochondrial

Chain XX:  85% 10% 5%



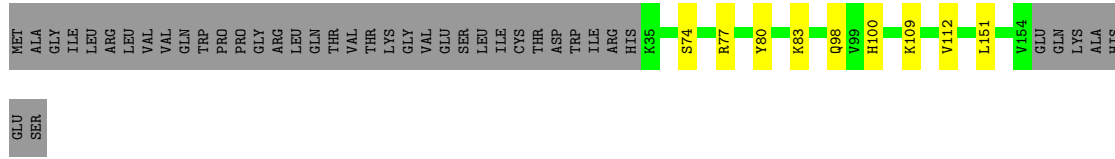
- Molecule 65: 39S ribosomal protein L47, mitochondrial

Chain XY:  58% 13% 29%

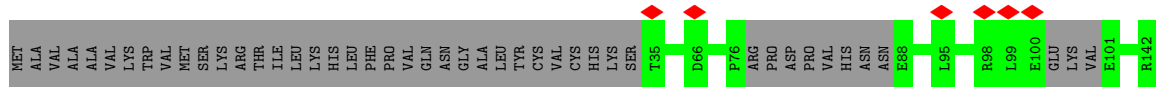


- Molecule 66: 39S ribosomal protein L30, mitochondrial

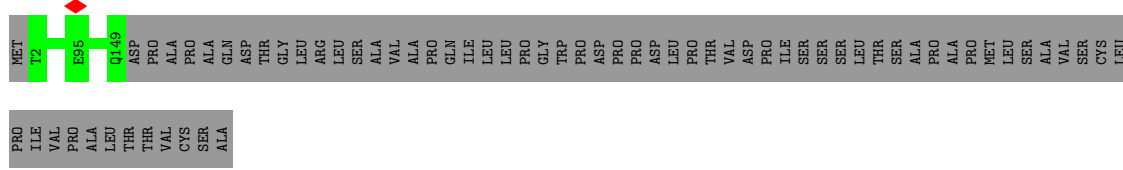




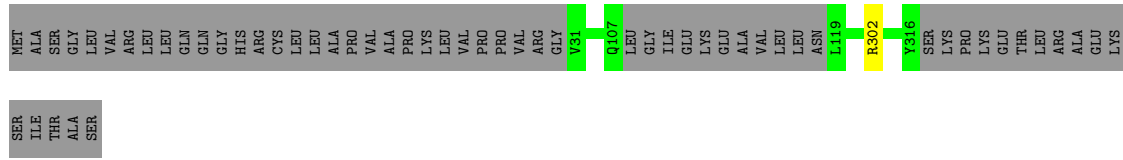
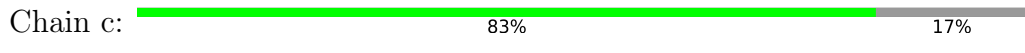
- Molecule 67: 39S ribosomal protein L42, mitochondrial



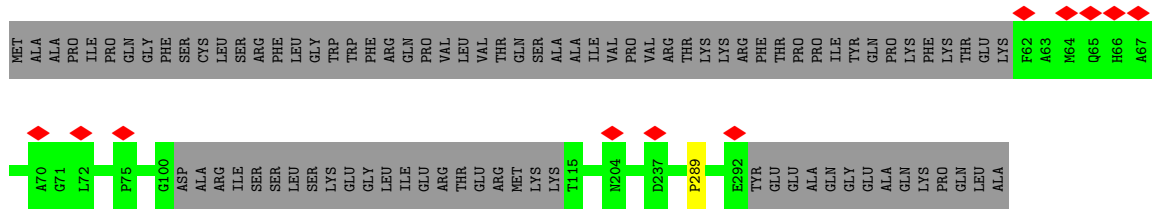
- Molecule 68: 39S ribosomal protein L43, mitochondrial



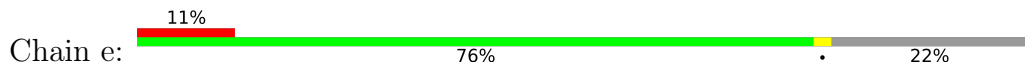
- Molecule 69: 39S ribosomal protein L44, mitochondrial

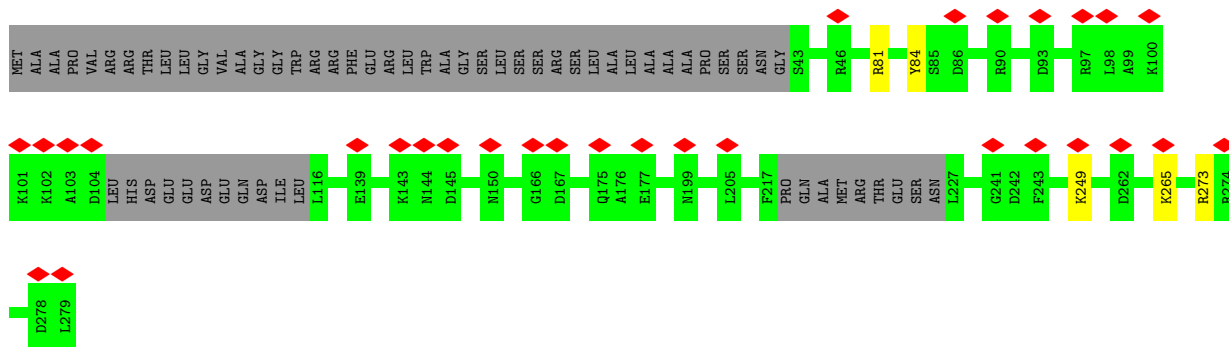


- Molecule 70: 39S ribosomal protein L45, mitochondrial

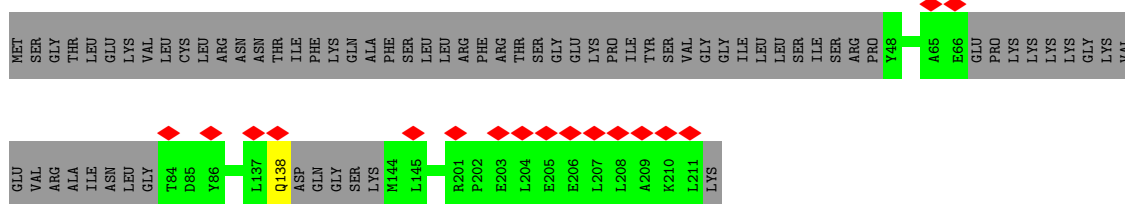


- Molecule 71: 39S ribosomal protein L46, mitochondrial

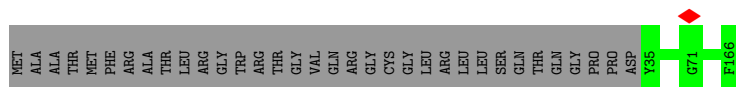
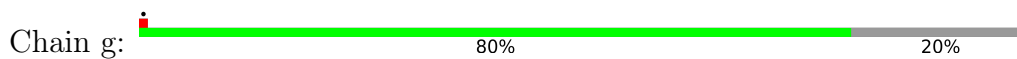




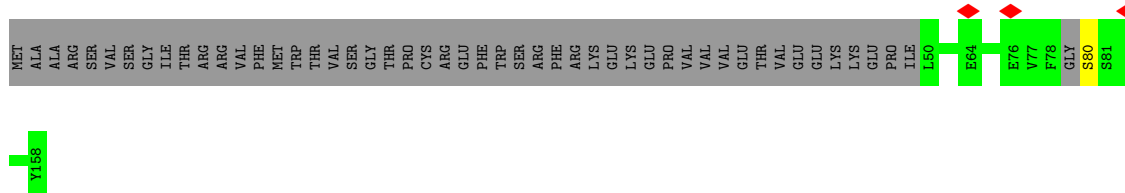
- Molecule 72: 39S ribosomal protein L48, mitochondrial



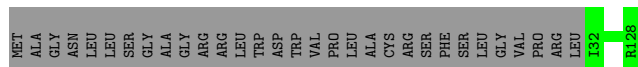
- Molecule 73: 39S ribosomal protein L49, mitochondrial



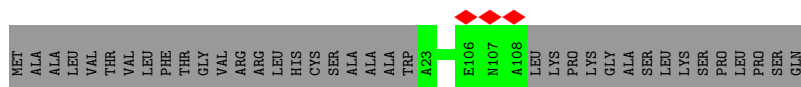
- Molecule 74: 39S ribosomal protein L50, mitochondrial



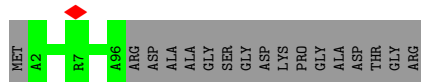
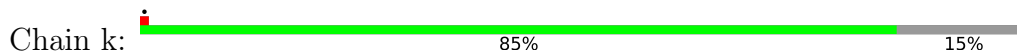
- Molecule 75: 39S ribosomal protein L51, mitochondrial



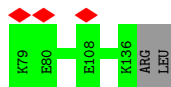
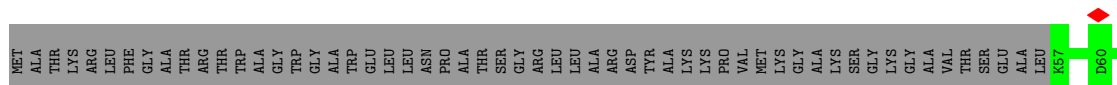
- Molecule 76: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA



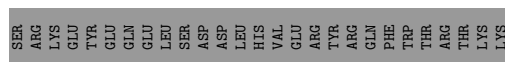
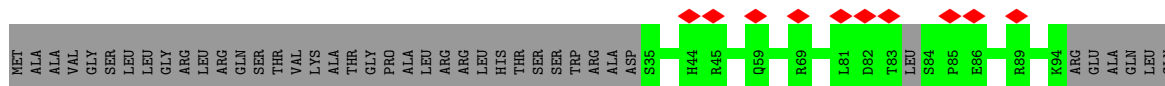
• Molecule 77: 39S ribosomal protein L53, mitochondrial



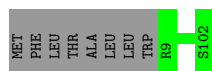
• Molecule 78: 39S ribosomal protein L54, mitochondrial



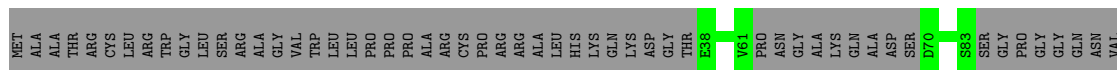
• Molecule 79: 39S ribosomal protein L55, mitochondrial

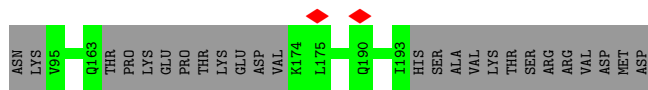


• Molecule 80: Ribosomal protein 63, mitochondrial

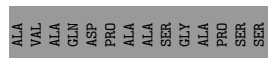
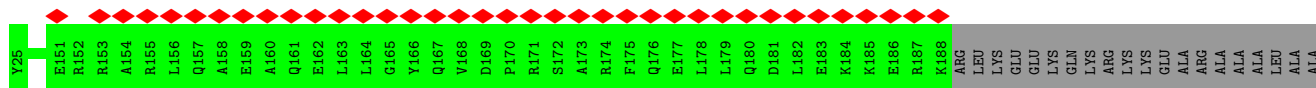
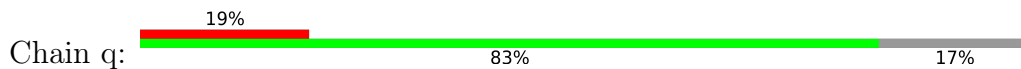


• Molecule 81: Peptidyl-tRNA hydrolase ICT1, mitochondrial

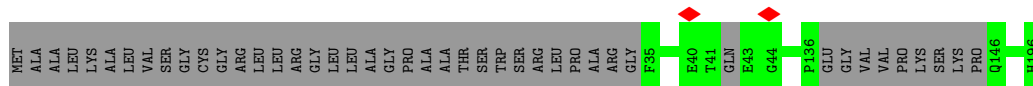
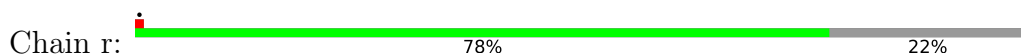




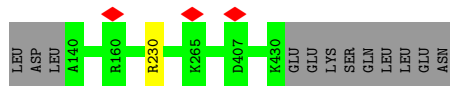
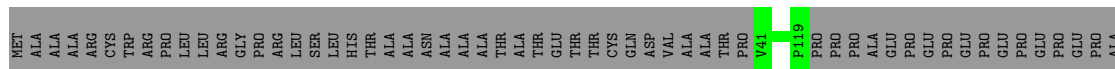
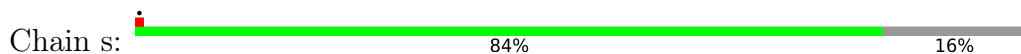
- Molecule 82: Growth arrest and DNA damage-inducible proteins-interacting protein 1



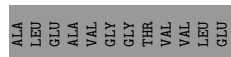
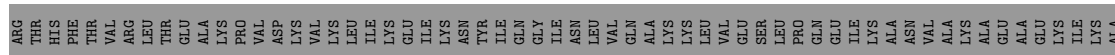
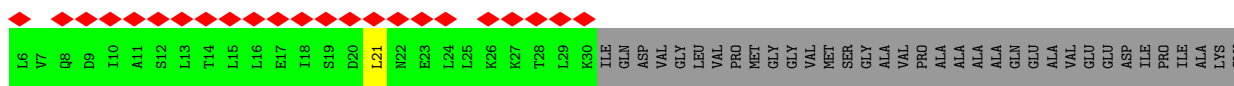
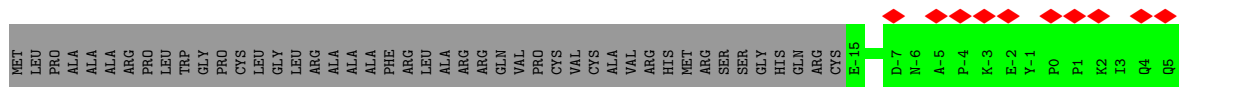
- Molecule 83: 39S ribosomal protein S18a, mitochondrial



- Molecule 84: 39S ribosomal protein S30, mitochondrial

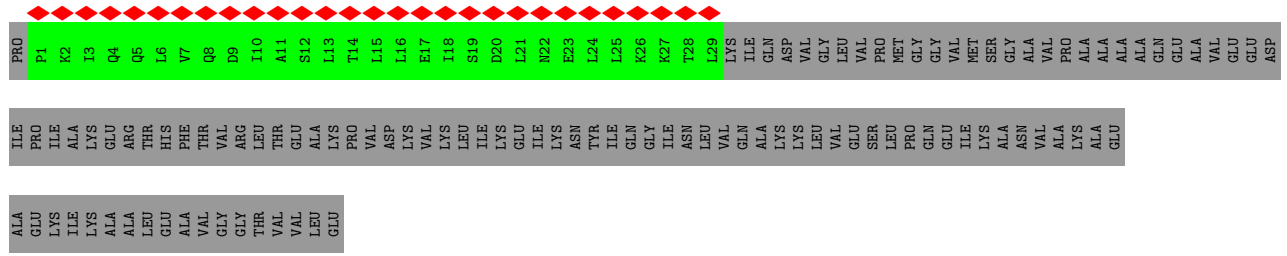


- Molecule 85: 39S ribosomal protein L12, mitochondrial

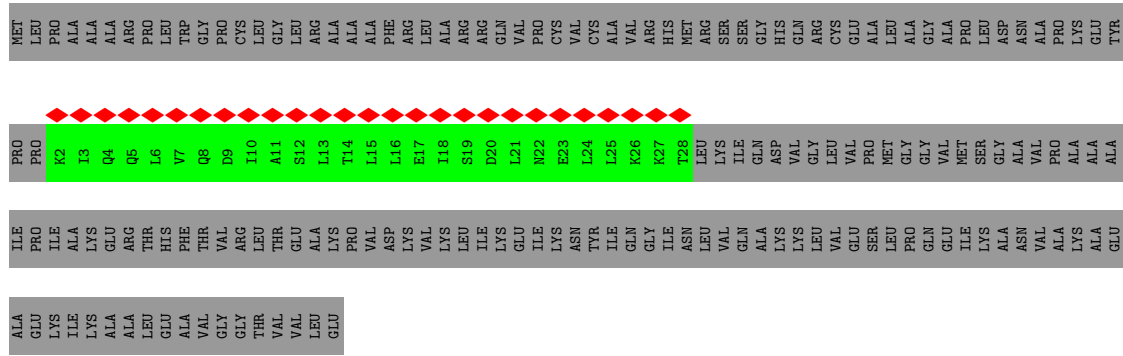


- Molecule 85: 39S ribosomal protein L12, mitochondrial

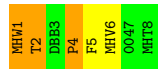
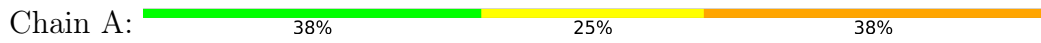




• Molecule 85: 39S ribosomal protein L12, mitochondrial



• Molecule 86: Quinupristin



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14502	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.154	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: MG, GTP, ZN, MHV, MHU, 004, MHW, DOL, DBB, MHT

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	0.31	0/895	0.46	0/1201
2	1	0.26	0/444	0.46	0/591
3	2	0.36	0/382	0.46	0/507
4	3	0.35	0/852	0.45	0/1136
5	4	0.32	0/349	0.46	0/461
6	5	0.27	0/3299	0.43	0/4495
7	6	0.28	0/3040	0.43	0/4134
8	7	0.26	0/2420	0.42	0/3270
9	8	1.83	1/1164 (0.1%)	0.46	2/1566 (0.1%)
10	9	0.29	0/1024	0.42	0/1379
11	XA	0.40	0/35662	0.80	13/55502 (0.0%)
12	A0	0.23	0/1727	0.42	0/2338
13	A1	0.24	0/2276	0.40	0/3079
14	A2	0.24	0/939	0.41	0/1256
15	A3	0.26	0/621	0.43	0/820
16	A4	0.24	0/4615	0.41	0/6228
17	A5	0.24	0/1497	0.40	0/2013
18	AA	0.21	0/22022	0.76	11/34275 (0.0%)
19	AB	0.24	0/1819	0.41	0/2462
20	AC	0.24	0/1112	0.41	0/1505
21	AD	0.24	0/2768	0.42	0/3707
22	AE	0.24	0/989	0.44	0/1335
23	AF	0.24	0/1708	0.39	0/2291
24	AG	0.25	0/2559	0.40	0/3429
25	AH	0.23	0/1128	0.42	0/1529
26	AI	0.25	0/1031	0.42	0/1390
27	AJ	0.25	0/854	0.46	0/1148
28	AK	0.22	0/879	0.40	0/1182
29	AL	0.25	0/1406	0.39	0/1878
30	AM	0.25	0/941	0.42	0/1265
31	AN	0.25	0/864	0.44	0/1169
32	AO	0.24	0/1580	0.39	0/2150



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	AP	0.25	0/782	0.38	0/1050
34	AQ	0.23	0/746	0.42	0/993
35	AR	0.24	0/2103	0.40	0/2842
36	AS	0.25	0/1127	0.40	0/1518
37	AT	0.25	0/1361	0.41	0/1829
38	AU	0.23	0/1482	0.39	0/1987
39	AV	0.24	0/2925	0.42	0/3948
40	AW	0.25	0/778	0.43	0/1048
41	AX	0.24	0/2884	0.43	0/3903
42	AY	0.24	0/985	0.37	0/1329
43	AZ	0.24	0/748	0.38	0/1000
44	XB	0.21	0/1400	0.73	0/2168
45	XD	0.29	0/1879	0.46	0/2527
46	XE	0.32	0/2465	0.45	0/3344
47	XF	0.34	0/2071	0.47	0/2817
48	XH	0.26	0/798	0.44	0/1073
49	XI	0.26	0/1727	0.43	0/2340
50	XJ	0.24	0/1309	0.40	0/1764
51	XK	0.31	0/1495	0.44	0/2029
52	XL	0.29	0/904	0.44	0/1218
53	XM	0.31	0/2359	0.44	0/3185
54	XN	0.30	0/1825	0.45	0/2458
55	XO	0.29	0/1269	0.45	0/1708
56	XP	0.26	0/1190	0.44	0/1611
57	XQ	0.27	0/2026	0.44	0/2734
58	XR	0.36	0/1174	0.49	0/1572
59	XS	0.32	0/1311	0.47	0/1778
60	XT	0.33	0/1402	0.44	0/1886
61	XU	0.31	0/1200	0.43	0/1623
62	XV	0.28	0/1693	0.44	0/2297
63	XW	0.33	0/893	0.46	0/1204
64	XX	0.28	0/2090	0.41	0/2825
65	XY	0.28	0/1571	0.41	0/2106
66	XZ	0.32	0/1003	0.44	0/1354
67	a	0.29	0/838	0.45	0/1138
68	b	0.30	0/1202	0.48	0/1626
69	c	0.28	0/2264	0.43	0/3059
70	d	0.26	0/1811	0.43	0/2454
71	e	1.43	6/1797 (0.3%)	0.42	0/2422
72	f	0.27	0/1159	0.42	0/1565
73	g	0.30	0/1134	0.45	0/1547
74	h	0.26	0/905	0.43	0/1233
75	i	0.35	0/849	0.45	0/1135

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	j	0.28	0/703	0.42	0/947
77	k	0.24	0/743	0.44	0/1003
78	l	0.24	0/692	0.37	0/939
79	m	0.23	0/508	0.44	0/682
80	o	0.31	0/818	0.45	0/1097
81	p	0.24	0/1071	0.42	0/1433
82	q	0.26	0/1413	0.39	0/1906
83	r	0.30	0/1282	0.42	0/1734
84	s	0.29	0/3114	0.44	0/4225
85	t1	0.25	0/366	0.38	0/497
85	t2	0.22	0/238	0.38	0/319
85	t3	0.22	0/238	0.37	0/319
85	t4	0.23	0/229	0.37	0/308
85	t5	0.22	0/229	0.38	0/308
85	t6	0.22	0/213	0.38	0/286
86	A	4.68	2/13 (15.4%)	3.06	2/15 (13.3%)
All	All	0.36	9/177670 (0.0%)	0.58	28/251956 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
45	XD	0	1
49	XI	0	1
62	XV	0	1
71	e	0	1
72	f	0	1
74	h	0	1
86	A	1	0
All	All	1	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	99	ARG	CG-CD	61.78	3.06	1.51
71	e	84	TYR	CD2-CE2	31.82	1.87	1.39
71	e	84	TYR	CD1-CE1	31.25	1.86	1.39
71	e	84	TYR	CE2-CZ	21.80	1.66	1.38
71	e	84	TYR	CE1-CZ	21.25	1.66	1.38
71	e	84	TYR	CG-CD1	18.55	1.63	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	e	84	TYR	CG-CD2	17.19	1.61	1.39
86	A	4	PRO	CA-CB	-12.04	1.29	1.53
86	A	4	PRO	N-CA	6.89	1.58	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	XA	2758	G	N3-C4-N9	-9.29	120.43	126.00
11	XA	2758	G	C5-C6-O6	7.38	133.03	128.60
11	XA	2789	C	C5-C4-N4	7.27	125.29	120.20
86	A	4	PRO	N-CA-CB	7.05	111.77	103.30
11	XA	2758	G	N3-C4-C5	6.88	132.04	128.60
18	AA	1488	C	OP1-P-OP2	-6.76	109.45	119.60
18	AA	1192	C	N3-C2-O2	-6.73	117.19	121.90
11	XA	2789	C	C6-N1-C1'	6.63	128.75	120.80
18	AA	1463	G	C5-C6-O6	6.62	132.57	128.60
86	A	4	PRO	CA-N-CD	-6.27	102.72	111.50
9	8	99	ARG	CG-CD-NE	5.79	123.97	111.80
11	XA	2758	G	N1-C6-O6	-5.75	116.45	119.90
18	AA	1561	C	N1-C2-O2	5.75	122.35	118.90
9	8	99	ARG	CB-CG-CD	5.74	126.51	111.60
18	AA	1561	C	N3-C2-O2	-5.72	117.90	121.90
11	XA	2789	C	C2-N1-C1'	-5.69	112.54	118.80
11	XA	2758	G	C6-C5-N7	5.69	133.81	130.40
18	AA	1191	C	N1-C2-O2	5.49	122.19	118.90
11	XA	2789	C	N3-C4-N4	-5.42	114.21	118.00
18	AA	1463	G	N1-C6-O6	-5.37	116.68	119.90
18	AA	765	C	C2-N1-C1'	5.35	124.69	118.80
11	XA	2758	G	N9-C4-C5	5.33	107.53	105.40
11	XA	2992	G	O5'-P-OP2	-5.28	100.95	105.70
11	XA	2758	G	C8-N9-C1'	5.23	133.80	127.00
18	AA	1463	G	N3-C4-N9	-5.16	122.90	126.00
11	XA	2758	G	C4-N9-C1'	-5.15	119.81	126.50
18	AA	1487	C	OP1-P-O3'	5.07	116.36	105.20
18	AA	1487	C	OP1-P-OP2	5.00	127.10	119.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
86	A	2	THR	CB

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	XD	206	TYR	Peptide
49	XI	197	LEU	Peptide
62	XV	148	THR	Peptide
71	e	265	LYS	Peptide
72	f	138	GLN	Peptide
74	h	80	SER	Peptide

## 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	880	902	902	16	0
2	1	439	480	480	4	0
3	2	376	406	406	8	0
4	3	831	883	883	15	0
5	4	341	361	361	3	0
6	5	3204	3201	3201	32	0
7	6	2947	2839	2839	38	0
8	7	2365	2373	2372	22	0
9	8	1140	1171	1171	8	0
10	9	996	987	987	12	0
11	XA	31875	16183	16192	283	0
12	A0	1684	1685	1685	15	0
13	A1	2230	2261	2261	24	0
14	A2	925	964	964	16	0
15	A3	610	682	682	6	0
16	A4	4521	4546	4545	46	0
17	A5	1489	1577	1577	11	0
18	AA	19690	9997	10003	163	0
19	AB	1776	1769	1769	19	0
20	AC	1082	1088	1088	17	0
21	AD	2716	2785	2785	25	0
22	AE	972	1001	1001	14	0
23	AF	1668	1716	1716	21	0
24	AG	2505	2492	2490	27	0
25	AH	1105	1136	1136	14	0
26	AI	1011	1052	1052	11	0
27	AJ	838	887	887	10	0
28	AK	861	885	885	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	AL	1382	1473	1472	13	0
30	AM	920	951	951	12	0
31	AN	846	908	908	11	0
32	AO	1528	1490	1490	20	0
33	AP	765	796	796	7	0
34	AQ	734	749	749	2	0
35	AR	2060	2074	2074	19	0
36	AS	1100	1103	1103	12	0
37	AT	1330	1343	1343	18	0
38	AU	1461	1471	1471	19	0
39	AV	2867	2862	2862	24	0
40	AW	766	785	785	9	0
41	AX	2814	2802	2802	23	0
42	AY	956	912	911	9	0
43	AZ	731	734	734	6	0
44	XB	1255	635	640	9	0
45	XD	1842	1896	1896	29	0
46	XE	2396	2402	2402	25	0
47	XF	2013	2045	2044	31	0
48	XH	784	832	832	10	0
49	XI	1691	1783	1783	16	0
50	XJ	1291	1367	1364	12	0
51	XK	1451	1448	1448	12	0
52	XL	889	941	941	8	0
53	XM	2305	2378	2378	37	0
54	XN	1778	1808	1808	21	0
55	XO	1245	1283	1283	25	0
56	XP	1164	1162	1162	14	0
57	XQ	1978	2022	2022	29	0
58	XR	1153	1214	1214	24	0
59	XS	1284	1354	1354	19	0
60	XT	1368	1410	1410	14	0
61	XU	1171	1164	1164	16	0
62	XV	1648	1656	1654	21	0
63	XW	871	898	898	10	0
64	XX	2035	2054	2054	20	0
65	XY	1534	1575	1575	26	0
66	XZ	978	1030	1030	7	0
67	a	813	777	777	0	0
68	b	1178	1180	1180	0	0
69	c	2217	2220	2220	0	0
70	d	1763	1747	1746	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	e	1762	1767	1767	0	0
72	f	1139	1152	1152	0	0
73	g	1097	1086	1085	0	0
74	h	882	867	867	0	0
75	i	827	857	857	0	0
76	j	689	678	678	0	0
77	k	732	745	745	0	0
78	l	673	654	653	0	0
79	m	500	525	525	0	0
80	o	797	804	804	0	0
81	p	1058	1083	1083	0	0
82	q	1379	1359	1359	0	0
83	r	1247	1267	1267	0	0
84	s	3036	3023	3022	0	0
85	t1	354	379	374	0	0
85	t2	238	268	270	0	0
85	t3	238	268	270	0	0
85	t4	229	255	257	0	0
85	t5	229	255	257	0	0
85	t6	214	236	236	0	0
86	A	73	67	64	2	0
87	0	1	0	0	0	0
87	4	1	0	0	0	0
87	AB	1	0	0	0	0
87	AO	1	0	0	0	0
87	AP	1	0	0	0	0
87	AT	1	0	0	0	0
87	r	1	0	0	0	0
88	2	1	0	0	0	0
88	9	1	0	0	0	0
88	AA	45	0	0	0	0
88	AH	1	0	0	0	0
88	XA	140	0	0	0	0
88	XD	1	0	0	0	0
88	XI	1	0	0	0	0
88	XM	2	0	0	0	0
88	XW	1	0	0	0	0
88	g	1	0	0	0	0
88	o	1	0	0	0	0
89	XA	48	50	50	4	0
90	AX	32	10	12	1	0
All	All	169107	144698	144704	1255	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 5.

All (1255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2721:G:O6	11:XA:2990:A:C6	1.84	1.30
11:XA:2724:G:OP1	47:XF:131:LYS:NZ	1.91	1.03
11:XA:3063:G:O2'	11:XA:3066:C:OP2	1.86	0.94
11:XA:2864:U:O5'	63:XW:50:ARG:NH1	2.04	0.91
11:XA:1777:A:N6	11:XA:1780:U:OP2	2.03	0.91
11:XA:1957:A:O4'	60:XT:163:ARG:NH1	2.04	0.91
11:XA:2721:G:O6	11:XA:2990:A:C5	2.23	0.90
18:AA:701:G:N2	18:AA:841:A:O2'	2.05	0.90
11:XA:1962:A:OP2	11:XA:2501:C:N4	2.05	0.89
49:XI:51:THR:O	54:XN:250:ARG:NH1	2.06	0.88
11:XA:2537:G:O2'	11:XA:2634:U:OP2	1.91	0.88
18:AA:826:A:OP1	27:AJ:55:ARG:NH1	2.07	0.87
30:AM:93:LEU:O	35:AR:175:ARG:NH2	2.08	0.87
45:XD:132:ASP:OD2	45:XD:135:ARG:NH1	2.08	0.86
11:XA:2517:U:OP1	45:XD:287:ARG:NH2	2.08	0.86
4:3:168:ARG:NH2	4:3:170:ASN:OD1	2.10	0.85
62:XV:184:GLU:O	65:XY:93:LYS:NZ	2.09	0.85
26:AI:71:SER:O	26:AI:74:ARG:NH1	2.09	0.85
7:6:27:ARG:N	11:XA:2832:A:N1	2.24	0.85
23:AF:79:ALA:O	24:AG:312:GLN:NE2	2.10	0.84
53:XM:72:THR:OG1	53:XM:77:ARG:NH2	2.11	0.84
4:3:179:LYS:O	7:6:370:ARG:NH2	2.11	0.84
1:0:84:ARG:NH2	11:XA:2306:A:O2'	2.10	0.83
11:XA:3068:G:N2	11:XA:3068:G:OP2	2.11	0.83
11:XA:2166:C:O2	11:XA:2214:A:N6	2.12	0.83
18:AA:1200:G:N2	18:AA:1418:G:O2'	2.12	0.83
57:XQ:70:GLU:OE2	57:XQ:213:GLN:NE2	2.12	0.83
11:XA:3082:G:N2	11:XA:3085:A:OP2	2.11	0.82
18:AA:860:A:N7	18:AA:919:A:O2'	2.12	0.82
27:AJ:84:ARG:NH1	27:AJ:85:LEU:O	2.12	0.82
11:XA:2987:U:O2'	11:XA:2991:U:OP1	1.97	0.82
15:A3:132:LYS:NZ	18:AA:939:A:OP1	2.13	0.82
11:XA:2191:A:N6	11:XA:2198:A:OP2	2.12	0.81
18:AA:1233:C:OP1	18:AA:1353:A:N6	2.12	0.81
38:AU:126:GLN:OE1	38:AU:129:ARG:NH2	2.13	0.81
11:XA:1696:C:OP2	65:XY:180:LYS:NZ	2.13	0.81
18:AA:825:U:N3	18:AA:827:A:OP1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AA:1141:C:O2	18:AA:1162:A:N6	2.14	0.81
12:A0:90:ASP:OD1	32:AO:215:ARG:NH1	2.13	0.81
11:XA:1882:A:N6	11:XA:1893:A:O4'	2.14	0.80
24:AG:103:ASP:OD1	24:AG:106:ARG:NH2	2.15	0.80
24:AG:198:ARG:N	24:AG:246:ARG:O	2.13	0.80
21:AD:127:ASN:O	43:AZ:72:ARG:NH1	2.15	0.80
11:XA:1674:A:N7	60:XT:47:ILE:N	2.29	0.79
54:XN:168:GLU:N	54:XN:171:GLU:OE2	2.15	0.79
19:AB:103:GLU:OE2	36:AS:52:ARG:NH2	2.15	0.79
25:AH:74:LYS:N	25:AH:175:THR:O	2.15	0.79
11:XA:1828:A:N6	11:XA:2683:C:O2	2.14	0.79
53:XM:185:ASP:OD1	53:XM:186:ILE:N	2.14	0.79
24:AG:276:ARG:NH1	24:AG:373:ASP:OD2	2.15	0.78
35:AR:176:GLU:OE2	35:AR:182:ARG:NE	2.17	0.78
14:A2:38:ARG:NH2	18:AA:1184:U:OP1	2.16	0.78
12:A0:49:ARG:NH2	38:AU:41:ARG:O	2.17	0.78
16:A4:336:ASN:ND2	16:A4:409:ASP:OD2	2.16	0.78
13:A1:169:ARG:O	13:A1:218:ASN:ND2	2.16	0.78
23:AF:126:TYR:O	23:AF:134:GLN:NE2	2.16	0.78
57:XQ:118:ARG:NH2	57:XQ:202:VAL:O	2.17	0.78
38:AU:138:GLU:OE2	38:AU:141:ARG:NH2	2.16	0.77
21:AD:178:GLU:OE2	21:AD:181:ARG:NH2	2.18	0.77
11:XA:2721:G:C6	11:XA:2990:A:C6	2.72	0.77
8:7:155:GLU:OE1	8:7:156:ARG:NH1	2.17	0.77
11:XA:1680:A:OP1	65:XY:230:LYS:NZ	2.17	0.77
15:A3:155:ARG:NH2	18:AA:1154:A:OP2	2.18	0.77
18:AA:1220:A:O2'	24:AG:395:LYS:O	2.01	0.77
18:AA:1557:A:O2'	27:AJ:72:LYS:NZ	2.18	0.77
32:AO:185:SER:O	35:AR:183:LYS:NZ	2.18	0.77
28:AK:41:ARG:NH2	28:AK:88:ARG:O	2.18	0.76
11:XA:1747:G:OP2	11:XA:1749:C:N4	2.17	0.76
18:AA:1429:C:O2	18:AA:1460:C:N4	2.18	0.76
38:AU:77:GLU:OE1	38:AU:81:LYS:NZ	2.18	0.76
7:6:367:ASP:OD1	7:6:370:ARG:NH1	2.18	0.76
21:AD:108:ALA:O	21:AD:114:ARG:NH1	2.19	0.76
10:9:22:THR:OG1	10:9:36:ARG:NH1	2.18	0.76
11:XA:1781:A:OP1	61:XU:83:ARG:NH2	2.18	0.76
11:XA:2039:A:N6	11:XA:2729:U:O2	2.18	0.76
13:A1:129:PHE:O	16:A4:63:LYS:NZ	2.18	0.76
11:XA:1689:C:OP2	64:XX:5:LYS:NZ	2.18	0.76
41:AX:53:GLU:N	41:AX:67:HIS:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:198:ALA:O	7:6:254:TYR:OH	2.03	0.75
30:AM:55:ASP:OD2	37:AT:146:GLN:NE2	2.18	0.75
18:AA:752:C:O2'	18:AA:793:C:N4	2.18	0.75
28:AK:90:ARG:NH2	28:AK:95:SER:O	2.19	0.75
51:XK:10:GLN:NE2	60:XT:203:LEU:O	2.19	0.75
54:XN:201:ASP:OD1	54:XN:202:GLN:N	2.20	0.75
11:XA:2563:U:OP1	45:XD:284:ARG:NH1	2.18	0.75
13:A1:163:VAL:O	42:AY:317:ASN:ND2	2.19	0.75
11:XA:2515:U:O2'	45:XD:282:ALA:O	2.05	0.75
2:1:23:GLU:N	2:1:23:GLU:OE1	2.20	0.75
7:6:368:ARG:NH2	11:XA:2859:A:OP2	2.20	0.74
23:AF:122:GLN:NE2	23:AF:138:GLU:O	2.20	0.74
16:A4:198:TYR:O	16:A4:239:ARG:NH1	2.20	0.74
24:AG:117:PHE:O	24:AG:122:ARG:NH1	2.20	0.74
11:XA:1672:C:O2'	60:XT:149:ARG:O	2.04	0.74
13:A1:312:TYR:OH	41:AX:338:ASP:O	2.04	0.74
59:XS:72:GLU:O	59:XS:76:HIS:ND1	2.20	0.74
41:AX:206:GLU:OE1	41:AX:249:ARG:NH1	2.20	0.74
18:AA:1429:C:OP1	24:AG:388:ARG:NH2	2.20	0.74
34:AQ:55:GLU:OE2	34:AQ:59:ARG:NE	2.20	0.74
11:XA:1958:G:OP2	60:XT:160:GLY:N	2.19	0.73
57:XQ:71:PRO:O	57:XQ:73:ARG:NH1	2.20	0.73
11:XA:2167:A:N6	11:XA:2212:C:OP2	2.21	0.73
61:XU:16:GLN:NE2	61:XU:17:LEU:O	2.22	0.73
17:A5:136:ASN:OD1	17:A5:139:LYS:NZ	2.21	0.73
14:A2:42:GLU:N	23:AF:241:TRP:O	2.22	0.73
11:XA:2248:U:OP1	58:XR:99:ARG:NH2	2.22	0.73
6:5:30:ALA:N	45:XD:201:GLY:O	2.22	0.73
22:AE:48:PRO:O	33:AP:124:TYR:OH	2.05	0.72
11:XA:3217:A:O4'	57:XQ:86:ARG:NH2	2.22	0.72
16:A4:269:HIS:O	16:A4:270:ARG:NE	2.22	0.72
18:AA:949:U:O3'	31:AN:29:ARG:NH1	2.23	0.72
6:5:33:TRP:O	6:5:39:ARG:NH2	2.22	0.72
60:XT:126:ASP:OD1	60:XT:127:MET:N	2.22	0.72
11:XA:1749:C:OP2	11:XA:2899:C:O2'	2.07	0.72
11:XA:1877:U:O3'	53:XM:30:ASN:ND2	2.22	0.72
18:AA:1014:A:O2'	18:AA:1031:G:O4'	2.07	0.72
4:3:175:ASP:O	4:3:178:GLN:NE2	2.23	0.72
18:AA:659:U:OP1	21:AD:226:ARG:NH2	2.21	0.72
57:XQ:252:GLN:OE1	57:XQ:253:GLN:NE2	2.23	0.72
50:XJ:154:ARG:NH1	50:XJ:155:VAL:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:191:ASN:ND2	56:XP:137:GLU:O	2.23	0.71
11:XA:1800:G:N1	11:XA:1803:A:OP2	2.23	0.71
11:XA:2714:A:OP2	46:XE:239:ARG:NH1	2.23	0.71
26:AI:158:ARG:NH2	26:AI:177:ASP:OD1	2.23	0.71
11:XA:2262:C:O2	59:XS:175:ARG:NH2	2.24	0.71
13:A1:100:GLU:O	20:AC:156:GLN:NE2	2.22	0.71
18:AA:722:C:N3	18:AA:798:C:O2'	2.23	0.71
49:XI:224:HIS:O	49:XI:228:GLN:N	2.24	0.71
11:XA:2744:U:O2	11:XA:2745:A:N6	2.24	0.71
18:AA:1231:A:O2'	18:AA:1236:C:N4	2.24	0.71
39:AV:189:CYS:SG	39:AV:277:ARG:NH1	2.64	0.71
11:XA:2721:G:O6	11:XA:2990:A:N1	2.24	0.71
18:AA:1454:G:OP2	24:AG:377:ARG:NH2	2.24	0.71
19:AB:111:LEU:O	19:AB:113:HIS:ND1	2.24	0.71
1:0:181:ARG:NH1	1:0:186:THR:O	2.24	0.70
11:XA:2139:U:OP2	66:XZ:74:SER:N	2.22	0.70
13:A1:81:VAL:O	13:A1:99:LYS:NZ	2.23	0.70
33:AP:140:TYR:O	33:AP:141:ARG:NE	2.24	0.70
47:XF:75:GLU:OE2	47:XF:210:ARG:NE	2.24	0.70
7:6:114:ARG:NH1	44:XB:1643:A:OP1	2.25	0.70
21:AD:111:LYS:O	21:AD:114:ARG:NH1	2.25	0.70
52:XL:31:ALA:N	52:XL:91:MET:SD	2.65	0.70
3:2:82:ARG:NH2	11:XA:1791:G:OP2	2.24	0.69
9:8:110:GLU:OE2	9:8:114:ARG:NE	2.24	0.69
11:XA:3220:A:OP1	46:XE:260:LYS:NZ	2.25	0.69
48:XH:103:GLU:OE1	48:XH:104:ASN:ND2	2.24	0.69
10:9:83:GLU:OE2	65:XY:91:ARG:NH2	2.24	0.69
47:XF:126:LYS:NZ	47:XF:130:GLN:OE1	2.24	0.69
41:AX:111:TYR:O	41:AX:115:THR:OG1	2.09	0.69
10:9:127:LEU:O	10:9:134:ASN:ND2	2.25	0.69
18:AA:1008:A:OP1	22:AE:50:ARG:NE	2.25	0.69
11:XA:3078:C:N4	11:XA:3079:G:O6	2.25	0.69
11:XA:1883:G:N7	47:XF:281:ARG:NH1	2.41	0.69
11:XA:2581:A:O2'	11:XA:2583:C:N4	2.26	0.69
18:AA:780:C:N3	29:AL:197:ARG:NH2	2.40	0.69
41:AX:266:ASN:ND2	41:AX:311:SER:O	2.25	0.68
11:XA:2822:C:O2'	11:XA:2915:C:OP2	2.10	0.68
14:A2:12:ARG:NH2	18:AA:1125:A:O4'	2.26	0.68
11:XA:1761:A:O2'	11:XA:1762:A:O5'	2.12	0.68
28:AK:89:ASN:OD1	28:AK:102:ARG:NH1	2.27	0.68
42:AY:340:SER:OG	42:AY:377:ARG:NH2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2457:A:N3	55:XO:17:ARG:NH2	2.41	0.68
53:XM:246:ASP:OD1	53:XM:249:LYS:NZ	2.27	0.68
62:XV:150:SER:O	62:XV:152:ARG:NH1	2.27	0.68
17:A5:109:ARG:NH2	17:A5:179:LEU:O	2.26	0.67
20:AC:37:ASN:OD1	20:AC:41:ARG:NH1	2.27	0.67
62:XV:136:ARG:O	62:XV:143:ARG:NH2	2.26	0.67
18:AA:769:G:OP2	31:AN:73:ARG:NH2	2.28	0.67
24:AG:312:GLN:OE1	24:AG:345:ARG:NH2	2.27	0.67
18:AA:826:A:N7	27:AJ:55:ARG:NE	2.43	0.67
50:XJ:27:GLY:O	50:XJ:58:LYS:NZ	2.28	0.66
58:XR:96:GLU:O	59:XS:105:GLN:NE2	2.27	0.66
6:5:72:ARG:NH2	11:XA:1712:A:OP2	2.28	0.66
11:XA:3059:A:OP1	11:XA:3061:G:O2'	2.12	0.66
11:XA:3127:G:O2'	11:XA:3130:A:N6	2.28	0.66
39:AV:201:GLU:OE2	39:AV:237:GLN:NE2	2.28	0.66
18:AA:703:A:OP2	38:AU:43:ASN:ND2	2.29	0.66
27:AJ:96:PRO:O	27:AJ:127:ARG:NH2	2.29	0.66
22:AE:53:ALA:N	22:AE:56:GLN:O	2.28	0.66
26:AI:81:GLU:O	26:AI:148:ARG:NH1	2.28	0.66
7:6:282:SER:OG	7:6:283:GLU:OE1	2.13	0.66
25:AH:135:GLU:N	28:AK:124:GLN:O	2.28	0.66
11:XA:2187:C:O3'	50:XJ:106:LYS:NZ	2.29	0.66
12:A0:180:LYS:NZ	32:AO:180:SER:OG	2.29	0.66
18:AA:798:C:OP1	30:AM:10:LYS:N	2.29	0.66
48:XH:108:ARG:NH1	48:XH:143:GLU:OE2	2.28	0.66
11:XA:1692:A:O2'	65:XY:175:ARG:NH1	2.29	0.66
11:XA:2830:A:N6	11:XA:2837:A:OP2	2.28	0.66
11:XA:2016:C:O2	11:XA:2931:A:O2'	2.14	0.65
18:AA:1280:C:O3'	19:AB:210:ARG:NH2	2.29	0.65
57:XQ:262:GLN:OE1	57:XQ:262:GLN:N	2.29	0.65
18:AA:1483:C:N3	18:AA:1567:A:N1	2.44	0.65
7:6:239:ASN:OD1	7:6:275:GLN:NE2	2.30	0.65
14:A2:99:LEU:O	18:AA:1600:A:N6	2.28	0.65
55:XO:100:GLN:NE2	55:XO:102:GLY:O	2.29	0.65
14:A2:17:ARG:NH2	18:AA:1022:A:OP2	2.29	0.65
46:XE:54:SER:OG	46:XE:57:ASN:OD1	2.14	0.65
11:XA:1708:A:O5'	65:XY:192:LYS:NZ	2.30	0.65
11:XA:2499:U:OP2	11:XA:2504:A:N6	2.27	0.65
11:XA:3151:A:N6	11:XA:3163:G:O2'	2.30	0.65
18:AA:710:U:OP2	30:AM:13:ARG:NH1	2.29	0.65
11:XA:1700:U:O4	65:XY:193:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AA:868:C:OP2	18:AA:870:C:N4	2.29	0.65
18:AA:668:U:O2'	32:AO:83:GLY:O	2.13	0.65
42:AY:292:GLN:OE1	42:AY:292:GLN:N	2.29	0.65
11:XA:2239:A:OP2	51:XK:75:LYS:NZ	2.30	0.64
52:XL:120:LYS:O	52:XL:143:ASN:ND2	2.30	0.64
5:4:84:ARG:NE	11:XA:3188:U:OP2	2.30	0.64
7:6:308:GLN:NE2	7:6:311:MET:SD	2.71	0.64
11:XA:2192:A:OP1	50:XJ:142:ARG:NE	2.30	0.64
18:AA:1314:C:N3	23:AF:36:ARG:NH2	2.44	0.64
54:YN:234:ASP:O	54:YN:238:LYS:HA	1.96	0.64
11:XA:2400:C:O2'	11:XA:2401:A:O5'	2.14	0.64
11:XA:3012:U:O4'	11:XA:3173:G:N2	2.29	0.64
35:AR:208:ILE:O	35:AR:214:ASN:ND2	2.29	0.64
39:AV:132:LYS:O	39:AV:136:GLY:N	2.28	0.64
7:6:117:VAL:O	7:6:121:ARG:NH2	2.30	0.64
11:XA:1805:A:OP2	62:XV:94:HIS:NE2	2.31	0.64
46:XE:69:ASP:OD1	46:XE:154:ARG:NH1	2.30	0.64
8:7:279:GLU:N	8:7:279:GLU:OE1	2.29	0.64
10:9:74:VAL:O	65:XY:83:ALA:N	2.31	0.64
37:AT:89:ASP:OD1	38:AU:120:ARG:NH2	2.31	0.64
21:AD:192:GLY:O	32:AO:78:ARG:NH2	2.30	0.64
18:AA:1050:C:OP2	29:AL:198:ARG:NH1	2.31	0.63
38:AU:110:GLN:O	38:AU:114:ARG:NE	2.29	0.63
21:AD:254:ALA:O	21:AD:280:HIS:N	2.31	0.63
57:XQ:103:ARG:NH2	57:XQ:167:TYR:OH	2.31	0.63
31:AN:62:ASP:OD1	31:AN:88:VAL:N	2.29	0.63
62:XV:147:SER:OG	62:XV:152:ARG:N	2.32	0.63
24:AG:272:SER:OG	24:AG:347:ALA:O	2.17	0.63
51:XK:52:ASP:OD2	51:XK:124:ARG:NH2	2.32	0.63
55:XO:124:GLU:OE1	55:XO:128:ASN:ND2	2.31	0.63
11:XA:1755:A:O2'	48:XH:64:LEU:O	2.14	0.63
11:XA:2618:U:O4	11:XA:3043:C:N4	2.31	0.63
18:AA:1347:G:OP1	28:AK:36:ARG:NH1	2.31	0.63
48:XH:58:ARG:NH1	48:XH:77:HIS:O	2.32	0.63
11:XA:2403:G:OP2	45:XD:105:ARG:NH2	2.31	0.62
18:AA:897:C:OP1	27:AJ:114:ARG:NH2	2.33	0.62
47:XF:114:THR:O	47:XF:156:ARG:NH2	2.31	0.62
8:7:190:ASP:O	8:7:295:ARG:NH1	2.32	0.62
36:AS:7:GLU:N	36:AS:7:GLU:OE1	2.32	0.62
35:AR:70:PHE:O	35:AR:76:GLN:NE2	2.33	0.62
38:AU:58:GLU:OE2	38:AU:62:HIS:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:XP:61:ALA:O	56:XP:176:ARG:NE	2.32	0.62
11:XA:2147:G:OP1	59:XS:104:ARG:NE	2.32	0.62
11:XA:2727:C:O2'	11:XA:2815:G:N2	2.31	0.62
18:AA:1212:U:O2'	18:AA:1214:A:N6	2.33	0.62
18:AA:1322:C:OP1	20:AC:43:ARG:NH1	2.32	0.62
7:6:286:ARG:NE	7:6:295:GLN:O	2.33	0.62
18:AA:942:A:N6	18:AA:1047:A:OP1	2.33	0.62
24:AG:129:GLU:N	24:AG:129:GLU:OE1	2.31	0.62
33:AP:134:LYS:O	38:AU:193:ARG:NE	2.31	0.62
42:AY:303:GLN:NE2	42:AY:307:GLU:OE1	2.32	0.62
11:XA:1885:A:OP2	47:XF:168:LYS:NZ	2.32	0.62
41:AX:174:ASN:OD1	41:AX:177:ARG:NH1	2.31	0.62
11:XA:1918:G:N2	11:XA:1998:U:O4	2.32	0.61
46:XE:103:LYS:NZ	46:XE:291:GLY:O	2.29	0.61
62:XV:54:TRP:NE1	62:XV:56:LEU:O	2.33	0.61
11:XA:2990:A:O2'	89:XA:5141:DOL:O18	2.10	0.61
62:XV:66:GLU:N	62:XV:66:GLU:OE1	2.33	0.61
47:XF:167:MET:SD	47:XF:276:GLN:NE2	2.73	0.61
49:XI:101:ASN:OD1	49:XI:151:ASN:N	2.33	0.61
64:XX:80:TRP:O	64:XX:131:THR:OG1	2.18	0.61
2:1:23:GLU:OE2	2:1:57:VAL:N	2.33	0.61
4:3:169:ARG:NH2	11:XA:1892:A:OP1	2.33	0.61
10:9:134:ASN:OD1	10:9:135:PHE:N	2.34	0.61
2:1:53:ARG:NH2	11:XA:2879:A:O2'	2.33	0.61
11:XA:1953:A:O2'	11:XA:2463:A:OP1	2.19	0.61
18:AA:945:G:O2'	29:AL:154:ARG:NH2	2.33	0.61
40:AW:78:GLU:N	40:AW:78:GLU:OE2	2.33	0.61
59:XS:91:GLN:N	59:XS:91:GLN:OE1	2.32	0.61
16:A4:99:SER:N	16:A4:102:GLU:OE2	2.33	0.61
53:XM:148:PHE:O	53:XM:170:ASN:ND2	2.32	0.61
11:XA:2643:G:O2'	11:XA:2645:G:OP2	2.18	0.61
13:A1:74:ALA:O	13:A1:110:ASN:ND2	2.34	0.61
37:AT:109:ASN:ND2	37:AT:111:GLU:OE2	2.32	0.60
41:AX:161:TRP:NE1	41:AX:183:GLU:OE2	2.33	0.60
11:XA:2268:G:N7	53:XM:44:ARG:NH1	2.48	0.60
22:AE:5:GLU:OE2	22:AE:96:HIS:ND1	2.33	0.60
47:XF:97:HIS:NE2	47:XF:101:MET:SD	2.74	0.60
11:XA:2262:C:OP2	59:XS:182:LYS:NZ	2.29	0.60
7:6:360:ARG:NH2	11:XA:2869:A:N7	2.49	0.60
24:AG:382:PRO:O	25:AH:131:ARG:NH1	2.34	0.60
33:AP:65:CYS:SG	33:AP:68:CYS:N	2.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A4:537:ARG:O	16:A4:539:LYS:NZ	2.34	0.60
33:AP:49:ASP:OD2	40:AW:82:SER:N	2.35	0.60
11:XA:2187:C:O2'	50:XJ:106:LYS:NZ	2.35	0.60
11:XA:2826:G:OP1	63:XW:49:ARG:NH1	2.33	0.60
62:XV:49:ILE:O	62:XV:81:ARG:NH1	2.33	0.60
39:AV:173:PHE:O	39:AV:178:THR:OG1	2.17	0.59
63:XW:62:HIS:N	63:XW:65:ASN:OD1	2.34	0.59
18:AA:702:C:O2'	18:AA:842:C:O2	2.17	0.59
18:AA:869:C:OP2	32:AO:97:ARG:NH2	2.35	0.59
29:AL:149:ASP:OD2	29:AL:152:HIS:ND1	2.35	0.59
40:AW:132:GLU:O	40:AW:135:GLN:NE2	2.34	0.59
15:A3:187:GLU:O	29:AL:212:ARG:NH2	2.36	0.59
18:AA:993:A:OP1	26:AI:192:ARG:NH2	2.34	0.59
61:XU:71:ARG:NH2	61:XU:73:GLN:OE1	2.36	0.59
21:AD:293:ASP:OD1	21:AD:307:LYS:N	2.33	0.59
18:AA:1483:C:N4	18:AA:1567:A:C2	2.70	0.59
40:AW:103:ARG:O	40:AW:115:ASP:N	2.35	0.59
10:9:52:GLN:NE2	11:XA:2416:U:O3'	2.36	0.59
11:XA:1673:U:O2'	60:XT:149:ARG:NH2	2.36	0.59
18:AA:1320:G:OP1	20:AC:41:ARG:NH1	2.36	0.59
37:AT:130:GLY:N	37:AT:135:CYS:SG	2.76	0.59
44:XB:1625:A:N7	56:XP:86:GLN:NE2	2.45	0.59
62:XV:181:ASP:O	65:XY:93:LYS:NZ	2.34	0.59
16:A4:247:ILE:O	16:A4:254:LYS:NZ	2.35	0.58
39:AV:87:HIS:ND1	39:AV:90:TYR:OH	2.33	0.58
4:3:182:ASP:OD1	4:3:183:ARG:N	2.34	0.58
14:A2:9:ARG:NH2	18:AA:1021:U:OP2	2.34	0.58
14:A2:24:ASN:ND2	18:AA:1597:C:OP2	2.36	0.58
18:AA:1389:G:N1	18:AA:1416:A:OP2	2.35	0.58
8:7:262:ASP:OD1	8:7:263:VAL:N	2.35	0.58
11:XA:2144:A:OP1	58:XR:57:ARG:NH1	2.36	0.58
53:XM:264:GLN:NE2	53:XM:266:PHE:O	2.36	0.58
11:XA:2240:C:OP2	51:XK:71:LYS:NZ	2.33	0.58
11:XA:1864:A:OP1	58:XR:17:ARG:NH1	2.36	0.58
24:AG:362:GLU:OE2	24:AG:365:ARG:NH1	2.35	0.58
57:XQ:268:ASP:OD1	57:XQ:269:MET:N	2.37	0.58
7:6:119:GLU:N	7:6:119:GLU:OE1	2.35	0.58
6:5:334:LYS:O	6:5:362:THR:OG1	2.20	0.58
11:XA:2370:A:OP1	61:XU:41:GLN:NE2	2.36	0.58
14:A2:24:ASN:OD1	14:A2:25:LYS:N	2.36	0.58
1:0:96:ASN:ND2	11:XA:2709:A:O2'	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:XO:129:CYS:SG	55:XO:130:LEU:N	2.77	0.58
6:5:149:ASN:ND2	6:5:152:GLU:OE2	2.34	0.58
11:XA:2954:C:O2	54:XN:182:LYS:NZ	2.32	0.58
57:XQ:254:MET:SD	57:XQ:255:LYS:N	2.77	0.58
12:A0:96:ARG:N	12:A0:117:ILE:O	2.35	0.57
51:XK:24:LYS:O	51:XK:26:GLN:NE2	2.37	0.57
6:5:381:LEU:O	6:5:407:LYS:NZ	2.36	0.57
11:XA:2195:A:O2'	11:XA:2196:A:O5'	2.19	0.57
47:XF:215:SER:OG	47:XF:257:GLN:N	2.35	0.57
49:XI:48:MET:O	54:XN:250:ARG:NH1	2.36	0.57
63:XW:115:ASP:OD1	63:XW:116:LEU:N	2.38	0.57
65:XY:151:ASP:OD1	65:XY:154:ARG:NH2	2.32	0.57
18:AA:782:A:O2'	31:AN:46:ARG:NH1	2.38	0.57
29:AL:169:ASN:OD1	29:AL:170:LEU:N	2.37	0.57
32:AO:196:GLY:O	35:AR:146:LYS:NZ	2.37	0.57
43:AZ:54:ASN:ND2	43:AZ:57:THR:OG1	2.37	0.57
7:6:283:GLU:OE1	7:6:283:GLU:N	2.38	0.57
13:A1:118:ALA:O	13:A1:122:HIS:ND1	2.38	0.57
58:XR:36:ASN:OD1	58:XR:37:ARG:N	2.38	0.56
11:XA:2029:A:O2'	11:XA:2030:U:OP1	2.23	0.56
26:AI:79:LYS:N	26:AI:82:GLU:OE2	2.33	0.56
39:AV:132:LYS:NZ	39:AV:166:GLU:OE1	2.38	0.56
11:XA:2755:A:O2'	64:XX:112:ARG:NH2	2.38	0.56
61:XU:9:LEU:N	65:XY:183:GLN:OE1	2.39	0.56
18:AA:1233:C:O2'	28:AK:86:ARG:NH1	2.38	0.56
16:A4:134:GLU:HB3	16:A4:135:PRO:HD3	1.86	0.56
19:AB:137:TYR:O	19:AB:264:ARG:NH2	2.35	0.56
65:XY:154:ARG:NH1	65:XY:160:GLN:O	2.39	0.56
7:6:206:TYR:OH	7:6:242:GLY:O	2.16	0.56
15:A3:184:GLU:OE1	15:A3:184:GLU:N	2.39	0.56
64:XX:207:THR:HG1	64:XX:210:GLU:CD	2.09	0.56
11:XA:1770:G:OP2	58:XR:11:ARG:NH1	2.39	0.56
18:AA:918:A:O2'	18:AA:919:A:O4'	2.23	0.56
45:XD:187:LEU:O	45:XD:219:LYS:NZ	2.35	0.56
18:AA:1483:C:C4	18:AA:1567:A:N1	2.74	0.56
39:AV:141:ASN:OD1	39:AV:142:PHE:N	2.39	0.56
18:AA:1142:A:N6	18:AA:1161:A:OP2	2.34	0.55
23:AF:116:GLU:OE1	23:AF:120:ARG:NH2	2.40	0.55
30:AM:68:LEU:O	35:AR:161:ILE:N	2.37	0.55
55:XO:18:MET:HE1	55:XO:48:ARG:HE	1.72	0.55
7:6:37:ASN:ND2	63:XW:125:VAL:O	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AA:1367:A:O3'	23:AF:194:LYS:NZ	2.39	0.55
23:AF:151:ASN:O	23:AF:223:LYS:NZ	2.38	0.55
47:XF:220:ASP:O	47:XF:245:ALA:N	2.39	0.55
26:AI:83:ILE:O	26:AI:148:ARG:NH1	2.35	0.55
37:AT:97:GLU:N	37:AT:97:GLU:OE1	2.36	0.55
18:AA:766:G:OP2	31:AN:76:HIS:NE2	2.35	0.55
18:AA:1401:G:N1	18:AA:1404:C:OP2	2.35	0.55
23:AF:129:ALA:O	23:AF:134:GLN:NE2	2.39	0.55
48:XH:95:GLU:OE2	48:XH:112:VAL:N	2.39	0.55
53:XM:231:GLU:OE1	53:XM:231:GLU:N	2.39	0.55
1:0:139:ARG:NH2	11:XA:2322:C:OP1	2.34	0.55
18:AA:917:C:OP2	32:AO:91:ARG:NH2	2.39	0.55
41:AX:272:THR:OG1	41:AX:282:ILE:O	2.23	0.55
12:A0:61:GLU:OE2	12:A0:139:TRP:N	2.40	0.55
44:XB:1644:G:O6	56:XP:87:HIS:NE2	2.38	0.55
8:7:94:HIS:NE2	60:XT:135:GLU:OE2	2.38	0.55
14:A2:102:ASN:OD1	14:A2:103:LYS:N	2.39	0.55
11:XA:2531:U:O4	45:XD:246:ARG:NH2	2.39	0.55
41:AX:246:GLU:OE2	41:AX:250:GLN:NE2	2.39	0.55
11:XA:2990:A:H2'	11:XA:2992:G:OP2	2.07	0.55
18:AA:1199:G:N2	18:AA:1423:A:OP2	2.34	0.55
30:AM:18:THR:N	30:AM:37:ALA:O	2.37	0.55
39:AV:47:HIS:N	39:AV:78:ASN:OD1	2.40	0.55
53:XM:260:LYS:NZ	53:XM:265:ILE:O	2.35	0.55
57:XQ:227:LYS:O	57:XQ:229:TRP:N	2.40	0.54
11:XA:1728:U:O2	64:XX:96:LYS:NZ	2.40	0.54
37:AT:95:ASN:OD1	37:AT:96:LYS:N	2.38	0.54
11:XA:2066:C:O2'	11:XA:2067:C:OP1	2.25	0.54
18:AA:1106:C:O2'	18:AA:1108:C:OP2	2.20	0.54
37:AT:9:ILE:O	37:AT:12:THR:OG1	2.22	0.54
47:XF:191:ASP:OD1	47:XF:192:SER:N	2.41	0.54
48:XH:136:ASN:OD1	48:XH:137:LYS:N	2.40	0.54
8:7:247:ASN:ND2	8:7:251:ILE:O	2.39	0.54
16:A4:247:ILE:O	16:A4:247:ILE:HG22	2.06	0.54
41:AX:206:GLU:OE2	41:AX:208:TYR:OH	2.25	0.54
86:A:1:MHW:O	86:A:2:THR:HG23	2.08	0.54
13:A1:154:THR:OG1	25:AH:171:GLU:OE2	2.25	0.54
58:XR:96:GLU:OE1	58:XR:96:GLU:N	2.41	0.54
16:A4:591:GLU:N	16:A4:591:GLU:OE1	2.40	0.54
18:AA:1008:A:OP2	22:AE:50:ARG:NH1	2.40	0.54
36:AS:92:PHE:O	40:AW:91:GLN:NE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:XF:70:ARG:NE	47:XF:194:GLU:OE1	2.41	0.54
7:6:282:SER:O	7:6:283:GLU:N	2.41	0.54
6:5:337:GLU:N	6:5:337:GLU:OE1	2.41	0.54
10:9:126:LYS:O	10:9:129:GLN:NE2	2.40	0.54
11:XA:2305:U:OP1	60:XT:149:ARG:NH1	2.40	0.54
18:AA:1048:C:O2'	18:AA:1049:A:OP1	2.23	0.54
48:XH:120:ARG:NH2	64:XX:136:ASP:OD2	2.40	0.54
53:XM:119:THR:O	53:XM:123:ASN:ND2	2.40	0.54
11:XA:1725:C:O2	11:XA:2921:A:N6	2.37	0.54
31:AN:12:TRP:NE1	37:AT:81:ASP:O	2.41	0.54
11:XA:2138:U:O2'	11:XA:2151:A:N3	2.39	0.53
11:XA:2511:C:O2'	45:XD:257:ILE:O	2.23	0.53
18:AA:1108:C:N4	18:AA:1125:A:N7	2.56	0.53
12:A0:132:GLU:OE1	12:A0:205:ALA:N	2.41	0.53
6:5:300:ARG:HA	6:5:303:ARG:HE	1.73	0.53
7:6:114:ARG:NH2	56:XP:116:TYR:O	2.41	0.53
11:XA:2756:C:OP1	48:XH:121:ASN:ND2	2.36	0.53
64:XX:83:GLU:N	64:XX:83:GLU:OE1	2.42	0.53
1:0:95:ARG:NH1	11:XA:1821:A:OP2	2.42	0.53
25:AH:66:SER:OG	25:AH:68:GLU:OE1	2.25	0.53
38:AU:52:GLU:N	38:AU:52:GLU:OE1	2.42	0.53
32:AO:125:GLN:N	32:AO:125:GLN:OE1	2.41	0.53
19:AB:153:TYR:O	19:AB:157:ASN:ND2	2.42	0.53
23:AF:176:ASP:OD1	23:AF:179:ARG:NH2	2.39	0.53
5:4:88:TRP:NE1	11:XA:2160:A:OP2	2.37	0.53
7:6:274:LYS:NZ	7:6:276:ASP:OD1	2.39	0.53
11:XA:2990:A:C4	11:XA:2992:G:OP2	2.61	0.53
11:XA:1844:A:OP2	58:XR:48:ARG:NH2	2.40	0.53
12:A0:50:LEU:O	12:A0:55:TRP:NE1	2.41	0.53
13:A1:156:TYR:O	13:A1:167:ARG:NH1	2.41	0.53
47:XF:292:ASP:OD1	47:XF:293:PHE:N	2.42	0.53
10:9:72:PRO:O	65:XY:85:TRP:NE1	2.42	0.53
11:XA:2182:G:N2	11:XA:2199:A:N3	2.57	0.53
11:XA:2721:G:C6	11:XA:2990:A:C5	2.96	0.53
50:XJ:126:GLN:OE1	50:XJ:126:GLN:N	2.42	0.53
11:XA:2990:A:HO2'	89:XA:5141:DOL:HO18	1.51	0.52
18:AA:1192:C:C5	18:AA:1193:U:C6	2.97	0.52
14:A2:113:ASN:OD1	14:A2:114:LYS:N	2.42	0.52
18:AA:1191:C:H2'	18:AA:1192:C:C6	2.44	0.52
28:AK:28:HIS:NE2	43:AZ:60:GLU:OE2	2.38	0.52
32:AO:65:GLN:O	32:AO:69:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:XR:17:ARG:HA	58:XR:20:ARG:HG2	1.91	0.52
46:XE:334:ASP:OD1	46:XE:335:GLU:N	2.43	0.52
11:XA:3148:C:OP1	46:XE:211:ILE:HG12	2.09	0.52
12:A0:30:ASP:OD1	12:A0:31:SER:N	2.42	0.52
41:AX:51:THR:O	41:AX:67:HIS:N	2.42	0.52
4:3:113:ARG:NH2	11:XA:2898:U:O2'	2.43	0.52
11:XA:2453:G:O6	11:XA:2672:A:N6	2.42	0.52
46:XE:327:GLU:OE1	46:XE:327:GLU:N	2.43	0.52
63:XW:96:ILE:O	63:XW:134:VAL:N	2.37	0.52
18:AA:1189:U:HO2'	18:AA:1190:C:P	2.33	0.52
18:AA:1430:A:OP1	24:AG:388:ARG:NH2	2.38	0.52
31:AN:53:ASP:OD2	31:AN:57:GLN:N	2.42	0.52
12:A0:60:ARG:O	39:AV:245:HIS:NE2	2.42	0.51
18:AA:1225:C:O2'	18:AA:1449:G:O2'	2.28	0.51
27:AJ:61:VAL:O	27:AJ:84:ARG:N	2.38	0.51
16:A4:339:LEU:O	16:A4:374:HIS:NE2	2.44	0.51
16:A4:472:ASP:OD1	16:A4:505:ARG:NE	2.44	0.51
18:AA:990:U:OP1	26:AI:96:GLN:NE2	2.43	0.51
59:XS:196:ASN:OD1	59:XS:197:SER:N	2.42	0.51
14:A2:9:ARG:O	14:A2:20:VAL:N	2.41	0.51
19:AB:156:GLU:OE1	24:AG:163:HIS:ND1	2.44	0.51
19:AB:162:CYS:O	19:AB:261:LYS:NZ	2.41	0.51
7:6:124:ARG:NH2	9:8:112:GLU:OE1	2.39	0.51
16:A4:98:ALA:N	16:A4:102:GLU:OE2	2.43	0.51
18:AA:1084:C:OP1	26:AI:193:LYS:N	2.42	0.51
53:XM:255:MET:O	53:XM:258:THR:OG1	2.29	0.51
35:AR:202:ARG:NE	35:AR:233:ALA:O	2.37	0.51
46:XE:316:PHE:HB3	46:XE:317:PRO:HD3	1.91	0.51
55:XO:18:MET:CE	55:XO:48:ARG:HE	2.23	0.51
11:XA:2939:C:H2'	11:XA:2940:A:O4'	2.10	0.51
25:AH:161:GLN:HA	25:AH:164:LEU:CD1	2.41	0.51
53:XM:53:HIS:O	53:XM:58:GLN:NE2	2.43	0.51
18:AA:1148:A:O3'	29:AL:202:ARG:NH2	2.44	0.51
32:AO:76:ASP:OD1	32:AO:77:TYR:N	2.44	0.51
45:XD:264:ARG:HE	45:XD:270:PRO:HD3	1.74	0.51
11:XA:1742:G:O2'	11:XA:1754:G:O6	2.29	0.50
18:AA:1234:C:O2'	18:AA:1235:U:OP1	2.28	0.50
39:AV:271:GLU:N	39:AV:271:GLU:OE1	2.43	0.50
6:5:112:ARG:NH1	6:5:301:PRO:O	2.42	0.50
18:AA:1366:C:O2'	18:AA:1419:G:O4'	2.23	0.50
19:AB:119:GLU:OE1	19:AB:119:GLU:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AE:54:HIS:NE2	22:AE:83:SER:O	2.44	0.50
62:XV:19:TYR:OH	62:XV:31:ASP:OD1	2.30	0.50
22:AE:56:GLN:OE1	22:AE:56:GLN:N	2.44	0.50
56:XP:146:GLN:O	56:XP:146:GLN:HG2	2.11	0.50
13:A1:59:LYS:NZ	16:A4:83:THR:O	2.43	0.50
51:XK:130:ASP:OD1	51:XK:131:GLU:N	2.44	0.50
4:3:180:TYR:OH	7:6:367:ASP:OD2	2.23	0.50
11:XA:2443:C:O2	11:XA:2444:A:N6	2.45	0.50
11:XA:2614:U:O3'	52:XL:53:ARG:NH1	2.45	0.50
38:AU:178:GLU:N	38:AU:178:GLU:OE1	2.45	0.50
8:7:51:GLU:OE2	8:7:54:ARG:NH2	2.44	0.50
35:AR:247:HIS:O	35:AR:251:GLU:OE1	2.30	0.50
11:XA:2529:U:O2'	45:XD:206:TYR:O	2.29	0.50
11:XA:2955:U:OP2	11:XA:2963:A:N6	2.44	0.50
45:XD:194:ASN:ND2	45:XD:245:GLY:O	2.44	0.50
46:XE:56:GLU:OE2	55:XO:141:HIS:ND1	2.45	0.50
11:XA:2928:C:OP2	11:XA:3073:C:O2'	2.27	0.50
11:XA:3160:A:OP1	46:XE:213:LYS:NZ	2.35	0.50
11:XA:2472:A:N3	11:XA:2474:C:N4	2.60	0.49
11:XA:2575:U:O2	11:XA:2582:A:N6	2.45	0.49
11:XA:2802:A:H2'	11:XA:2803:A:O4'	2.12	0.49
22:AE:14:GLN:N	22:AE:17:GLU:OE2	2.40	0.49
44:XB:1615:A:O2'	44:XB:1616:A:O4'	2.21	0.49
59:XS:166:SER:OG	59:XS:188:THR:N	2.45	0.49
39:AV:79:ILE:HD11	39:AV:88:ALA:HB2	1.94	0.49
44:XB:1640:A:OP2	56:XP:84:ARG:NH2	2.45	0.49
11:XA:2721:G:C6	11:XA:2990:A:N6	2.80	0.49
11:XA:2813:U:N3	11:XA:2817:G:OP2	2.45	0.49
18:AA:1310:C:O2'	28:AK:128:TRP:NE1	2.42	0.49
31:AN:66:LEU:HD13	31:AN:79:HIS:HB3	1.94	0.49
61:XU:49:THR:O	61:XU:52:ASP:OD1	2.30	0.49
6:5:264:ASP:OD1	45:XD:148:LYS:NZ	2.43	0.49
11:XA:2172:A:OP2	50:XJ:21:ARG:NH1	2.39	0.49
11:XA:2667:U:C4	11:XA:2668:A:C8	3.00	0.49
57:XQ:226:PRO:O	57:XQ:229:TRP:NE1	2.45	0.49
18:AA:1390:A:H1'	18:AA:1392:A:N7	2.28	0.49
60:XT:157:ARG:HB2	60:XT:167:MET:HG3	1.94	0.49
86:A:1:MHW:C	86:A:2:THR:HG23	2.43	0.49
1:0:138:ARG:NH1	11:XA:2320:A:O3'	2.45	0.49
11:XA:1799:U:H2'	11:XA:1800:G:O4'	2.11	0.49
11:XA:2349:G:H2'	11:XA:2350:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2419:C:OP2	61:XU:50:ARG:NH2	2.45	0.49
35:AR:89:LYS:O	35:AR:92:LYS:NZ	2.40	0.49
18:AA:1261:C:OP1	21:AD:108:ALA:N	2.46	0.49
50:XJ:107:GLU:OE1	50:XJ:109:ALA:N	2.44	0.49
62:XV:103:ASP:OD1	62:XV:104:TYR:N	2.45	0.49
4:3:138:PRO:HA	4:3:141:LYS:HZ2	1.78	0.49
11:XA:1847:U:OP1	53:XM:47:ARG:NE	2.45	0.49
13:A1:256:SER:O	13:A1:260:ARG:NH1	2.45	0.49
18:AA:682:A:N6	18:AA:865:A:H61	2.09	0.49
23:AF:77:ALA:N	24:AG:368:GLY:O	2.44	0.49
53:XM:168:GLU:OE2	53:XM:220:ARG:NH2	2.44	0.49
6:5:80:ARG:NH2	6:5:82:TYR:OH	2.46	0.49
11:XA:2381:A:N6	11:XA:2412:A:N1	2.61	0.49
6:5:343:GLN:NE2	6:5:417:LEU:O	2.46	0.48
10:9:54:LYS:NZ	11:XA:2415:C:O3'	2.45	0.48
26:AI:94:ASN:OD1	26:AI:95:THR:N	2.44	0.48
45:XD:204:ALA:HB1	45:XD:208:ARG:HE	1.77	0.48
11:XA:3066:C:H2'	11:XA:3067:U:H5'	1.95	0.48
45:XD:216:LEU:HD23	45:XD:216:LEU:H	1.77	0.48
6:5:334:LYS:N	6:5:362:THR:OG1	2.46	0.48
11:XA:1729:U:OP1	64:XX:100:ARG:NH1	2.40	0.48
18:AA:1460:C:OP1	23:AF:177:ARG:NH2	2.39	0.48
46:XE:219:MET:O	46:XE:223:GLY:N	2.41	0.48
54:XN:99:TRP:NE1	54:XN:103:GLU:OE2	2.46	0.48
58:XR:149:HIS:O	66:XZ:151:LEU:N	2.47	0.48
6:5:143:PRO:HA	6:5:146:HIS:HD1	1.78	0.48
39:AV:108:THR:O	39:AV:111:THR:OG1	2.27	0.48
47:XF:94:ASP:OD1	47:XF:95:ILE:N	2.44	0.48
65:XY:94:SER:OG	65:XY:95:ASN:N	2.45	0.48
1:0:138:ARG:HA	1:0:141:ILE:HG12	1.95	0.48
11:XA:2259:C:O2'	11:XA:2261:C:OP2	2.28	0.48
18:AA:657:G:O4'	18:AA:1480:A:O2'	2.26	0.48
47:XF:142:ARG:HA	47:XF:149:GLY:HA2	1.95	0.48
55:XO:86:ILE:HB	55:XO:87:PRO:HD3	1.95	0.48
18:AA:1193:U:O2'	23:AF:178:ARG:NH1	2.46	0.48
21:AD:257:SER:OG	21:AD:271:ALA:O	2.28	0.48
46:XE:133:THR:HG1	46:XE:144:THR:HG1	1.57	0.48
47:XF:248:LEU:HD21	47:XF:253:MET:HE1	1.95	0.48
11:XA:2520:C:OP2	45:XD:295:TYR:OH	2.30	0.48
13:A1:164:ARG:CD	16:A4:134:GLU:HG2	2.44	0.48
16:A4:148:GLN:NE2	16:A4:151:ASP:OD1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AA:1559:G:H2'	18:AA:1560:U:C6	2.49	0.48
21:AD:191:ARG:NH1	32:AO:79:ARG:O	2.47	0.48
30:AM:20:ARG:NH1	30:AM:42:PRO:O	2.40	0.48
53:XM:100:ARG:O	53:XM:104:LEU:HD23	2.14	0.48
57:XQ:225:LYS:NZ	57:XQ:228:PRO:O	2.43	0.48
18:AA:1433:A:N3	18:AA:1458:A:N6	2.62	0.48
11:XA:2692:G:N1	11:XA:2696:A:OP2	2.38	0.48
45:XD:128:GLN:NE2	45:XD:129:VAL:O	2.47	0.48
45:XD:232:ARG:NH1	45:XD:291:PRO:O	2.43	0.48
46:XE:163:GLU:OE1	46:XE:166:ARG:NH1	2.46	0.48
57:XQ:107:HIS:O	57:XQ:108:ILE:HG13	2.14	0.48
11:XA:3149:C:N4	11:XA:3161:G:N7	2.62	0.48
23:AF:110:LEU:HD13	23:AF:201:MET:HE3	1.96	0.48
6:5:270:ILE:HG22	6:5:270:ILE:O	2.14	0.47
20:AC:75:ASN:O	28:AK:103:ARG:NH2	2.47	0.47
46:XE:102:LEU:N	46:XE:123:GLN:O	2.42	0.47
49:XI:181:ILE:O	49:XI:184:THR:N	2.46	0.47
61:XU:44:ILE:HB	61:XU:45:PRO:CD	2.44	0.47
18:AA:836:A:N1	18:AA:854:U:O2'	2.44	0.47
18:AA:1232:A:C2	18:AA:1404:C:N3	2.82	0.47
18:AA:1430:A:N6	18:AA:1459:A:OP2	2.46	0.47
41:AX:121:ALA:N	41:AX:299:ASN:OD1	2.47	0.47
46:XE:310:LEU:HG	46:XE:310:LEU:O	2.14	0.47
11:XA:3066:C:C2'	11:XA:3067:U:H5'	2.44	0.47
24:AG:203:GLU:O	24:AG:207:GLU:OE1	2.32	0.47
35:AR:260:ASP:HA	35:AR:263:ARG:HG2	1.96	0.47
45:XD:111:ARG:NE	45:XD:165:ASN:OD1	2.47	0.47
46:XE:145:LEU:HD13	46:XE:181:ILE:HG21	1.95	0.47
49:XI:163:GLU:O	49:XI:166:ARG:HG3	2.14	0.47
18:AA:1323:G:N7	20:AC:36:LYS:NZ	2.52	0.47
56:XP:109:TRP:HA	56:XP:112:LYS:HG2	1.97	0.47
61:XU:31:PRO:O	65:XY:121:ARG:NH2	2.48	0.47
11:XA:2331:C:H4'	11:XA:2332:C:O4'	2.15	0.47
16:A4:372:TYR:O	16:A4:376:ILE:HG12	2.15	0.47
18:AA:770:C:O2'	18:AA:771:A:OP1	2.31	0.47
18:AA:1431:G:N1	18:AA:1458:A:OP2	2.42	0.47
23:AF:70:LYS:O	24:AG:365:ARG:NH1	2.47	0.47
18:AA:1508:C:N3	18:AA:1542:U:O4	2.48	0.47
58:XR:38:CYS:SG	58:XR:39:TYR:N	2.88	0.47
58:XR:51:VAL:HG11	59:XS:174:PHE:HB3	1.97	0.47
4:3:185:ASN:ND2	7:6:371:ASP:OD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2139:U:O4	66:XZ:77:ARG:NH1	2.48	0.47
11:XA:2171:U:N3	11:XA:2198:A:N7	2.56	0.47
11:XA:2545:U:O2'	11:XA:2633:A:OP2	2.20	0.47
16:A4:116:VAL:O	16:A4:120:ILE:HD12	2.14	0.47
22:AE:38:ASP:OD1	22:AE:39:LEU:N	2.47	0.47
47:XF:121:ARG:O	47:XF:142:ARG:NE	2.46	0.47
52:XL:101:ASP:OD2	57:XQ:152:ARG:NH2	2.42	0.47
55:XO:94:ALA:HB3	55:XO:95:PRO:HD3	1.97	0.47
1:O:86:THR:OG1	11:XA:2684:C:OP1	2.23	0.47
11:XA:2621:G:C2	11:XA:2622:G:C8	3.03	0.47
18:AA:689:U:OP1	18:AA:827:A:O2'	2.31	0.47
18:AA:949:U:O2'	31:AN:29:ARG:NH1	2.48	0.47
18:AA:1462:G:HO2'	18:AA:1463:G:H8	1.62	0.47
20:AC:45:SER:N	20:AC:167:LEU:O	2.45	0.47
35:AR:162:SER:O	35:AR:170:ARG:NH1	2.46	0.47
49:XI:50:VAL:O	54:YN:211:ASN:ND2	2.48	0.47
54:YN:177:ASP:OD1	54:YN:178:GLN:N	2.48	0.47
9:8:186:GLN:N	9:8:186:GLN:OE1	2.47	0.47
11:XA:1787:G:N2	11:XA:1790:A:OP2	2.44	0.47
14:A2:46:ILE:HG13	14:A2:47:THR:N	2.30	0.47
24:AG:351:ALA:O	24:AG:354:SER:OG	2.32	0.47
3:2:70:LEU:O	65:XY:198:ARG:NH2	2.48	0.46
17:A5:117:LYS:NZ	17:A5:121:ASN:OD1	2.48	0.46
18:AA:1247:G:N2	18:AA:1342:C:OP2	2.48	0.46
20:AC:89:ASP:OD2	20:AC:90:VAL:N	2.48	0.46
22:AE:37:ARG:NH2	38:AU:163:GLU:OE1	2.47	0.46
58:XR:104:ASP:OD1	60:XT:211:THR:OG1	2.30	0.46
6:5:119:GLN:NE2	6:5:261:PRO:O	2.45	0.46
53:XM:44:ARG:HD3	53:XM:45:ARG:HG3	1.97	0.46
37:AT:7:PHE:HB2	37:AT:10:ARG:HE	1.79	0.46
44:XB:1642:G:H2'	44:XB:1643:A:C8	2.51	0.46
49:XI:34:THR:OG1	49:XI:36:HIS:O	2.31	0.46
64:XX:141:LEU:O	64:XX:145:ILE:HD12	2.14	0.46
4:3:138:PRO:HA	4:3:141:LYS:HG2	1.96	0.46
16:A4:526:ASP:OD2	16:A4:526:ASP:N	2.48	0.46
54:YN:71:ASP:N	54:YN:71:ASP:OD1	2.48	0.46
6:5:160:HIS:HA	6:5:164:TRP:HB2	1.97	0.46
11:XA:1671:G:C6	11:XA:1818:A:N1	2.83	0.46
11:XA:2978:U:O2'	11:XA:3057:C:OP1	2.31	0.46
11:XA:3011:A:O2'	11:XA:3173:G:N2	2.48	0.46
24:AG:379:ARG:NH2	25:AH:133:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:AV:75:LEU:O	39:AV:79:ILE:HG13	2.16	0.46
42:AY:277:LEU:O	42:AY:281:GLU:OE1	2.32	0.46
60:XT:99:ILE:O	60:XT:103:LEU:HD23	2.16	0.46
6:5:92:PRO:O	6:5:96:HIS:ND1	2.48	0.46
10:9:129:GLN:OE1	10:9:134:ASN:ND2	2.48	0.46
23:AF:201:MET:N	23:AF:202:PRO:HD2	2.31	0.46
42:AY:344:GLN:N	42:AY:344:GLN:OE1	2.48	0.46
8:7:192:TRP:O	8:7:295:ARG:NH1	2.49	0.46
11:XA:2458:A:OP2	55:XO:9:ILE:N	2.48	0.46
11:XA:2472:A:O2'	11:XA:2478:G:N7	2.41	0.46
16:A4:443:ASP:O	16:A4:446:LYS:NZ	2.49	0.46
18:AA:1068:A:N6	18:AA:1089:U:OP2	2.48	0.46
39:AV:193:LYS:HE3	39:AV:193:LYS:HA	1.97	0.46
47:XF:278:SER:O	47:XF:278:SER:OG	2.32	0.46
53:XM:264:GLN:NE2	53:XM:269:LEU:O	2.49	0.46
64:XX:207:THR:N	64:XX:210:GLU:OE2	2.37	0.46
65:XY:215:LYS:O	65:XY:219:ILE:HD12	2.14	0.46
3:2:82:ARG:HD2	3:2:90:LEU:O	2.16	0.46
11:XA:3195:A:OP2	11:XA:3196:G:O2'	2.27	0.46
11:XA:2214:A:OP1	54:YN:31:LYS:NZ	2.48	0.46
14:A2:95:GLU:OE1	14:A2:95:GLU:N	2.45	0.46
18:AA:1234:C:O2	18:AA:1234:C:H2'	2.16	0.46
19:AB:186:THR:HG23	19:AB:186:THR:O	2.16	0.46
23:AF:155:MET:SD	23:AF:179:ARG:NH1	2.88	0.46
27:AJ:50:GLY:O	27:AJ:89:ARG:NH1	2.48	0.46
57:XQ:199:THR:O	57:XQ:199:THR:HG23	2.16	0.46
7:6:108:GLN:O	7:6:112:GLU:OE1	2.34	0.46
9:8:137:ARG:O	9:8:141:GLU:OE1	2.34	0.46
18:AA:769:G:N2	18:AA:772:A:OP2	2.37	0.46
30:AM:97:PHE:HE2	38:AU:63:TYR:HH	1.62	0.46
64:XX:207:THR:OG1	64:XX:210:GLU:OE1	2.34	0.46
4:3:113:ARG:HD2	53:XM:80:LYS:HG2	1.97	0.45
11:XA:2674:U:H2'	11:XA:2675:G:O4'	2.16	0.45
16:A4:290:ASP:OD2	16:A4:291:VAL:N	2.48	0.45
57:XQ:108:ILE:HG13	57:XQ:108:ILE:O	2.16	0.45
6:5:306:PRO:O	6:5:310:ARG:NE	2.43	0.45
6:5:393:LYS:O	6:5:396:VAL:HG12	2.16	0.45
11:XA:2665:U:OP2	55:XO:17:ARG:HD2	2.16	0.45
19:AB:202:ILE:O	19:AB:202:ILE:HG22	2.16	0.45
25:AH:77:SER:HB2	25:AH:173:THR:OG1	2.17	0.45
35:AR:176:GLU:N	35:AR:176:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:98:GLN:NE2	11:XA:2709:A:N3	2.52	0.45
11:XA:1961:A:O4'	60:XT:161:ARG:HA	2.16	0.45
11:XA:2548:C:C2	11:XA:2568:G:N2	2.85	0.45
22:AE:115:GLU:OE2	22:AE:115:GLU:HA	2.17	0.45
39:AV:134:GLN:NE2	57:XQ:56:PRO:O	2.50	0.45
65:XY:161:GLU:OE1	65:XY:161:GLU:N	2.49	0.45
11:XA:3066:C:O2'	46:XE:233:GLN:OE1	2.32	0.45
16:A4:260:CYS:HB2	16:A4:293:THR:HG21	1.99	0.45
18:AA:1464:G:O2'	18:AA:1465:C:O4'	2.33	0.45
27:AJ:47:ARG:HE	27:AJ:48:LYS:H	1.63	0.45
36:AS:75:TYR:OH	40:AW:91:GLN:O	2.35	0.45
53:XM:153:ASN:ND2	53:XM:256:LEU:O	2.50	0.45
11:XA:2875:A:H4'	56:XP:178:TYR:CE2	2.51	0.45
13:A1:83:LEU:O	13:A1:99:LYS:NZ	2.44	0.45
13:A1:211:ARG:NH2	42:AY:359:SER:OG	2.50	0.45
18:AA:1053:A:N1	18:AA:1100:C:O2'	2.50	0.45
18:AA:1132:U:H2'	18:AA:1133:C:C6	2.51	0.45
24:AG:200:LEU:O	24:AG:218:TYR:OH	2.31	0.45
31:AN:30:VAL:N	31:AN:47:LYS:O	2.50	0.45
41:AX:130:LYS:O	41:AX:130:LYS:HG3	2.17	0.45
11:XA:2550:A:C5	11:XA:2590:A:C6	3.05	0.45
16:A4:543:GLU:OE1	16:A4:543:GLU:N	2.45	0.45
35:AR:221:GLN:OE1	35:AR:223:ARG:NE	2.48	0.45
41:AX:157:ASP:OD1	41:AX:158:ALA:N	2.50	0.45
41:AX:297:MET:O	41:AX:297:MET:HG2	2.16	0.45
6:5:200:ARG:NH1	6:5:234:ASP:OD2	2.50	0.45
11:XA:1718:A:H2'	11:XA:1719:G:O4'	2.17	0.45
11:XA:1884:G:O2'	11:XA:1895:C:O2	2.34	0.45
11:XA:2646:G:C2	11:XA:2647:G:C8	3.04	0.45
17:A5:131:ARG:O	17:A5:135:MET:HG2	2.16	0.45
18:AA:982:A:N6	18:AA:1007:G:O6	2.49	0.45
20:AC:48:ASP:OD2	20:AC:48:ASP:N	2.49	0.45
21:AD:94:THR:OG1	21:AD:97:GLU:OE1	2.33	0.45
21:AD:400:GLU:N	21:AD:400:GLU:OE1	2.49	0.45
25:AH:70:ASP:OD2	25:AH:151:SER:N	2.44	0.45
56:XP:71:PHE:HB3	56:XP:72:PRO:HD3	1.98	0.45
57:XQ:165:GLU:OE2	57:XQ:170:ARG:NH2	2.50	0.45
30:AM:84:SER:O	30:AM:87:MET:HG3	2.17	0.45
36:AS:62:ASP:OD2	36:AS:64:TRP:NE1	2.50	0.45
47:XF:77:VAL:O	47:XF:77:VAL:HG13	2.17	0.45
57:XQ:61:VAL:HG22	57:XQ:62:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:3007:C:N4	11:XA:3054:G:C5	2.84	0.45
13:A1:256:SER:OG	13:A1:257:SER:N	2.49	0.45
13:A1:274:LYS:HD2	13:A1:274:LYS:N	2.32	0.45
16:A4:335:PHE:HA	16:A4:338:ILE:HG12	1.99	0.45
18:AA:1367:A:N1	18:AA:1388:C:O4'	2.50	0.45
47:XF:177:ALA:HB1	47:XF:253:MET:SD	2.57	0.45
63:XW:112:GLU:O	63:XW:115:ASP:OD1	2.34	0.45
3:2:82:ARG:NH2	11:XA:1790:A:O5'	2.50	0.45
7:6:291:TYR:O	56:XP:40:ASN:ND2	2.50	0.45
10:9:23:SER:OG	11:XA:2420:U:O2'	2.28	0.45
11:XA:2574:G:O2'	11:XA:2575:U:P	2.75	0.45
17:A5:-3:LEU:O	17:A5:-1:GLU:N	2.50	0.45
18:AA:1061:A:O5'	45:XD:254:LYS:NZ	2.40	0.45
18:AA:1235:U:H5''	18:AA:1236:C:OP2	2.17	0.45
23:AF:229:MET:O	23:AF:233:ASN:ND2	2.50	0.45
24:AG:143:ASP:OD1	24:AG:144:GLY:N	2.50	0.45
26:AI:181:ILE:O	26:AI:181:ILE:HG13	2.18	0.45
42:AY:377:ARG:O	42:AY:381:ASN:ND2	2.50	0.45
44:XB:1620:A:N3	44:XB:1620:A:H2'	2.32	0.45
11:XA:3115:U:H2'	11:XA:3116:C:H6	1.82	0.44
11:XA:3169:C:O2'	11:XA:3170:C:O4'	2.28	0.44
18:AA:1489:G:N2	18:AA:1583:A:N3	2.65	0.44
20:AC:113:ARG:NE	25:AH:164:LEU:O	2.51	0.44
57:XQ:153:ASN:OD1	57:XQ:154:VAL:N	2.50	0.44
61:XU:16:GLN:N	62:XV:206:GLU:OE2	2.48	0.44
6:5:409:GLU:OE1	6:5:409:GLU:N	2.48	0.44
8:7:306:LEU:O	8:7:306:LEU:HG	2.17	0.44
11:XA:2290:A:O2'	11:XA:2291:A:H5'	2.18	0.44
18:AA:1282:G:N2	18:AA:1286:A:OP2	2.41	0.44
50:XJ:113:THR:OG1	50:XJ:116:HIS:ND1	2.40	0.44
53:XM:141:VAL:HG12	53:XM:143:GLU:H	1.82	0.44
65:XY:175:ARG:NH2	65:XY:176:ILE:O	2.51	0.44
11:XA:3180:A:C4	11:XA:3190:A:C6	3.06	0.44
16:A4:133:ALA:HB2	20:AC:148:LYS:HB2	1.98	0.44
16:A4:613:GLU:HA	16:A4:616:ASP:OD1	2.17	0.44
55:XO:149:LEU:HA	55:XO:152:LEU:CD2	2.47	0.44
65:XY:130:GLU:O	65:XY:133:ASP:OD1	2.36	0.44
6:5:185:ILE:HA	6:5:188:CYS:SG	2.58	0.44
11:XA:1672:C:H2'	11:XA:1673:U:O4'	2.18	0.44
11:XA:1795:A:H2'	11:XA:1796:A:O4'	2.17	0.44
11:XA:2726:C:C4	11:XA:2727:C:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:3151:A:C5	11:XA:3152:C:C5	3.06	0.44
11:XA:3175:A:OP2	11:XA:3187:C:N4	2.50	0.44
16:A4:111:LYS:HD3	16:A4:111:LYS:N	2.33	0.44
19:AB:57:ASP:OD2	19:AB:58:PHE:N	2.50	0.44
51:XK:133:ILE:CG2	51:XK:137:ILE:HG23	2.48	0.44
4:3:116:ARG:NH2	4:3:159:ASP:OD1	2.51	0.44
11:XA:1878:U:O2'	47:XF:92:ARG:NH2	2.51	0.44
11:XA:2166:C:N4	11:XA:2212:C:OP2	2.50	0.44
16:A4:556:LYS:HD3	16:A4:595:MET:HE1	1.99	0.44
18:AA:990:U:H2'	18:AA:991:G:O4'	2.16	0.44
23:AF:35:SER:OG	23:AF:36:ARG:N	2.51	0.44
49:XI:181:ILE:O	49:XI:182:ASP:OD1	2.36	0.44
62:XV:77:VAL:N	62:XV:87:VAL:O	2.46	0.44
11:XA:2955:U:C5	11:XA:2963:A:N1	2.86	0.44
11:XA:3228:U:OP2	46:XE:156:ARG:NH2	2.50	0.44
18:AA:1526:U:O2'	18:AA:1527:A:O4'	2.36	0.44
32:AO:143:CYS:SG	32:AO:146:GLN:OE1	2.75	0.44
32:AO:163:LEU:HD23	32:AO:163:LEU:H	1.83	0.44
47:XF:141:ILE:O	47:XF:142:ARG:HB2	2.18	0.44
50:XJ:85:PRO:O	50:XJ:124:LYS:NZ	2.51	0.44
55:XO:33:LEU:HD13	55:XO:52:MET:HE1	1.99	0.44
11:XA:2148:A:OP1	58:XR:99:ARG:HD3	2.17	0.44
28:AK:69:ASP:O	28:AK:73:GLU:OE1	2.35	0.44
41:AX:108:LEU:HD23	41:AX:112:LEU:HD23	1.99	0.44
53:XM:156:VAL:HG22	53:XM:157:GLN:H	1.82	0.44
59:XS:127:ARG:NH2	59:XS:157:GLU:OE1	2.51	0.44
11:XA:1808:A:O2'	11:XA:1810:A:OP1	2.22	0.44
11:XA:2182:G:H2'	11:XA:2183:C:C6	2.53	0.44
18:AA:650:U:OP1	21:AD:427:ARG:NH1	2.50	0.44
53:XM:270:ALA:HB1	53:XM:271:PRO:HD2	2.00	0.44
54:XM:171:GLU:OE1	54:XM:171:GLU:N	2.41	0.44
59:XS:175:ARG:HB2	59:XS:180:PHE:HB3	2.00	0.44
65:XY:94:SER:O	65:XY:98:LEU:HD23	2.17	0.44
11:XA:2054:U:O2'	11:XA:2055:U:O4'	2.32	0.44
11:XA:2331:C:H4'	11:XA:2332:C:C6	2.52	0.44
11:XA:3071:U:H2'	89:XA:5141:DOL:H483	2.00	0.44
20:AC:88:GLU:O	20:AC:92:LEU:HD23	2.18	0.44
36:AS:67:GLU:OE2	40:AW:85:ARG:NE	2.50	0.44
46:XE:183:ASP:OD1	46:XE:183:ASP:N	2.48	0.44
53:XM:192:PRO:O	53:XM:196:ARG:HG3	2.18	0.44
63:XW:60:TYR:OH	63:XW:137:LYS:NZ	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:87:ILE:H	1:0:87:ILE:HD12	1.83	0.43
12:A0:63:ARG:NH1	12:A0:110:ASP:OD2	2.46	0.43
17:A5:35:LEU:O	17:A5:50:ASN:N	2.51	0.43
18:AA:1567:A:N6	18:AA:1569:G:C2	2.85	0.43
32:AO:81:HIS:ND1	32:AO:82:LYS:O	2.51	0.43
37:AT:36:THR:O	37:AT:45:ARG:NE	2.51	0.43
42:AY:327:GLU:O	42:AY:331:HIS:ND1	2.51	0.43
55:XO:113:ARG:HG2	55:XO:114:SER:N	2.33	0.43
11:XA:1939:G:O2'	11:XA:1973:G:H4'	2.18	0.43
11:XA:2619:A:O4'	11:XA:3038:U:O2'	2.37	0.43
11:XA:3008:C:C2	11:XA:3032:G:N2	2.86	0.43
11:XA:3212:C:O4'	11:XA:3212:C:O2	2.35	0.43
18:AA:1151:C:OP2	29:AL:201:ARG:NH1	2.44	0.43
18:AA:1210:U:H2'	18:AA:1211:G:C8	2.53	0.43
20:AC:116:GLN:OE1	20:AC:152:ARG:NH1	2.50	0.43
37:AT:101:HIS:O	37:AT:105:ILE:HD12	2.19	0.43
46:XE:248:ILE:HG13	46:XE:250:ARG:HG2	2.00	0.43
4:3:153:THR:HG21	11:XA:2044:A:OP1	2.19	0.43
6:5:391:VAL:O	6:5:391:VAL:HG13	2.19	0.43
8:7:207:HIS:HA	8:7:210:ILE:HG12	2.00	0.43
11:XA:2121:G:H2'	11:XA:2122:A:O4'	2.18	0.43
11:XA:2604:A:H2'	11:XA:2605:C:O4'	2.19	0.43
16:A4:134:GLU:CB	16:A4:135:PRO:HD3	2.46	0.43
39:AV:83:GLU:O	39:AV:87:HIS:CD2	2.71	0.43
53:XM:252:LEU:HD23	53:XM:252:LEU:H	1.83	0.43
55:XO:29:LEU:HD21	55:XO:51:GLU:HB3	1.99	0.43
57:XQ:70:GLU:N	57:XQ:71:PRO:HD2	2.33	0.43
58:XR:85:ALA:O	58:XR:89:ASN:OD1	2.36	0.43
64:XX:40:PRO:HB3	64:XX:43:TYR:CZ	2.53	0.43
3:2:60:ARG:HD2	3:2:92:HIS:CE1	2.53	0.43
7:6:134:ALA:O	7:6:138:GLU:OE1	2.37	0.43
12:A0:57:ASP:OD1	18:AA:704:U:N3	2.51	0.43
18:AA:1024:G:C4	18:AA:1026:A:OP2	2.72	0.43
41:AX:170:GLN:OE1	41:AX:175:LYS:NZ	2.50	0.43
1:0:163:GLU:OE1	1:0:181:ARG:NH2	2.50	0.43
11:XA:2143:G:C6	11:XA:2258:A:C2	3.06	0.43
18:AA:1404:C:C2	18:AA:1407:U:C5	3.06	0.43
19:AB:111:LEU:O	19:AB:112:ASP:OD1	2.36	0.43
25:AH:75:ARG:N	25:AH:175:THR:OG1	2.51	0.43
39:AV:144:PHE:CZ	39:AV:167:VAL:HG21	2.54	0.43
41:AX:100:MET:HB3	90:AX:500:GTP:HN1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:XD:248:SER:OG	45:XD:249:ASN:N	2.52	0.43
46:XE:325:GLU:OE1	46:XE:325:GLU:N	2.40	0.43
66:XZ:98:GLN:OE1	66:XZ:100:HIS:NE2	2.52	0.43
8:7:143:TRP:HE3	8:7:179:PHE:HB3	1.83	0.43
11:XA:2470:G:O2'	52:XL:36:THR:HG22	2.19	0.43
18:AA:805:C:O2	18:AA:805:C:O4'	2.36	0.43
18:AA:922:C:H1'	18:AA:923:A:N7	2.33	0.43
18:AA:1360:G:C2	18:AA:1361:G:C5	3.07	0.43
23:AF:49:GLU:OE2	23:AF:49:GLU:N	2.44	0.43
55:XO:115:LEU:HD23	55:XO:115:LEU:H	1.84	0.43
56:XP:70:VAL:HG12	56:XP:72:PRO:HD2	2.01	0.43
58:XR:20:ARG:HA	58:XR:23:GLU:OE1	2.17	0.43
61:XU:127:TYR:O	61:XU:131:GLU:OE1	2.37	0.43
7:6:144:GLY:N	7:6:145:PRO:CD	2.82	0.43
17:A5:-2:VAL:O	17:A5:-1:GLU:C	2.56	0.43
29:AL:126:GLU:HB2	29:AL:181:ILE:HD11	2.01	0.43
39:AV:106:ASN:OD1	39:AV:107:TRP:N	2.52	0.43
41:AX:337:LEU:HG	41:AX:337:LEU:O	2.18	0.43
48:XH:117:SER:O	48:XH:121:ASN:ND2	2.52	0.43
51:XK:37:ILE:HG13	51:XK:38:ARG:N	2.34	0.43
53:XM:203:ARG:NH2	53:XM:261:ASP:O	2.52	0.43
62:XV:190:CYS:O	62:XV:191:LEU:HB3	2.19	0.43
6:5:177:CYS:O	6:5:180:ILE:HG22	2.18	0.43
11:XA:2279:U:OP1	47:XF:255:LYS:NZ	2.46	0.43
14:A2:50:SER:O	14:A2:53:MET:HG2	2.19	0.43
19:AB:222:ILE:HG13	19:AB:222:ILE:O	2.19	0.43
37:AT:25:ASP:N	37:AT:25:ASP:OD2	2.51	0.43
49:XI:66:PRO:O	49:XI:67:SER:OG	2.34	0.43
1:0:166:SER:N	1:0:169:ASP:OD1	2.52	0.43
11:XA:1837:C:O2	11:XA:1837:C:O4'	2.36	0.43
11:XA:1917:A:C8	11:XA:1983:U:C4	3.07	0.43
11:XA:2025:C:OP1	59:XS:182:LYS:HD2	2.19	0.43
11:XA:2552:U:C2	11:XA:2553:G:C8	3.06	0.43
11:XA:3127:G:N2	11:XA:3130:A:OP2	2.48	0.43
13:A1:291:GLU:OE1	13:A1:315:SER:OG	2.36	0.43
16:A4:294:PHE:O	16:A4:298:ILE:HG12	2.18	0.43
16:A4:479:GLU:HA	16:A4:482:ILE:HD11	2.00	0.43
18:AA:889:G:N1	18:AA:905:A:OP2	2.41	0.43
18:AA:1268:C:OP2	18:AA:1269:U:O2'	2.27	0.43
18:AA:1374:A:N6	18:AA:1379:A:C6	2.87	0.43
20:AC:62:ILE:HA	20:AC:66:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AS:90:PRO:O	36:AS:91:ASN:OD1	2.36	0.43
45:XD:126:VAL:O	45:XD:160:GLY:N	2.50	0.43
53:XM:285:PRO:O	53:XM:286:THR:OG1	2.34	0.43
5:4:69:LYS:HD2	5:4:100:GLN:OE1	2.19	0.43
8:7:167:VAL:HG13	8:7:168:ARG:N	2.34	0.43
11:XA:1799:U:P	62:XV:41:ARG:HE	2.42	0.43
16:A4:162:GLU:OE1	16:A4:164:ARG:NH1	2.47	0.43
16:A4:616:ASP:HA	16:A4:619:LYS:HG2	2.00	0.43
43:AZ:52:TYR:HE2	43:AZ:55:HIS:HD1	1.67	0.43
64:XX:93:ASN:O	64:XX:94:ASN:OD1	2.36	0.43
11:XA:2021:U:O4	53:XM:41:ARG:NH2	2.52	0.42
11:XA:2538:C:H2'	11:XA:2539:A:O4'	2.19	0.42
11:XA:2729:U:O4	11:XA:2730:A:N6	2.52	0.42
19:AB:110:ARG:NH1	36:AS:68:ASP:OD2	2.48	0.42
47:XF:91:PRO:O	47:XF:176:VAL:HG21	2.18	0.42
6:5:414:PHE:O	6:5:417:LEU:HD23	2.20	0.42
11:XA:2379:C:O4'	11:XA:2379:C:O2	2.35	0.42
11:XA:2546:G:C2	11:XA:2547:C:C5	3.07	0.42
11:XA:3035:C:O2'	52:XL:34:LYS:NZ	2.52	0.42
89:XA:5141:DOL:H311	89:XA:5141:DOL:H343	2.02	0.42
16:A4:634:ALA:HB3	16:A4:641:ILE:HG21	2.01	0.42
17:A5:101:ILE:O	17:A5:101:ILE:HG23	2.19	0.42
18:AA:865:A:H2'	18:AA:866:A:N9	2.34	0.42
18:AA:1275:A:O2'	18:AA:1300:A:N6	2.50	0.42
18:AA:1411:G:C2	18:AA:1412:G:C5	3.07	0.42
53:XM:74:PHE:HA	53:XM:77:ARG:HG2	2.00	0.42
61:XU:11:ARG:HH21	62:XV:211:LYS:HB3	1.84	0.42
11:XA:2376:A:C6	11:XA:2421:G:O6	2.73	0.42
13:A1:91:VAL:O	13:A1:94:GLY:N	2.52	0.42
16:A4:243:ASN:O	16:A4:247:ILE:HG12	2.19	0.42
18:AA:1486:C:O2'	18:AA:1487:C:H5'	2.18	0.42
21:AD:202:SER:OG	21:AD:220:THR:O	2.37	0.42
37:AT:116:GLU:O	37:AT:119:GLU:HG3	2.19	0.42
50:XJ:59:ASP:N	50:XJ:59:ASP:OD1	2.50	0.42
11:XA:2099:U:H2'	11:XA:2100:C:C6	2.54	0.42
11:XA:2295:C:O2'	11:XA:2297:A:OP1	2.33	0.42
11:XA:2336:U:C2	11:XA:2337:A:C8	3.08	0.42
11:XA:2727:C:H2'	11:XA:2728:C:H6	1.83	0.42
11:XA:2877:C:H2'	11:XA:2878:G:O4'	2.19	0.42
11:XA:2939:C:O2'	11:XA:2940:A:H5'	2.18	0.42
18:AA:839:A:OP1	30:AM:84:SER:OG	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AA:889:G:O4'	18:AA:891:C:N4	2.53	0.42
18:AA:1211:G:N1	18:AA:1354:A:C6	2.87	0.42
18:AA:1517:A:O2'	18:AA:1518:C:O4'	2.37	0.42
21:AD:147:PRO:O	21:AD:155:GLN:NE2	2.52	0.42
24:AG:115:GLY:N	25:AH:84:ASP:OD1	2.52	0.42
39:AV:321:GLU:O	39:AV:326:LYS:NZ	2.53	0.42
45:XD:180:ASP:OD1	45:XD:180:ASP:N	2.51	0.42
54:YN:174:GLY:O	54:YN:177:ASP:OD1	2.37	0.42
7:6:233:LEU:HD21	7:6:236:LEU:HD12	2.01	0.42
9:8:165:ASP:OD1	9:8:165:ASP:N	2.49	0.42
13:A1:188:LYS:HA	13:A1:191:ILE:HG22	2.01	0.42
16:A4:628:ILE:HA	16:A4:631:VAL:HG22	2.02	0.42
19:AB:265:GLN:O	19:AB:268:GLU:HG3	2.20	0.42
51:XK:175:ASP:OD1	51:XK:175:ASP:N	2.50	0.42
53:XM:247:ILE:HG22	53:XM:247:ILE:O	2.20	0.42
3:2:69:ARG:HD2	3:2:78:VAL:HG21	2.01	0.42
8:7:189:LEU:HD23	8:7:189:LEU:H	1.84	0.42
11:XA:1722:A:H2'	11:XA:1723:A:O4'	2.20	0.42
11:XA:2182:G:O2'	11:XA:2183:C:O4'	2.22	0.42
11:XA:2954:C:H2'	11:XA:2955:U:O4'	2.19	0.42
16:A4:247:ILE:O	16:A4:247:ILE:CG2	2.68	0.42
39:AV:235:GLU:O	39:AV:239:GLY:N	2.50	0.42
53:XM:133:LYS:C	53:XM:134:ARG:HG2	2.39	0.42
62:XV:196:GLU:O	62:XV:200:GLU:OE1	2.37	0.42
1:0:79:ALA:N	11:XA:3099:C:O2	2.52	0.42
2:1:20:MET:HA	2:1:58:GLU:HA	2.02	0.42
12:A0:115:TRP:CG	12:A0:130:GLU:HA	2.54	0.42
17:A5:31:SER:N	17:A5:32:PRO:HD3	2.35	0.42
18:AA:746:A:C4	18:AA:747:A:C8	3.07	0.42
18:AA:1152:A:C2	18:AA:1153:C:C6	3.07	0.42
18:AA:1271:C:N4	18:AA:1320:G:O2'	2.46	0.42
24:AG:214:SER:O	24:AG:217:ASP:OD1	2.38	0.42
25:AH:149:THR:HG22	25:AH:150:GLY:N	2.35	0.42
26:AI:194:LEU:H	26:AI:194:LEU:HD23	1.84	0.42
38:AU:162:GLU:OE2	38:AU:162:GLU:N	2.52	0.42
54:YN:198:MET:O	54:YN:201:ASP:OD1	2.37	0.42
57:XQ:97:LYS:O	57:XQ:101:GLU:HG3	2.20	0.42
61:XU:47:GLU:OE1	61:XU:47:GLU:N	2.53	0.42
65:XY:133:ASP:OD1	65:XY:134:LYS:N	2.52	0.42
6:5:177:CYS:HA	6:5:180:ILE:HG22	2.01	0.42
6:5:214:ASN:OD1	6:5:214:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:38:THR:O	8:7:42:GLU:OE1	2.38	0.42
11:XA:1861:U:H2'	11:XA:1862:U:C6	2.55	0.42
11:XA:1977:U:H2'	11:XA:1978:A:H8	1.84	0.42
11:XA:2013:U:H2'	11:XA:2014:A:O4'	2.20	0.42
11:XA:2580:U:HO2'	11:XA:2581:A:P	2.42	0.42
11:XA:2743:U:O4'	64:XX:99:LYS:NZ	2.41	0.42
16:A4:295:ASN:O	16:A4:299:GLU:OE1	2.37	0.42
18:AA:701:G:OP1	38:AU:38:LYS:NZ	2.48	0.42
18:AA:939:A:O2'	18:AA:940:A:O4'	2.25	0.42
18:AA:1161:A:C2	18:AA:1162:A:C8	3.08	0.42
18:AA:1278:C:OP2	21:AD:269:ARG:NH1	2.47	0.42
37:AT:150:PRO:HA	37:AT:153:VAL:O	2.20	0.42
41:AX:393:ARG:O	41:AX:397:TYR:CD2	2.72	0.42
47:XF:215:SER:HA	47:XF:239:THR:HG22	2.01	0.42
55:XO:139:ASP:OD1	55:XO:140:SER:N	2.53	0.42
57:XQ:262:GLN:O	57:XQ:265:LEU:HD22	2.19	0.42
64:XX:82:GLY:N	64:XX:83:GLU:OE1	2.52	0.42
11:XA:1884:G:N7	47:XF:281:ARG:HD2	2.35	0.42
11:XA:2372:U:O2	11:XA:2372:U:O4'	2.37	0.42
12:A0:126:SER:N	12:A0:127:GLU:OE2	2.53	0.42
18:AA:952:A:N3	18:AA:954:C:N4	2.66	0.42
24:AG:98:THR:HG23	24:AG:98:THR:O	2.19	0.42
29:AL:72:LEU:HD12	29:AL:73:LEU:O	2.20	0.42
35:AR:162:SER:O	35:AR:170:ARG:NH2	2.53	0.42
37:AT:91:GLU:OE2	38:AU:123:ARG:NH1	2.53	0.42
37:AT:96:LYS:O	37:AT:100:GLU:OE1	2.37	0.42
46:XE:271:LEU:HB3	46:XE:285:VAL:HG13	2.01	0.42
53:XM:203:ARG:NE	53:XM:264:GLN:O	2.53	0.42
6:5:114:LEU:HD21	45:XD:127:ILE:HG12	2.02	0.42
11:XA:2016:C:OP1	11:XA:2039:A:O2'	2.30	0.42
11:XA:2145:G:H1'	59:XS:104:ARG:NH2	2.35	0.42
11:XA:3223:A:C4	11:XA:3224:G:C8	3.07	0.42
16:A4:104:ARG:HA	16:A4:107:LEU:CD2	2.50	0.42
18:AA:906:C:OP1	21:AD:117:ARG:NE	2.53	0.42
19:AB:194:ILE:HA	19:AB:220:VAL:O	2.20	0.42
38:AU:102:HIS:O	38:AU:106:MET:SD	2.78	0.42
44:XB:1623:G:OP2	56:XP:87:HIS:HB2	2.20	0.42
7:6:379:ILE:O	7:6:380:TYR:CG	2.73	0.41
8:7:147:ALA:O	8:7:150:MET:HG2	2.21	0.41
11:XA:2125:C:OP2	59:XS:178:LYS:HE3	2.20	0.41
11:XA:2289:G:O4'	47:XF:101:MET:CE	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A4:487:PHE:HB2	16:A4:519:TYR:HB3	2.01	0.41
21:AD:93:LEU:HG	21:AD:94:THR:H	1.84	0.41
22:AE:21:THR:O	22:AE:24:ARG:HG2	2.19	0.41
30:AM:50:GLN:NE2	37:AT:129:PHE:O	2.47	0.41
36:AS:15:ARG:O	36:AS:18:ASP:OD1	2.37	0.41
58:XR:23:GLU:HG2	58:XR:24:VAL:N	2.34	0.41
61:XU:27:GLN:HB2	61:XU:43:ARG:HB3	2.01	0.41
64:XX:226:LEU:HD12	65:XY:155:LEU:HB3	2.01	0.41
3:2:49:ARG:NH2	11:XA:2500:A:N1	2.69	0.41
11:XA:2293:A:C6	53:XM:39:ARG:HD2	2.55	0.41
11:XA:2690:G:O2'	11:XA:2691:U:H5'	2.20	0.41
13:A1:295:SER:O	13:A1:299:LEU:HD23	2.20	0.41
18:AA:700:A:OP2	38:AU:27:ARG:NH2	2.53	0.41
21:AD:135:GLY:O	21:AD:165:GLN:NE2	2.54	0.41
29:AL:176:ASP:N	29:AL:176:ASP:OD1	2.52	0.41
41:AX:371:ALA:N	41:AX:372:PRO:CD	2.84	0.41
52:XL:43:ASN:ND2	52:XL:117:THR:OG1	2.53	0.41
61:XU:52:ASP:OD1	61:XU:53:LEU:N	2.53	0.41
1:0:90:ASN:O	1:0:94:ARG:HG2	2.19	0.41
3:2:88:LYS:NZ	10:9:18:MET:SD	2.77	0.41
8:7:53:ALA:HA	8:7:56:LEU:CD2	2.50	0.41
9:8:116:LEU:O	9:8:119:LYS:HG3	2.20	0.41
11:XA:1678:C:N4	11:XA:1773:A:OP2	2.42	0.41
11:XA:2292:G:N1	58:XR:10:LEU:N	2.69	0.41
11:XA:2292:G:OP1	58:XR:11:ARG:NH1	2.53	0.41
11:XA:2752:C:C2	11:XA:2753:A:C8	3.09	0.41
11:XA:2952:U:C2	11:XA:2953:U:C5	3.08	0.41
18:AA:1343:A:N3	18:AA:1343:A:H2'	2.35	0.41
21:AD:232:THR:HG22	21:AD:233:ALA:N	2.35	0.41
28:AK:50:GLU:O	28:AK:54:ILE:HD12	2.20	0.41
32:AO:106:PRO:HA	32:AO:109:ARG:HG2	2.02	0.41
49:XI:137:ASP:OD1	49:XI:137:ASP:N	2.53	0.41
55:XO:26:ILE:HG13	55:XO:27:HIS:N	2.36	0.41
58:XR:10:LEU:HB2	58:XR:13:ARG:HD2	2.02	0.41
58:XR:95:VAL:HG23	58:XR:95:VAL:O	2.20	0.41
59:XS:153:LEU:O	59:XS:201:ALA:N	2.45	0.41
7:6:288:SER:OG	7:6:289:PRO:HD2	2.20	0.41
7:6:379:ILE:O	7:6:379:ILE:HG13	2.20	0.41
11:XA:2060:A:O2'	11:XA:2061:C:OP2	2.34	0.41
11:XA:2287:U:C4	11:XA:2288:A:N7	2.88	0.41
11:XA:2451:A:OP2	11:XA:2452:A:OP2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2558:A:C4'	11:XA:2559:U:OP2	2.68	0.41
11:XA:3039:U:C2	11:XA:3041:U:H5''	2.56	0.41
13:A1:144:GLU:OE2	13:A1:144:GLU:HA	2.20	0.41
18:AA:1060:A:O2'	45:XD:254:LYS:NZ	2.54	0.41
18:AA:1104:A:OP1	18:AA:1591:C:O2'	2.24	0.41
32:AO:105:CYS:HB2	32:AO:106:PRO:HD2	2.02	0.41
36:AS:18:ASP:OD1	36:AS:19:LEU:N	2.53	0.41
49:XI:166:ARG:HA	49:XI:169:ARG:HG2	2.02	0.41
51:XK:161:GLU:O	51:XK:164:ASP:OD1	2.38	0.41
52:XL:133:GLU:OE1	52:XL:133:GLU:N	2.53	0.41
54:YN:172:VAL:HG13	54:YN:175:PHE:CZ	2.55	0.41
58:XR:108:TYR:OH	60:XT:208:ILE:HD11	2.20	0.41
64:XX:180:ASP:N	64:XX:181:PRO:HD3	2.35	0.41
11:XA:2139:U:OP2	66:XZ:74:SER:CB	2.68	0.41
11:XA:2307:U:H2'	11:XA:2308:A:O4'	2.21	0.41
11:XA:2696:A:O2'	11:XA:2698:G:OP1	2.27	0.41
11:XA:2726:C:O2	11:XA:2726:C:H2'	2.19	0.41
11:XA:2833:A:OP1	63:XW:74:ARG:NH1	2.45	0.41
12:A0:184:THR:OG1	12:A0:185:SER:N	2.54	0.41
15:A3:166:GLN:O	15:A3:170:GLU:OE1	2.39	0.41
18:AA:1452:U:H2'	18:AA:1453:A:C8	2.54	0.41
35:AR:259:TYR:O	35:AR:263:ARG:HG2	2.21	0.41
36:AS:47:GLN:NE2	36:AS:48:ARG:O	2.54	0.41
44:XB:1607:U:O2'	44:XB:1608:G:H5'	2.21	0.41
46:XE:142:MET:HG2	46:XE:181:ILE:O	2.19	0.41
49:XI:198:PRO:O	49:XI:199:SER:C	2.59	0.41
54:YN:103:GLU:OE1	54:YN:106:ARG:NH2	2.49	0.41
61:XU:26:ILE:HD13	61:XU:56:TYR:CZ	2.55	0.41
64:XX:226:LEU:HA	64:XX:229:ILE:HG12	2.01	0.41
1:0:121:VAL:HG12	1:0:122:LEU:N	2.36	0.41
8:7:199:LEU:O	8:7:203:THR:HG23	2.21	0.41
9:8:169:PHE:HB2	9:8:170:PRO:HD3	2.03	0.41
11:XA:2216:A:N3	49:XI:150:HIS:NE2	2.65	0.41
13:A1:140:ASP:OD1	13:A1:141:GLU:N	2.53	0.41
20:AC:45:SER:OG	20:AC:46:LYS:N	2.52	0.41
29:AL:140:GLU:O	29:AL:144:GLU:OE1	2.38	0.41
35:AR:140:ASP:OD2	35:AR:141:VAL:N	2.54	0.41
45:XD:251:ASP:OD1	45:XD:251:ASP:C	2.58	0.41
49:XI:112:MET:O	49:XI:116:LEU:HD23	2.21	0.41
55:XO:23:GLU:HG2	55:XO:24:SER:N	2.35	0.41
55:XO:140:SER:O	55:XO:146:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:XY:220:LYS:O	65:XY:224:GLU:OE1	2.38	0.41
11:XA:2055:U:H2'	11:XA:2056:G:H8	1.85	0.41
11:XA:2951:A:H2'	11:XA:2952:U:H6	1.86	0.41
13:A1:189:LYS:O	13:A1:193:LEU:HD23	2.20	0.41
14:A2:32:ARG:NH1	18:AA:1599:A:OP2	2.44	0.41
18:AA:893:G:OP2	27:AJ:79:LYS:NZ	2.52	0.41
18:AA:1173:C:H2'	18:AA:1174:U:C6	2.55	0.41
18:AA:1516:G:C6	18:AA:1517:A:N6	2.89	0.41
21:AD:407:ASP:OD1	21:AD:407:ASP:N	2.49	0.41
21:AD:422:TRP:HA	21:AD:425:LEU:HD21	2.03	0.41
31:AN:39:LEU:O	37:AT:11:ARG:NH1	2.53	0.41
36:AS:104:THR:O	36:AS:107:GLN:HG3	2.21	0.41
43:AZ:66:ARG:NH1	43:AZ:80:ASP:OD1	2.53	0.41
54:XN:59:VAL:HG13	54:XN:59:VAL:O	2.21	0.41
62:XV:132:GLU:O	62:XV:148:THR:OG1	2.39	0.41
65:XY:202:LEU:HB3	65:XY:203:PRO:CD	2.50	0.41
1:0:85:ARG:NH2	11:XA:3102:U:H5''	2.36	0.41
7:6:89:ASP:N	7:6:89:ASP:OD1	2.54	0.41
7:6:379:ILE:HD13	11:XA:1882:A:C5	2.56	0.41
11:XA:3181:U:OP2	11:XA:3182:A:O2'	2.32	0.41
18:AA:687:G:O2'	18:AA:688:A:O5'	2.34	0.41
18:AA:1143:C:N4	18:AA:1576:G:OP1	2.54	0.41
21:AD:217:ASP:OD1	21:AD:218:PHE:N	2.53	0.41
29:AL:75:ASP:OD2	38:AU:153:LYS:NZ	2.42	0.41
39:AV:192:LYS:HG3	39:AV:193:LYS:N	2.35	0.41
39:AV:247:MET:HG3	39:AV:249:LEU:CD1	2.51	0.41
40:AW:109:GLU:O	40:AW:126:ARG:NH1	2.49	0.41
59:XS:161:ILE:HD11	59:XS:194:ARG:CB	2.50	0.41
66:XZ:80:TYR:HA	66:XZ:83:LYS:HG2	2.03	0.41
6:5:68:PRO:HB2	11:XA:1713:A:N6	2.36	0.41
6:5:292:TYR:CD1	6:5:345:VAL:HG12	2.56	0.41
9:8:104:VAL:HG23	9:8:104:VAL:O	2.20	0.41
11:XA:2289:G:O4'	47:XF:101:MET:HE1	2.20	0.41
11:XA:2670:C:O2'	11:XA:2671:C:H5'	2.20	0.41
11:XA:3013:G:O6	11:XA:3025:A:C6	2.74	0.41
11:XA:3122:U:O2	11:XA:3122:U:O4'	2.37	0.41
11:XA:3126:C:H2'	11:XA:3127:G:O4'	2.21	0.41
12:A0:130:GLU:OE1	12:A0:130:GLU:N	2.54	0.41
14:A2:44:THR:HG22	14:A2:45:CYS:N	2.36	0.41
16:A4:162:GLU:HB2	16:A4:167:LYS:HE2	2.02	0.41
16:A4:420:MET:HG2	16:A4:457:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A5:89:ASN:O	17:A5:100:PRO:HD2	2.21	0.41
18:AA:1302:C:OP1	20:AC:165:LYS:NZ	2.41	0.41
18:AA:1359:U:H2'	18:AA:1360:G:H8	1.86	0.41
18:AA:1397:U:C2	18:AA:1410:G:C2	3.09	0.41
18:AA:1433:A:C4	18:AA:1434:A:C8	3.09	0.41
19:AB:230:CYS:SG	19:AB:231:LEU:N	2.94	0.41
21:AD:161:SER:OG	21:AD:162:LYS:N	2.53	0.41
24:AG:211:GLU:OE1	24:AG:211:GLU:N	2.54	0.41
32:AO:161:GLY:O	35:AR:223:ARG:NH2	2.54	0.41
33:AP:124:TYR:HB3	34:AQ:9:ALA:HB2	2.02	0.41
39:AV:39:LYS:O	39:AV:43:ARG:CB	2.69	0.41
46:XE:277:ASN:HB3	46:XE:282:ILE:CG1	2.51	0.41
47:XF:175:LYS:HG2	47:XF:273:LEU:HD13	2.03	0.41
49:XI:111:LEU:O	49:XI:115:GLN:OE1	2.39	0.41
51:XK:7:ALA:HB3	51:XK:8:PRO:HD3	2.02	0.41
53:XM:156:VAL:HG22	53:XM:157:GLN:N	2.36	0.41
54:XN:203:GLU:O	54:XN:206:GLU:HG3	2.21	0.41
56:XP:176:ARG:HG2	56:XP:178:TYR:HD1	1.86	0.41
57:XQ:70:GLU:N	57:XQ:71:PRO:CD	2.84	0.41
58:XR:54:THR:HG21	59:XS:172:MET:H	1.86	0.41
66:XZ:109:LYS:HA	66:XZ:112:VAL:HG12	2.02	0.41
4:3:139:ALA:O	4:3:142:LYS:HG2	2.21	0.41
7:6:282:SER:O	7:6:284:ASP:N	2.52	0.41
8:7:252:VAL:HG22	8:7:253:LYS:N	2.36	0.41
11:XA:1737:A:N6	11:XA:1760:G:O2'	2.51	0.41
11:XA:1828:A:H4'	11:XA:1829:A:C8	2.56	0.41
11:XA:2471:G:N2	11:XA:2655:G:OP2	2.48	0.41
17:A5:135:MET:HE3	17:A5:154:GLU:OE2	2.20	0.41
18:AA:920:G:C2	18:AA:921:U:C4	3.09	0.41
19:AB:162:CYS:SG	19:AB:254:GLN:HA	2.61	0.41
22:AE:115:GLU:HG3	22:AE:116:LYS:H	1.86	0.41
47:XF:49:ARG:NH1	47:XF:270:GLU:OE1	2.44	0.41
54:XN:201:ASP:OD1	54:XN:201:ASP:C	2.58	0.41
57:XQ:225:LYS:HG2	57:XQ:226:PRO:HD2	2.02	0.41
62:XV:148:THR:O	62:XV:150:SER:N	2.54	0.41
8:7:210:ILE:HG21	8:7:275:CYS:SG	2.61	0.40
8:7:225:VAL:O	8:7:229:ILE:HG12	2.20	0.40
11:XA:2330:U:H2'	11:XA:2445:U:O4	2.21	0.40
15:A3:174:ARG:HA	15:A3:177:TRP:CE2	2.56	0.40
16:A4:639:LEU:N	16:A4:640:PRO:HD2	2.36	0.40
18:AA:663:A:H2'	18:AA:664:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AA:1433:A:C4	18:AA:1458:A:N6	2.89	0.40
30:AM:111:ARG:NH2	32:AO:232:PRO:O	2.54	0.40
35:AR:67:LYS:N	35:AR:68:PRO:CD	2.84	0.40
40:AW:162:VAL:HG12	40:AW:162:VAL:O	2.21	0.40
45:XD:206:TYR:O	45:XD:208:ARG:HD2	2.21	0.40
47:XF:280:TYR:CE2	53:XM:125:ARG:HD3	2.56	0.40
55:XO:43:GLU:OE1	55:XO:43:GLU:N	2.54	0.40
58:XR:122:ARG:NH2	58:XR:126:GLU:OE2	2.54	0.40
65:XY:132:LEU:O	65:XY:135:VAL:HG22	2.20	0.40
6:5:113:LEU:HD23	6:5:113:LEU:H	1.86	0.40
11:XA:2245:A:H1'	11:XA:2246:A:C8	2.55	0.40
11:XA:2401:A:OP2	45:XD:262:ARG:NH1	2.54	0.40
16:A4:373:HIS:HE1	16:A4:418:SER:HB2	1.86	0.40
18:AA:1131:C:H2'	18:AA:1132:U:H6	1.85	0.40
18:AA:1554:G:H2'	18:AA:1555:A:O4'	2.22	0.40
33:AP:127:PRO:HA	33:AP:130:LEU:HD23	2.02	0.40
41:AX:243:VAL:O	41:AX:247:LEU:HD23	2.21	0.40
45:XD:194:ASN:OD1	45:XD:243:THR:HG23	2.22	0.40
54:YN:201:ASP:O	54:YN:204:GLU:HG3	2.22	0.40
54:YN:215:PHE:CD1	54:YN:238:LYS:HB3	2.56	0.40
55:XO:41:ARG:NH2	55:XO:131:PRO:O	2.47	0.40
55:XO:60:ILE:HD11	55:XO:104:TYR:CG	2.56	0.40
57:XQ:136:ILE:O	57:XQ:151:LEU:HA	2.21	0.40
59:XS:162:GLU:HG2	59:XS:164:THR:HG23	2.03	0.40
62:XV:27:GLY:O	62:XV:32:LYS:NZ	2.39	0.40
63:XW:105:VAL:O	63:XW:105:VAL:HG23	2.21	0.40
7:6:147:HIS:O	7:6:151:LEU:HD23	2.22	0.40
7:6:288:SER:O	7:6:289:PRO:C	2.60	0.40
8:7:312:ILE:HA	8:7:315:LYS:HG2	2.03	0.40
11:XA:1687:A:H2'	11:XA:1688:A:O4'	2.22	0.40
11:XA:1732:C:O2'	11:XA:1733:C:OP1	2.28	0.40
11:XA:2025:C:H2'	11:XA:2026:A:O4'	2.22	0.40
11:XA:3127:G:C2	11:XA:3129:A:OP2	2.74	0.40
18:AA:1319:A:H4'	20:AC:60:HIS:NE2	2.37	0.40
18:AA:1462:G:O2'	18:AA:1463:G:H8	2.04	0.40
22:AE:15:ARG:HA	22:AE:18:THR:OG1	2.21	0.40
23:AF:116:GLU:O	23:AF:120:ARG:HG2	2.21	0.40
28:AK:56:SER:HB3	43:AZ:36:LEU:HD23	2.04	0.40
48:XH:92:GLU:OE1	48:XH:92:GLU:N	2.54	0.40
51:XK:76:VAL:HG23	51:XK:76:VAL:O	2.21	0.40
59:XS:144:LEU:HD23	59:XS:144:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:107:VAL:O	4:3:107:VAL:HG23	2.21	0.40
11:XA:2537:G:H2'	11:XA:2538:C:C6	2.56	0.40
11:XA:2847:C:H2'	11:XA:2848:A:O4'	2.22	0.40
11:XA:2919:A:C6	64:XX:97:LEU:HD12	2.56	0.40
16:A4:68:VAL:O	16:A4:68:VAL:HG12	2.22	0.40
18:AA:835:C:N4	18:AA:851:A:OP2	2.44	0.40
19:AB:268:GLU:HA	19:AB:271:TYR:CE2	2.56	0.40
25:AH:135:GLU:OE2	25:AH:137:ARG:NH2	2.55	0.40
32:AO:58:TYR:O	32:AO:61:SER:OG	2.31	0.40
39:AV:158:LYS:HD2	39:AV:158:LYS:N	2.36	0.40
50:XJ:120:ILE:HA	50:XJ:123:ILE:HG22	2.04	0.40
53:XM:185:ASP:OD1	53:XM:185:ASP:C	2.57	0.40
55:XO:113:ARG:NH1	55:XO:116:ASP:OD2	2.54	0.40
57:XQ:108:ILE:HA	57:XQ:174:ILE:HD11	2.04	0.40
62:XV:194:LEU:O	62:XV:197:GLU:HG3	2.22	0.40
64:XX:134:LEU:O	64:XX:137:GLU:HG3	2.22	0.40
7:6:58:ARG:O	7:6:62:GLU:OE1	2.40	0.40
7:6:83:ASP:OD2	7:6:85:LYS:NZ	2.46	0.40
8:7:119:LEU:H	8:7:119:LEU:HD23	1.86	0.40
11:XA:2574:G:O2'	11:XA:2575:U:OP1	2.36	0.40
16:A4:296:ALA:HA	16:A4:299:GLU:OE2	2.22	0.40
18:AA:1067:A:H2'	18:AA:1068:A:O4'	2.21	0.40
24:AG:356:VAL:HG22	24:AG:360:GLU:HB2	2.04	0.40
41:AX:126:LEU:HD23	41:AX:343:ILE:HB	2.02	0.40
53:XM:150:ALA:HB1	53:XM:152:VAL:HG13	2.03	0.40
53:XM:182:ARG:O	53:XM:185:ASP:OD1	2.40	0.40
55:XO:64:LYS:NZ	55:XO:97:TYR:O	2.47	0.40
57:XQ:70:GLU:O	57:XQ:72:GLU:N	2.51	0.40
57:XQ:180:GLU:N	57:XQ:180:GLU:OE1	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
2	1	51/65 (78%)	47 (92%)	4 (8%)	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%)	35 (97%)	1 (3%)	0	100	100
6	5	391/423 (92%)	367 (94%)	24 (6%)	0	100	100
7	6	348/380 (92%)	325 (93%)	23 (7%)	0	100	100
8	7	285/338 (84%)	265 (93%)	20 (7%)	0	100	100
9	8	133/206 (65%)	126 (95%)	7 (5%)	0	100	100
10	9	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
12	A0	197/218 (90%)	190 (96%)	7 (4%)	0	100	100
13	A1	273/323 (84%)	260 (95%)	13 (5%)	0	100	100
14	A2	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
15	A3	67/199 (34%)	66 (98%)	1 (2%)	0	100	100
16	A4	536/634 (84%)	503 (94%)	33 (6%)	0	100	100
17	A5	188/192 (98%)	179 (95%)	9 (5%)	0	100	100
19	AB	216/296 (73%)	209 (97%)	7 (3%)	0	100	100
20	AC	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
21	AD	341/430 (79%)	328 (96%)	13 (4%)	0	100	100
22	AE	120/125 (96%)	115 (96%)	5 (4%)	0	100	100
23	AF	197/242 (81%)	192 (98%)	5 (2%)	0	100	100
24	AG	300/396 (76%)	292 (97%)	8 (3%)	0	100	100
25	AH	133/201 (66%)	125 (94%)	8 (6%)	0	100	100
26	AI	134/194 (69%)	133 (99%)	1 (1%)	0	100	100
27	AJ	106/138 (77%)	95 (90%)	11 (10%)	0	100	100
28	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
29	AL	162/257 (63%)	156 (96%)	6 (4%)	0	100	100
30	AM	114/137 (83%)	113 (99%)	1 (1%)	0	100	100
31	AN	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
32	AO	183/258 (71%)	178 (97%)	5 (3%)	0	100	100
33	AP	93/142 (66%)	85 (91%)	8 (9%)	0	100	100
34	AQ	83/86 (96%)	78 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	AR	248/360 (69%)	237 (96%)	11 (4%)	0	100	100
36	AS	131/190 (69%)	124 (95%)	7 (5%)	0	100	100
37	AT	160/173 (92%)	149 (93%)	11 (7%)	0	100	100
38	AU	171/205 (83%)	167 (98%)	4 (2%)	0	100	100
39	AV	341/414 (82%)	322 (94%)	19 (6%)	0	100	100
40	AW	95/187 (51%)	92 (97%)	3 (3%)	0	100	100
41	AX	342/348 (98%)	324 (95%)	18 (5%)	0	100	100
42	AY	111/395 (28%)	104 (94%)	7 (6%)	0	100	100
43	AZ	84/106 (79%)	83 (99%)	1 (1%)	0	100	100
45	XD	234/305 (77%)	223 (95%)	9 (4%)	2 (1%)	17	55
46	XE	302/348 (87%)	290 (96%)	12 (4%)	0	100	100
47	XF	248/311 (80%)	238 (96%)	10 (4%)	0	100	100
48	XH	93/267 (35%)	87 (94%)	6 (6%)	0	100	100
49	XI	209/261 (80%)	194 (93%)	15 (7%)	0	100	100
50	XJ	168/192 (88%)	156 (93%)	12 (7%)	0	100	100
51	XK	175/178 (98%)	168 (96%)	7 (4%)	0	100	100
52	XL	113/145 (78%)	107 (95%)	6 (5%)	0	100	100
53	XM	285/296 (96%)	271 (95%)	14 (5%)	0	100	100
54	XN	219/251 (87%)	206 (94%)	13 (6%)	0	100	100
55	XO	150/175 (86%)	142 (95%)	8 (5%)	0	100	100
56	XP	141/179 (79%)	131 (93%)	10 (7%)	0	100	100
57	XQ	236/292 (81%)	222 (94%)	14 (6%)	0	100	100
58	XR	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
59	XS	158/205 (77%)	152 (96%)	6 (4%)	0	100	100
60	XT	164/212 (77%)	160 (98%)	4 (2%)	0	100	100
61	XU	137/153 (90%)	130 (95%)	7 (5%)	0	100	100
62	XV	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
63	XW	109/148 (74%)	105 (96%)	4 (4%)	0	100	100
64	XX	241/256 (94%)	230 (95%)	11 (5%)	0	100	100
65	XY	176/250 (70%)	169 (96%)	7 (4%)	0	100	100
66	XZ	118/161 (73%)	116 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	a	93/142 (66%)	83 (89%)	10 (11%)	0	100	100
68	b	146/215 (68%)	135 (92%)	11 (8%)	0	100	100
69	c	271/332 (82%)	259 (96%)	12 (4%)	0	100	100
70	d	211/306 (69%)	201 (95%)	9 (4%)	1 (0%)	29	67
71	e	211/279 (76%)	206 (98%)	5 (2%)	0	100	100
72	f	138/212 (65%)	131 (95%)	7 (5%)	0	100	100
73	g	130/166 (78%)	122 (94%)	8 (6%)	0	100	100
74	h	106/158 (67%)	101 (95%)	5 (5%)	0	100	100
75	i	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
76	j	84/123 (68%)	83 (99%)	1 (1%)	0	100	100
77	k	93/112 (83%)	87 (94%)	6 (6%)	0	100	100
78	l	78/138 (56%)	72 (92%)	6 (8%)	0	100	100
79	m	58/128 (45%)	53 (91%)	5 (9%)	0	100	100
80	o	92/102 (90%)	87 (95%)	5 (5%)	0	100	100
81	p	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
82	q	162/198 (82%)	159 (98%)	3 (2%)	0	100	100
83	r	144/196 (74%)	136 (94%)	8 (6%)	0	100	100
84	s	366/439 (83%)	352 (96%)	14 (4%)	0	100	100
85	t1	45/198 (23%)	42 (93%)	3 (7%)	0	100	100
85	t2	28/198 (14%)	28 (100%)	0	0	100	100
85	t3	28/198 (14%)	28 (100%)	0	0	100	100
85	t4	27/198 (14%)	25 (93%)	2 (7%)	0	100	100
85	t5	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
85	t6	25/198 (13%)	25 (100%)	0	0	100	100
86	A	2/8 (25%)	0	0	2 (100%)	0	0
All	All	13976/19235 (73%)	13324 (95%)	647 (5%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
86	A	2	THR
86	A	4	PRO
45	XD	207	ILE

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Mol	Chain	Res	Type
45	XD	208	ARG
70	d	289	PRO

### 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	97/164 (59%)	97 (100%)	0	100	100
2	1	50/60 (83%)	50 (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%)	351 (99%)	2 (1%)	86	92
7	6	313/332 (94%)	312 (100%)	1 (0%)	92	95
8	7	267/303 (88%)	267 (100%)	0	100	100
9	8	124/190 (65%)	123 (99%)	1 (1%)	81	89
10	9	104/112 (93%)	104 (100%)	0	100	100
12	A0	176/190 (93%)	175 (99%)	1 (1%)	86	92
13	A1	253/291 (87%)	250 (99%)	3 (1%)	71	84
14	A2	99/101 (98%)	96 (97%)	3 (3%)	41	64
15	A3	63/166 (38%)	63 (100%)	0	100	100
16	A4	500/566 (88%)	498 (100%)	2 (0%)	91	94
17	A5	171/171 (100%)	171 (100%)	0	100	100
19	AB	192/249 (77%)	192 (100%)	0	100	100
20	AC	115/143 (80%)	115 (100%)	0	100	100
21	AD	283/357 (79%)	281 (99%)	2 (1%)	84	90
22	AE	104/107 (97%)	104 (100%)	0	100	100
23	AF	178/209 (85%)	178 (100%)	0	100	100
24	AG	264/342 (77%)	264 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AH	125/180 (69%)	125 (100%)	0	100	100
26	AI	104/147 (71%)	104 (100%)	0	100	100
27	AJ	93/118 (79%)	92 (99%)	1 (1%)	73	85
28	AK	91/113 (80%)	91 (100%)	0	100	100
29	AL	152/226 (67%)	152 (100%)	0	100	100
30	AM	95/113 (84%)	95 (100%)	0	100	100
31	AN	93/115 (81%)	93 (100%)	0	100	100
32	AO	166/230 (72%)	166 (100%)	0	100	100
33	AP	86/123 (70%)	85 (99%)	1 (1%)	71	84
34	AQ	77/78 (99%)	77 (100%)	0	100	100
35	AR	229/318 (72%)	227 (99%)	2 (1%)	78	88
36	AS	115/164 (70%)	114 (99%)	1 (1%)	78	88
37	AT	150/157 (96%)	150 (100%)	0	100	100
38	AU	149/174 (86%)	148 (99%)	1 (1%)	84	90
39	AV	315/364 (86%)	314 (100%)	1 (0%)	92	95
40	AW	84/158 (53%)	84 (100%)	0	100	100
41	AX	307/308 (100%)	304 (99%)	3 (1%)	76	86
42	AY	104/357 (29%)	104 (100%)	0	100	100
43	AZ	79/95 (83%)	79 (100%)	0	100	100
45	XD	190/245 (78%)	189 (100%)	1 (0%)	88	93
46	XE	259/290 (89%)	259 (100%)	0	100	100
47	XF	217/262 (83%)	217 (100%)	0	100	100
48	XH	86/228 (38%)	86 (100%)	0	100	100
49	XI	194/232 (84%)	194 (100%)	0	100	100
50	XJ	133/150 (89%)	132 (99%)	1 (1%)	81	89
51	XK	155/156 (99%)	155 (100%)	0	100	100
52	XL	98/124 (79%)	98 (100%)	0	100	100
53	XM	245/249 (98%)	244 (100%)	1 (0%)	91	94
54	XN	188/211 (89%)	188 (100%)	0	100	100
55	XO	133/150 (89%)	133 (100%)	0	100	100
56	XP	125/154 (81%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	XQ	220/256 (86%)	220 (100%)	0	100	100
58	XR	118/126 (94%)	117 (99%)	1 (1%)	81	89
59	XS	145/180 (81%)	145 (100%)	0	100	100
60	XT	146/182 (80%)	144 (99%)	2 (1%)	67	81
61	XU	126/135 (93%)	126 (100%)	0	100	100
62	XV	179/191 (94%)	177 (99%)	2 (1%)	73	85
63	XW	91/119 (76%)	89 (98%)	2 (2%)	52	71
64	XX	219/229 (96%)	219 (100%)	0	100	100
65	XY	161/223 (72%)	161 (100%)	0	100	100
66	XZ	111/147 (76%)	111 (100%)	0	100	100
67	a	93/133 (70%)	93 (100%)	0	100	100
68	b	130/186 (70%)	130 (100%)	0	100	100
69	c	241/288 (84%)	240 (100%)	1 (0%)	91	94
70	d	196/273 (72%)	196 (100%)	0	100	100
71	e	188/236 (80%)	185 (98%)	3 (2%)	62	79
72	f	127/188 (68%)	127 (100%)	0	100	100
73	g	122/148 (82%)	122 (100%)	0	100	100
74	h	103/148 (70%)	103 (100%)	0	100	100
75	i	86/110 (78%)	86 (100%)	0	100	100
76	j	68/97 (70%)	68 (100%)	0	100	100
77	k	80/90 (89%)	80 (100%)	0	100	100
78	l	74/116 (64%)	74 (100%)	0	100	100
79	m	54/113 (48%)	54 (100%)	0	100	100
80	o	80/87 (92%)	80 (100%)	0	100	100
81	p	117/181 (65%)	117 (100%)	0	100	100
82	q	141/163 (86%)	141 (100%)	0	100	100
83	r	138/169 (82%)	138 (100%)	0	100	100
84	s	326/381 (86%)	325 (100%)	1 (0%)	92	95
85	t1	41/158 (26%)	40 (98%)	1 (2%)	49	69
85	t2	29/158 (18%)	29 (100%)	0	100	100
85	t3	29/158 (18%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
85	t4	28/158 (18%)	28 (100%)	0	100	100
85	t5	28/158 (18%)	28 (100%)	0	100	100
85	t6	26/158 (16%)	26 (100%)	0	100	100
86	A	2/2 (100%)	2 (100%)	0	100	100
All	All	12571/16582 (76%)	12530 (100%)	41 (0%)	92	95

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	5	144	ARG
6	5	310	ARG
7	6	99	ARG
9	8	119	LYS
12	A0	113	LYS
13	A1	51	LYS
13	A1	167	ARG
13	A1	294	LYS
14	A2	37	ARG
14	A2	40	LYS
14	A2	68	LYS
16	A4	158	LYS
16	A4	403	LYS
21	AD	186	LYS
21	AD	272	LYS
27	AJ	138	LYS
33	AP	139	ARG
35	AR	81	LYS
35	AR	99	LYS
36	AS	123	LYS
38	AU	114	ARG
39	AV	64	LYS
41	AX	189	LYS
41	AX	232	ARG
41	AX	275	LYS
45	XD	208	ARG
50	XJ	154	ARG
53	XM	44	ARG
58	XR	44	ARG
60	XT	154	LYS
60	XT	163	ARG
62	XV	149	ARG

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Mol	Chain	Res	Type
62	XV	212	LYS
63	XW	56	MET
63	XW	119	ARG
69	c	302	ARG
71	e	81	ARG
71	e	249	LYS
71	e	273	ARG
84	s	230	ARG
85	t1	21[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	52	GLN
7	6	174	HIS
13	A1	275	ASN
13	A1	279	ASN
16	A4	285	ASN
16	A4	504	ASN
23	AF	72	GLN
23	AF	233	ASN
28	AK	60	ASN
34	AQ	85	GLN
39	AV	246	ASN
41	AX	364	ASN
57	XQ	55	GLN
57	XQ	158	GLN
60	XT	210	HIS
70	d	66	HIS
77	k	15	GLN
78	l	135	ASN
82	q	147	GLN
85	t5	4	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	XA	1492/1559 (95%)	261 (17%)	7 (0%)
18	AA	920/951 (96%)	164 (17%)	3 (0%)
44	XB	54/73 (73%)	9 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2466/2583 (95%)	434 (17%)	10 (0%)

All (434) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	XA	1672	C
11	XA	1674	A
11	XA	1681	G
11	XA	1685	C
11	XA	1689	C
11	XA	1692	A
11	XA	1693	C
11	XA	1695	C
11	XA	1699	C
11	XA	1700	U
11	XA	1704	U
11	XA	1707	C
11	XA	1708	A
11	XA	1709	G
11	XA	1710	A
11	XA	1711	C
11	XA	1712	A
11	XA	1715	C
11	XA	1724	A
11	XA	1727	A
11	XA	1733	C
11	XA	1734	C
11	XA	1736	A
11	XA	1737	A
11	XA	1741	A
11	XA	1748	G
11	XA	1762	A
11	XA	1763	A
11	XA	1764	C
11	XA	1765	C
11	XA	1770	G
11	XA	1777	A
11	XA	1804	A
11	XA	1805	A
11	XA	1809	U
11	XA	1810	A
11	XA	1811	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	XA	1821	A
11	XA	1823	A
11	XA	1827	C
11	XA	1828	A
11	XA	1832	A
11	XA	1836	A
11	XA	1844	A
11	XA	1853	A
11	XA	1854	U
11	XA	1856	A
11	XA	1869	A
11	XA	1872	U
11	XA	1878	U
11	XA	1882	A
11	XA	1887	A
11	XA	1893	A
11	XA	1902	C
11	XA	1903	C
11	XA	1909	A
11	XA	1918	G
11	XA	1919	C
11	XA	1940	A
11	XA	1944	C
11	XA	1950	U
11	XA	1958	G
11	XA	1974	A
11	XA	1975	U
11	XA	1985	G
11	XA	1986	A
11	XA	1992	C
11	XA	1993	A
11	XA	1994	A
11	XA	2000	C
11	XA	2001	C
11	XA	2002	G
11	XA	2003	A
11	XA	2010	U
11	XA	2015	G
11	XA	2022	G
11	XA	2030	U
11	XA	2036	C
11	XA	2037	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	XA	2039	A
11	XA	2055	U
11	XA	2067	C
11	XA	2079	C
11	XA	2099	U
11	XA	2111	C
11	XA	2113	G
11	XA	2125	C
11	XA	2126	U
11	XA	2135	A
11	XA	2138	U
11	XA	2147	G
11	XA	2159	U
11	XA	2168	U
11	XA	2169	A
11	XA	2176	C
11	XA	2177	U
11	XA	2178	A
11	XA	2179	A
11	XA	2180	A
11	XA	2181	A
11	XA	2182	G
11	XA	2188	A
11	XA	2195	A
11	XA	2196	A
11	XA	2198	A
11	XA	2200	A
11	XA	2237	A
11	XA	2241	A
11	XA	2243	A
11	XA	2244	U
11	XA	2245	A
11	XA	2251	A
11	XA	2260	A
11	XA	2262	C
11	XA	2283	C
11	XA	2284	C
11	XA	2285	U
11	XA	2297	A
11	XA	2299	U
11	XA	2300	G
11	XA	2316	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	XA	2322	C
11	XA	2332	C
11	XA	2345	G
11	XA	2359	C
11	XA	2374	A
11	XA	2381	A
11	XA	2390	A
11	XA	2407	U
11	XA	2414	C
11	XA	2415	C
11	XA	2418	A
11	XA	2432	A
11	XA	2446	A
11	XA	2451	A
11	XA	2458	A
11	XA	2478	G
11	XA	2493	C
11	XA	2520	C
11	XA	2523	C
11	XA	2527	A
11	XA	2530	A
11	XA	2540	C
11	XA	2557	C
11	XA	2558	A
11	XA	2559	U
11	XA	2560	G
11	XA	2570	C
11	XA	2575	U
11	XA	2576	A
11	XA	2577	C
11	XA	2578	C
11	XA	2579	C
11	XA	2581	A
11	XA	2592	G
11	XA	2594	U
11	XA	2618	U
11	XA	2626	U
11	XA	2627	G
11	XA	2628	U
11	XA	2630	U
11	XA	2633	A
11	XA	2635	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	XA	2654	U
11	XA	2656	U
11	XA	2659	C
11	XA	2683	C
11	XA	2686	G
11	XA	2694	A
11	XA	2695	G
11	XA	2696	A
11	XA	2706	A
11	XA	2715	A
11	XA	2718	C
11	XA	2719	G
11	XA	2723	A
11	XA	2724	G
11	XA	2725	A
11	XA	2732	G
11	XA	2733	G
11	XA	2740	A
11	XA	2745	A
11	XA	2758	G
11	XA	2788	C
11	XA	2789	C
11	XA	2810	G
11	XA	2832	A
11	XA	2833	A
11	XA	2847	C
11	XA	2854	U
11	XA	2859	A
11	XA	2864	U
11	XA	2865	C
11	XA	2869	A
11	XA	2871	U
11	XA	2879	A
11	XA	2906	C
11	XA	2910	A
11	XA	2913	A
11	XA	2916	G
11	XA	2917	G
11	XA	2918	A
11	XA	2921	A
11	XA	2928	C
11	XA	2934	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	XA	2935	A
11	XA	2939	C
11	XA	2946	A
11	XA	2952	U
11	XA	2956	A
11	XA	2962	C
11	XA	2963	A
11	XA	2971	A
11	XA	2989	G
11	XA	2990	A
11	XA	2992	G
11	XA	3000	A
11	XA	3005	A
11	XA	3007	C
11	XA	3016	G
11	XA	3021	C
11	XA	3041	U
11	XA	3049	U
11	XA	3053	A
11	XA	3054	G
11	XA	3065	U
11	XA	3067	U
11	XA	3069	A
11	XA	3073	C
11	XA	3089	A
11	XA	3090	G
11	XA	3096	U
11	XA	3100	U
11	XA	3122	U
11	XA	3124	U
11	XA	3129	A
11	XA	3150	U
11	XA	3151	A
11	XA	3154	U
11	XA	3157	C
11	XA	3158	A
11	XA	3160	A
11	XA	3162	C
11	XA	3168	C
11	XA	3169	C
11	XA	3172	C
11	XA	3177	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	XA	3182	A
11	XA	3184	C
11	XA	3189	C
11	XA	3190	A
11	XA	3194	U
11	XA	3196	G
11	XA	3208	C
11	XA	3209	A
11	XA	3210	C
11	XA	3212	C
11	XA	3217	A
11	XA	3218	A
11	XA	3219	G
11	XA	3228	U
18	AA	651	A
18	AA	680	U
18	AA	688	A
18	AA	694	C
18	AA	704	U
18	AA	721	U
18	AA	722	C
18	AA	730	A
18	AA	753	A
18	AA	757	A
18	AA	761	A
18	AA	766	G
18	AA	771	A
18	AA	791	G
18	AA	792	C
18	AA	794	U
18	AA	796	G
18	AA	811	G
18	AA	812	A
18	AA	814	A
18	AA	825	U
18	AA	829	C
18	AA	830	U
18	AA	832	U
18	AA	835	C
18	AA	836	A
18	AA	844	A
18	AA	851	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	AA	856	A
18	AA	860	A
18	AA	861	U
18	AA	865	A
18	AA	866	A
18	AA	868	C
18	AA	869	C
18	AA	880	C
18	AA	881	A
18	AA	890	C
18	AA	893	G
18	AA	897	C
18	AA	899	G
18	AA	903	U
18	AA	917	C
18	AA	919	A
18	AA	922	C
18	AA	923	A
18	AA	932	C
18	AA	933	G
18	AA	938	A
18	AA	939	A
18	AA	942	A
18	AA	950	A
18	AA	967	A
18	AA	975	A
18	AA	992	U
18	AA	993	A
18	AA	994	A
18	AA	1001	C
18	AA	1002	C
18	AA	1009	C
18	AA	1015	A
18	AA	1031	G
18	AA	1042	U
18	AA	1049	A
18	AA	1062	G
18	AA	1069	A
18	AA	1081	U
18	AA	1082	A
18	AA	1103	A
18	AA	1105	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	AA	1106	C
18	AA	1109	A
18	AA	1121	A
18	AA	1128	C
18	AA	1142	A
18	AA	1143	C
18	AA	1151	C
18	AA	1167	A
18	AA	1188	A
18	AA	1189	U
18	AA	1190	C
18	AA	1193	U
18	AA	1194	C
18	AA	1213	A
18	AA	1214	A
18	AA	1215	U
18	AA	1220	A
18	AA	1223	C
18	AA	1225	C
18	AA	1226	C
18	AA	1227	G
18	AA	1228	A
18	AA	1229	U
18	AA	1235	U
18	AA	1236	C
18	AA	1237	A
18	AA	1248	C
18	AA	1250	C
18	AA	1251	A
18	AA	1261	C
18	AA	1268	C
18	AA	1271	C
18	AA	1284	U
18	AA	1290	C
18	AA	1293	C
18	AA	1294	A
18	AA	1295	A
18	AA	1296	A
18	AA	1297	G
18	AA	1307	G
18	AA	1326	A
18	AA	1327	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	AA	1330	C
18	AA	1331	A
18	AA	1341	C
18	AA	1342	C
18	AA	1343	A
18	AA	1344	U
18	AA	1349	U
18	AA	1353	A
18	AA	1354	A
18	AA	1356	A
18	AA	1365	A
18	AA	1369	U
18	AA	1378	C
18	AA	1390	A
18	AA	1391	U
18	AA	1402	A
18	AA	1404	C
18	AA	1405	U
18	AA	1406	A
18	AA	1407	U
18	AA	1416	A
18	AA	1422	G
18	AA	1423	A
18	AA	1430	A
18	AA	1448	U
18	AA	1459	A
18	AA	1461	A
18	AA	1463	G
18	AA	1478	A
18	AA	1482	A
18	AA	1486	C
18	AA	1488	C
18	AA	1489	G
18	AA	1503	G
18	AA	1525	C
18	AA	1526	U
18	AA	1527	A
18	AA	1528	A
18	AA	1531	C
18	AA	1537	C
18	AA	1539	C
18	AA	1551	G

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Mol	Chain	Res	Type
18	AA	1557	A
18	AA	1568	U
18	AA	1571	U
18	AA	1582	G
18	AA	1584	A
18	AA	1585	A
18	AA	1594	G
18	AA	1595	G
18	AA	1598	G
18	AA	1599	A
44	XB	1608	G
44	XB	1611	G
44	XB	1615	A
44	XB	1619	C
44	XB	1620	A
44	XB	1621	A
44	XB	1646	U
44	XB	1649	C
44	XB	1659	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	XA	2066	C
11	XA	2195	A
11	XA	2417	C
11	XA	2558	A
11	XA	2574	G
11	XA	2961	C
11	XA	2962	C
18	AA	770	C
18	AA	1048	C
18	AA	1234	C

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

5 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
86	DBB	A	3	86	4,5,6	0.81	0	1,5,7	0.81	0
86	MHW	A	1	86	9,9,10	2.62	3 (33%)	10,11,13	2.58	2 (20%)
86	MHU	A	5	86	14,15,16	2.19	4 (28%)	18,19,21	1.49	3 (16%)
86	MHV	A	6	86	7,9,10	6.01	1 (14%)	7,11,13	6.05	5 (71%)
86	004	A	7	86	9,10,11	1.03	0	9,12,14	0.90	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
86	DBB	A	3	86	-	3/3/4/6	-
86	MHW	A	1	86	-	2/2/2/4	0/1/1/1
86	MHU	A	5	86	-	0/9/12/14	0/1/1/1
86	MHV	A	6	86	-	0/1/12/14	0/1/1/1
86	004	A	7	86	-	2/4/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	A	6	MHV	OD1-CG	15.69	1.48	1.21
86	A	5	MHU	CZ-NZ	6.19	1.52	1.37
86	A	1	MHW	CA-C	5.81	1.54	1.48
86	A	1	MHW	OG1-CB	4.21	1.45	1.36
86	A	1	MHW	CB-CA	-2.39	1.36	1.40
86	A	5	MHU	CD1-CG	2.22	1.43	1.38
86	A	5	MHU	CB-CG	2.11	1.56	1.51
86	A	5	MHU	CD2-CE2	2.11	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	A	6	MHV	OD1-CG-CB	-12.24	106.43	121.96
86	A	6	MHV	OD1-CG-CD2	-8.64	107.29	122.05
86	A	1	MHW	O-C-CA	-7.21	117.39	124.22
86	A	5	MHU	CM-N-CA	3.50	124.52	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	A	6	MHV	CB-CA-N	-3.45	105.36	112.50
86	A	6	MHV	CD2-CG-CB	2.92	120.24	115.89
86	A	6	MHV	CE-CD2-CG	2.91	116.77	111.89
86	A	1	MHW	CD-CG2-CB	-2.76	116.56	120.05
86	A	5	MHU	CB-CA-C	-2.48	106.95	111.65
86	A	5	MHU	O-C-CA	-2.03	119.47	124.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	A	1	MHW	O-C-CA-N
86	A	1	MHW	O-C-CA-CB
86	A	3	DBB	O-C-CA-CB
86	A	3	DBB	C-CA-CB-CG
86	A	3	DBB	N-CA-CB-CG
86	A	7	004	C-CA-CB-CG1
86	A	7	004	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A	1	MHW	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 204 ligands modelled in this entry, 202 are monoatomic - leaving 2 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
89	DOL	XA	5141	-	43,50,50	3.48	14 (32%)	51,70,70	2.75	13 (25%)
90	GTP	AX	500	-	26,34,34	1.11	2 (7%)	32,54,54	1.49	6 (18%)

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
89	DOL	XA	5141	-	-	16/58/77/77	0/2/3/3
90	GTP	AX	500	-	-	8/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	XA	5141	DOL	C28-C29	10.18	1.56	1.32
89	XA	5141	DOL	C22-C23	9.53	1.56	1.32
89	XA	5141	DOL	C19-C20	7.15	1.56	1.34
89	XA	5141	DOL	C26-N25	6.58	1.48	1.34
89	XA	5141	DOL	C6-N5	6.42	1.49	1.34
89	XA	5141	DOL	C22-C20	5.41	1.57	1.45
89	XA	5141	DOL	O36-C37	5.38	1.46	1.34
89	XA	5141	DOL	C42-S39	5.16	1.86	1.78
89	XA	5141	DOL	C13-C10	4.48	1.57	1.50
90	AX	500	GTP	C5-C6	-3.93	1.39	1.47
89	XA	5141	DOL	C16-C14	3.71	1.56	1.51
89	XA	5141	DOL	C28-C26	3.68	1.55	1.48
89	XA	5141	DOL	O27-C26	-2.85	1.19	1.24
89	XA	5141	DOL	C8-C6	2.71	1.55	1.50
89	XA	5141	DOL	O18-C17	-2.66	1.38	1.43
90	AX	500	GTP	C2-N3	2.14	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	XA	5141	DOL	O40-S39-O41	-14.72	101.41	118.19
89	XA	5141	DOL	C24-N25-C26	-6.43	111.63	122.03
89	XA	5141	DOL	C4-N5-C1	-3.69	107.91	112.45
90	AX	500	GTP	PA-O3A-PB	-3.65	120.31	132.83
89	XA	5141	DOL	C32-O36-C37	-3.61	111.58	117.78
89	XA	5141	DOL	C23-C22-C20	-3.24	121.00	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	AX	500	GTP	C5-C6-N1	3.20	119.59	113.95
90	AX	500	GTP	PB-O3B-PG	-3.02	122.47	132.83
90	AX	500	GTP	C8-N7-C5	2.99	108.68	102.99
90	AX	500	GTP	C2-N1-C6	-2.96	119.64	125.10
89	XA	5141	DOL	O15-C14-C16	2.93	125.73	121.55
89	XA	5141	DOL	O36-C32-C30	2.83	111.82	107.09
89	XA	5141	DOL	C3-C4-N5	2.73	106.14	103.33
89	XA	5141	DOL	O15-C14-C13	2.66	124.74	120.77
89	XA	5141	DOL	C21-C20-C22	2.52	122.04	118.08
89	XA	5141	DOL	C8-C6-N5	-2.49	116.89	119.76
89	XA	5141	DOL	C16-C17-C19	-2.47	106.46	111.10
89	XA	5141	DOL	C30-C29-C28	-2.44	119.79	126.44
90	AX	500	GTP	O6-C6-C5	-2.14	120.20	124.37

There are no chirality outliers.

All (24) torsion outliers are listed below:

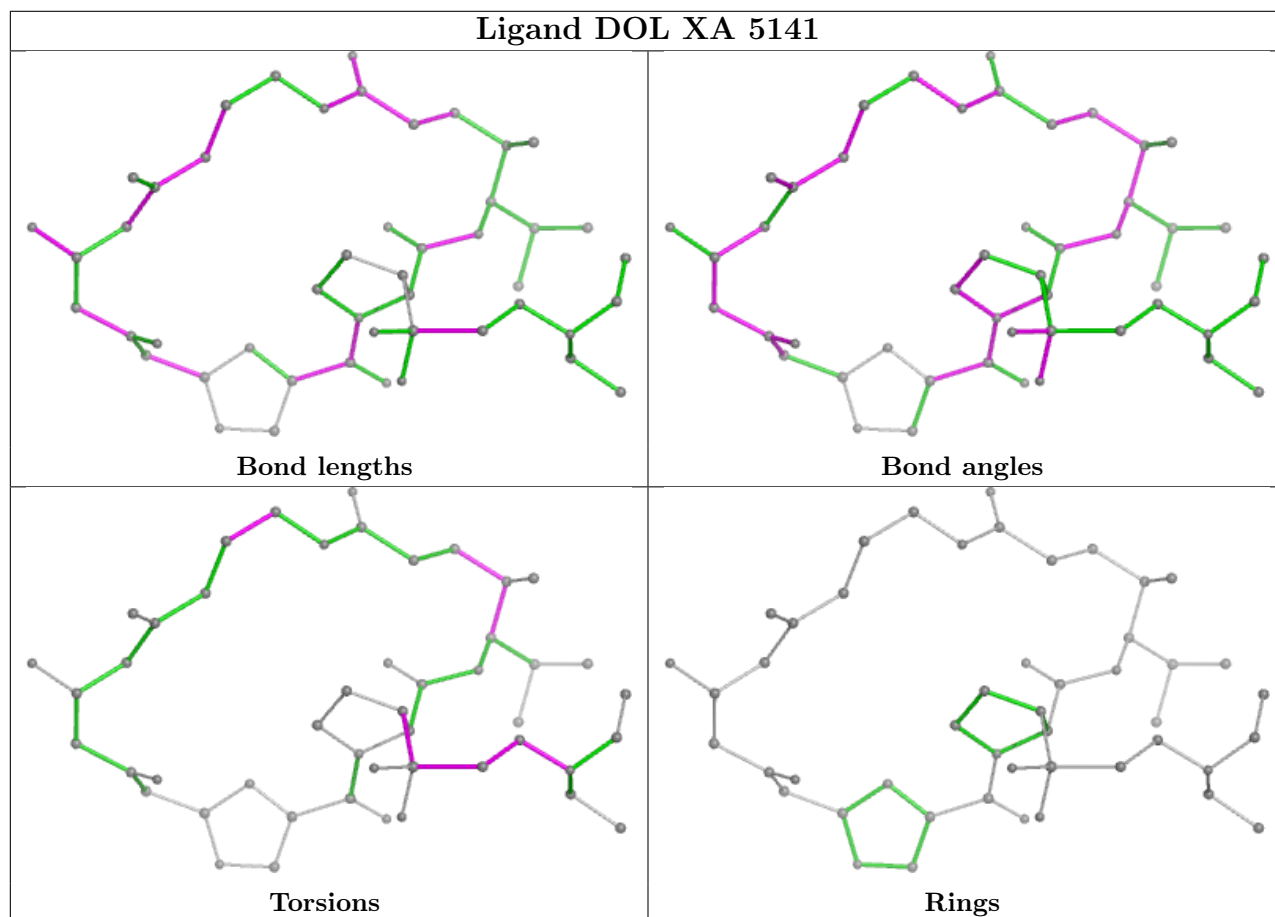
Mol	Chain	Res	Type	Atoms
89	XA	5141	DOL	C1-C2-S39-O41
89	XA	5141	DOL	C1-C2-S39-O40
89	XA	5141	DOL	C43-C42-S39-C2
89	XA	5141	DOL	C43-C42-S39-O41
89	XA	5141	DOL	C29-C30-C32-C33
89	XA	5141	DOL	C31-C30-C32-C33
90	AX	500	GTP	PB-O3B-PG-O3G
90	AX	500	GTP	C5'-O5'-PA-O3A
89	XA	5141	DOL	C3-C2-S39-O41
89	XA	5141	DOL	C3-C2-S39-C42
89	XA	5141	DOL	S39-C42-C43-N44
89	XA	5141	DOL	C28-C29-C30-C31
90	AX	500	GTP	O4'-C4'-C5'-O5'
89	XA	5141	DOL	C3-C2-S39-O40
89	XA	5141	DOL	C31-C30-C32-O36
90	AX	500	GTP	C5'-O5'-PA-O1A
90	AX	500	GTP	C5'-O5'-PA-O2A
89	XA	5141	DOL	C29-C30-C32-O36
89	XA	5141	DOL	C22-C23-C24-N25
89	XA	5141	DOL	C43-C42-S39-O40
90	AX	500	GTP	C3'-C4'-C5'-O5'
90	AX	500	GTP	PB-O3B-PG-O1G
90	AX	500	GTP	PB-O3B-PG-O2G
89	XA	5141	DOL	C42-C43-N44-C47

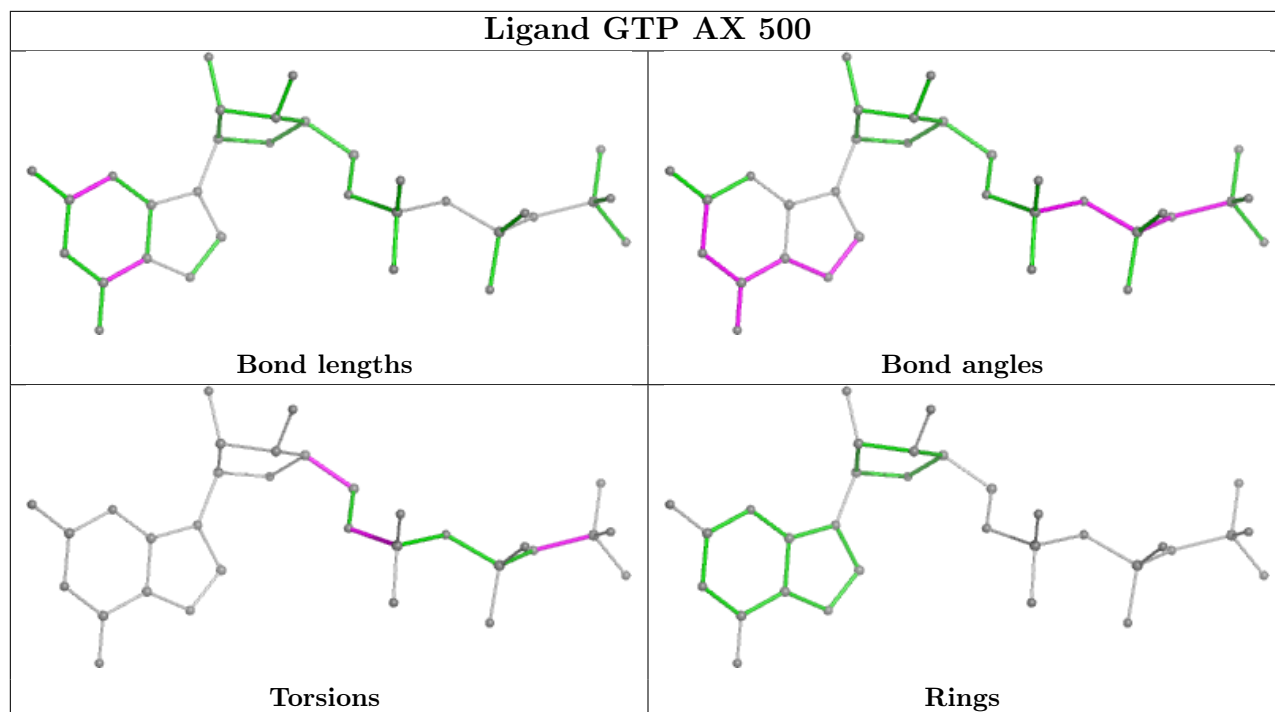
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	XA	5141	DOL	4	0
90	AX	500	GTP	1	0

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





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	7	2
41	AX	2
7	6	2
18	AA	1
16	A4	1
83	r	1
39	AV	1
17	A5	1
70	d	1
86	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1383:A	O3'	1388:C	P	8.11
1	A4	537:ARG	C	538:ASP	N	6.58

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	285:ASN	C	286:LEU	N	5.98
1	r	134:ARG	C	135:LEU	N	5.36
1	AV	269:SER	C	270:PRO	N	5.00
1	A5	105:THR	C	106:ARG	N	4.31
1	AX	168:LEU	C	169:LEU	N	3.23
1	6	79:GLY	C	80:GLU	N	3.17
1	7	185:LEU	C	186:ASP	N	3.11
1	d	252:LEU	C	253:THR	N	3.06
1	AX	195:ASN	C	196:GLU	N	3.03
1	6	282:SER	C	283:GLU	N	3.01
1	A	5:MHU	C	6:MHV	N	1.62

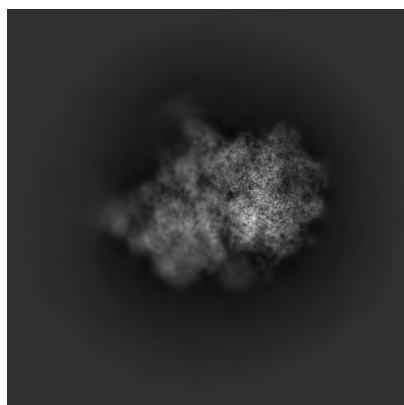
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11390. These allow visual inspection of the internal detail of the map and identification of artifacts.

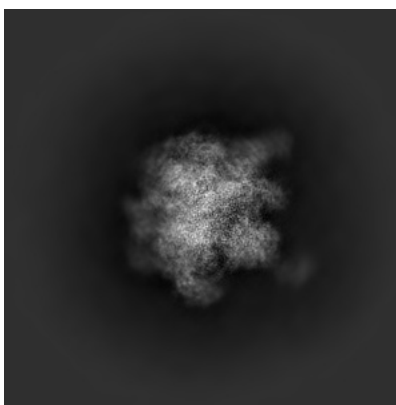
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

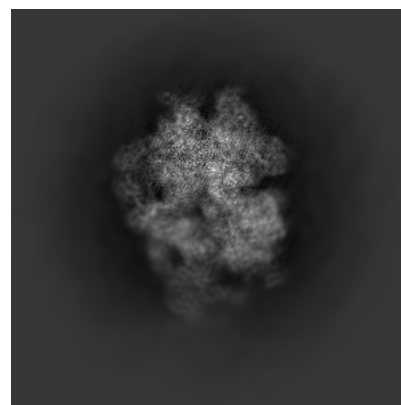
#### 6.1.1 Primary map



X



Y

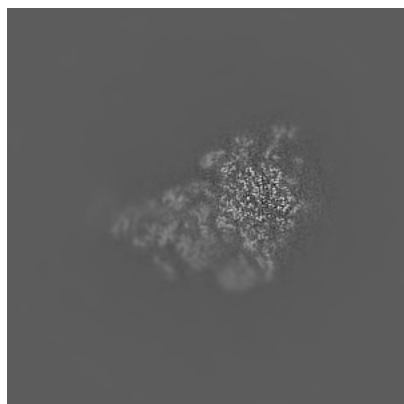


Z

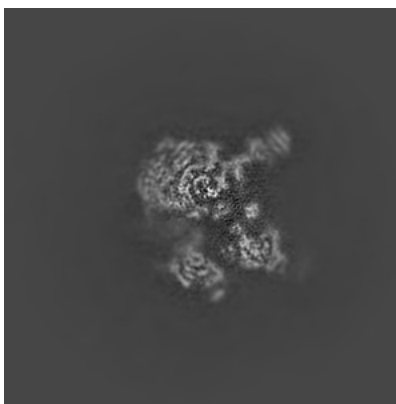
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

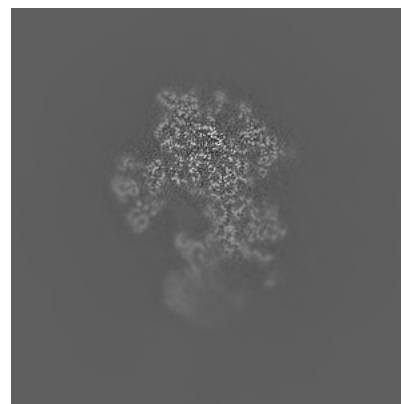
#### 6.2.1 Primary map



X Index: 260



Y Index: 260



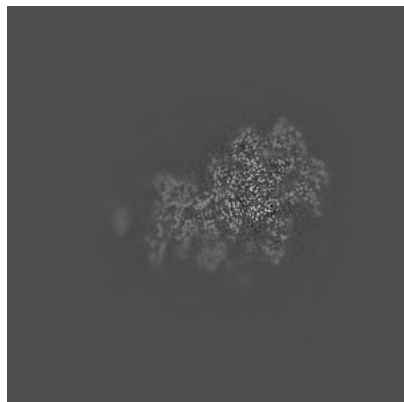
Z Index: 260



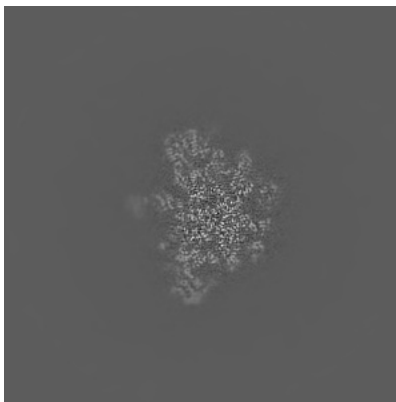
The images above show central slices of the map in three orthogonal directions.

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

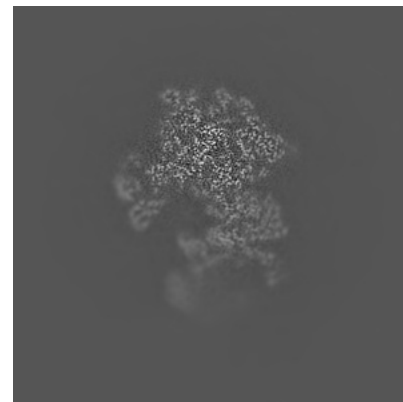
### 6.3.1 Primary map



X Index: 278



Y Index: 321

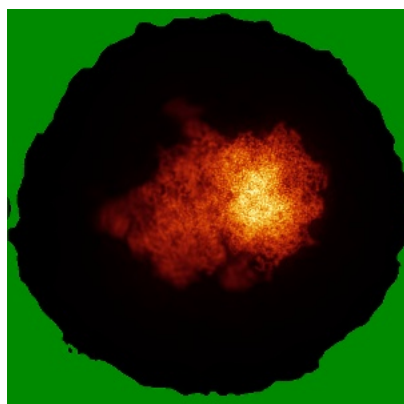


Z Index: 264

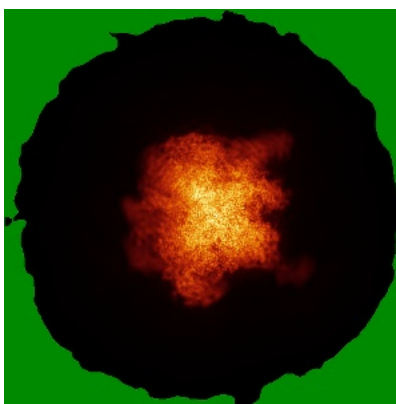
The images above show the largest variance slices of the map in three orthogonal directions.

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

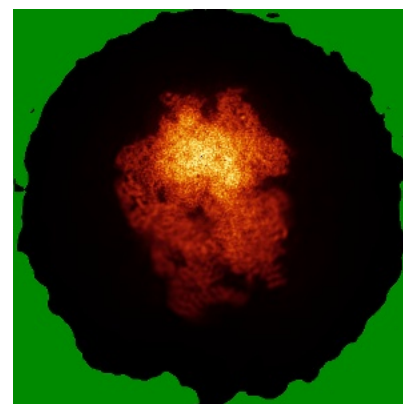
### 6.4.1 Primary map



X



Y

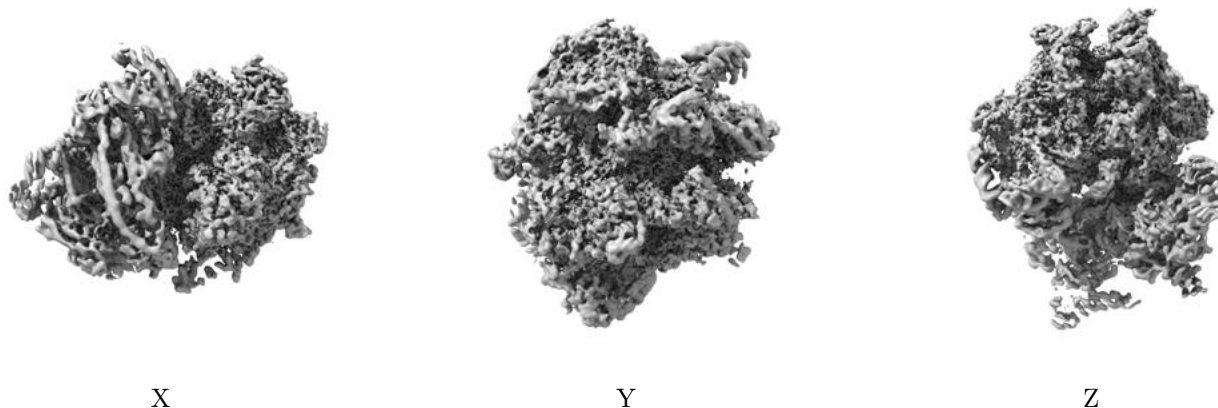


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

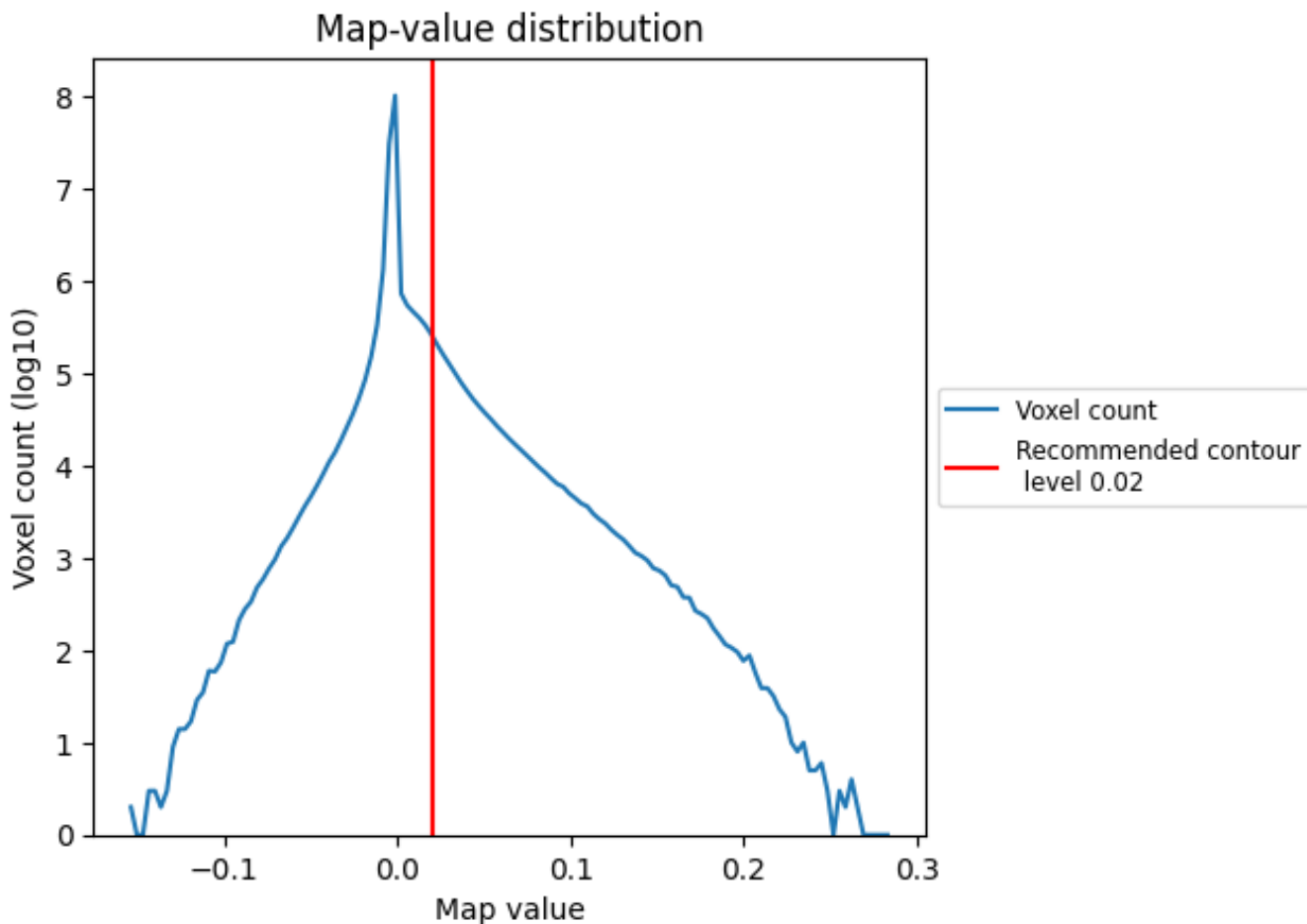
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

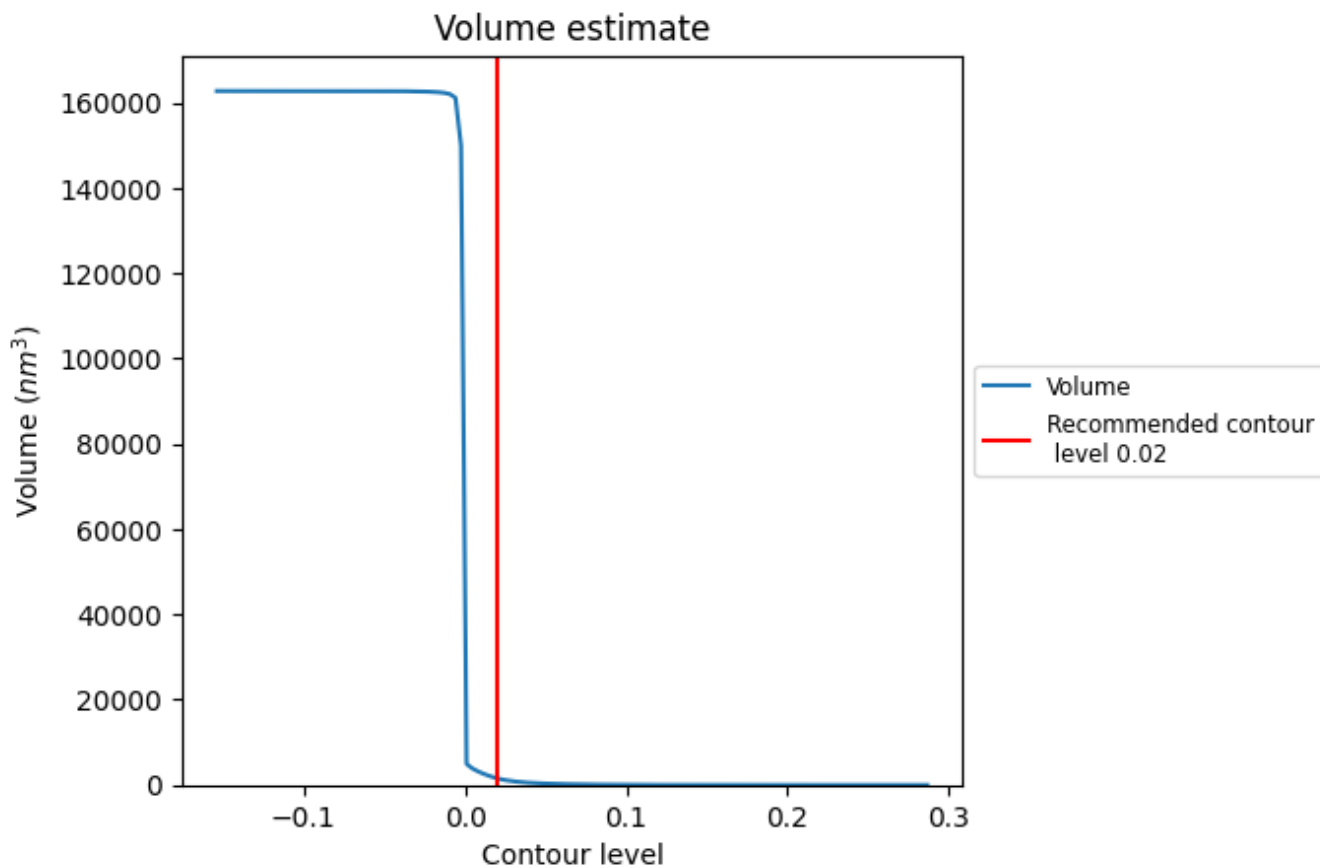
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

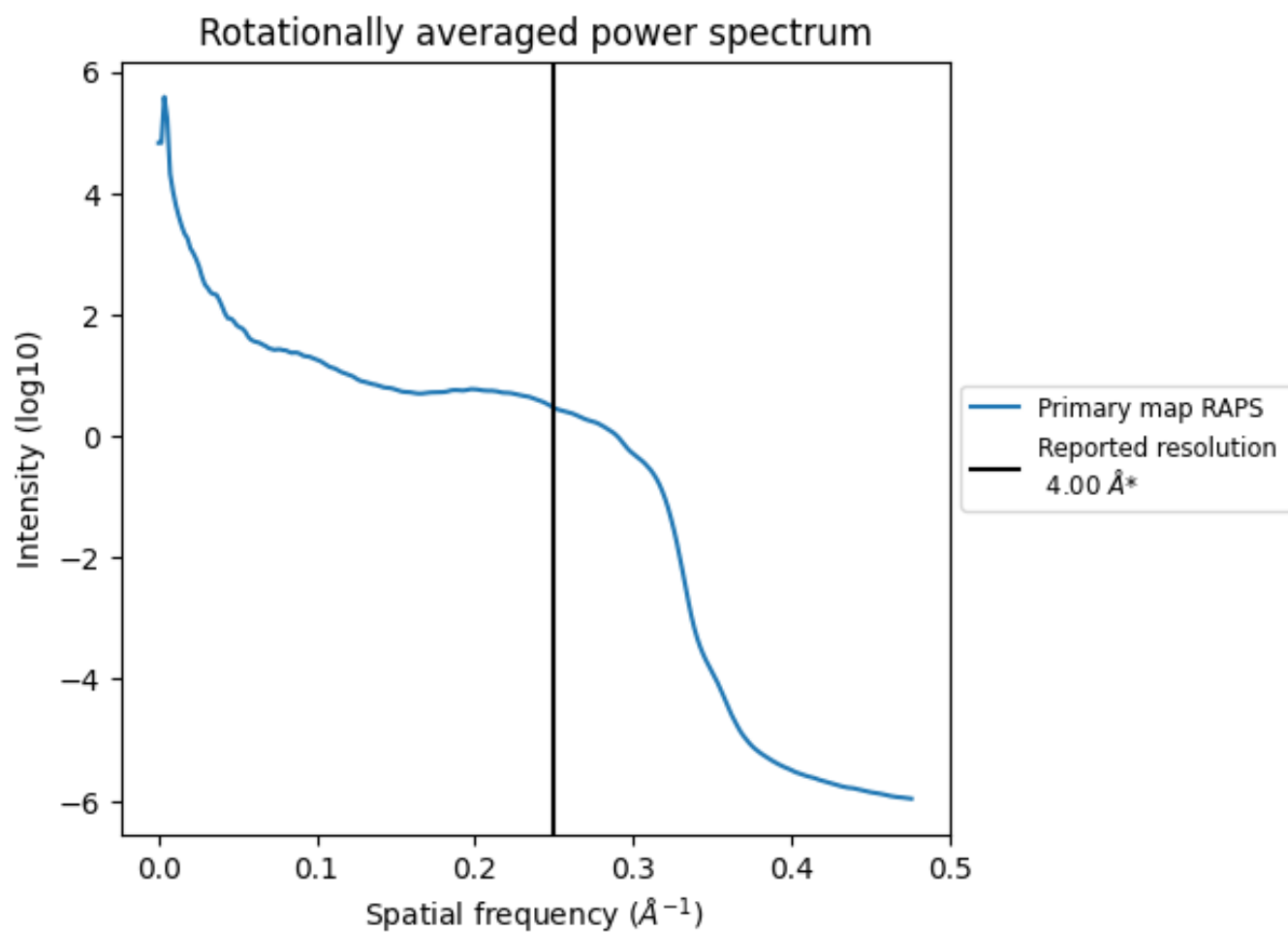
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1563  $\text{nm}^3$ ; this corresponds to an approximate mass of 1412 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  $0.250 \text{\AA}^{-1}$

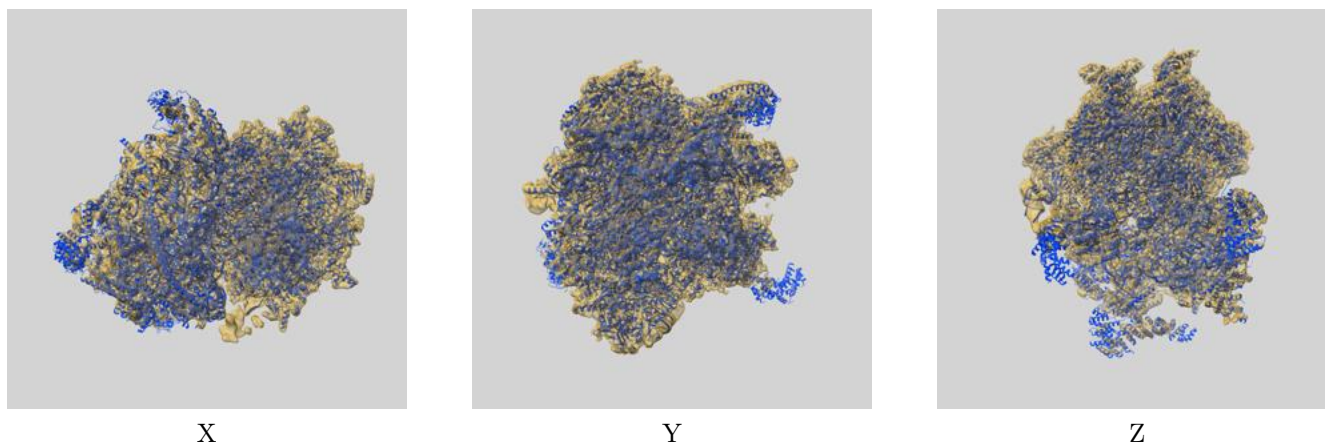
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

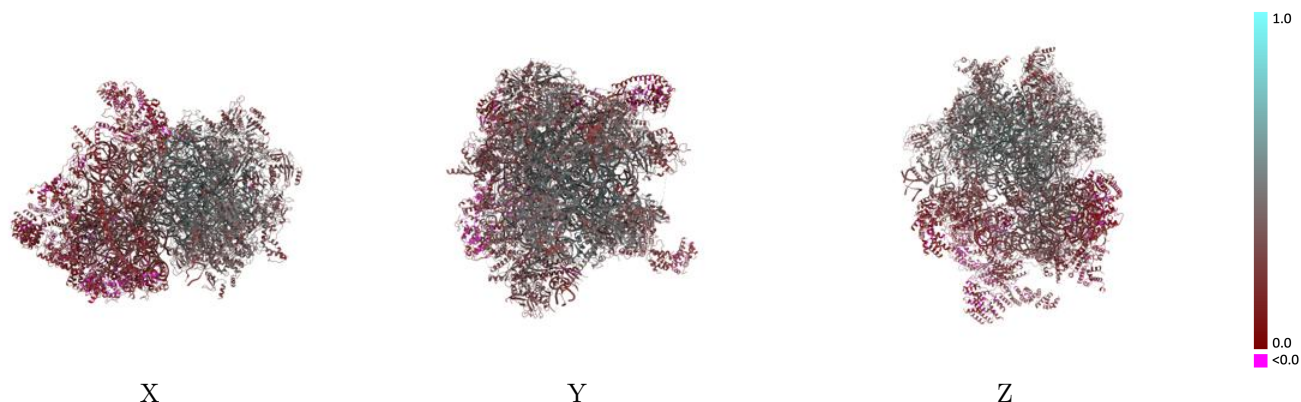
This section contains information regarding the fit between EMDB map EMD-11390 and PDB model 6ZS9. Per-residue inclusion information can be found in section 3 on page 22.

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



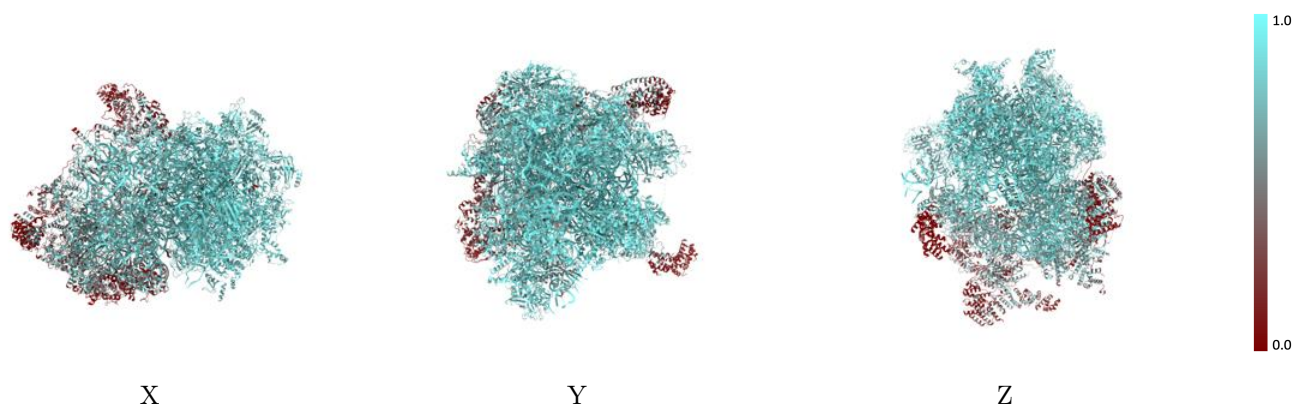
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

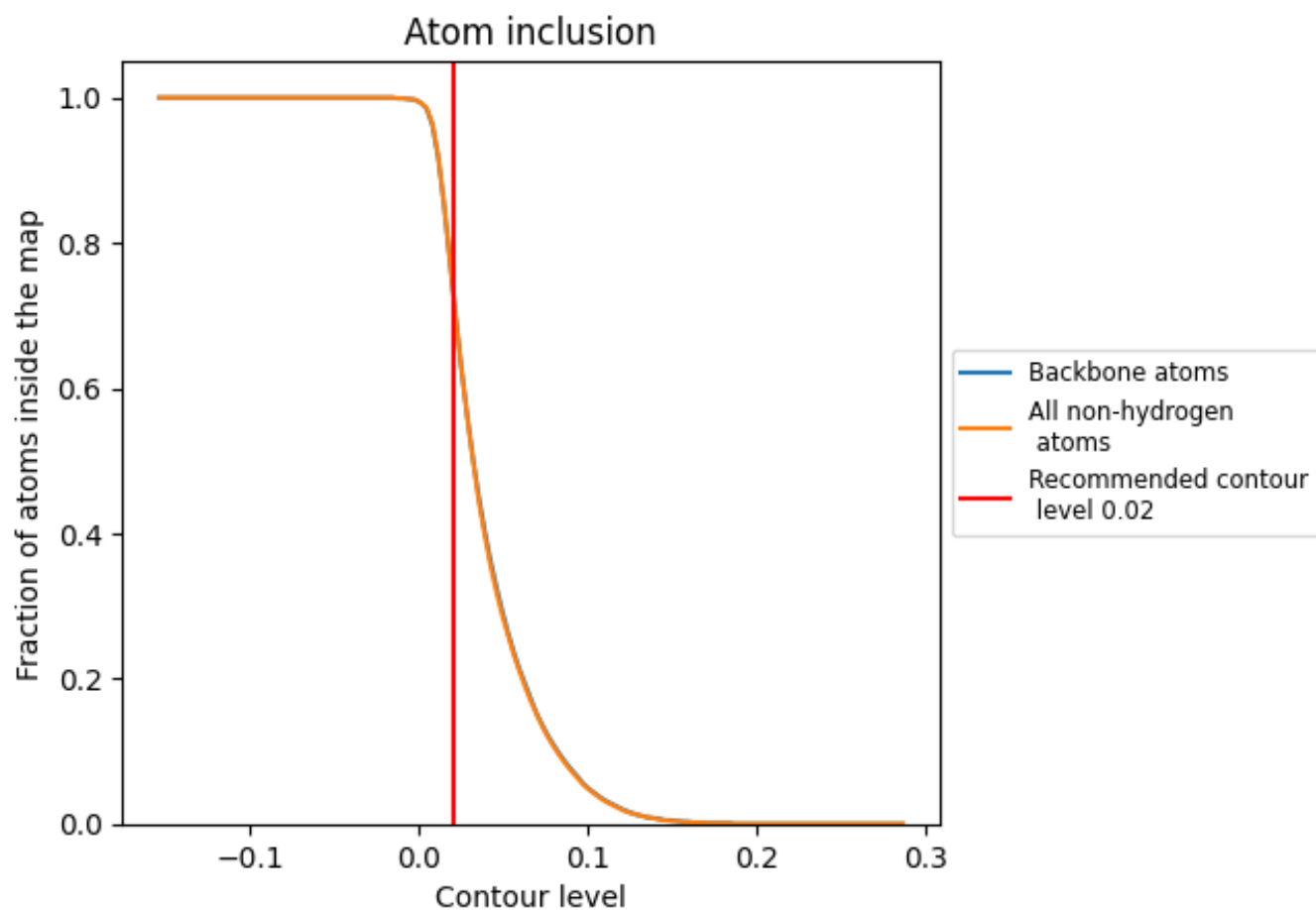
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 73% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7340	 0.3220
0	 0.8690	 0.4080
1	 0.8380	 0.3940
2	 0.9170	 0.5100
3	 0.8950	 0.4860
4	 0.9110	 0.4660
5	 0.8290	 0.3750
6	 0.8140	 0.3390
7	 0.7920	 0.3450
8	 0.5980	 0.2100
9	 0.8230	 0.3920
A	 0.8900	 0.4820
A0	 0.5810	 0.1780
A1	 0.2490	 0.1060
A2	 0.3720	 0.1990
A3	 0.7870	 0.3580
A4	 0.2210	 0.1310
A5	 0.5650	 0.2350
AA	 0.8810	 0.2660
AB	 0.6390	 0.1850
AC	 0.4620	 0.1490
AD	 0.5750	 0.2260
AE	 0.4920	 0.1860
AF	 0.3010	 0.1090
AG	 0.4580	 0.1420
AH	 0.2400	 0.1200
AI	 0.5450	 0.1730
AJ	 0.7230	 0.3000
AK	 0.4830	 0.0970
AL	 0.5550	 0.1820
AM	 0.5870	 0.1950
AN	 0.6480	 0.2110
AO	 0.6160	 0.2230
AP	 0.5320	 0.1890
AQ	 0.6700	 0.2480

































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Chain	Atom inclusion	Q-score
AR	0.5380	0.1660
AS	0.5060	0.1830
AT	0.6470	0.2290
AU	0.5110	0.1810
AV	0.3200	0.1320
AW	0.5490	0.1580
AX	0.1840	0.0640
AY	0.2640	0.1160
AZ	0.3230	0.1370
XA	0.9540	0.4670
XB	0.9580	0.3160
XD	0.8580	0.4280
XE	0.8690	0.4320
XF	0.8810	0.4510
XH	0.7950	0.3670
XI	0.5960	0.2500
XJ	0.6560	0.2080
XK	0.8680	0.4460
XL	0.8720	0.4420
XM	0.8690	0.4280
XN	0.8540	0.4310
XO	0.8580	0.4160
XP	0.8330	0.3680
XQ	0.7620	0.3760
XR	0.8660	0.4470
XS	0.8630	0.4440
XT	0.8720	0.4470
XU	0.8650	0.4200
XV	0.8210	0.3660
XW	0.8930	0.4700
XX	0.8300	0.3870
XY	0.8700	0.4200
XZ	0.8870	0.4600
a	0.8320	0.3980
b	0.8870	0.4390
c	0.8410	0.3820
d	0.7640	0.3340
e	0.6470	0.1870
f	0.6570	0.2440
g	0.8480	0.4110
h	0.8000	0.3470
i	0.8690	0.4730

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Chain	Atom inclusion	Q-score
j	 0.8500	 0.4030
k	 0.7660	 0.2760
l	 0.7220	 0.2560
m	 0.6570	 0.2000
o	 0.9070	 0.4700
p	 0.7970	 0.3320
q	 0.6440	 0.3000
r	 0.8670	 0.4100
s	 0.8610	 0.4140
t1	 0.2520	 0.2020
t2	 0.2020	 0.1940
t3	 0.0000	 0.1650
t4	 0.0000	 0.1480
t5	 0.0000	 0.1500
t6	 0.0000	 0.1200