



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:29 AM UTC

PDB ID : 6ZS9 / pdb_00006zs9
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

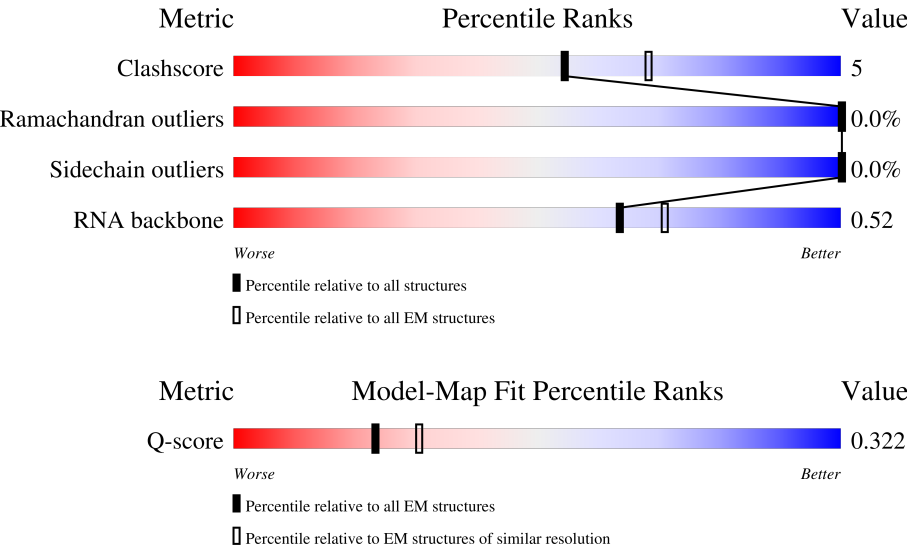
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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.



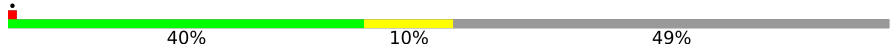
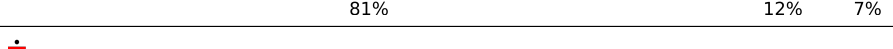
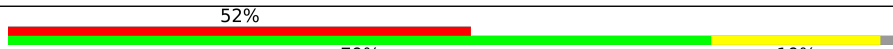
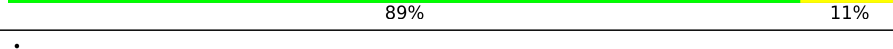
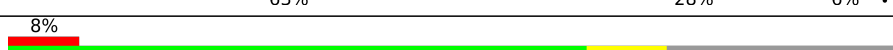
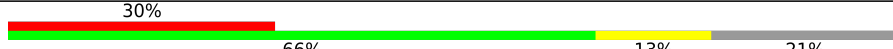
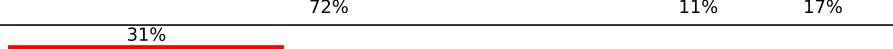
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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

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

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

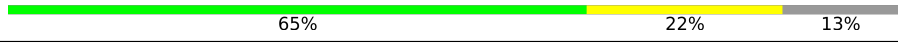
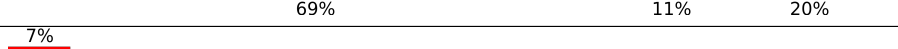
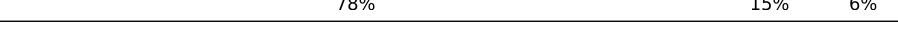
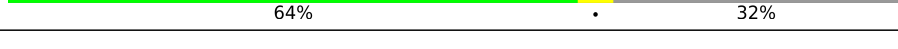
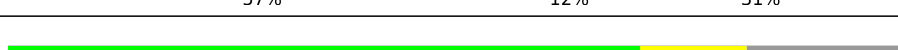
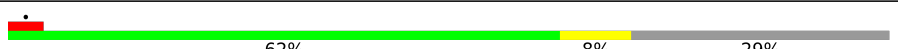
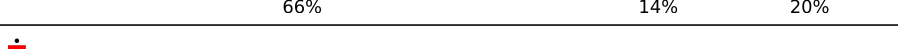
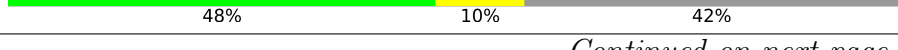
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Mol	Chain	Length	Quality of chain
29	AL	257	
30	AM	137	
31	AN	130	
32	AO	258	
33	AP	142	
34	AQ	86	
35	AR	360	
36	AS	190	
37	AT	173	
38	AU	205	
39	AV	414	
40	AW	187	
41	AX	348	
42	AY	395	
43	AZ	106	
44	XB	73	
45	XD	305	
46	XE	348	
47	XF	311	
48	XH	267	
49	XI	261	
50	XJ	192	
51	XK	178	
52	XL	145	
53	XM	296	

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Mol	Chain	Length	Quality of chain
54	XN	251	
55	XO	175	
56	XP	179	
57	XQ	292	
58	XR	149	
59	XS	205	
60	XT	212	
61	XU	153	
62	XV	216	
63	XW	148	
64	XX	256	
65	XY	250	
66	XZ	161	
67	a	142	
68	b	215	
69	c	332	
70	d	306	
71	e	279	
72	f	212	
73	g	166	
74	h	158	
75	i	128	
76	j	123	
77	k	112	
78	l	138	

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Mol	Chain	Length	Quality of chain
79	m	128	
80	o	102	
81	p	206	
82	q	198	
83	r	196	
84	s	439	
85	t1	198	
85	t2	198	
85	t3	198	
85	t4	198	
85	t5	198	
85	t6	198	
86	A	8	

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
1	0	108	Total	C	H	N	O	S	0	0
			1782	545	902	172	157	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
35	AR	250	Total	C	H	N	O	S	0	0
			4134	1314	2074	353	385	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
55	XO	152	Total	C	H	N	O	S	0	0
			2528	784	1283	239	215	7		

- Molecule 56 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
71	e	217	Total	C	H	N	O	S	0	0
			3529	1124	1767	310	323	5		

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

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

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

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

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

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

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

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

- 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
76	j	86	Total	C	H	N	O	S	0	0
			1367	426	678	134	127	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 86 is a protein called Quinupristin.

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

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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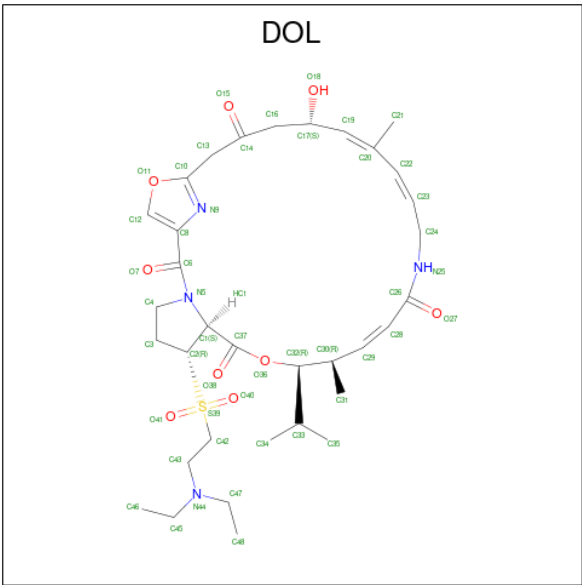
Continued from previous page...

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 (CCD ID: MG) (formula: Mg).

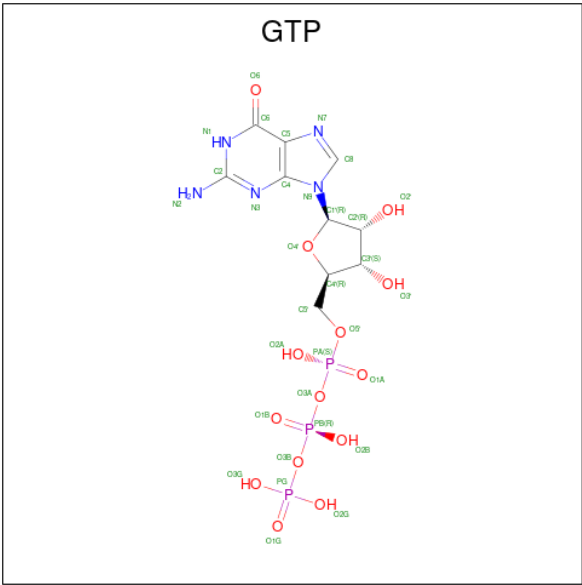
Mol	Chain	Residues	Atoms		AltConf
88	2	1	Total 1	Mg 1	0
88	9	1	Total 1	Mg 1	0
88	XA	140	Total 140	Mg 140	0
88	AA	45	Total 45	Mg 45	0
88	AH	1	Total 1	Mg 1	0
88	XD	1	Total 1	Mg 1	0
88	XI	1	Total 1	Mg 1	0
88	XM	2	Total 2	Mg 2	0
88	XW	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	o	1	Total 1	Mg 1	0

- 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 (CCD ID: DOL) (formula: C₃₄H₅₀N₄O₉S).



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

- Molecule 90 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

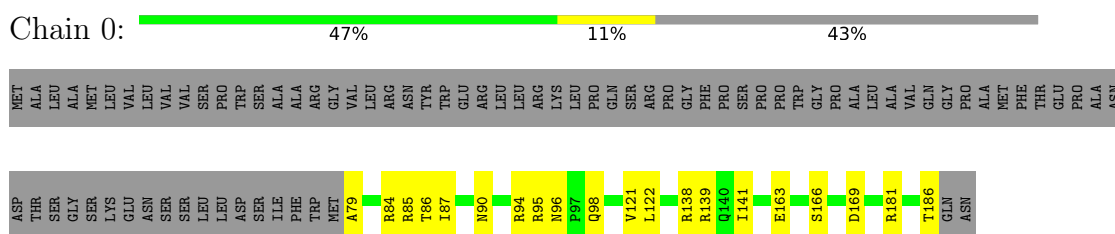


Mol	Chain	Residues	Atoms						AltConf
90	AX	1	Total	C	H	N	O	P	0
			42	10	10	5	14	3	

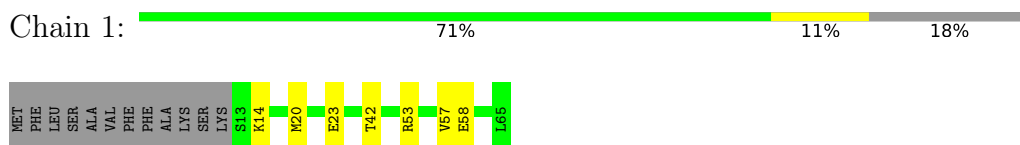
3 Residue-property plots

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.

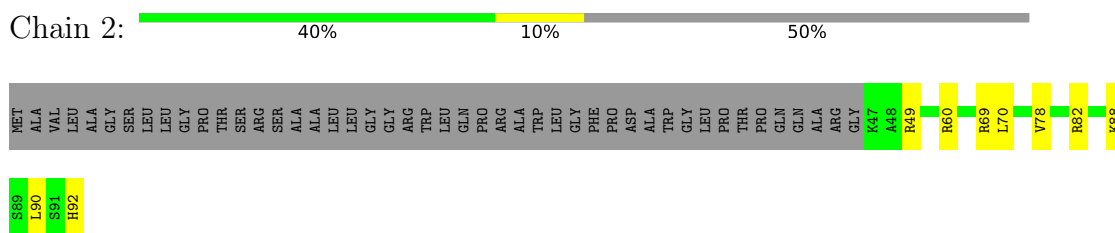
- Molecule 1: 39S ribosomal protein L32, mitochondrial



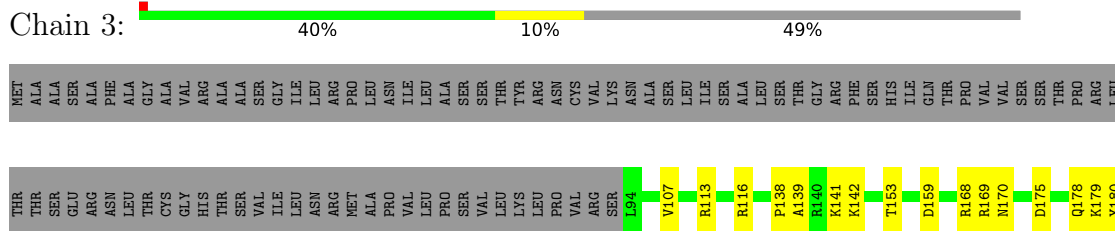
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial



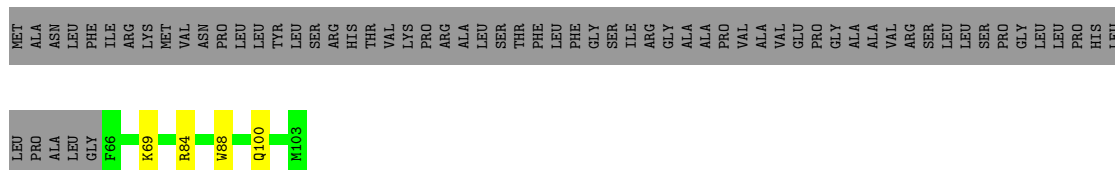
- Molecule 4: 39S ribosomal protein L35, mitochondrial





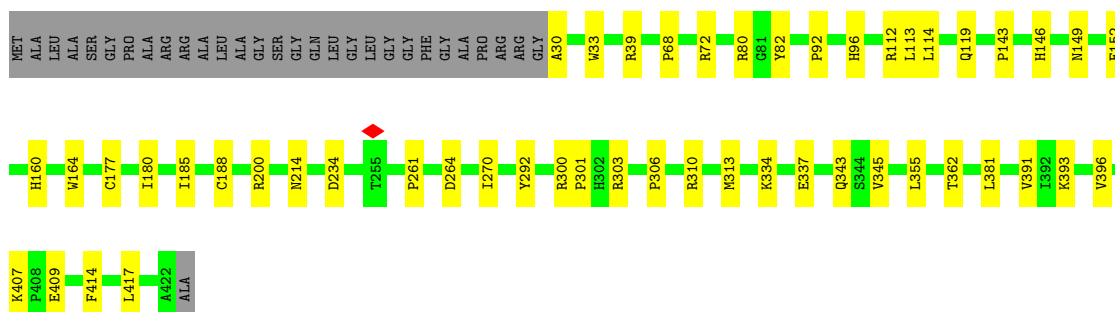
- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4: 33% 63%



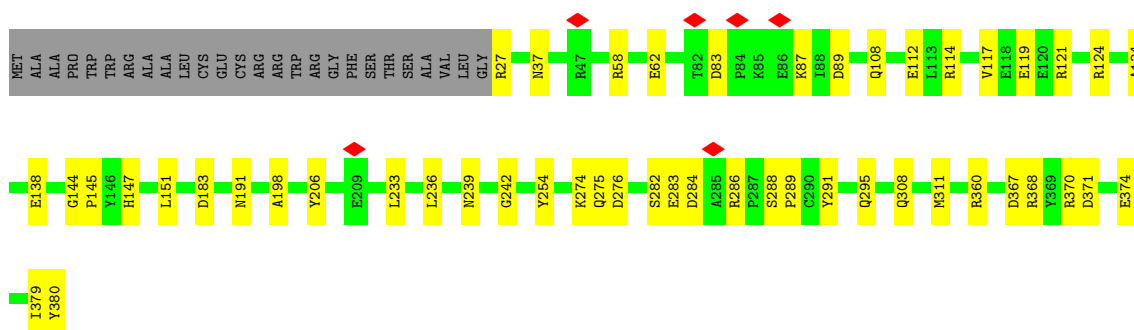
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5: 81% 12% 7%



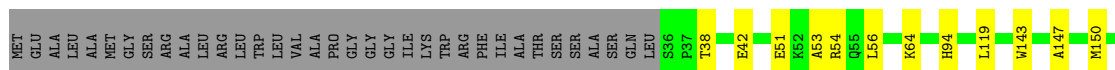
- Molecule 7: 39S ribosomal protein L38, mitochondrial

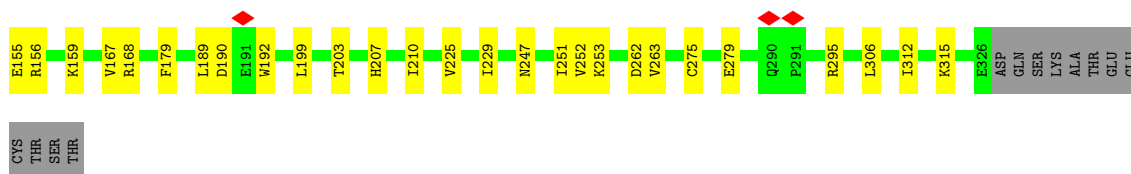
Chain 6: 80% 13% 7%



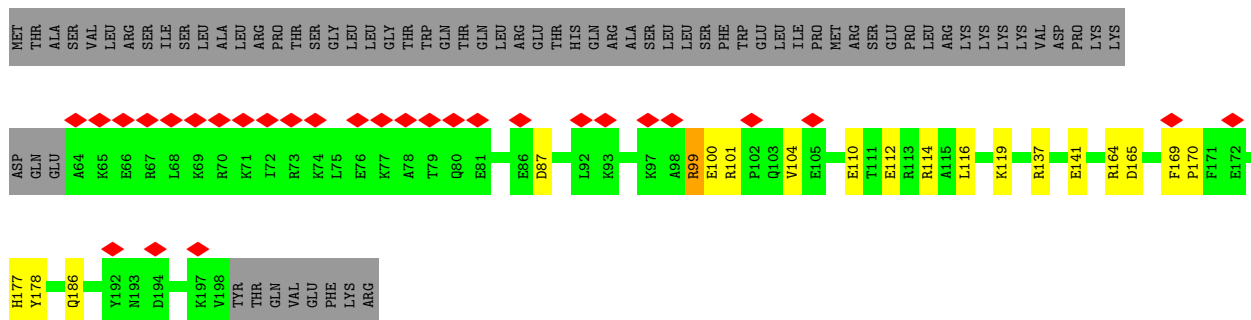
- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7: 75% 12% 14%

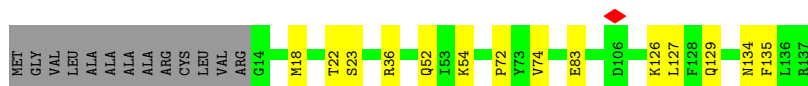
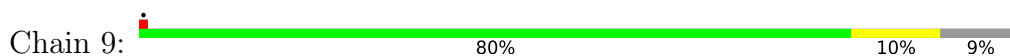




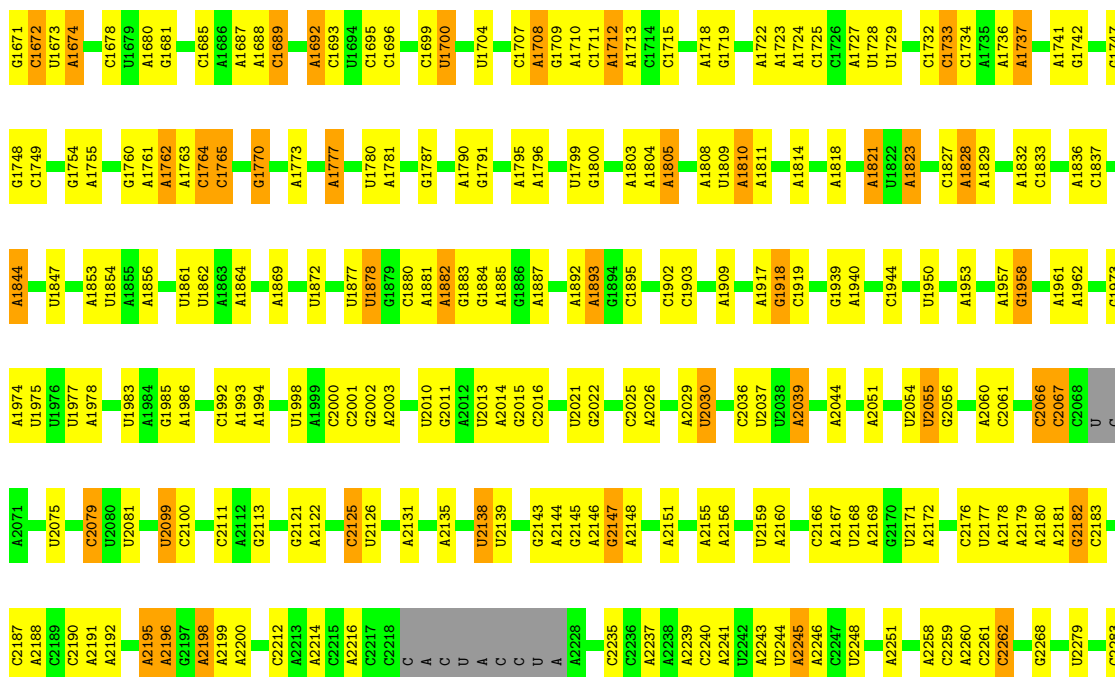
- Molecule 9: 39S ribosomal protein L40, mitochondrial

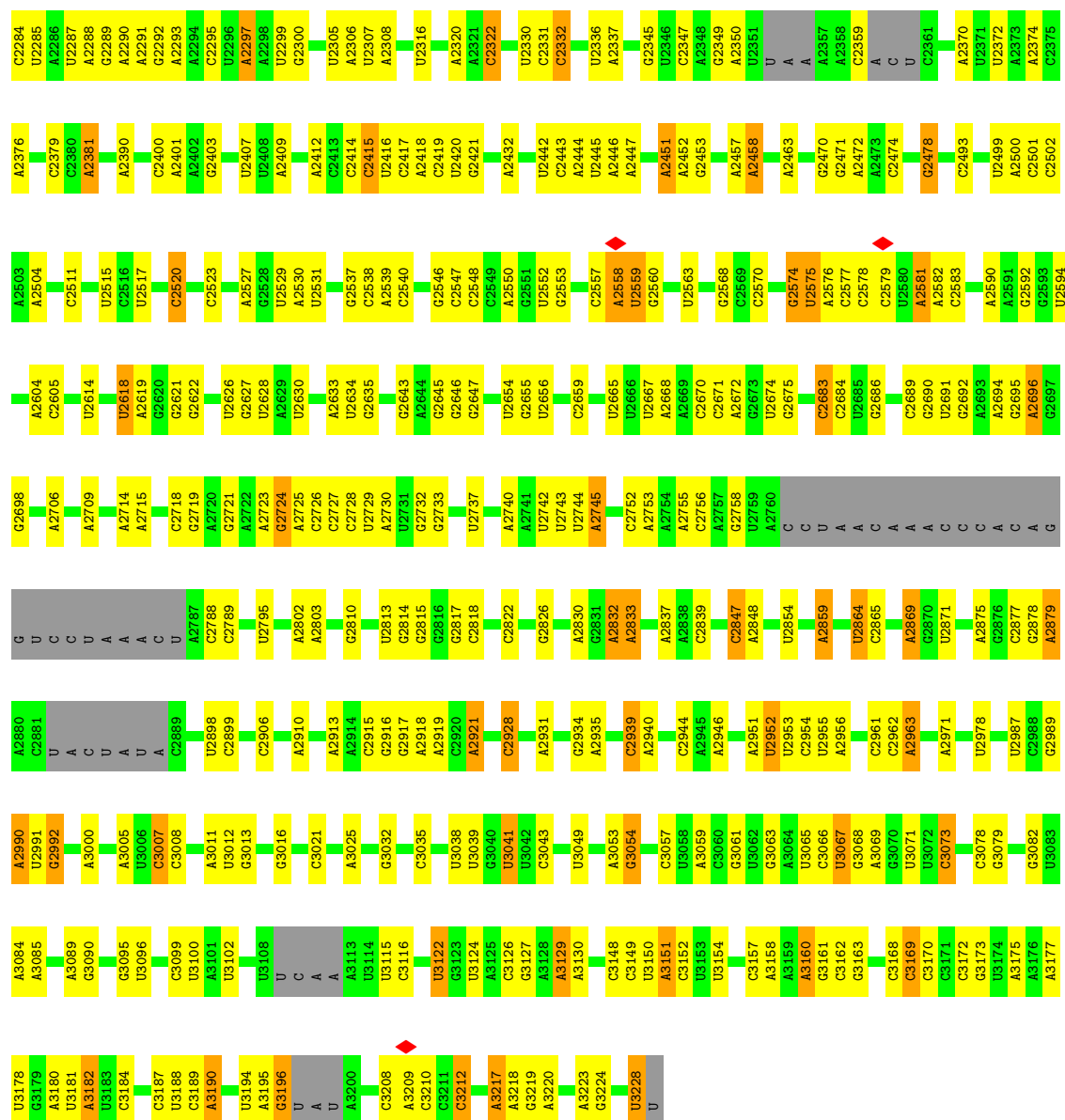


- Molecule 10: 39S ribosomal protein L41, mitochondrial

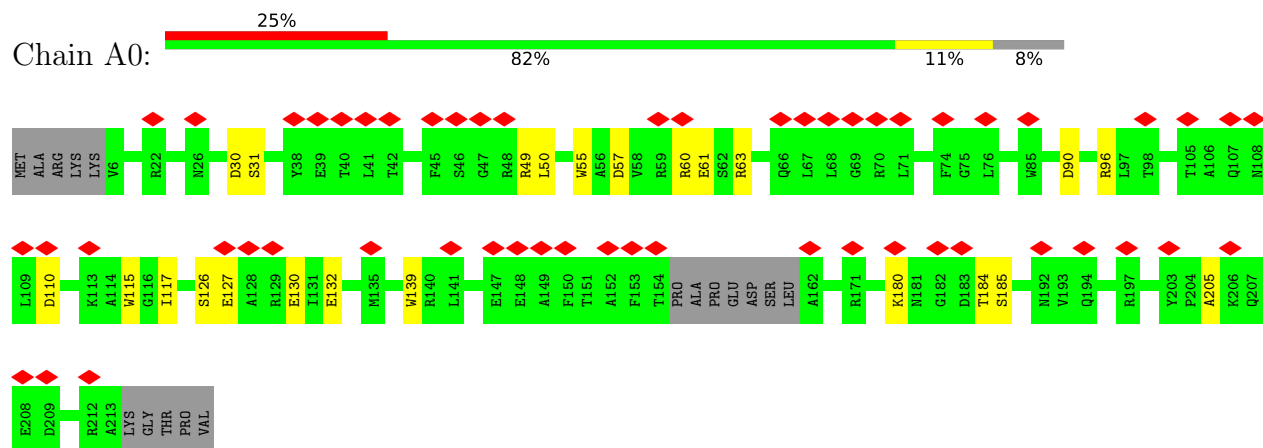


- Molecule 11: 16S rRNA



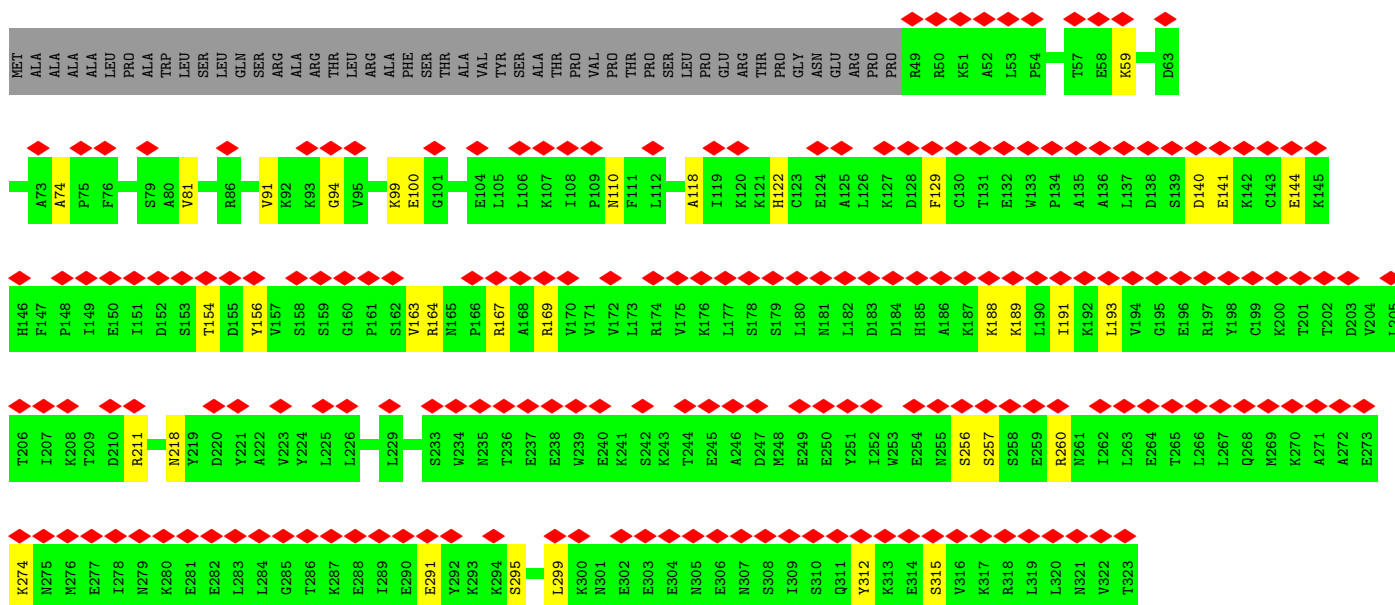


- Molecule 12: 28S ribosomal protein S34, mitochondrial

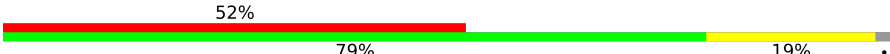


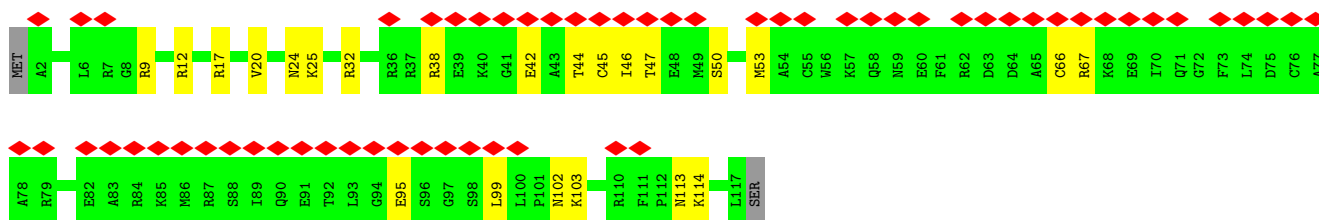
- Molecule 13: 28S ribosomal protein S35, mitochondrial

Chain A1: 



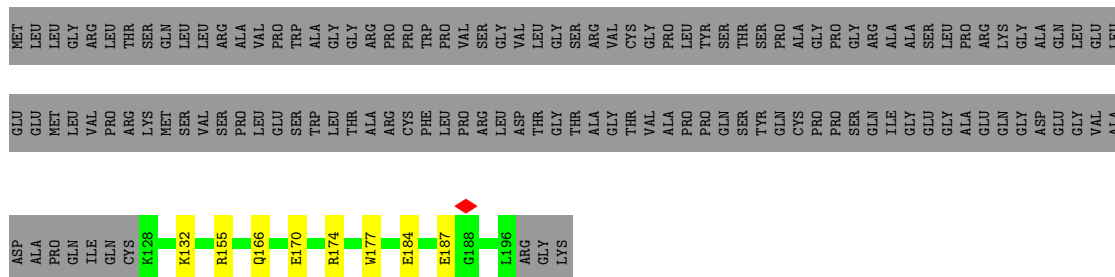
- Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2: 



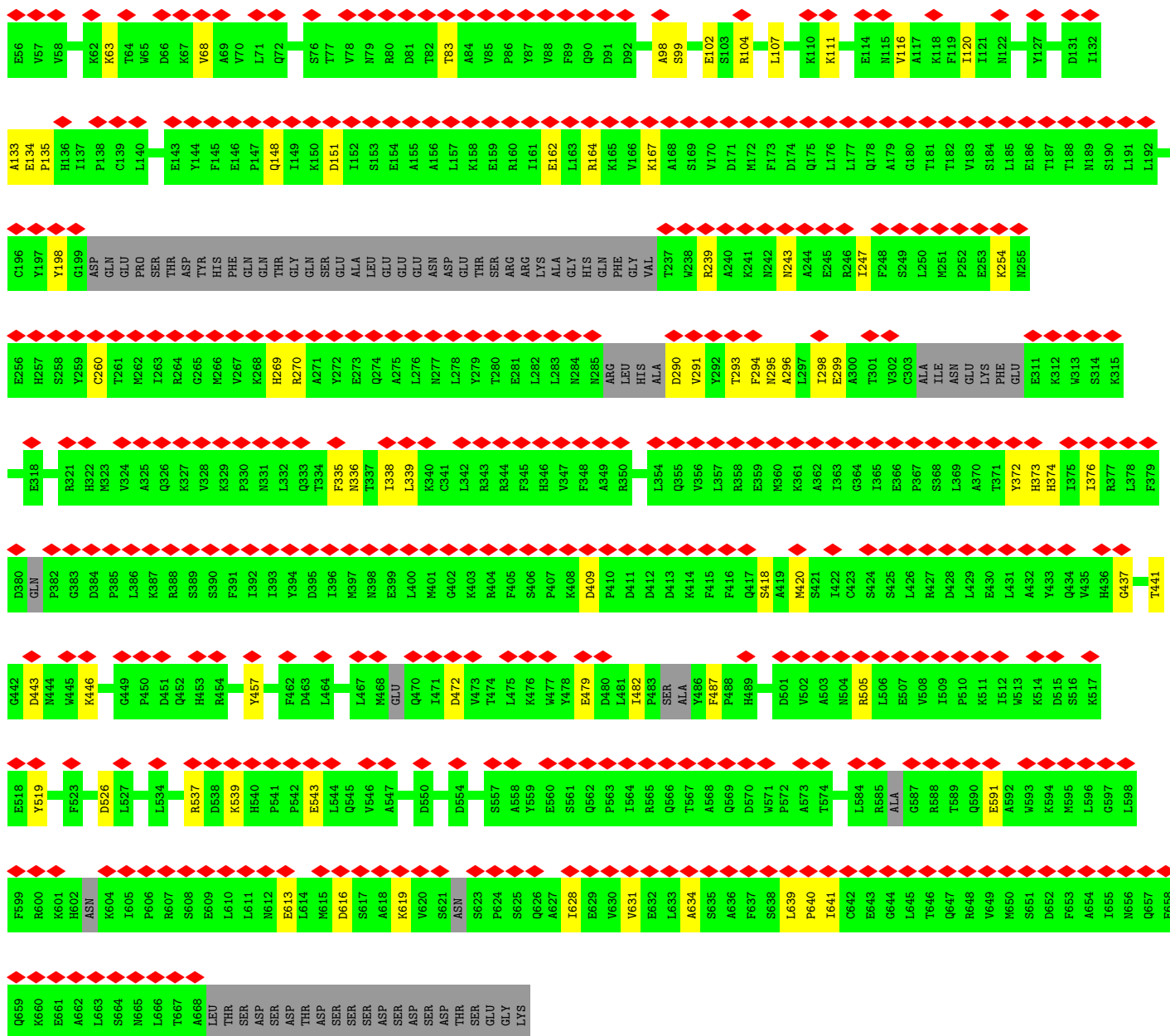
- Molecule 15: Aurora kinase A-interacting protein

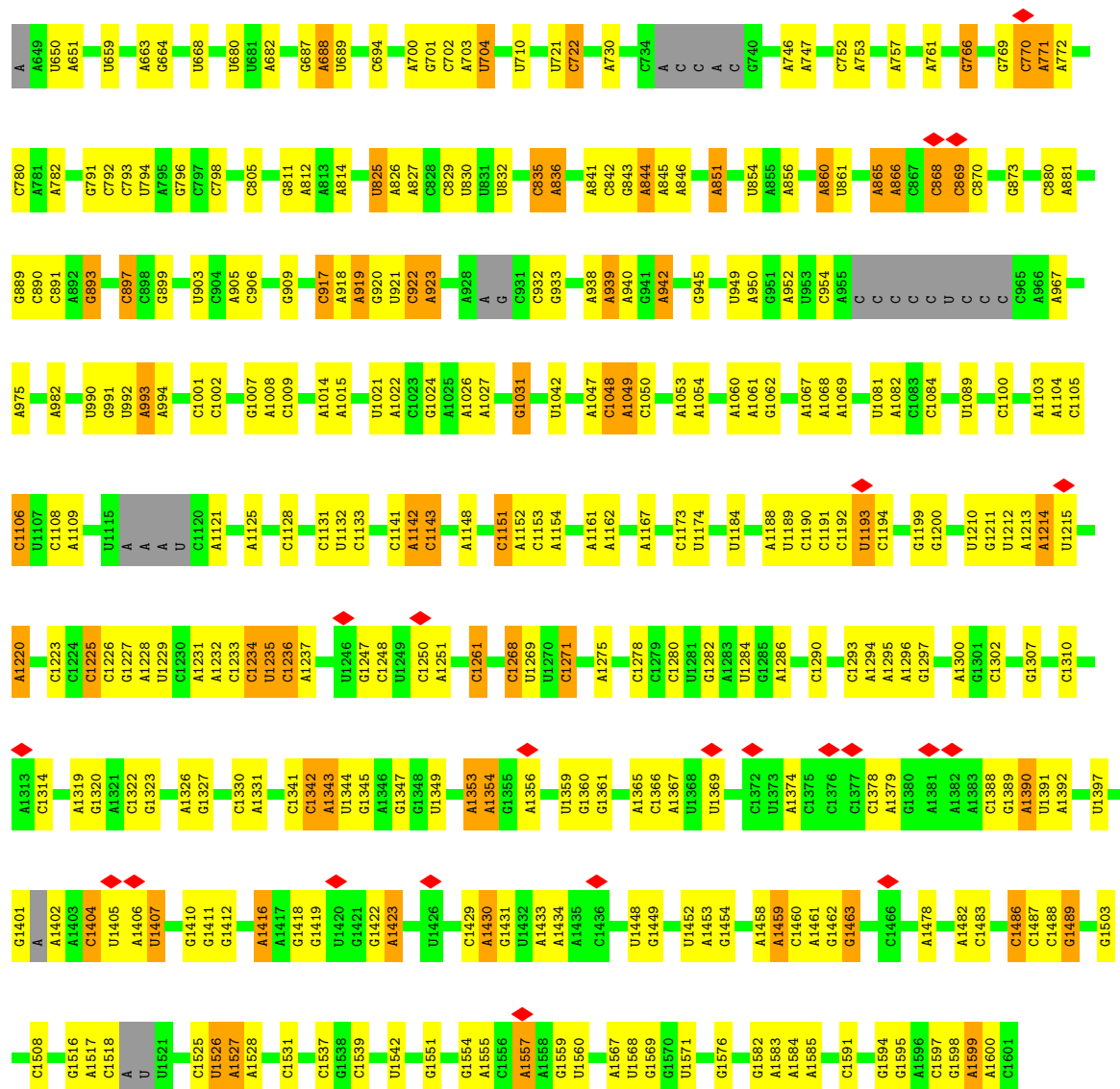
Chain A3: 



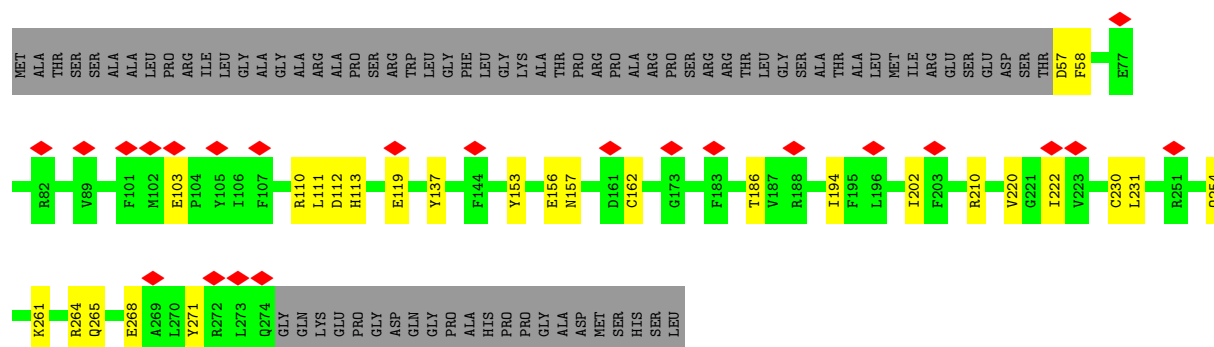
- Molecule 16: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4: 

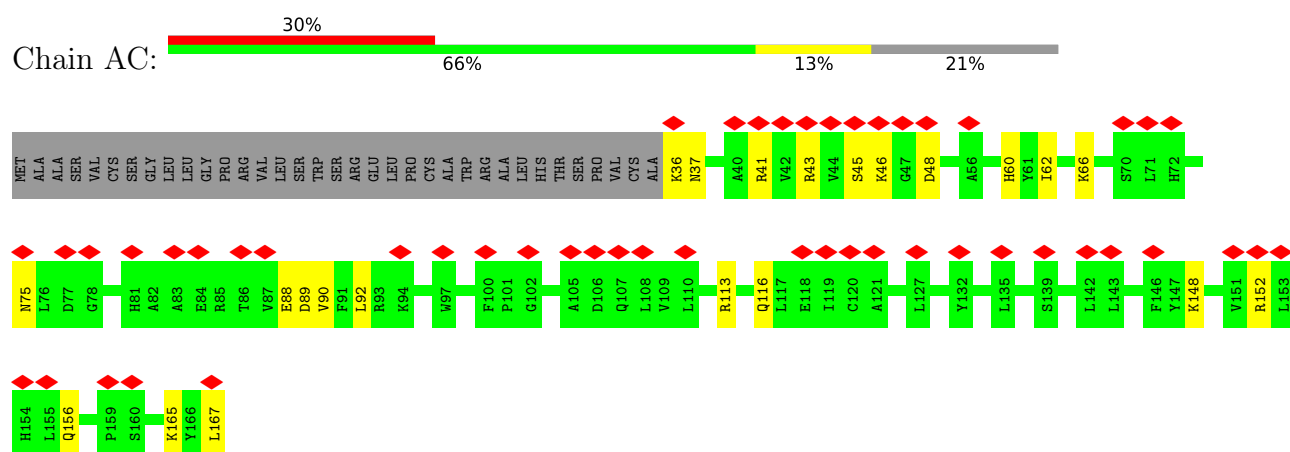




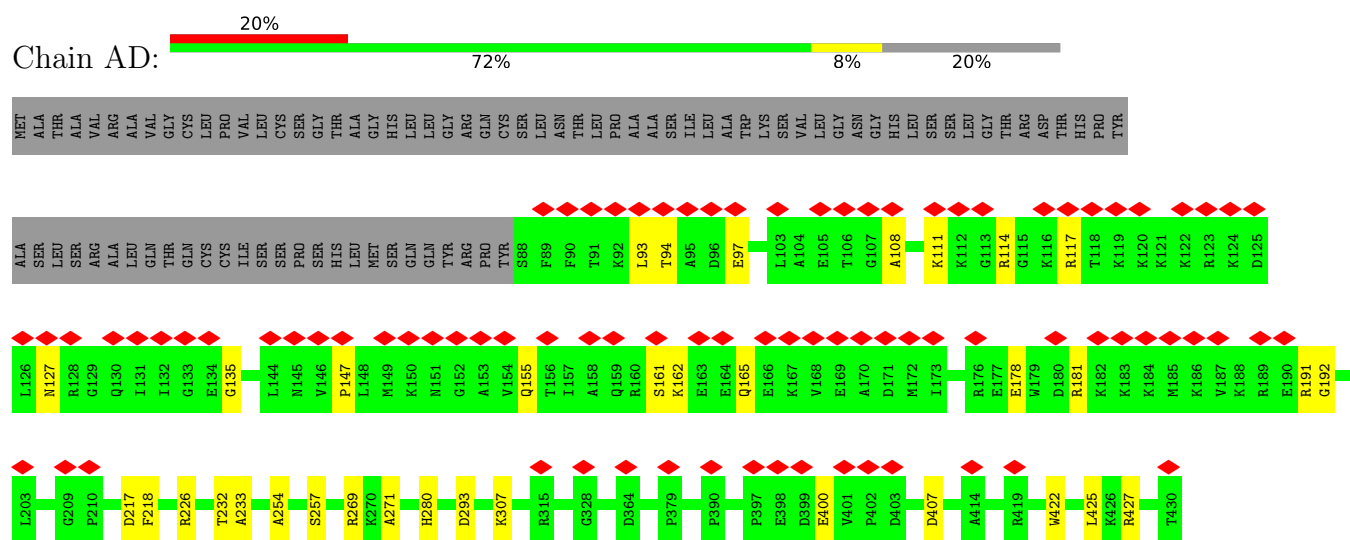
- Molecule 19: 28S ribosomal protein S2, mitochondrial



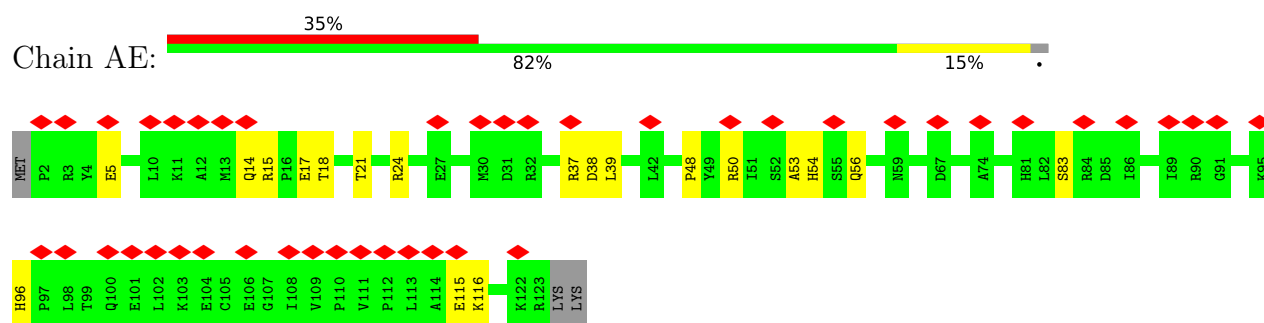
- Molecule 20: 28S ribosomal protein S24, mitochondrial



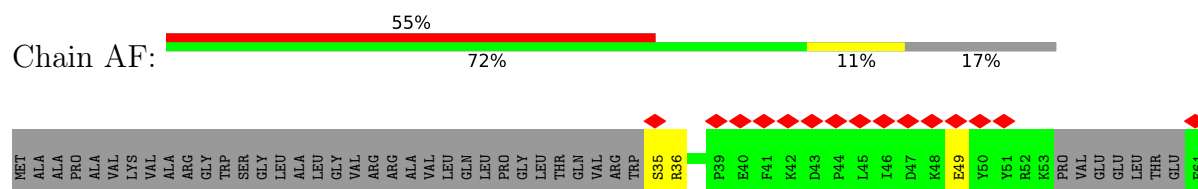
- Molecule 21: 28S ribosomal protein S5, mitochondrial



- Molecule 22: 28S ribosomal protein S6, mitochondrial



- Molecule 23: 28S ribosomal protein S7, mitochondrial





LEU
SER
GLU
GLU
LYS
GLU
GLU
SER
LYS
SER

- Molecule 26: 28S ribosomal protein S11, mitochondrial

Chain AI: 

MET GLN ALA VAL ARG ASN ALA SER LEU PHE ARG LEU ARG SER TRP TRP TRP PRO GLN THR GLY ILE CYS THR GLY ALA ARG GLN LEU ASP ALA ALA LYS GLN LYS VAL GLU GLN ASN ALA ALA PRO SER HIS THR K59 F60

S61 P67 G68 E69 E70 S71 S72 L73 R74 W75 A76 G77 K78 K79 F80 E81 I83 P84 I85 I88 K89 H92 N93 N94 T95 Q96 V99 A102 S103 N104 E115 R118 A127 T130 A131 G132 I133 A134 A137 K140 Q141 K142 G143 R148 L154

R158 L159 H163 G164 M167 D177 N178 I181 K190 A191 R192 K193 L194

- Molecule 27: 28S ribosomal protein S12, mitochondrial

Chain AJ: 

MET SER TRP GLY LEU LEU HIS LEU LEU THR ASN THR LEU THR CYS GLY PRO PRO ALA VAL ARG LEU TRP ALA CYS SER MET A31 R44 R47 K48 L49 G50 P51 T52 E53 G54 R55 V61 K72 K79 R84 L85 R89 P96 L102 R114

R127 Y130 K137 K138

- Molecule 28: 28S ribosomal protein S14, mitochondrial

Chain AK: 

MET ALA ALA PHE MET LEU MET GLY SER LEU LEU ARG THR PHE LYS GLN MET GLN VAL PRO PRO SER SER ALA ALA SER GLY GLN VAL ARG H28 R36 K39 R40 R41 K42 M43 E46 Y47 E50 R51 I54 N55 S56 L57 R58 T61 I62 L63 P64 K65 I66 L67 Q68 D69 A71

D72 E73 E74 I75 A76 A77 L78 P79 R80 D81 R86 I87 R88 N89 R90 M93 T94 S95 G99 R102 R103 I109 H113 G118 Q119 Q124 W128

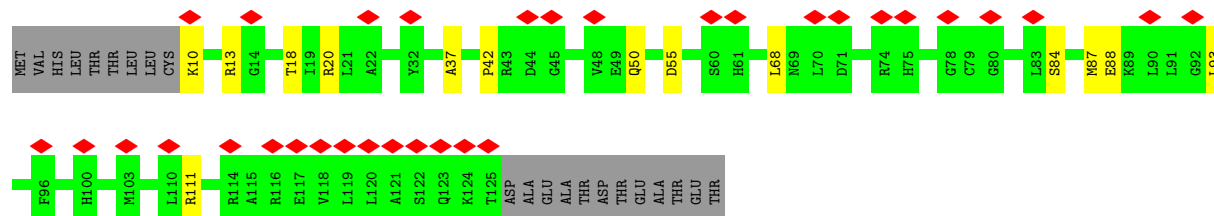
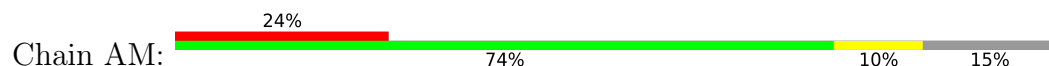
- Molecule 29: 28S ribosomal protein S15, mitochondrial

Chain AL: 

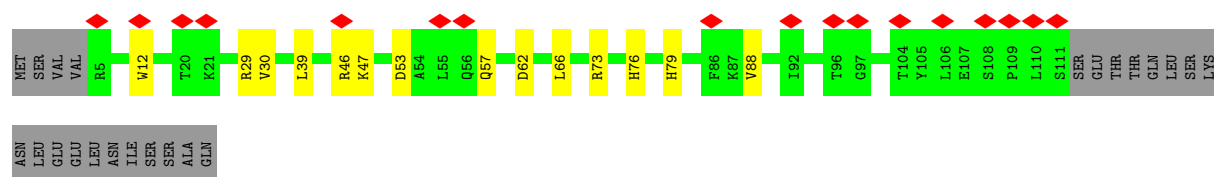
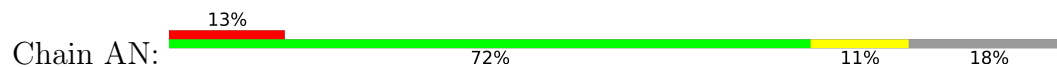
MET LEU ARG VAL TRP ARG THR SER LEU LEU SER LEU ILE ARG THR ARG ALA VAL THR GLN VAL VAL PRO PRO GLY GLY SER LYS PHE PRO PHE ASN GLN TRP GLY LEU GLN PRO ARG SER LEU LEU LEU GLN ALA ALA ARG GLY TYR VAL VAL ARG LYS PRO PRO ALA GLN

SER ARG ASP ASP D66 S70 T71 L72 L73 K74 D75 Y76 Q77 W78 V79 P80 G81 I82 E83 K84 V85 D86 D87 D88 R91 E96 M97 A98 N99 K113 A117 M118 P119 E120 D121 T122 R123 E126 A127 V134 R137 E140 E144 D149 H152 K153 R154

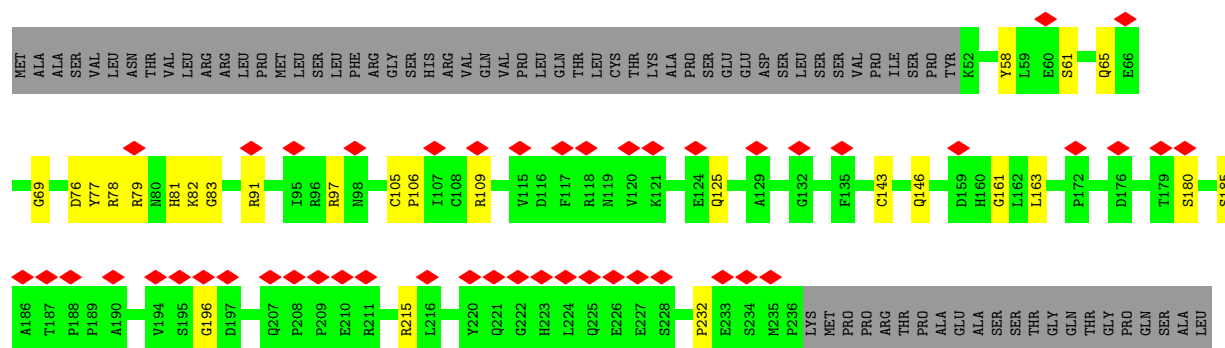
- Molecule 30: 28S ribosomal protein S16, mitochondrial



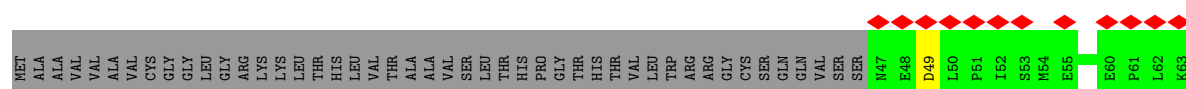
- Molecule 31: 28S ribosomal protein S17, mitochondrial

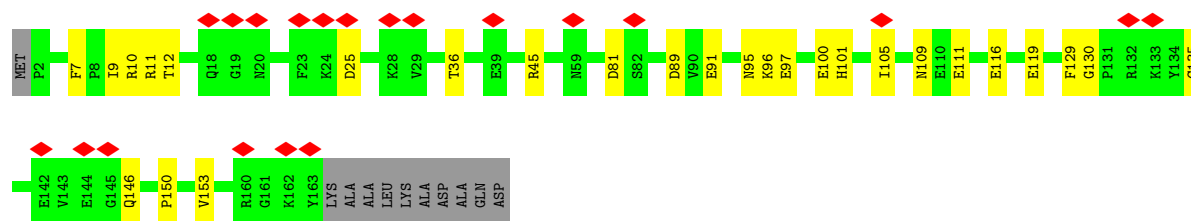


- Molecule 32: 28S ribosomal protein S18b, mitochondrial

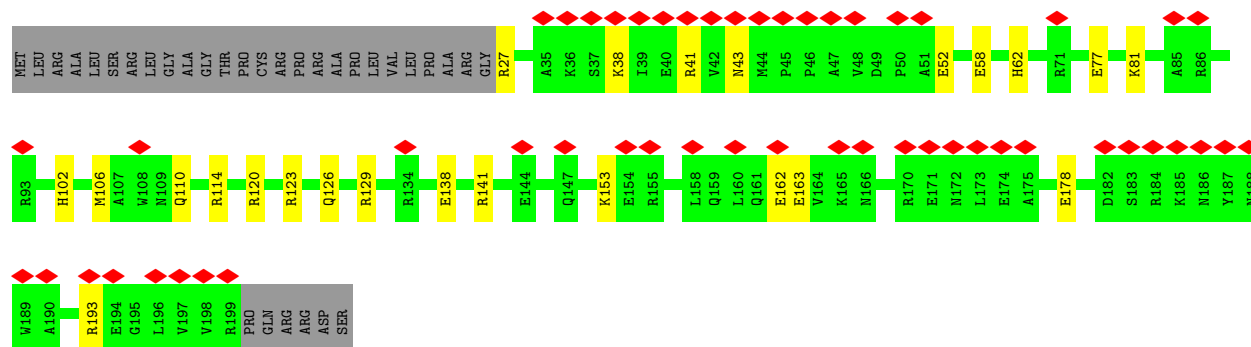
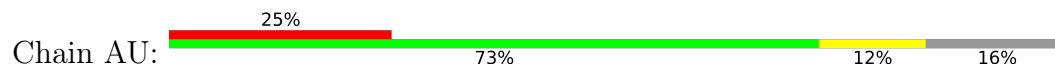


- Molecule 33: 28S ribosomal protein S18c, mitochondrial

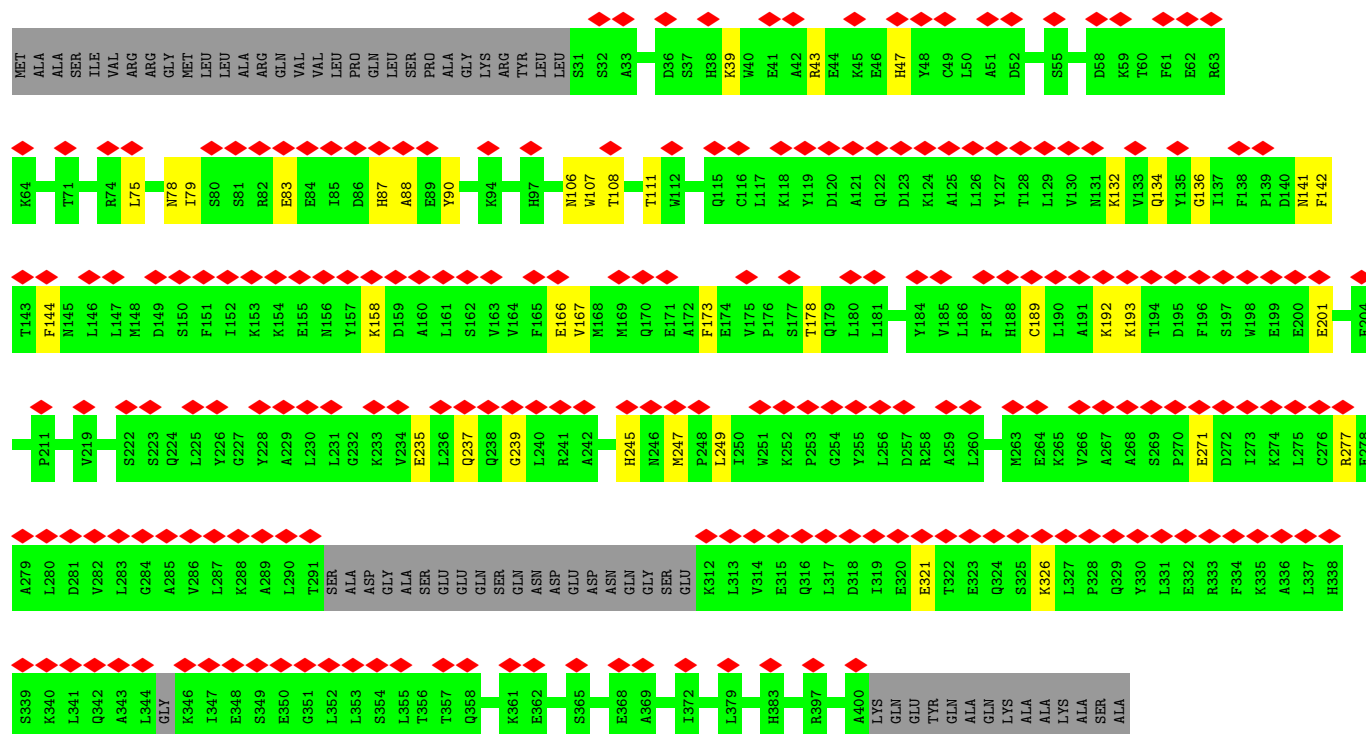
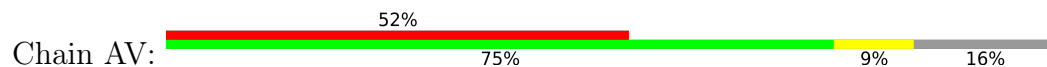




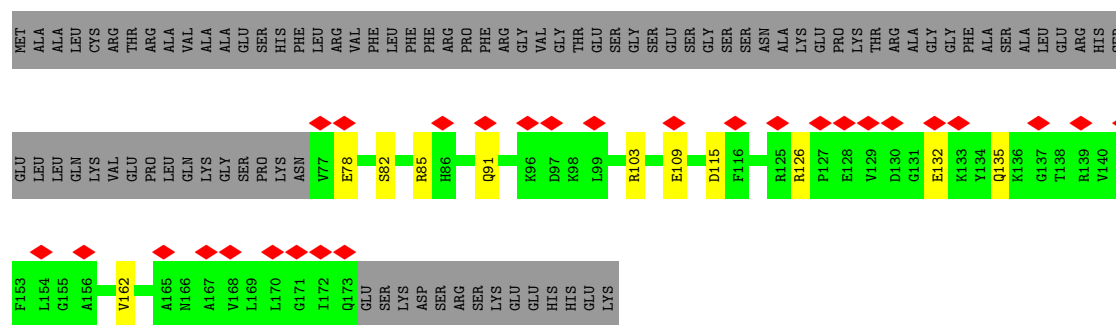
- Molecule 38: 28S ribosomal protein S26, mitochondrial

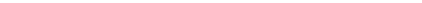


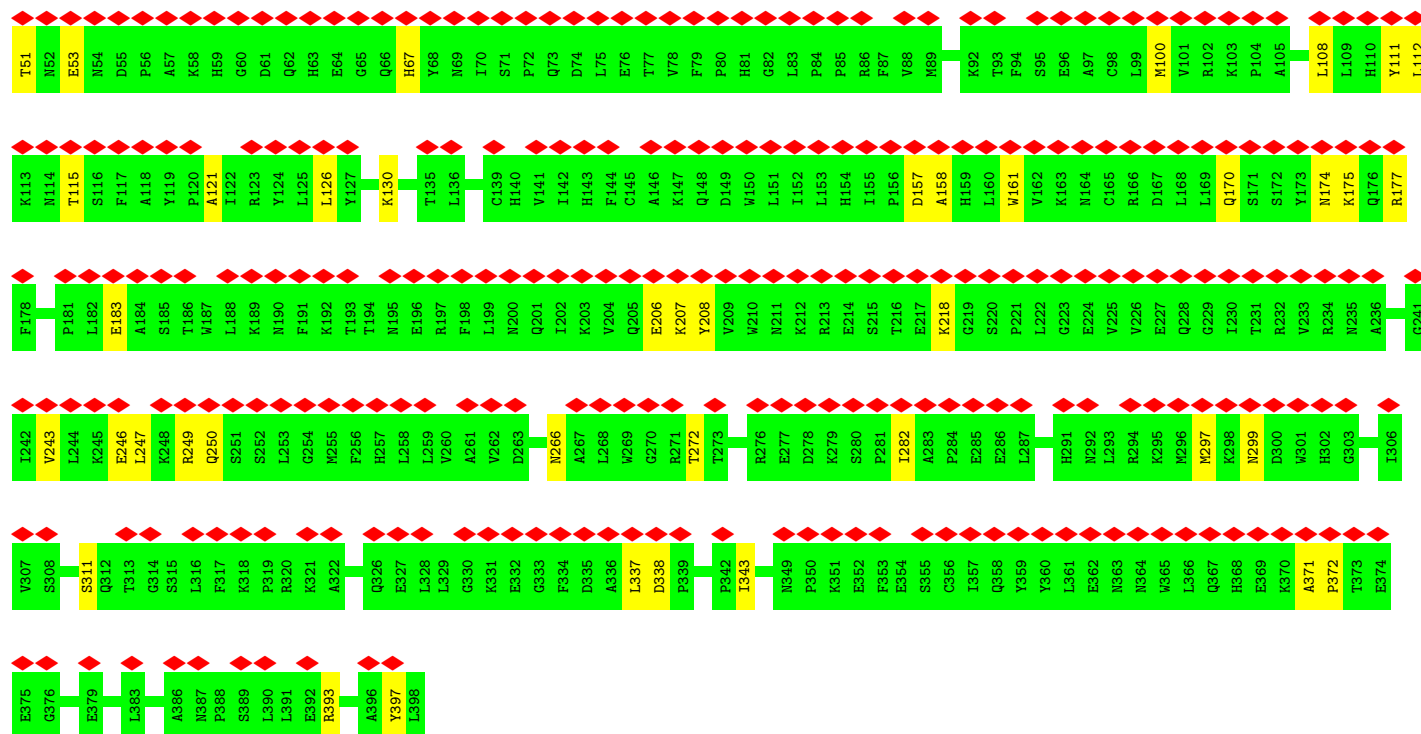
- Molecule 39: 28S ribosomal protein S27, mitochondrial

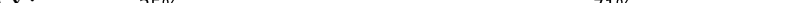


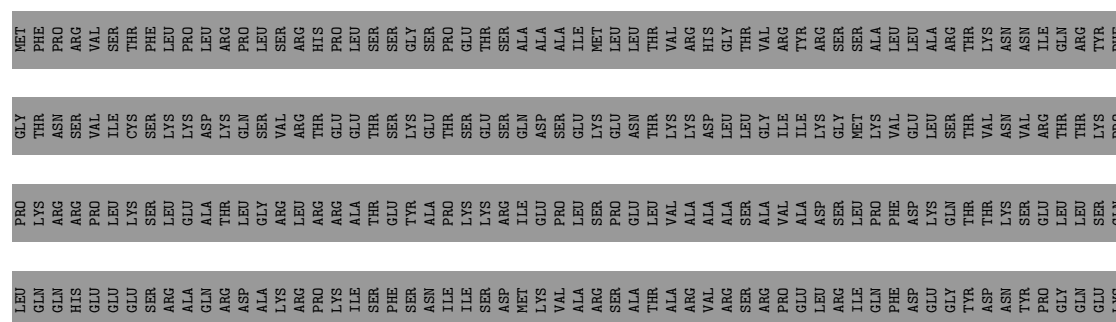
- Molecule 40: 28S ribosomal protein S28, mitochondrial

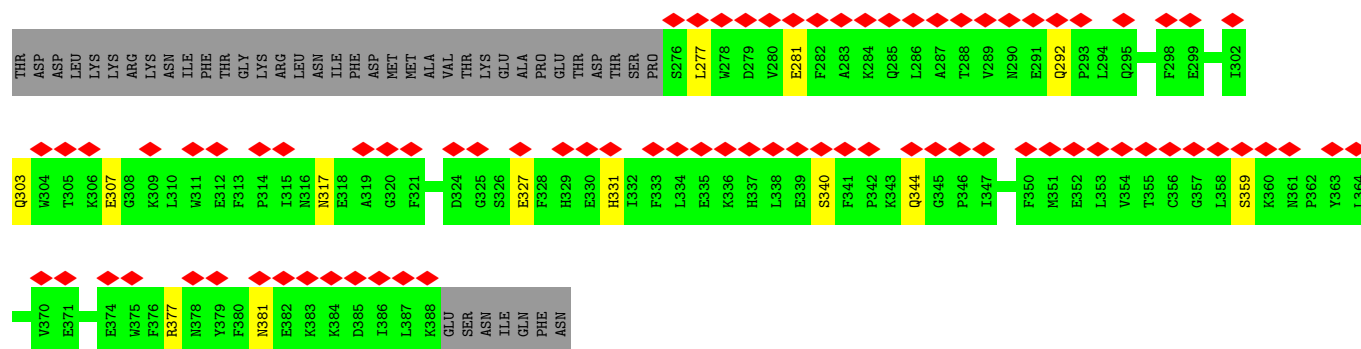


- Chain AX:  79% 88% 12%

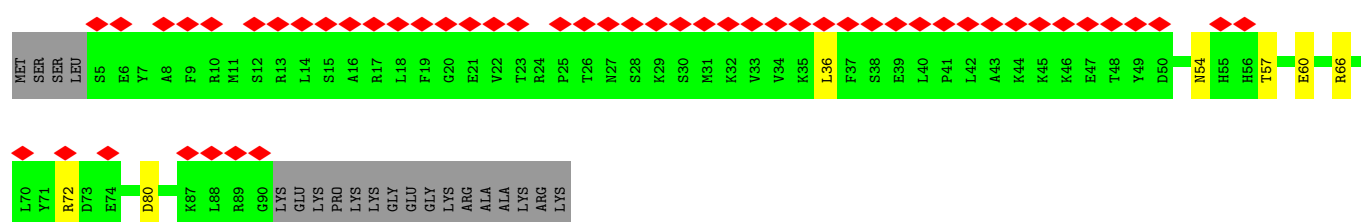


- Chain AY:  21% 25% 71%





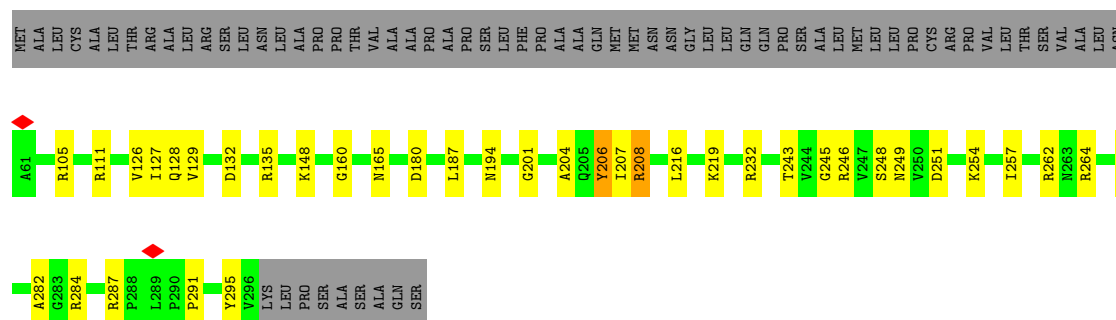
- Molecule 43: 28S ribosomal protein S33, mitochondrial



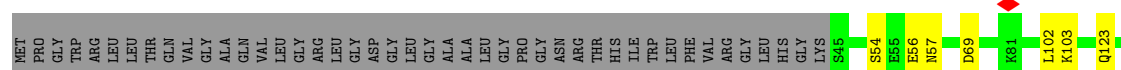
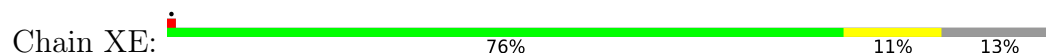
- Molecule 44: mt-tRNAVal

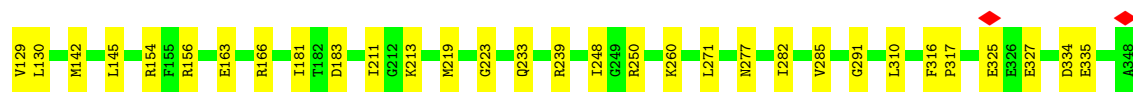


- Molecule 45: 39S ribosomal protein L2, mitochondrial



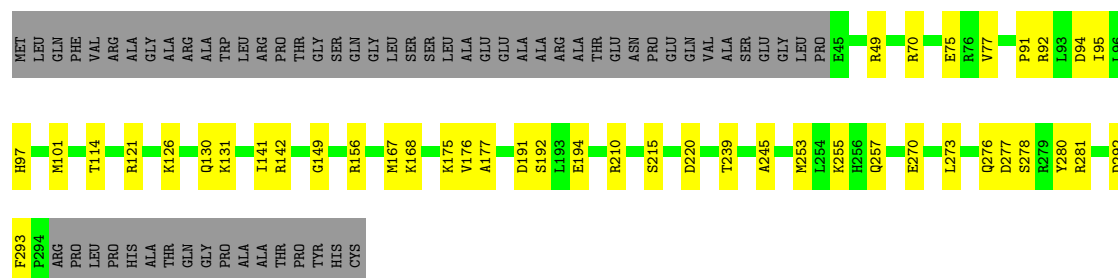
- Molecule 46: 39S ribosomal protein L3, mitochondrial





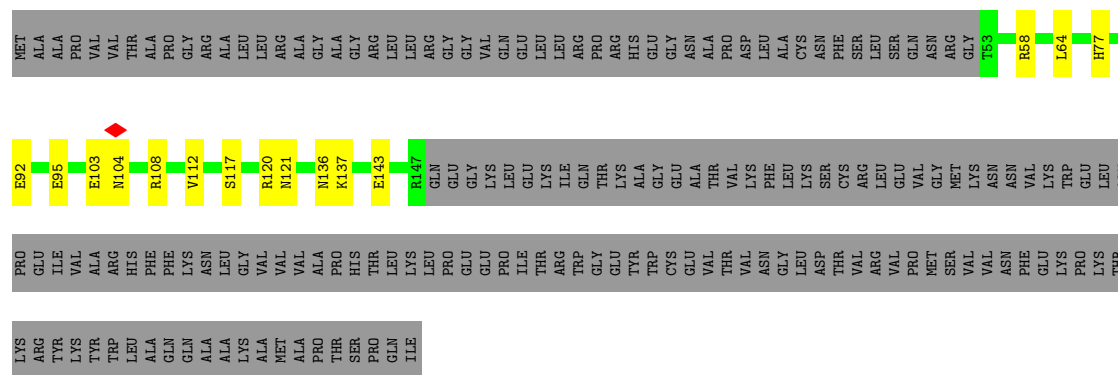
- Molecule 47: 39S ribosomal protein L4, mitochondrial

Chain XF: 66% 14% 20%



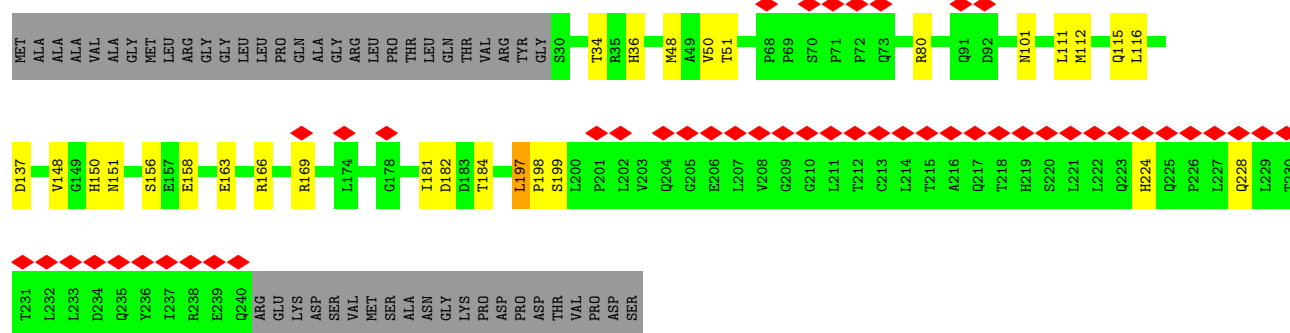
- Molecule 48: 39S ribosomal protein L9, mitochondrial

Chain XH: 30% 6% 64%



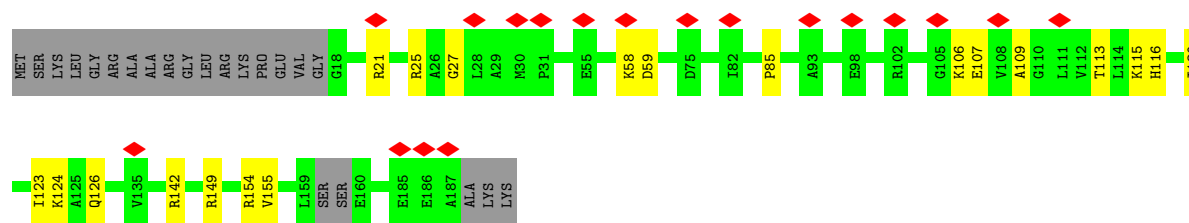
- Molecule 49: 39S ribosomal protein L10, mitochondrial

Chain XI: 19% 70% 10% 19%



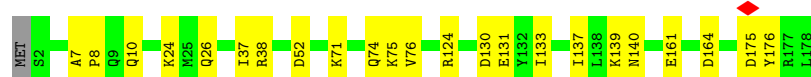
- Molecule 50: 39S ribosomal protein L11, mitochondrial

Chain XJ: 9% 78% 10% 11%



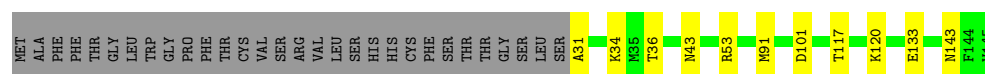
- Molecule 51: 39S ribosomal protein L13, mitochondrial

Chain XK: 87% 13% .



- Molecule 52: 39S ribosomal protein L14, mitochondrial

Chain XL: 72% 8% 21%



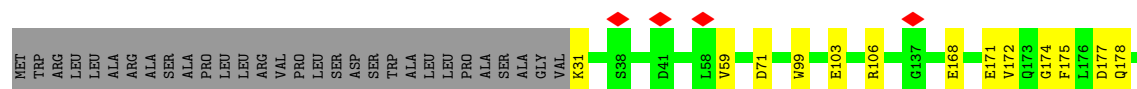
- Molecule 53: 39S ribosomal protein L15, mitochondrial

Chain XM: 77% 20% .



- Molecule 54: 39S ribosomal protein L16, mitochondrial

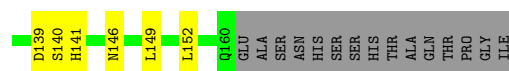
Chain XN: 78% 10% 12%



- Molecule 55: 39S ribosomal protein L17, mitochondrial

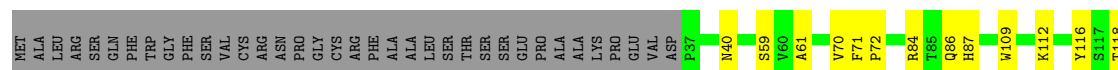
Chain XO: 65% 22% 13%





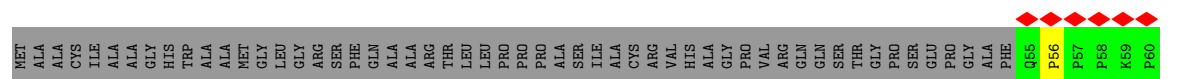
- Molecule 56: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain XP: 69% 11% 20%



- Molecule 57: 39S ribosomal protein L19, mitochondrial

Chain XQ: 7% 68% 14% 18%



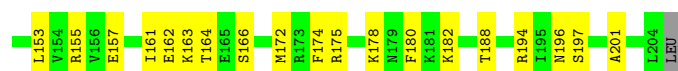
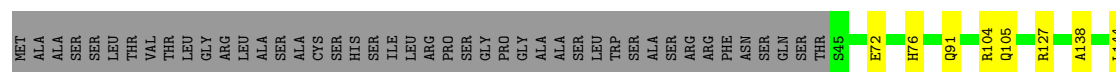
- Molecule 58: 39S ribosomal protein L20, mitochondrial

Chain XR: 76% 18% 6%



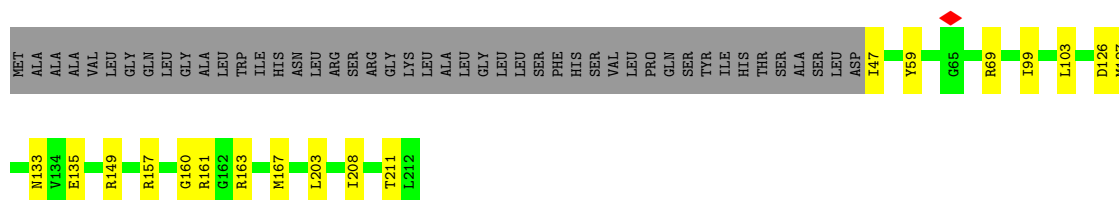
- Molecule 59: 39S ribosomal protein L21, mitochondrial

Chain XS: 65% 13% 22%

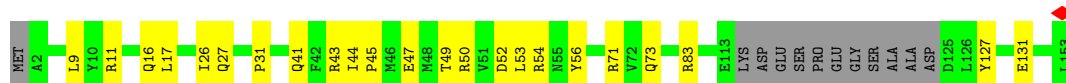
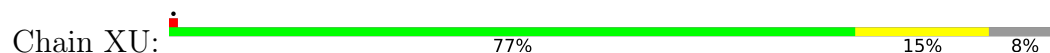


- Molecule 60: 39S ribosomal protein L22, mitochondrial

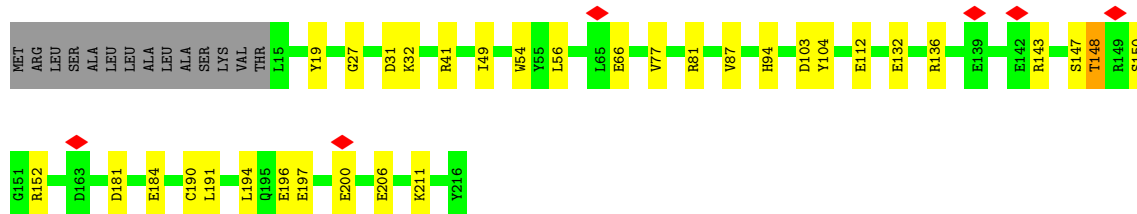
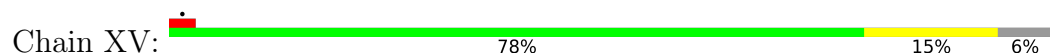
Chain XT: 70% 8% 22%



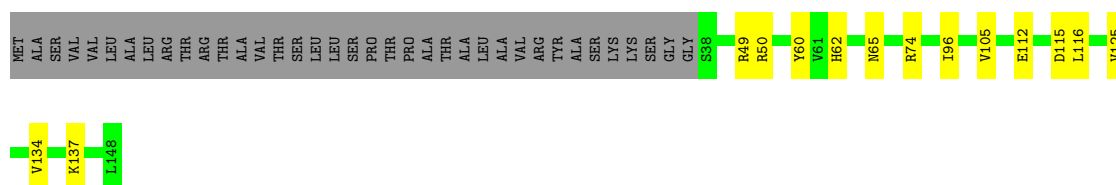
- Molecule 61: 39S ribosomal protein L23, mitochondrial



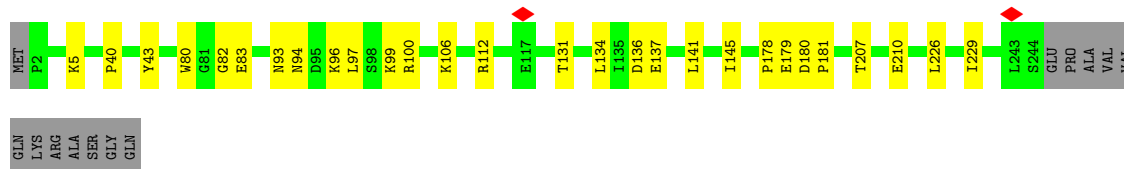
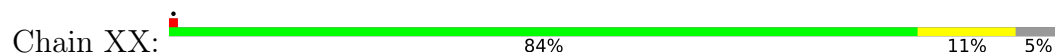
- Molecule 62: 39S ribosomal protein L24, mitochondrial



- Molecule 63: 39S ribosomal protein L27, mitochondrial

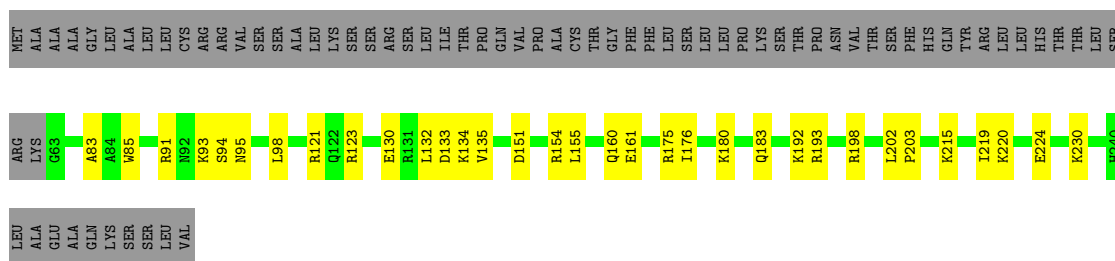


- Molecule 64: 39S ribosomal protein L28, mitochondrial



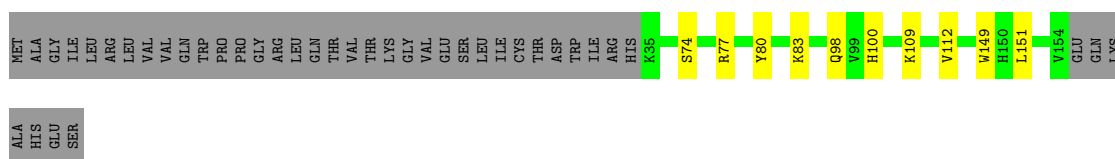
- Molecule 65: 39S ribosomal protein L47, mitochondrial





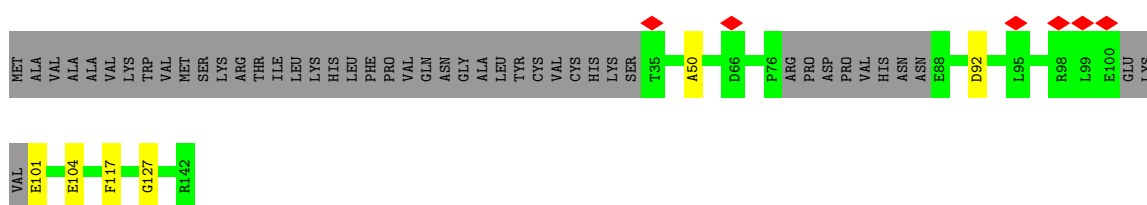
- Molecule 66: 39S ribosomal protein L30, mitochondrial

Chain XZ: 68% 6% 25%



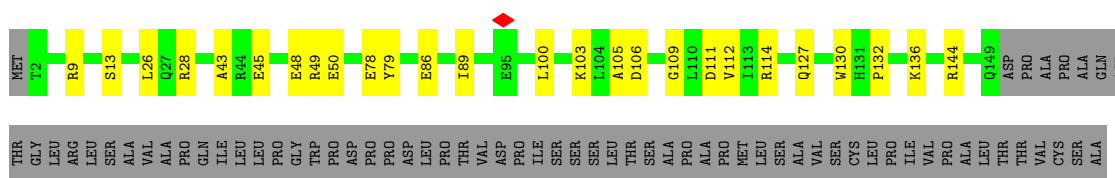
- Molecule 67: 39S ribosomal protein L42, mitochondrial

Chain a: 64% 32%



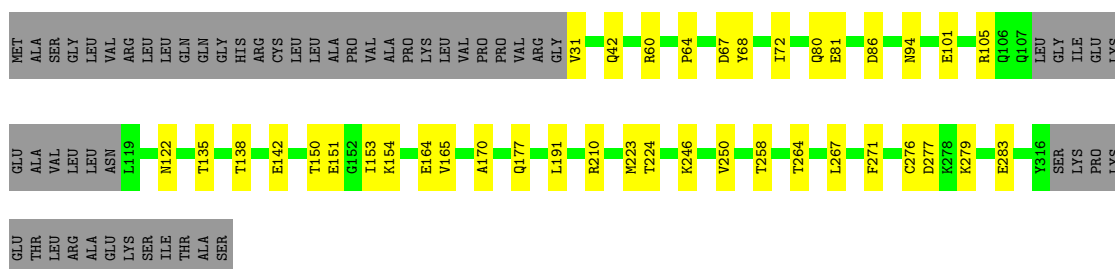
- Molecule 68: 39S ribosomal protein L43, mitochondrial

Chain b: 57% 12% 31%



- Molecule 69: 39S ribosomal protein L44, mitochondrial

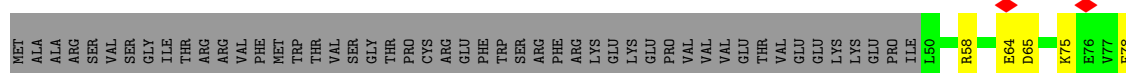
Chain c: 71% 12% 17%



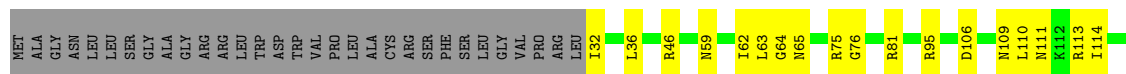
- | | | | | | |
|------|------|------|------|------|------|
| MET | ALA | THR | PHE | ARG | ALA | THR | LEU | ARG | GLY | TRP | ARG | GLY | CYS | GLY | ARG | LEU | LEU | LEU | SER | GLN | THR | GLN | GLY | PRO | ASP | P36 | P95 | R37 | F38 | T65 | G71 | R76 | R90 | N93 | K98 | N104 | R105 | Q106 | R111 | Q121 | V124 |
|------|------|------|------|------|------|



- Molecule 74: 39S ribosomal protein L50, mitochondrial



- Molecule 75: 39S ribosomal protein L51, mitochondrial



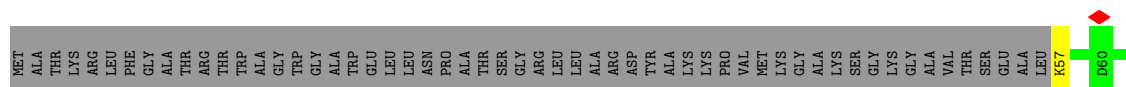
- Molecule 76: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA

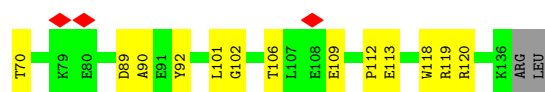


- Molecule 77: 39S ribosomal protein L53, mitochondrial

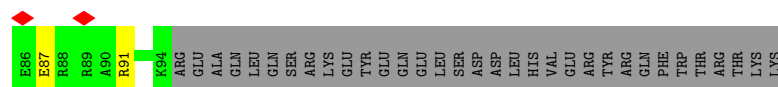
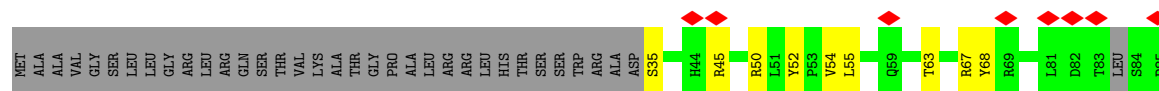
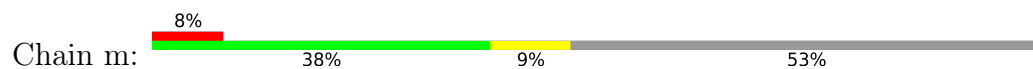


- Molecule 78: 39S ribosomal protein L54, mitochondrial

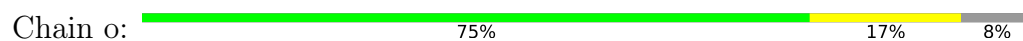




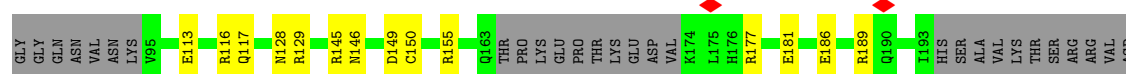
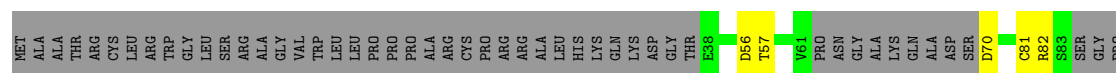
- Molecule 79: 39S ribosomal protein L55, mitochondrial



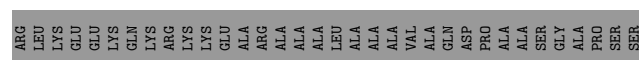
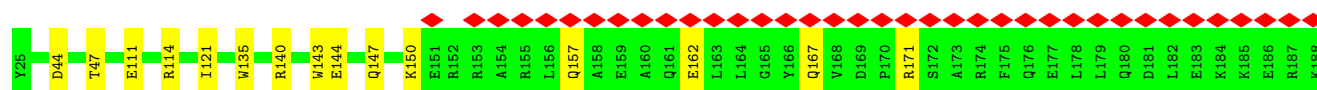
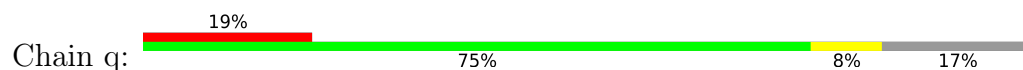
- Molecule 80: Ribosomal protein 63, mitochondrial



- Molecule 81: Peptidyl-tRNA hydrolase ICT1, mitochondrial

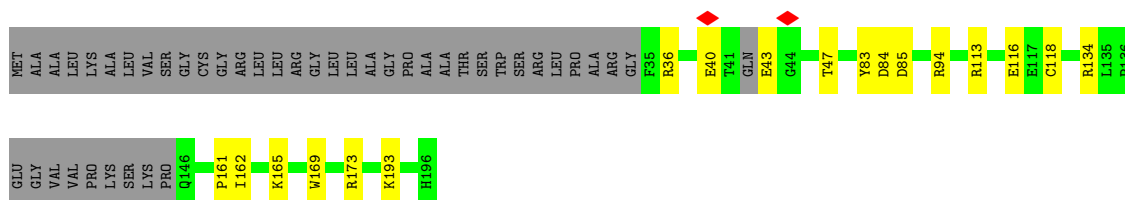


- Molecule 82: Growth arrest and DNA damage-inducible proteins-interacting protein 1



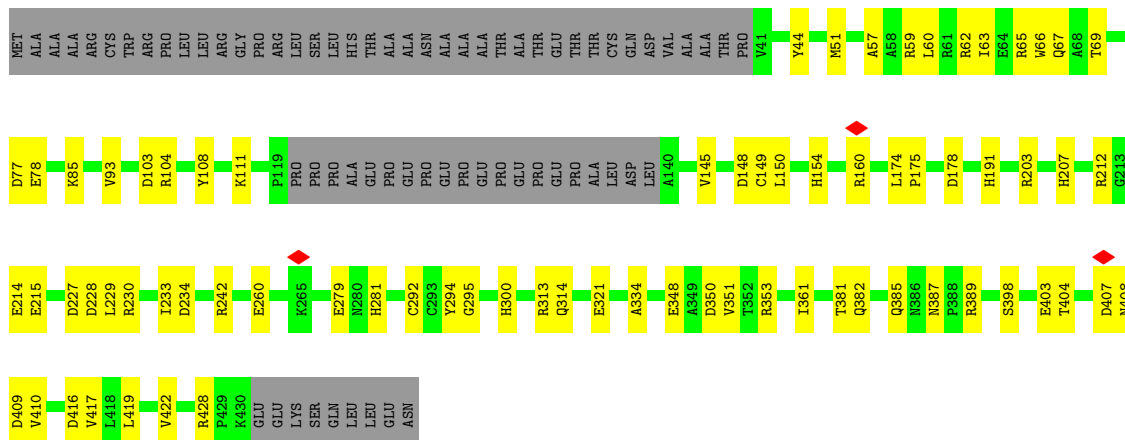
- Molecule 83: 39S ribosomal protein S18a, mitochondrial





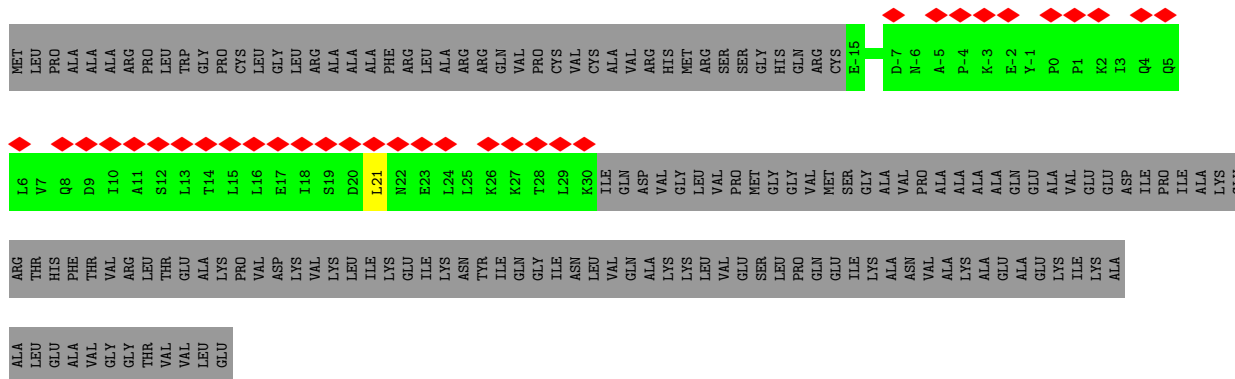
• Molecule 84: 39S ribosomal protein S30, mitochondrial

Chain s: 67% 17% 16%



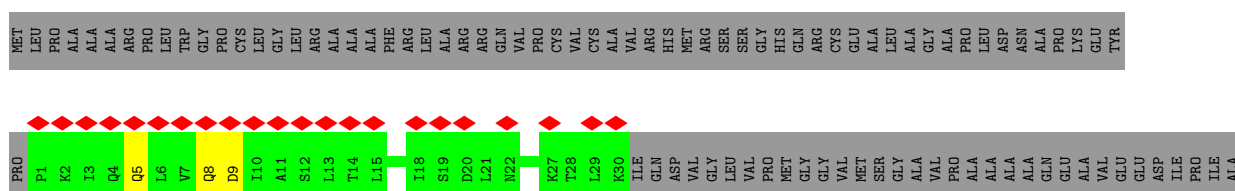
• Molecule 85: 39S ribosomal protein L12, mitochondrial

Chain t1: 17% 23% 77%

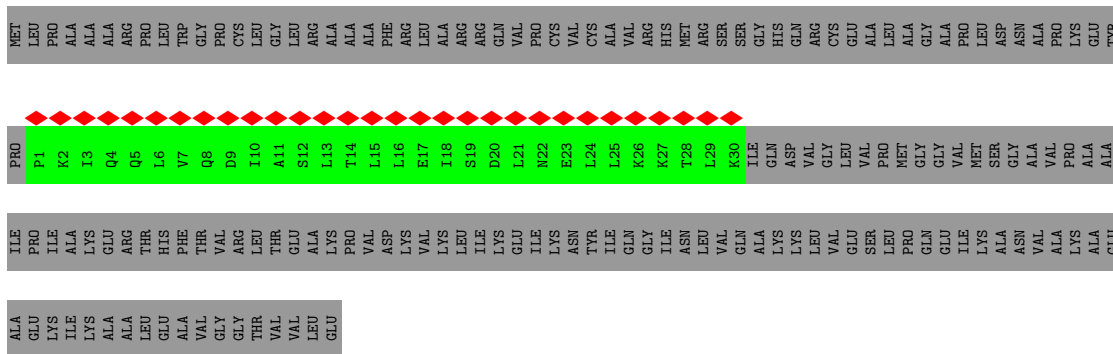


• Molecule 85: 39S ribosomal protein L12, mitochondrial

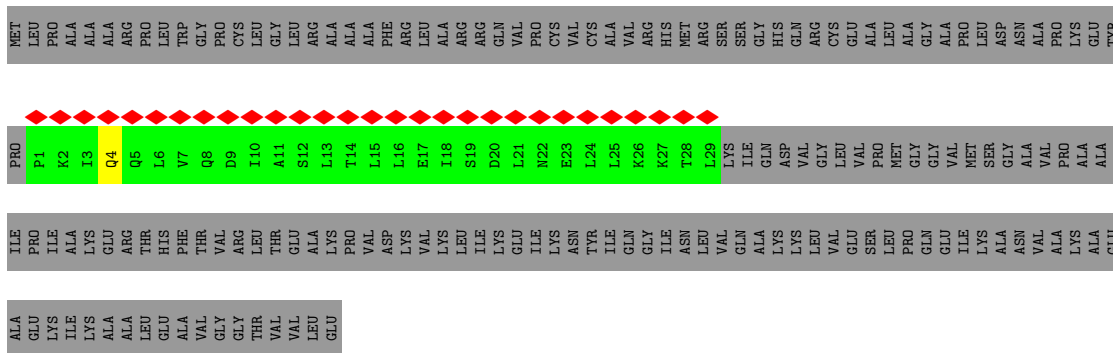
Chain t2: 11% 14% 85%



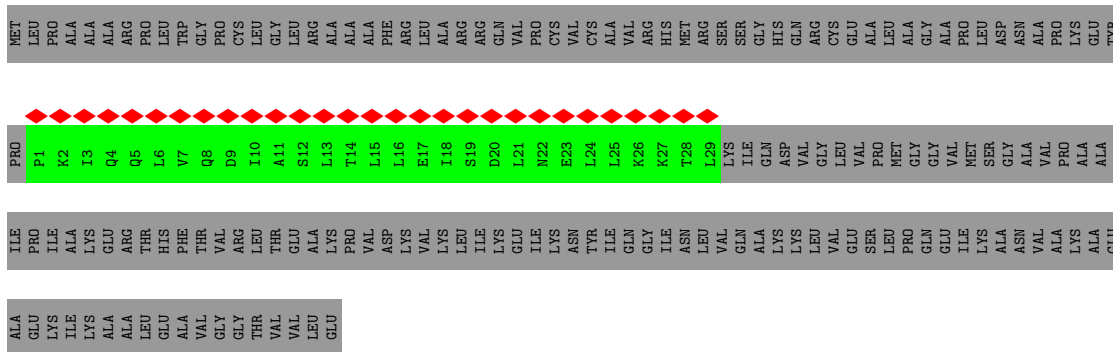
- Molecule 85: 39S ribosomal protein L12, mitochondrial



- Molecule 85: 39S ribosomal protein L12, mitochondrial



- Molecule 85: 39S ribosomal protein L12, mitochondrial



- Molecule 85: 39S ribosomal protein L12, mitochondrial



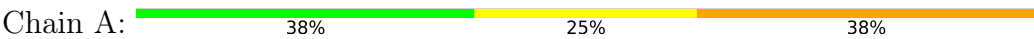
MET LEU PRO ALA ALA ARG PRO TRP GLY PRO CYS LEU GLY LEU ARG ALA ALA PHE ARG ARG ARG GLN VAL PRO CYS VAL CYS ALA VAL ARG HIS MET ARG SER SER GLY HIS ARG CYS GLU ALA LEU ALA GLY ALA PRO ASP ASN ALA PRO LYS GLU TYR

PRO PRO K2 K3 K4 K5 K6 K7 K8 K9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 LEU LYS ILE GLN ASP VAL GLY LEU VAL PRO MET GLY VAL MET SER GLY VAL PRO ALA ALA ALA ALA GLN GLU ALA VAL ASP

ILE PRO ILE ALA LYS GLU ARG THR HIS PHE THR VAL ARG LEU THR GLU THR ALA LYS PRO VAL ASP LYS VAL LYS LEU ILE LYS GLU ILE ILE ASN TYR ILE GLN GLY ILE ASN LEU VAL GLN ALA LYS LYS LEU VAL GLU SER LEU PRO GLN GLU ILE LYS ALA ASN VAL ALA LYS ALA GLU

ALA GLU LYS ILE LYS ALA ALA LEU GLU VAL GLY THR VAL LEU GLU

● Molecule 86: Quinupristin



MHV1 T2 DBE3 P4 F5 MHV6 Q047 MHV8

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MHW, DBB, 004, DOL, GTP, MG, MHV, MHU, 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	0.22	0/895	0.32	0/1201
2	1	0.15	0/444	0.33	0/591
3	2	0.31	0/382	0.42	0/507
4	3	0.27	0/852	0.36	0/1136
5	4	0.22	0/349	0.33	0/461
6	5	0.16	0/3299	0.32	0/4495
7	6	0.15	0/3040	0.32	0/4134
8	7	0.14	0/2420	0.30	0/3270
9	8	1.51	1/1164 (0.1%)	0.38	2/1566 (0.1%)
10	9	0.16	0/1024	0.30	0/1379
11	XA	0.19	0/35662	0.28	0/55502
12	A0	0.10	0/1727	0.29	0/2338
13	A1	0.11	0/2276	0.27	0/3079
14	A2	0.12	0/939	0.32	0/1256
15	A3	0.17	0/621	0.36	0/820
16	A4	0.12	0/4615	0.31	0/6228
17	A5	0.12	0/1497	0.31	0/2013
18	AA	0.10	0/22022	0.23	0/34275
19	AB	0.11	0/1819	0.29	0/2462
20	AC	0.10	0/1112	0.26	0/1505
21	AD	0.11	0/2768	0.28	0/3707
22	AE	0.11	0/989	0.31	0/1335
23	AF	0.10	0/1708	0.27	0/2291
24	AG	0.10	0/2559	0.28	0/3429
25	AH	0.11	0/1128	0.29	0/1529
26	AI	0.10	0/1031	0.27	0/1390
27	AJ	0.12	0/854	0.30	0/1148
28	AK	0.12	0/879	0.33	0/1182
29	AL	0.12	0/1406	0.30	0/1878
30	AM	0.11	0/941	0.31	0/1265
31	AN	0.11	0/864	0.29	0/1169
32	AO	0.10	0/1580	0.27	0/2150

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AP	0.09	0/782	0.23	0/1050
34	AQ	0.12	0/746	0.28	0/993
35	AR	0.11	0/2103	0.28	0/2842
36	AS	0.11	0/1127	0.27	0/1518
37	AT	0.10	0/1361	0.29	0/1829
38	AU	0.13	0/1482	0.30	0/1987
39	AV	0.11	0/2925	0.30	0/3948
40	AW	0.10	0/778	0.25	0/1048
41	AX	0.11	0/2884	0.30	0/3903
42	AY	0.11	0/985	0.29	0/1329
43	AZ	0.11	0/748	0.27	0/1000
44	XB	0.09	0/1400	0.20	0/2168
45	XD	0.19	0/1879	0.34	0/2527
46	XE	0.21	0/2465	0.30	0/3344
47	XF	0.26	0/2071	0.37	0/2817
48	XH	0.15	0/798	0.31	0/1073
49	XI	0.15	0/1727	0.31	0/2340
50	XJ	0.11	0/1309	0.29	0/1764
51	XK	0.22	0/1495	0.34	0/2029
52	XL	0.19	0/904	0.29	0/1218
53	XM	0.21	0/2359	0.34	0/3185
54	XN	0.19	0/1825	0.34	0/2458
55	XO	0.21	0/1269	0.37	0/1708
56	XP	0.15	0/1190	0.32	0/1611
57	XQ	0.17	0/2026	0.33	0/2734
58	XR	0.28	0/1174	0.38	0/1572
59	XS	0.23	0/1311	0.34	0/1778
60	XT	0.23	0/1402	0.35	0/1886
61	XU	0.20	0/1200	0.33	0/1623
62	XV	0.15	0/1693	0.33	0/2297
63	XW	0.21	0/893	0.31	0/1204
64	XX	0.17	0/2090	0.31	0/2825
65	XY	0.19	0/1571	0.32	0/2106
66	XZ	0.23	0/1003	0.35	0/1354
67	a	0.18	0/838	0.35	0/1138
68	b	0.22	0/1202	0.40	0/1626
69	c	0.17	0/2264	0.31	0/3059
70	d	0.12	0/1811	0.28	0/2454
71	e	0.77	6/1797 (0.3%)	0.29	0/2422
72	f	0.17	0/1159	0.31	0/1565
73	g	0.21	0/1134	0.38	0/1547
74	h	0.14	0/905	0.30	0/1233
75	i	0.28	0/849	0.39	0/1135

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	j	0.18	0/703	0.35	0/947
77	k	0.12	0/743	0.30	0/1003
78	l	0.10	0/692	0.28	0/939
79	m	0.13	0/508	0.33	0/682
80	o	0.23	0/818	0.38	0/1097
81	p	0.13	0/1071	0.29	0/1433
82	q	0.15	0/1413	0.31	0/1906
83	r	0.19	0/1282	0.31	0/1734
84	s	0.18	0/3114	0.34	0/4225
85	t1	0.14	0/366	0.25	0/497
85	t2	0.08	0/238	0.23	0/319
85	t3	0.09	0/238	0.23	0/319
85	t4	0.08	0/229	0.20	0/308
85	t5	0.09	0/229	0.23	0/308
85	t6	0.08	0/213	0.22	0/286
86	A	4.80	2/13 (15.4%)	3.49	3/15 (20.0%)
All	All	0.22	9/177670 (0.0%)	0.30	5/251956 (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	51.32	3.06	1.52
71	e	84	TYR	CD2-CE2	16.14	1.87	1.38
71	e	84	TYR	CD1-CE1	15.86	1.86	1.38
86	A	4	PRO	CA-CB	-11.99	1.29	1.53
71	e	84	TYR	CE2-CZ	11.94	1.66	1.38
71	e	84	TYR	CE1-CZ	11.64	1.66	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	e	84	TYR	CG-CD1	11.39	1.63	1.39
71	e	84	TYR	CG-CD2	10.55	1.61	1.39
86	A	4	PRO	N-CA	7.94	1.58	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	A	4	PRO	N-CA-CB	7.97	111.77	103.00
86	A	4	PRO	CB-CA-C	7.15	123.68	110.10
86	A	4	PRO	CA-N-CD	-6.63	102.72	112.00
9	8	99	ARG	CB-CG-CD	6.61	126.51	111.30
9	8	99	ARG	CG-CD-NE	5.44	123.97	112.00

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	6	0
3	2	376	406	406	8	0
4	3	831	883	883	14	0
5	4	341	361	361	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	5	3204	3201	3201	33	0
7	6	2947	2839	2839	42	0
8	7	2365	2373	2372	24	0
9	8	1140	1171	1171	44	0
10	9	996	987	987	12	0
11	XA	31875	16183	16192	324	0
12	A0	1684	1685	1685	15	0
13	A1	2230	2261	2261	23	0
14	A2	925	964	964	17	0
15	A3	610	682	682	6	0
16	A4	4521	4546	4545	46	0
17	A5	1489	1577	1577	12	0
18	AA	19690	9997	10003	165	0
19	AB	1776	1769	1769	19	0
20	AC	1082	1088	1088	17	0
21	AD	2716	2785	2785	24	0
22	AE	972	1001	1001	14	0
23	AF	1668	1716	1716	20	0
24	AG	2505	2492	2490	29	0
25	AH	1105	1136	1136	15	0
26	AI	1011	1052	1052	11	0
27	AJ	838	887	887	11	0
28	AK	861	885	885	12	0
29	AL	1382	1473	1472	14	0
30	AM	920	951	951	10	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	20	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	24	0
42	AY	956	912	911	9	0
43	AZ	731	734	734	5	0
44	XB	1255	635	640	10	0
45	XD	1842	1896	1896	29	0
46	XE	2396	2402	2402	25	0
47	XF	2013	2045	2044	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	XH	784	832	832	10	0
49	XI	1691	1783	1783	20	0
50	XJ	1291	1367	1364	17	0
51	XK	1451	1448	1448	17	0
52	XL	889	941	941	8	0
53	XM	2305	2378	2378	42	0
54	XN	1778	1808	1808	21	0
55	XO	1245	1283	1283	25	0
56	XP	1164	1162	1162	18	0
57	XQ	1978	2022	2022	29	0
58	XR	1153	1214	1214	26	0
59	XS	1284	1354	1354	25	0
60	XT	1368	1410	1410	19	0
61	XU	1171	1164	1164	17	0
62	XV	1648	1656	1654	22	0
63	XW	871	898	898	11	0
64	XX	2035	2054	2054	22	0
65	XY	1534	1575	1575	27	0
66	XZ	978	1030	1030	8	0
67	a	813	777	777	6	0
68	b	1178	1180	1180	18	0
69	c	2217	2220	2220	27	0
70	d	1763	1747	1746	19	0
71	e	1762	1767	1767	45	0
72	f	1139	1152	1152	9	0
73	g	1097	1086	1085	19	0
74	h	882	867	867	11	0
75	i	827	857	857	16	0
76	j	689	678	678	10	0
77	k	732	745	745	9	0
78	l	673	654	653	12	0
79	m	500	525	525	8	0
80	o	797	804	804	13	0
81	p	1058	1083	1083	15	0
82	q	1379	1359	1359	8	0
83	r	1247	1267	1267	14	0
84	s	3036	3023	3022	47	0
85	t1	354	379	374	0	0
85	t2	238	268	270	2	0
85	t3	238	268	270	0	0
85	t4	229	255	257	1	0
85	t5	229	255	257	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	t6	214	236	236	0	0
86	A	73	67	65	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	144705	1578	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 (1578) 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)
71:e:84:TYR:CE1	71:e:84:TYR:CD1	1.86	1.58
71:e:84:TYR:CD2	71:e:84:TYR:CE2	1.87	1.56
11:XA:2721:G:O6	11:XA:2990:A:C6	1.84	1.30
9:8:99:ARG:CD	71:e:84:TYR:CD1	2.25	1.19
9:8:99:ARG:CD	71:e:84:TYR:CD2	2.28	1.16
9:8:99:ARG:CG	71:e:84:TYR:CE2	2.27	1.16
9:8:99:ARG:CD	71:e:84:TYR:CE1	2.28	1.15
9:8:99:ARG:CD	71:e:84:TYR:CE2	2.30	1.15
9:8:99:ARG:CG	71:e:84:TYR:CD2	2.29	1.15
9:8:99:ARG:CG	71:e:84:TYR:CD1	2.30	1.14
9:8:99:ARG:CG	71:e:84:TYR:CE1	2.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:99:ARG:CD	71:e:84:TYR:CZ	2.30	1.14
9:8:99:ARG:CD	71:e:84:TYR:CG	2.33	1.11
9:8:99:ARG:CG	71:e:84:TYR:CZ	2.34	1.11
9:8:99:ARG:CG	71:e:84:TYR:CG	2.35	1.09
11:XA:2724:G:OP1	47:XF:131:LYS:NZ	1.91	1.03
9:8:99:ARG:HD3	71:e:84:TYR:CG	1.98	0.98
9:8:99:ARG:HD2	71:e:84:TYR:CE1	1.97	0.97
9:8:99:ARG:HG2	71:e:84:TYR:CD2	1.98	0.96
9:8:99:ARG:HG3	71:e:84:TYR:CZ	1.99	0.96
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
68:b:9:ARG:NH1	68:b:111:ASP:O	2.05	0.90
18:AA:701:G:N2	18:AA:841:A:O2'	2.05	0.90
59:XS:138:ALA:O	68:b:127:GLN:NE2	2.05	0.89
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
71:e:264:LEU:O	71:e:273:ARG:NH2	2.07	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
9:8:87:ASP:O	79:m:45:ARG:NH1	2.06	0.86
11:XA:2517:U:OP1	45:XD:287:ARG:NH2	2.08	0.86
9:8:99:ARG:NE	71:e:84:TYR:CE2	2.43	0.86
68:b:45:GLU:OE2	68:b:49:ARG:NE	2.06	0.86
9:8:99:ARG:CB	71:e:84:TYR:CD1	2.58	0.85
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
51:XK:124:ARG:NH1	67:a:117:PHE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:XQ:70:GLU:OE2	57:XQ:213:GLN:NE2	2.12	0.83
11:XA:1881:A:OP2	73:g:111:ARG:NH2	2.11	0.82
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
84:s:51:MET:O	84:s:62:ARG:NH2	2.13	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
77:k:56:ARG:NH2	77:k:61:GLU:O	2.13	0.81
9:8:164:ARG:NH1	72:f:84:THR:O	2.13	0.81
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
44:XB:1635:C:OP1	72:f:108:GLN:NE2	2.14	0.80
24:AG:198:ARG:N	24:AG:246:ARG:O	2.13	0.80
11:XA:1880:C:OP2	73:g:111:ARG:NH1	2.15	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
9:8:164:ARG:NH1	72:f:87:GLU:O	2.15	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
11:XA:2011:G:O6	75:i:113:ARG:NH1	2.16	0.79
53:XM:185:ASP:OD1	53:XM:186:ILE:N	2.14	0.79
72:f:176:SER:O	79:m:35:SER:N	2.16	0.78
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
50:XJ:25:ARG:NH2	78:l:57:LYS:O	2.17	0.78
57:XQ:118:ARG:NH2	57:XQ:202:VAL:O	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
84:s:228:ASP:O	84:s:230:ARG:NH1	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
30:AM:55:ASP:OD2	37:AT:146:GLN:NE2	2.18	0.75
84:s:279:GLU:OE2	84:s:281:HIS:NE2	2.19	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
69:c:42:GLN:NE2	75:i:36:LEU:O	2.18	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
7:6:198:ALA:O	7:6:254:TYR:OH	2.03	0.74
9:8:99:ARG:HB3	71:e:84:TYR:CD1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
70:d:288:LYS:O	70:d:290:GLU:N	2.19	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
82:q:111:GLU:OE2	82:q:114:ARG:NH1	2.21	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
9:8:99:ARG:HG2	71:e:84:TYR:CE2	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
60:XT:133:ASN:O	70:d:230: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:69:ARG:NH1	70:d:228:PHE:O	2.22	0.72
11:XA:2347:C:O3'	70:d:69:LYS:NZ	2.23	0.72
60:XT:126:ASP:OD1	60:XT:127:MET:N	2.22	0.72
68:b:132:PRO:O	68:b:136:LYS:NZ	2.23	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
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
13:A1:81:VAL:O	13:A1:99:LYS:NZ	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
71:e:177:GLU:O	71:e:190:ARG:NH2	2.24	0.70
47:XF:277:ASP:O	73:g:90:ARG:NH2	2.24	0.70
82:q:157:GLN:NE2	82:q:162:GLU:OE1	2.24	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
67:a:101:GLU:OE1	67:a:101:GLU:N	2.25	0.70
9:8:99:ARG:HD2	71:e:84:TYR:CD1	2.23	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
85:t2:5:GLN:NE2	85:t2:9:ASP:OD2	2.25	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
7:6:183:ASP:OD2	81:p:189:ARG:NH1	2.26	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:2990:A:O2'	89:XA:5141:DOL:O18	2.10	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
76:j:50:SER:OG	76:j:55:ARG:O	2.10	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
11:XA:2416:U:OP1	84:s:313:ARG:NH1	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:AY:340:SER:OG	42:AY:377:ARG:NH2	2.27	0.68
69:c:60:ARG:NH2	69:c:64:PRO:O	2.26	0.68
72:f:92:ASN:ND2	72:f:193:ASP:OD2	2.27	0.68
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
82:q:143:TRP:O	82:q:147:GLN:NE2	2.26	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
68:b:28:ARG:NH2	68:b:78:GLU:OE1	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
84:s:148:ASP:OD1	84:s:149:CYS:N	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
73:g:98:LYS:NZ	73:g:154:ASP:OD2	2.29	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
81:p:113:GLU:OE1	81:p:116:ARG:NH2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:AA:868:C:OP2	18:AA:870:C:N4	2.29	0.65
50:XJ:115:LYS:N	78:l:92:TYR:OH	2.29	0.65
84:s:348:GLU:OE2	84:s:382:GLN:NE2	2.30	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
9:8:99:ARG:HD3	71:e:84:TYR:CD2	2.24	0.65
11:XA:2239:A:OP2	51:XK:75:LYS:NZ	2.30	0.64
11:XA:2262:C:OP2	59:XS:182:LYS:NZ	2.29	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
72:f:101:THR:OG1	79:m:67:ARG:NH1	2.30	0.64
18:AA:1314:C:N3	23:AF:36:ARG:NH2	2.44	0.64
54:XN:234:ASP:O	54:XN:238:LYS:HA	1.96	0.64
11:XA:2400:C:O2'	11:XA:2401:A:O5'	2.14	0.64
11:XA:2447:A:OP1	84:s:59:ARG:NE	2.28	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:1765:C:OP2	75:i:75: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
2:1:42:THR:O	82:q:135:TRP:NE1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:8:101:ARG:NH1	71:e:82:SER:O	2.32	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:1733:C:OP2	75:i:111:ASN:ND2	2.32	0.62
11:XA:1733:C:O4'	75:i:95:ARG:NH2	2.32	0.62
11:XA:2403:G:OP2	45:XD:105:ARG:NH2	2.31	0.62
61:XU:54:ARG:NH2	84:s:314:GLN:OE1	2.32	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
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:702:C:O2'	18:AA:842:C:O2	2.17	0.62
18:AA:942:A:N6	18:AA:1047:A:OP1	2.33	0.62
59:XS:155:ARG:NH1	76:j:52:ALA:O	2.33	0.62
9:8:99:ARG:HG3	71:e:84:TYR:CE1	2.26	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
84:s:191:HIS:O	84:s:428:ARG:NH2	2.33	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
62:XV:66:GLU:N	62:XV:66:GLU:OE1	2.33	0.61
85:t4:4:GLN:N	85:t4:4:GLN:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:XA:2279:U:OP2	75:i:46:ARG:NH2	2.33	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
76:j:103:ARG:NE	76:j:106:GLU:OE2	2.35	0.60
11:XA:2268:G:N7	53:XM:44:ARG:NH1	2.48	0.60
71:e:203:LYS:N	71:e:237:LEU:O	2.35	0.60
84:s:350:ASP:OD2	84:s:389:ARG:NH2	2.33	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
68:b:86:GLU:OE1	68:b:86:GLU:N	2.35	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
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
69:c:80:GLN:O	69:c:210:ARG:NH2	2.32	0.60
39:AV:173:PHE:O	39:AV:178:THR:OG1	2.17	0.59
53:XM:238:ARG:NH1	81:p:70:ASP:OD1	2.34	0.59
63:XW:62:HIS:N	63:XW:65:ASN:OD1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AA:993:A:OP1	26:AI:192:ARG:NH2	2.34	0.59
51:XK:139:LYS:O	68:b:144:ARG:NE	2.35	0.59
61:XU:71:ARG:NH2	61:XU:73:GLN:OE1	2.36	0.59
84:s:321:GLU:OE2	84:s:398:SER:N	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
69:c:81:GLU:OE2	69:c:210:ARG:NE	2.35	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
70:d:157:HIS:O	70:d:161:HIS:ND1	2.36	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
11:XA:1878:U:OP1	73:g:141:ASN:ND2	2.37	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
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:YN: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2195:A:O2'	11:XA:2196:A:O5'	2.19	0.57
37:AT:9:ILE:O	37:AT:12:THR:OG1	2.22	0.57
70:d:158:ASP:OD1	70:d:159:ARG:N	2.37	0.57
11:XA:2990:A:HO2'	89:XA:5141:DOL:HO18	1.51	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
84:s:62:ARG:O	84:s:65:ARG:HG2	2.05	0.57
9:8:99:ARG:HG3	71:e:84:TYR:CE2	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
71:e:139:GLU:OE1	71:e:143:LYS:NZ	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
74:h:78:PHE:O	74:h:80:SER:C	2.47	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
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
77:k:56:ARG:NH1	77:k:58:ASP:O	2.34	0.55
7:6:37:ASN:ND2	63:XW:125:VAL:O	2.35	0.55
18:AA:1367:A:O3'	23:AF:194:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
82:q:44:ASP:O	82:q:47:THR:OG1	2.23	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
77:k:24:GLU:OE2	77:k:26:ASN:N	2.39	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
62:XV:112:GLU:OE1	70:d:81:ARG:NH2	2.39	0.55
1:0:139:ARG:NH2	11:XA:2322:C:OP1	2.34	0.55
9:8:99:ARG:CB	71:e:84:TYR:CG	2.89	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
69:c:283:GLU:N	69:c:283:GLU:OE1	2.39	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
9:8:99:ARG:NE	71:e:84:TYR:CZ	2.73	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
60:XT:135:GLU:OE2	70:d:279:THR:OG1	2.21	0.55
11:XA:2944:C:O3'	80:o:20:LYS:NZ	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
66:XZ:149:TRP:NE1	76:j:45:GLU:OE1	2.38	0.55
9:8:178:TYR:N	79:m:63:THR:O	2.37	0.54
11:XA:3178:U:O2'	83:r:134:ARG:NH1	2.40	0.54
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:AA:845:A:O2'	18:AA:846:A:O4'	2.25	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
11:XA:2156:A:N7	83:r:173:ARG:NH2	2.56	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
81:p:149:ASP:OD1	81:p:150:CYS:N	2.40	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
47:XF:70:ARG:NE	47:XF:194:GLU:OE1	2.41	0.54
84:s:294:TYR:OH	84:s:353:ARG:NH2	2.41	0.54
7:6:282:SER:O	7:6:283:GLU:N	2.41	0.54
11:XA:2190:C:OP2	78:l:120:ARG:NH2	2.38	0.54
73:g:104:ASN:OD1	73:g:105:ARG:N	2.40	0.54
84:s:214:GLU:OE2	84:s:227:ASP: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:1061:A:O5'	45:XD:254:LYS:NZ	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
56:XP:59:SER:OG	81:p:177:ARG:NH1	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
69:c:267:LEU:O	69:c:267:LEU:HD12	2.09	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
8:7:64:LYS:NZ	70:d:278:LYS:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AO:125:GLN:N	32:AO:125:GLN:OE1	2.41	0.53
55:XO:91:GLN:NE2	84:s:44:TYR:OH	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
78:l:112:PRO:O	78:l:118:TRP:NE1	2.42	0.53
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
51:XK:140:ASN:ND2	69:c:264:THR:OG1	2.43	0.52
81:p:81:CYS:SG	81:p:82:ARG:N	2.80	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
58:XR:17:ARG:HA	58:XR:20:ARG:HG2	1.91	0.52
78:l:89:ASP:OD1	78:l:90:ALA:N	2.43	0.52
46:XE:334:ASP:OD1	46:XE:335:GLU:N	2.43	0.52
9:8:99:ARG:HB3	71:e:84:TYR:CG	2.45	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
70:d:249:GLU:OE2	70:d:262:HIS:ND1	2.43	0.52
41:AX:51:THR:O	41:AX:67:HIS:N	2.42	0.52
69:c:67:ASP:OD2	74:h:153:LYS:NZ	2.35	0.52
76:j:76:ARG:O	76:j:80:LEU:HD23	2.10	0.52
4:3:113:ARG:NH2	11:XA:2898:U:O2'	2.43	0.52
11:XA:3169:C:O2'	11:XA:3170:C:O4'	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:AA:939:A:O2'	18:AA:940:A:O4'	2.25	0.51
69:c:246:LYS:NZ	69:c:250:VAL:O	2.39	0.51
11:XA:1764:C:OP1	75:i:75:ARG:NH2	2.43	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
77:k:80:HIS:O	83:r:36:ARG:NH1	2.44	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
73:g:38:PHE:CD1	73:g:38:PHE:O	2.64	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
71:e:158:VAL:O	71:e:255:VAL:N	2.35	0.51
76:j:101:GLU:OE2	76:j:102:GLN:NE2	2.44	0.51
84:s:381:THR:O	84:s:385:GLN:NE2	2.44	0.51
84:s:416:ASP:OD1	84:s:417:VAL:N	2.44	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
79:m:52:TYR:N	79:m:68:TYR:O	2.39	0.51
83:r:43:GLU:OE1	83:r:43:GLU:N	2.44	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
11:XA:2195:A:OP1	78:l:119:ARG:NE	2.44	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
22:AE:54:HIS:NE2	22:AE:83:SER:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:XV:19:TYR:OH	62:XV:31:ASP:OD1	2.30	0.50
81:p:186:GLU:OE1	81:p:189:ARG:NE	2.40	0.50
22:AE:56:GLN:OE1	22:AE:56:GLN:N	2.44	0.50
50:XJ:149:ARG:NH2	78:l:102:GLY:O	2.44	0.50
56:XP:146:GLN:O	56:XP:146:GLN:HG2	2.11	0.50
9:8:177:HIS:N	71:e:58:VAL:O	2.39	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
83:r:84:ASP:OD1	83:r:85:ASP:N	2.44	0.50
11:XA:1833:C:OP2	68:b:114:ARG:NH1	2.41	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
49:XI:148:VAL:O	77:k:31:ARG:NH1	2.37	0.50
69:c:258:THR:N	69:c:271:PHE:O	2.44	0.50
71:e:175:GLN:N	71:e:175:GLN:OE1	2.44	0.50
81:p:128:ASN:OD1	81:p:129:ARG:N	2.43	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
70:d:116:MET:SD	70:d:116:MET:N	2.84	0.50
11:XA:2529:U:O2'	45:XD:206:TYR:O	2.29	0.50
11:XA:2689:C:O3'	80:o:9:ARG:N	2.45	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
75:i:95:ARG:NH1	75:i:111:ASN:OD1	2.45	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
84:s:174:LEU:HB3	84:s:175:PRO:HD3	1.94	0.49
4:3:180:TYR:OH	7:6:367:ASP:OD2	2.23	0.49
24:AG:383:GLY:O	25:AH:129:LYS:NZ	2.44	0.49
39:AV:79:ILE:HD11	39:AV:88:ALA:HB2	1.94	0.49
11:XA:2240:C:N3	83:r:193:LYS:NZ	2.54	0.49
44:XB:1640:A:OP2	56:XP:84:ARG:NH2	2.45	0.49
84:s:242:ARG:NH2	84:s:292:CYS:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
49:XI:80:ARG:NH1	78:l:113:GLU:OE2	2.45	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
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
69:c:276:CYS:O	69:c:279:LYS:N	2.45	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
84:s:77:ASP:OD1	84:s:78:GLU:N	2.45	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
7:6:374:GLU:OE2	81:p:145:ARG:NH1	2.42	0.48
11:XA:3066:C:H2'	11:XA:3067:U:H5'	1.95	0.48
24:AG:200:LEU:O	24:AG:218:TYR:OH	2.31	0.48
45:XD:216:LEU:HD23	45:XD:216:LEU:H	1.77	0.48
67:a:104:GLU:OE1	67:a:104:GLU:N	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2442:U:O3'	84:s:85:LYS:NZ	2.39	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:YN:99:TRP:NE1	54:YN:103:GLU:OE2	2.46	0.48
58:XR:149:HIS:O	66:XZ:151:LEU:N	2.47	0.48
68:b:45:GLU:O	68:b:48:GLU:HG3	2.13	0.48
69:c:94:ASN:OD1	69:c:122:ASN:ND2	2.40	0.48
6:5:143:PRO:HA	6:5:146:HIS:HD1	1.78	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
84:s:60:LEU:O	84:s:63:ILE:HG22	2.12	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
47:XF:142:ARG:HA	47:XF:149:GLY:HA2	1.95	0.48
51:XK:176:TYR:OH	83:r:94:ARG:NH2	2.47	0.48
55:XO:86:ILE:HB	55:XO:87:PRO:HD3	1.95	0.48
75:i:76:GLY:O	75:i:81:ARG:NH2	2.47	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
69:c:164:GLU:OE1	69:c:164:GLU:N	2.39	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
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
69:c:68:TYR:O	69:c:72:ILE:HD12	2.14	0.48
71:e:65:PRO:O	71:e:69:GLU:OE1	2.31	0.48
11:XA:2190:C:OP2	78:l:120:ARG:NH1	2.44	0.48
18:AA:1433:A:N3	18:AA:1458:A:N6	2.62	0.48
81:p:56:ASP:OD2	81:p:57:THR:N	2.47	0.48
84:s:108:TYR:O	84:s:212:ARG:NE	2.47	0.48
11:XA:2692:G:N1	11:XA:2696:A:OP2	2.38	0.48
17:A5:-2:VAL:O	17:A5:-1:GLU:C	2.56	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
50:XJ:149:ARG:NH2	78:l:101:LEU:O	2.46	0.48
57:XQ:107:HIS:O	57:XQ:108:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:h:114:ASN:HA	74:h:117:LEU:HD22	1.95	0.48
11:XA:3149:C:N4	11:XA:3161:G:N7	2.62	0.48
39:AV:108:THR:O	39:AV:111:THR:OG1	2.27	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
84:s:350:ASP:OD1	84:s:351:VAL:N	2.47	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
53:XM:185:ASP:OD1	53:XM:185:ASP:C	2.57	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
83:r:83:TYR:HA	83:r:118:CYS:SG	2.54	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
32:AO:58:TYR:O	32:AO:61:SER:OG	2.31	0.47
73:g:160:TRP:O	73:g:164:LYS:NZ	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
84:s:178:ASP:OD2	84:s:203:ARG:NH1	2.47	0.47
4:3:185:ASN:ND2	7:6:371:ASP:OD2	2.43	0.47
11:XA:1823:A:OP2	67:a:127:GLY:N	2.48	0.47
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
16:A4:116:VAL:O	16:A4:120:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AA:1343:A:O2'	18:AA:1345:G:N7	2.45	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
72:f:104:GLU:OE2	72:f:155:ARG:NH2	2.47	0.47
74:h:64:GLU:OE2	74:h:64:GLU:HA	2.15	0.47
75:i:59:ASN:O	75:i:63:LEU:HD23	2.15	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:XN:211:ASN:ND2	2.48	0.47
54:XN:177:ASP:OD1	54:XN:178:GLN:N	2.48	0.47
74:h:65:ASP:C	74:h:65:ASP:OD1	2.58	0.47
82:q:167:GLN:O	82:q:171:ARG:NE	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
53:XM:238:ARG:O	81:p:155:ARG:NH2	2.44	0.47
11:XA:2131:A:OP1	80:o:23:ARG:NH1	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
53:XM:133:LYS:C	53:XM:134:ARG:HG2	2.39	0.47
3:2:70:LEU:O	65:XY:198:ARG:NH2	2.48	0.46
11:XA:2016:C:OP1	11:XA:2039:A:O2'	2.30	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
74:h:135:GLN:N	74:h:135:GLN:OE1	2.48	0.46
84:s:260:GLU:N	84:s:260:GLU:OE1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:XN:71:ASP:N	54:XN: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
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
71:e:201:GLU:N	71:e:201:GLU:OE1	2.49	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
71:e:185:ARG:O	71:e:189:GLU:OE1	2.34	0.46
71:e:269:LEU:O	71:e:273:ARG:HD3	2.14	0.46
73:g:106:GLN:O	73:g:151:GLY:N	2.49	0.46
82:q:140:ARG:O	82:q:144:GLU:OE1	2.33	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
49:XI:198:PRO:O	49:XI:199:SER:C	2.59	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
69:c:164:GLU:HG2	69:c:165:VAL:N	2.31	0.46
70:d:235:GLN:OE1	70:d:235:GLN:N	2.49	0.46
75:i:109:ASN:OD1	75:i:110:LEU:N	2.48	0.46
84:s:103:ASP:OD1	84:s:104:ARG:N	2.48	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
2:1:14:LYS:NZ	11:XA:2848:A:O3'	2.49	0.46
11:XA:2214:A:OP1	54:XN: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
70:d:64:MET:N	70:d:64:MET:SD	2.89	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
64:XX:207:THR:OG1	64:XX:210:GLU:OE1	2.34	0.46
76:j:98:LEU:O	76:j:101:GLU:HG3	2.16	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
74:h:58:ARG:NH1	74:h:136:ASP:OD2	2.49	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
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
54:XN:201:ASP:OD1	54:XN:201:ASP:C	2.58	0.45
65:XY:161:GLU:OE1	65:XY:161:GLU:N	2.49	0.45
81:p:113:GLU:OE2	81:p:117:GLN:NE2	2.49	0.45
7:6:83:ASP:OD2	7:6:87:LYS:NZ	2.42	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
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
79:m:87:GLU:OE1	79:m:91:ARG:NH2	2.49	0.45
81:p:149:ASP:OD1	81:p:149:ASP:C	2.60	0.45
84:s:233:ILE:HD11	84:s:334:ALA:CB	2.47	0.45
11:XA:2051:A:N3	73:g:104:ASN:ND2	2.62	0.45
11:XA:2081:U:OP1	80:o:64:ALA:N	2.50	0.45
11:XA:2875:A:H4'	56:XP:178:TYR:CE2	2.51	0.45
13:A1:211:ARG:NH2	42:AY:359:SER:OG	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
45:XD:251:ASP:OD1	45:XD:251:ASP:C	2.58	0.45
70:d:197:VAL:O	70:d:198:ARG:NE	2.50	0.45
72:f:138:GLN:HG3	72:f:144:MET:H	1.82	0.45
76:j:102:GLN:O	76:j:106:GLU:OE1	2.35	0.45
7:6:288:SER:O	7:6:289:PRO:C	2.60	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
69:c:135:THR:O	69:c:138:THR:OG1	2.34	0.45
80:o:69:GLU:O	80:o:72:GLU:HG3	2.17	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
11:XA:2054:U:H2'	80:o:75:LYS:NZ	2.32	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
53:XM:103:TYR:OH	73:g:93:ASN:OD1	2.33	0.45
57:XQ:61:VAL:HG22	57:XQ:62:ILE:N	2.31	0.45
11:XA:2235:C:O2'	83:r:165:LYS:N	2.49	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:XW:112:GLU:O	63:XW:115:ASP:OD1	2.34	0.45
84:s:207:HIS:ND1	84:s:234:ASP:OD1	2.50	0.45
84:s:300:HIS:HB2	84:s:361:ILE:HG22	1.98	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: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
69:c:101:GLU:OE1	69:c:105:ARG:NH1	2.50	0.45
11:XA:2146:A:C4	58:XR:64:MET:HE1	2.52	0.44
11:XA:3115:U:H2'	11:XA:3116:C:H6	1.82	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
8:7:159:LYS:HA	67:a:92:ASP:HB2	1.98	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
38:AU:110:GLN:C	38:AU:114:ARG:HE	2.23	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:2502:C:O2	11:XA:3095:G:O2'	2.32	0.44
11:XA:2726:C:C4	11:XA:2727:C:C5	3.06	0.44
11:XA:3151:A:C5	11:XA:3152:C:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:AA:1027:A:O2'	18:AA:1054:A:O4'	2.31	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
84:s:63:ILE:O	84:s:67:GLN:OE1	2.36	0.44
84:s:242:ARG:HA	84:s:295:GLY:HA2	1.98	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
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
80:o:33:GLN:HA	80:o:36:ILE:HG12	1.98	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
50:XJ:85:PRO:O	50:XJ:124:LYS:NZ	2.51	0.44
58:XR:107:ILE:O	68:b:130:TRP:HB2	2.17	0.44
71:e:145:ASP:O	71:e:148:SER:OG	2.34	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
11:XA:2814:G:OP1	11:XA:2839:C:O2'	2.30	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:XN:171:GLU:OE1	54:XN:171:GLU:N	2.41	0.44
55:XO:18:MET:HE1	55:XO:48:ARG:HE	1.83	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
72:f:90:VAL:HG13	72:f:189:HIS:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
49:XI:101:ASN:O	77:k:35:GLN:NE2	2.50	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
75:i:64:GLY:O	75:i:65:ASN:OD1	2.36	0.44
83:r:162:ILE:HG13	83:r:162:ILE:O	2.18	0.44
1:0:87:ILE:H	1:0:87:ILE:HD12	1.83	0.43
11:XA:2742:U:O2	64:XX:99:LYS:NZ	2.47	0.43
11:XA:2743:U:O4'	64:XX:99:LYS:NZ	2.41	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:1302:C:OP1	20:AC:165:LYS:NZ	2.41	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
56:XP:86:GLN:C	56:XP:119:ARG:HD3	2.44	0.43
65:XY:123:ARG:NE	70:d:68:ARG:O	2.37	0.43
71:e:198:ASN:ND2	71:e:242:ASP:OD1	2.51	0.43
71:e:265:LYS:N	71:e:266:PRO:HD3	2.33	0.43
81:p:146:ASN:O	81:p:149:ASP:OD1	2.34	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:873:G:O2'	18:AA:921:U:O2	2.33	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
41:AX:207:LYS:N	41:AX:218:LYS:HZ2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:AV:83:GLU:O	39:AV:87:HIS:CD2	2.71	0.43
47:XF:141:ILE:O	47:XF:142:ARG:HB2	2.18	0.43
53:XM:14:ASP:OD2	74:h:119:GLN:NE2	2.51	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
77:k:9:GLY:C	77:k:10:LEU:HD23	2.43	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
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
56:XP:87:HIS:O	56:XP:118:THR:OG1	2.32	0.43
66:XZ:98:GLN:OE1	66:XZ:100:HIS:NE2	2.52	0.43
84:s:111:LYS:NZ	84:s:387:ASN:O	2.48	0.43
85:t:2:5:GLN:O	85:t:2:8:GLN:HG3	2.18	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
73:g:121:GLN:HA	73:g:124:VAL:HG22	2.01	0.43
7:6:144:GLY:N	7:6:145:PRO:CD	2.82	0.43
9:8:99:ARG:O	9:8:100:GLU:C	2.61	0.43
29:AL:126:GLU:HB2	29:AL:181:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
80:o:30:ARG:O	80:o:33:GLN:HG2	2.18	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
17:A5:104:VAL:O	17:A5:105:THR:C	2.61	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
59:XS:194:ARG:NH2	68:b:13:SER:OG	2.52	0.43
68:b:112:VAL:O	68:b:112:VAL:HG23	2.18	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
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
56:XP:177:ILE:O	56:XP:178:TYR:C	2.61	0.43
75:i:111:ASN:HA	75:i:114:ILE:HG12	2.00	0.43
84:s:407:ASP:O	84:s:408:ASN:OD1	2.36	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
60:XT:59:TYR:N	70:d:227:ARG:O	2.51	0.43
64:XX:93:ASN:O	64:XX:94:ASN:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2155:A:N6	83:r:169:TRP:O	2.52	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
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
60:XT:126:ASP:OD1	60:XT:126:ASP:C	2.62	0.42
69:c:223:MET:O	69:c:224:THR:C	2.62	0.42
70:d:137:PHE:N	70:d:138:PRO:CD	2.83	0.42
84:s:57:ALA:O	84:s:60:LEU:HD23	2.19	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: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
54:XN:174:GLY:O	54:XN:177:ASP:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:g:142:GLU:HG3	80:o:88:ILE:HD12	2.02	0.42
84:s:145:VAL:O	84:s:148: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
24:AG:264:GLU:CD	24:AG:264:GLU:H	2.27	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
77:k:65:ASP:OD1	77:k:66:VAL:N	2.52	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
18:AA:843:G:O2'	18:AA:844:A:N7	2.50	0.42
39:AV:235:GLU:O	39:AV:239:GLY:N	2.50	0.42
62:XV:196:GLU:O	62:XV:200:GLU:OE1	2.37	0.42
68:b:79:TYR:HD2	68:b:109:GLY:HA2	1.84	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
7:6:236:LEU:HD23	7:6:236:LEU:C	2.45	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:909:G:H21	27:AJ:138:LYS:HZ1	1.68	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
29:AL:169:ASN:OD1	29:AL:169:ASN:C	2.62	0.42
38:AU:162:GLU:OE2	38:AU:162:GLU:N	2.52	0.42
54:XN:198:MET:O	54:XN: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
69:c:138:THR:O	69:c:142:GLU:CD	2.62	0.42
77:k:55:VAL:HG12	77:k:55:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
45:XD:180:ASP:OD1	45:XD:180:ASP:N	2.51	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
69:c:150:THR:HA	69:c:153:ILE:HG22	2.02	0.42
80:o:55:THR:HG22	80:o:56:ARG:N	2.34	0.42
82:q:147:GLN:HA	82:q:150:LYS:HG2	2.01	0.42
84:s:57:ALA:HA	84:s:60:LEU:CD2	2.50	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
84:s:66:TRP:O	84:s:69:THR:OG1	2.30	0.42
6:5:114:LEU:HD21	45:XD:127:ILE:HG12	2.02	0.42
9:8:99:ARG:HD3	71:e:84:TYR:CD1	2.28	0.42
9:8:101:ARG:HH12	79:m:50:ARG:HE	1.68	0.42
11:XA:2079:C:O2	80:o:60:ARG:NH2	2.46	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
14:A2:66:CYS:O	14:A2:67:ARG:C	2.62	0.42
16:A4:104:ARG:HA	16:A4:107:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
46:XE:129:VAL:C	46:XE:130:LEU:HD22	2.44	0.42
51:XK:74:GLN:HA	83:r:161:PRO:HA	2.02	0.42
80:o:13:PRO:HG2	80:o:21:HIS:HB2	2.02	0.42
80:o:66:ARG:O	80:o:69:GLU:HG3	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
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
47:XF:278:SER:O	47:XF:278:SER:OG	2.32	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
75:i:106:ASP:O	75:i:109:ASN:OD1	2.37	0.41
76:j:101:GLU:O	76:j:105:GLN:OE1	2.38	0.41
84:s:409:ASP:OD1	84:s:410:VAL:N	2.53	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
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
63:XW:115:ASP:OD1	63:XW:115:ASP:C	2.62	0.41
84:s:93:VAL:HB	84:s:233:ILE:HG22	2.02	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:1814:A:O4'	75:i:32:ILE:HD11	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
69:c:276:CYS:O	69:c:277:ASP:OD2	2.38	0.41
73:g:76:ARG:NH2	73:g:164:LYS:O	2.52	0.41
7:6:288:SER:OG	7:6:289:PRO:HD2	2.20	0.41
11:XA:2060:A:O2'	11:XA:2061:C:OP2	2.34	0.41
11:XA:2075:U:O2'	11:XA:2833:A:N7	2.44	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
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
16:A4:437:GLY:O	16:A4:441:THR:OG1	2.37	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
29:AL:176:ASP:N	29:AL:176:ASP:OD1	2.52	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
49:XI:197:LEU:O	49:XI:198:PRO:C	2.63	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:XN:172:VAL:HG13	54:XN:175:PHE:CZ	2.55	0.41
58:XR:108:TYR:OH	60:XT:208:ILE:HD11	2.20	0.41
64:XX:178:PRO:C	64:XX:179:GLU:HG3	2.45	0.41
64:XX:180:ASP:N	64:XX:181:PRO:HD3	2.35	0.41
68:b:43:ALA:HB2	68:b:89:ILE:HD12	2.03	0.41
73:g:141:ASN:O	73:g:145:GLY:N	2.54	0.41
76:j:98:LEU:O	76:j:102:GLN:OE1	2.39	0.41
11:XA:2139:U:OP2	66:XZ:74:SER:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
54:XN:103:GLU:OE1	54:XN: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
7:6:289:PRO:C	7:6:291:TYR:H	2.28	0.41
7:6:379:ILE:O	7:6:379:ILE:HG13	2.20	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
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
65:XY:220:LYS:O	65:XY:224:GLU:OE1	2.38	0.41
69:c:170:ALA:HB3	69:c:191:LEU:HD21	2.03	0.41
70:d:173:THR:HA	70:d:176:ILE:HG12	2.03	0.41
75:i:59:ASN:O	75:i:62:ILE:N	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
68:b:49:ARG:HG3	68:b:50:GLU:N	2.35	0.41
81:p:177:ARG:O	81:p:181:GLU:OE1	2.38	0.41
1:O: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:1773:A:OP1	69:c:31:VAL:N	2.53	0.41
11:XA:2727:C:HO2'	11:XA:2815:G:N2	2.18	0.41
11:XA:2737:U:O2'	11:XA:3084:A:N3	2.47	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:76:HIS:CD2	67:a:50:ALA:HA	2.56	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
74:h:75:LYS:O	74:h:80:SER:HA	2.20	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:2039:A:N7	11:XA:2729:U:O2'	2.46	0.41
11:XA:2670:C:O2'	11:XA:2671:C:H5'	2.20	0.41
11:XA:2818:C:O2	17:A5:146:SER:OG	2.38	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
17:A5:89:ASN:O	17:A5:100:PRO:HD2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:17:ARG:NH2	74:h:115:SER:O	2.54	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
69:c:86:ASP:OD2	69:c:86:ASP:N	2.53	0.41
79:m:54:VAL:HG12	79:m:55:LEU:N	2.36	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
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
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
68:b:26:LEU:HD13	68:b:105:ALA:HA	2.03	0.41
78:l:106:THR:N	78:l:109:GLU:OE2	2.43	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
18:AA:1433:A:C4	18:AA:1458:A:N6	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
50:XJ:115:LYS:NZ	78:l:70:THR:O	2.54	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
68:b:100:LEU:O	68:b:103:LYS:HG2	2.21	0.40
73:g:36:PRO:O	73:g:38:PHE:CD2	2.75	0.40
84:s:215:GLU:HB2	84:s:229:LEU:HD11	2.03	0.40
84:s:403:GLU:OE2	84:s:404:THR:OG1	2.37	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
11:XA:2409:A:OP1	84:s:160:ARG:NH2	2.47	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
49:XI:156:SER:OG	49:XI:158:GLU:O	2.39	0.40
54:XN:201:ASP:O	54:XN:204:GLU:HG3	2.22	0.40
54:XN:215:PHE:CD1	54:XN: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
73:g:55:THR:HG22	73:g:55:THR:O	2.21	0.40
83:r:40:GLU:OE2	83:r:47:THR:OG1	2.30	0.40
84:s:148:ASP:OD1	84:s:148:ASP:C	2.63	0.40
7:6:147:HIS:O	7:6:151:LEU:HD23	2.22	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:2795:U:O2'	64:XX:106:LYS:O	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
69:c:177:GLN:OE1	69:c:177:GLN:N	2.40	0.40
70:d:288:LYS:HG2	70:d:289:PRO:HD2	2.03	0.40
73:g:37:ARG:O	73:g:38:PHE:CG	2.74	0.40
73:g:129:SER:N	73:g:130:PRO:HD2	2.36	0.40
84:s:63:ILE:HA	84:s:66:TRP:CD1	2.56	0.40
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
35:AR:135:ARG:HE	35:AR:186:TRP:CG	2.39	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
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
59:XS:163:LYS:HB3	68:b:106:ASP:HB3	2.02	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
69:c:151:GLU:O	69:c:154:LYS:HG2	2.22	0.40
69:c:276:CYS:O	69:c:277:ASP:C	2.64	0.40
74:h:139:LYS:O	74:h:142:GLU:HG2	2.21	0.40
83:r:113:ARG:O	83:r:116:GLU:HG2	2.22	0.40
6:5:313:MET:HE2	6:5:355:LEU:CD2	2.52	0.40
7:6:58:ARG:O	7:6:62:GLU:OE1	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
59:XS:72:GLU:C	59:XS:76:HIS:HD1	2.28	0.40
84:s:150:LEU:O	84:s:154:HIS:ND1	2.53	0.40
84:s:419:LEU:HA	84:s:422:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	14	48
46	XE	302/348 (87%)	290 (96%)	12 (4%)	0	100	100
47	XF	248/311 (80%)	238 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	24	60
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
45	XD	208	ARG
70	d	289	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/164 (59%)	97 (100%)	0	100	100
2	1	50/60 (83%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	267/303 (88%)	267 (100%)	0	100	100
9	8	124/190 (65%)	124 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
12	A0	176/190 (93%)	176 (100%)	0	100	100
13	A1	253/291 (87%)	253 (100%)	0	100	100
14	A2	99/101 (98%)	99 (100%)	0	100	100
15	A3	63/166 (38%)	63 (100%)	0	100	100
16	A4	500/566 (88%)	500 (100%)	0	100	100
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%)	283 (100%)	0	100	100
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
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%)	93 (100%)	0	100	100
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%)	94 (99%)	1 (1%)	65	74
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%)	86 (100%)	0	100	100
34	AQ	77/78 (99%)	77 (100%)	0	100	100
35	AR	229/318 (72%)	229 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	AS	115/164 (70%)	115 (100%)	0	100	100
37	AT	150/157 (96%)	150 (100%)	0	100	100
38	AU	149/174 (86%)	149 (100%)	0	100	100
39	AV	315/364 (86%)	315 (100%)	0	100	100
40	AW	84/158 (53%)	84 (100%)	0	100	100
41	AX	307/308 (100%)	307 (100%)	0	100	100
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%)	190 (100%)	0	100	100
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%)	133 (100%)	0	100	100
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%)	245 (100%)	0	100	100
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
57	XQ	220/256 (86%)	220 (100%)	0	100	100
58	XR	118/126 (94%)	118 (100%)	0	100	100
59	XS	145/180 (81%)	145 (100%)	0	100	100
60	XT	146/182 (80%)	146 (100%)	0	100	100
61	XU	126/135 (93%)	126 (100%)	0	100	100
62	XV	179/191 (94%)	179 (100%)	0	100	100
63	XW	91/119 (76%)	91 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	b	130/186 (70%)	130 (100%)	0	100	100
69	c	241/288 (84%)	241 (100%)	0	100	100
70	d	196/273 (72%)	196 (100%)	0	100	100
71	e	188/236 (80%)	188 (100%)	0	100	100
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%)	140 (99%)	1 (1%)	76	79
83	r	138/169 (82%)	138 (100%)	0	100	100
84	s	326/381 (86%)	326 (100%)	0	100	100
85	t1	41/158 (26%)	40 (98%)	1 (2%)	43	63
85	t2	29/158 (18%)	29 (100%)	0	100	100
85	t3	29/158 (18%)	29 (100%)	0	100	100
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%)	12568 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	AM	88	GLU
82	q	121	ILE
85	t1	21[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79)

such sidechains are listed below:

Mol	Chain	Res	Type
6	5	156	ASN
6	5	380	GLN
7	6	108	GLN
7	6	224	HIS
7	6	308	GLN
7	6	373	HIS
8	7	69	HIS
12	A0	88	GLN
13	A1	275	ASN
15	A3	140	HIS
16	A4	90	GLN
16	A4	285	ASN
16	A4	504	ASN
20	AC	107	GLN
23	AF	72	GLN
23	AF	147	GLN
23	AF	233	ASN
25	AH	183	HIS
28	AK	60	ASN
28	AK	117	HIS
28	AK	119	GLN
29	AL	146	HIS
32	AO	204	ASN
34	AQ	73	ASN
34	AQ	79	ASN
34	AQ	85	GLN
35	AR	117	GLN
37	AT	51	ASN
39	AV	115	GLN
39	AV	246	ASN
39	AV	381	GLN
39	AV	388	GLN
41	AX	114	ASN
41	AX	176	GLN
41	AX	364	ASN
41	AX	394	HIS
42	AY	285	GLN
45	XD	263	ASN
46	XE	125	GLN
47	XF	83	HIS
47	XF	98	GLN
47	XF	103	GLN

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Mol	Chain	Res	Type
47	XF	105	ASN
49	XI	189	GLN
51	XK	56	HIS
51	XK	70	ASN
51	XK	117	HIS
51	XK	160	GLN
52	XL	59	HIS
52	XL	103	ASN
53	XM	123	ASN
53	XM	139	GLN
54	XN	101	HIS
54	XN	210	GLN
57	XQ	158	GLN
58	XR	94	GLN
60	XT	210	HIS
63	XW	59	HIS
65	XY	117	GLN
68	b	25	GLN
68	b	102	GLN
68	b	107	GLN
70	d	66	HIS
71	e	75	GLN
71	e	87	HIS
72	f	54	HIS
72	f	94	HIS
73	g	63	HIS
74	h	103	HIS
74	h	110	HIS
75	i	120	HIS
77	k	15	GLN
78	l	135	ASN
80	o	21	HIS
82	q	139	GLN
82	q	147	GLN
84	s	191	HIS
84	s	375	ASN
84	s	420	GLN

5.3.3 RNA ⓘ

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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	55/73 (75%)	10 (18%)	0
All	All	2467/2583 (95%)	435 (17%)	10 (0%)

All (435) 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

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Mol	Chain	Res	Type
11	XA	1805	A
11	XA	1809	U
11	XA	1810	A
11	XA	1811	A
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

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Mol	Chain	Res	Type
11	XA	2022	G
11	XA	2030	U
11	XA	2036	C
11	XA	2037	U
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

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Mol	Chain	Res	Type
11	XA	2297	A
11	XA	2299	U
11	XA	2300	G
11	XA	2316	U
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

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Mol	Chain	Res	Type
11	XA	2628	U
11	XA	2630	U
11	XA	2633	A
11	XA	2635	G
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

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Mol	Chain	Res	Type
11	XA	2918	A
11	XA	2921	A
11	XA	2928	C
11	XA	2934	G
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

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Mol	Chain	Res	Type
11	XA	3168	C
11	XA	3169	C
11	XA	3172	C
11	XA	3177	A
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

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Mol	Chain	Res	Type
18	AA	835	C
18	AA	836	A
18	AA	844	A
18	AA	851	A
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

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Mol	Chain	Res	Type
18	AA	1081	U
18	AA	1082	A
18	AA	1103	A
18	AA	1105	C
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

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Mol	Chain	Res	Type
18	AA	1297	G
18	AA	1307	G
18	AA	1326	A
18	AA	1327	G
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

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Mol	Chain	Res	Type
18	AA	1531	C
18	AA	1537	C
18	AA	1539	C
18	AA	1551	G
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
44	XB	1663	C

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	004	A	7	86	9,10,11	1.11	0	9,12,14	0.78	0
86	DBB	A	3	86	4,5,6	0.85	0	1,5,7	0.08	0
86	MHW	A	1	86	9,9,10	2.61	3 (33%)	10,11,13	2.11	2 (20%)
86	MHU	A	5	86	14,15,16	2.26	5 (35%)	18,19,21	1.52	3 (16%)
86	MHV	A	6	86	7,9,10	5.85	1 (14%)	8,11,13	5.25	5 (62%)

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	004	A	7	86	-	0/4/6/8	0/1/1/1
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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	A	6	MHV	OD1-CG	15.25	1.48	1.21
86	A	5	MHU	CZ-NZ	6.21	1.52	1.37
86	A	1	MHW	CA-C	5.58	1.54	1.48
86	A	1	MHW	OG1-CB	4.29	1.45	1.36
86	A	1	MHW	CB-CA	-2.46	1.36	1.40
86	A	5	MHU	CD1-CG	2.39	1.43	1.38
86	A	5	MHU	CD2-CE2	2.34	1.42	1.38
86	A	5	MHU	CB-CG	2.14	1.56	1.51
86	A	5	MHU	CE1-CZ	2.03	1.43	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	A	6	MHV	OD1-CG-CB	-11.34	106.43	121.95
86	A	6	MHV	OD1-CG-CD2	-7.91	107.29	122.07
86	A	1	MHW	O-C-CA	-5.56	117.39	124.37
86	A	5	MHU	CM-N-CA	3.62	124.52	113.70
86	A	6	MHV	CB-CA-N	-3.45	105.36	112.50
86	A	6	MHV	CD2-CG-CB	2.87	120.24	115.89
86	A	1	MHW	CD-CG2-CB	-2.83	116.56	120.05
86	A	5	MHU	CB-CA-C	-2.44	106.95	111.81
86	A	6	MHV	CE-CD2-CG	2.24	116.77	111.81
86	A	5	MHU	O-C-CA	-2.06	119.47	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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 oligosaccharides 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
90	GTP	AX	500	-	33,34,34	0.95	1 (3%)	50,54,54	1.56	8 (16%)
89	DOL	XA	5141	-	47,50,50	3.84	18 (38%)	57,70,70	3.02	15 (26%)

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
90	GTP	AX	500	-	-	8/22/38/38	0/3/3/3
89	DOL	XA	5141	-	-	19/64/77/77	0/2/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	XA	5141	DOL	C28-C29	10.69	1.56	1.32
89	XA	5141	DOL	C6-N5	10.11	1.49	1.34
89	XA	5141	DOL	C22-C23	8.96	1.56	1.32
89	XA	5141	DOL	C19-C20	8.47	1.56	1.34
89	XA	5141	DOL	C10-N9	8.28	1.38	1.29
89	XA	5141	DOL	C26-N25	6.98	1.48	1.34
89	XA	5141	DOL	C13-C10	5.55	1.57	1.50
89	XA	5141	DOL	O36-C37	5.49	1.46	1.34
89	XA	5141	DOL	C22-C20	5.43	1.57	1.46
89	XA	5141	DOL	C8-C6	3.96	1.55	1.49
89	XA	5141	DOL	C16-C14	3.69	1.56	1.51
89	XA	5141	DOL	C28-C26	3.64	1.55	1.48
89	XA	5141	DOL	C12-C8	3.64	1.38	1.34
89	XA	5141	DOL	O27-C26	-2.84	1.19	1.24
89	XA	5141	DOL	O18-C17	-2.82	1.38	1.43
89	XA	5141	DOL	C3-C2	-2.46	1.50	1.54
90	AX	500	GTP	C2-N3	2.14	1.38	1.33
89	XA	5141	DOL	C24-C23	2.10	1.57	1.49
89	XA	5141	DOL	O36-C32	-2.03	1.41	1.44

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	XA	5141	DOL	O40-S39-O41	-14.75	101.41	118.13
89	XA	5141	DOL	O11-C10-C13	9.12	126.13	117.70
89	XA	5141	DOL	C24-N25-C26	-6.50	111.63	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	XA	5141	DOL	O11-C10-N9	-5.25	108.41	114.09
90	AX	500	GTP	C5-C4-N3	-5.16	120.18	128.39
90	AX	500	GTP	C2-N3-C4	4.75	120.47	112.30
89	XA	5141	DOL	O40-S39-C2	4.53	112.87	108.50
89	XA	5141	DOL	C4-N5-C1	-3.92	107.91	112.51
89	XA	5141	DOL	C32-O36-C37	-3.73	111.58	117.76
89	XA	5141	DOL	C23-C22-C20	-3.24	121.00	125.89
90	AX	500	GTP	N9-C4-N3	3.20	132.36	125.95
90	AX	500	GTP	C2-N1-C6	-3.02	119.64	125.11
89	XA	5141	DOL	C13-C14-C16	-3.00	109.50	118.39
89	XA	5141	DOL	O36-C32-C30	2.84	111.82	107.12
89	XA	5141	DOL	C3-C4-N5	2.66	106.14	103.22
90	AX	500	GTP	N9-C8-N7	-2.63	108.52	113.40
89	XA	5141	DOL	C21-C20-C22	2.59	122.04	118.09
90	AX	500	GTP	C5-C6-N1	2.49	119.59	113.25
90	AX	500	GTP	C8-N7-C5	2.48	108.68	104.26
89	XA	5141	DOL	C30-C29-C28	-2.46	119.79	126.30
89	XA	5141	DOL	O15-C14-C16	2.46	125.73	121.53
90	AX	500	GTP	O6-C6-C5	-2.40	120.20	126.53
89	XA	5141	DOL	O15-C14-C13	2.29	124.74	121.20

There are no chirality outliers.

All (27) 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
90	AX	500	GTP	C5'-O5'-PA-O2A
89	XA	5141	DOL	C3-C2-S39-C42
89	XA	5141	DOL	N9-C10-C13-C14
89	XA	5141	DOL	C28-C29-C30-C31
90	AX	500	GTP	O4'-C4'-C5'-O5'
89	XA	5141	DOL	C22-C23-C24-N25
89	XA	5141	DOL	C43-C42-S39-O40
89	XA	5141	DOL	O11-C10-C13-C14
89	XA	5141	DOL	C29-C30-C32-O36

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Mol	Chain	Res	Type	Atoms
89	XA	5141	DOL	C31-C30-C32-O36
89	XA	5141	DOL	C3-C2-S39-O41
90	AX	500	GTP	C5'-O5'-PA-O1A
89	XA	5141	DOL	S39-C42-C43-N44
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
89	XA	5141	DOL	C42-C43-N44-C45
89	XA	5141	DOL	C28-C29-C30-C32

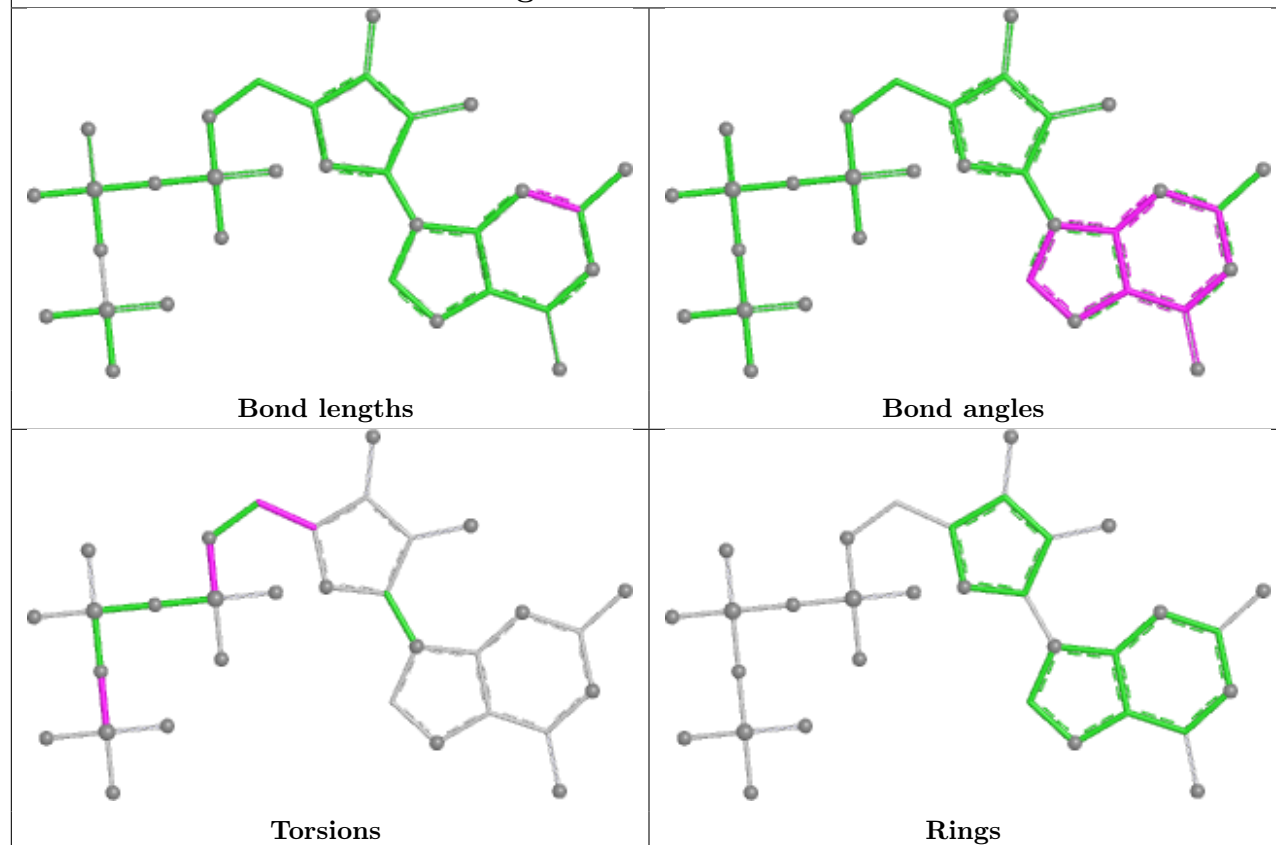
There are no ring outliers.

2 monomers are involved in 5 short contacts:

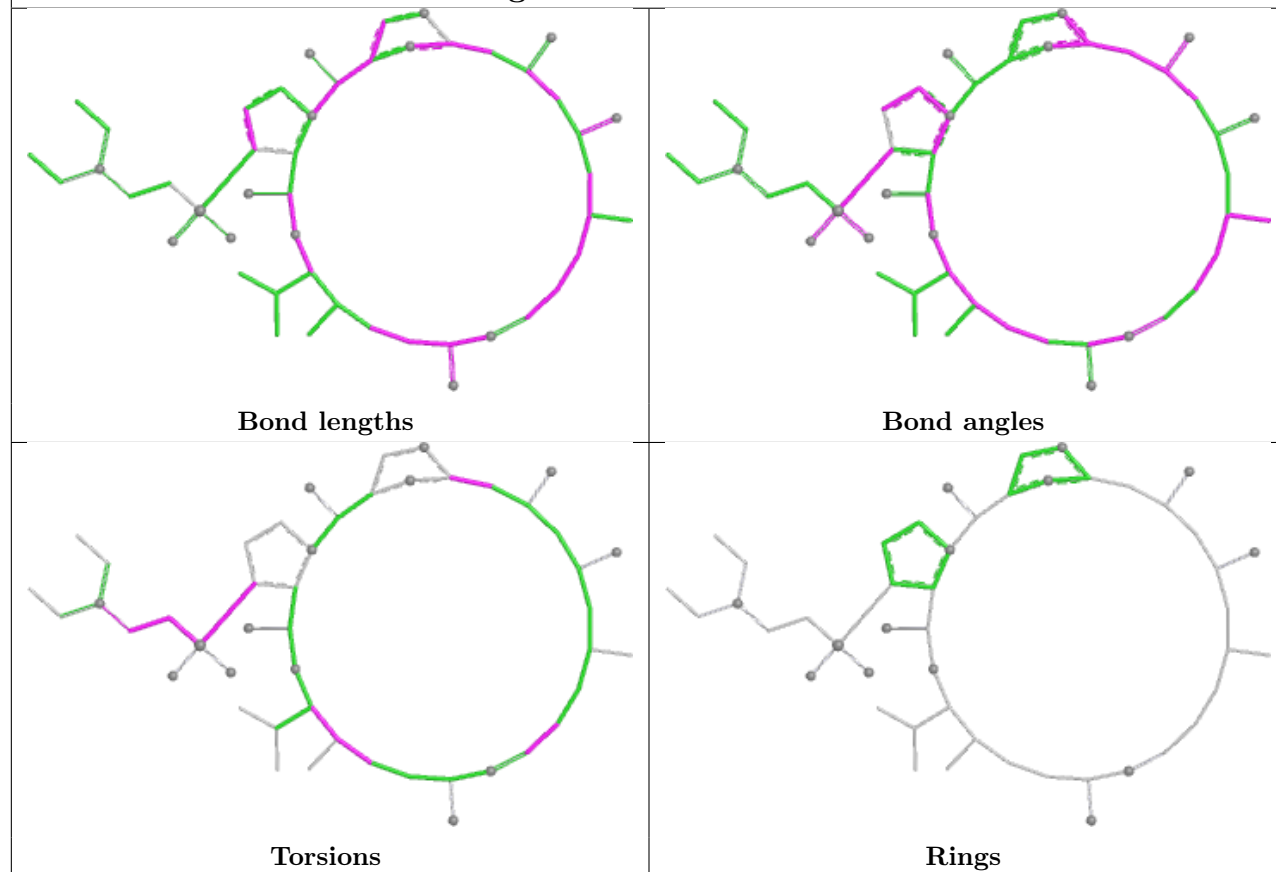
Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	AX	500	GTP	1	0
89	XA	5141	DOL	4	0

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

Ligand GTP AX 500



Ligand DOL XA 5141



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:ASP	O3'	1388:ASP	P	8.11
1	A4	537:ARG	C	538:ASP	N	6.58
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

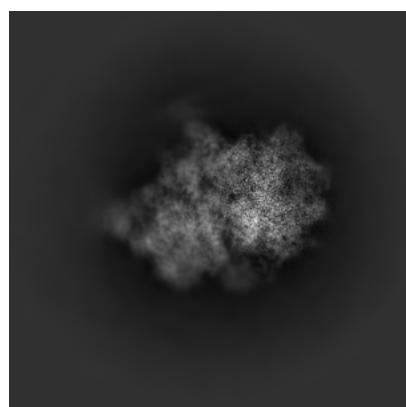
6 Map visualisation [i](#)

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.

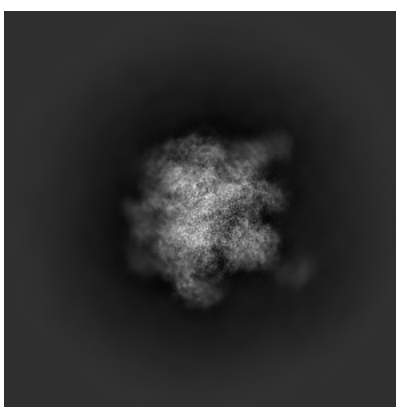
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

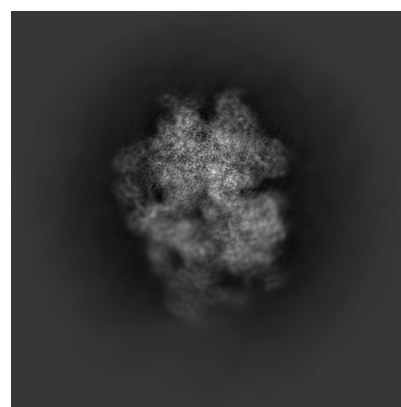
6.1.1 Primary map



X



Y

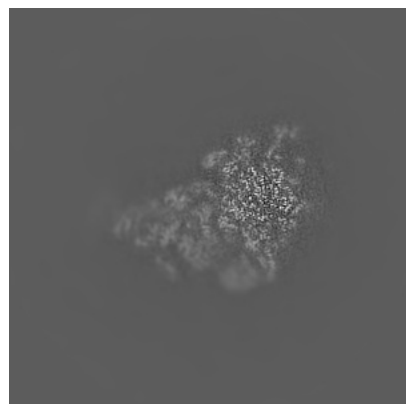


Z

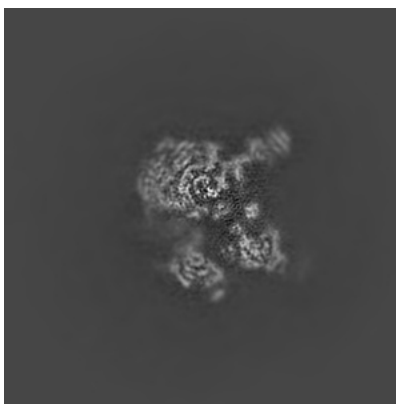
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

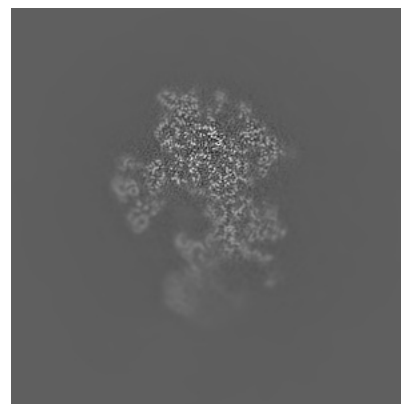
6.2.1 Primary map



X Index: 260



Y Index: 260

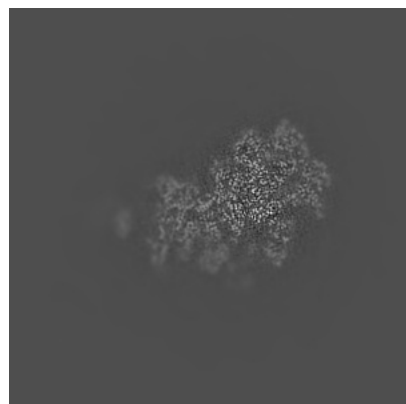


Z Index: 260

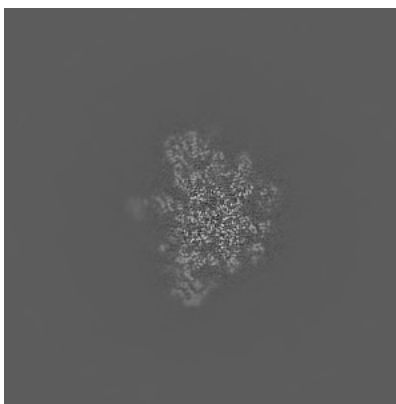
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

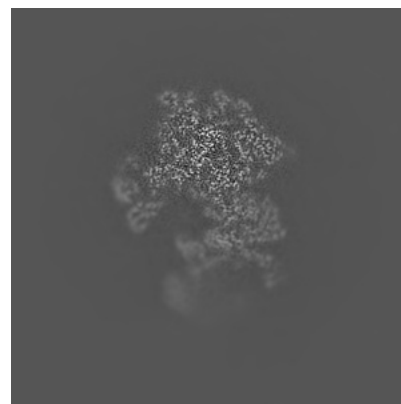
6.3.1 Primary map



X Index: 278



Y Index: 321

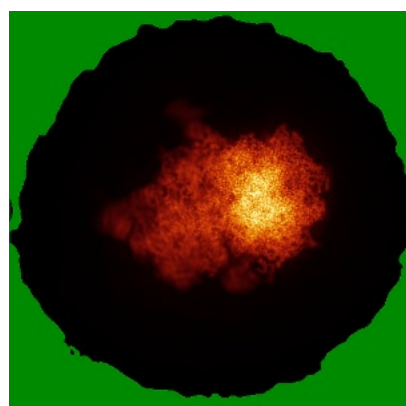


Z Index: 264

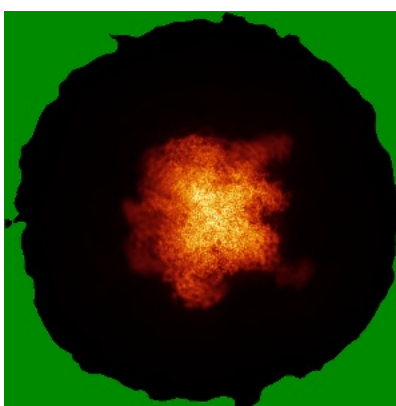
The images above show the largest variance slices of the map in three orthogonal directions.

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

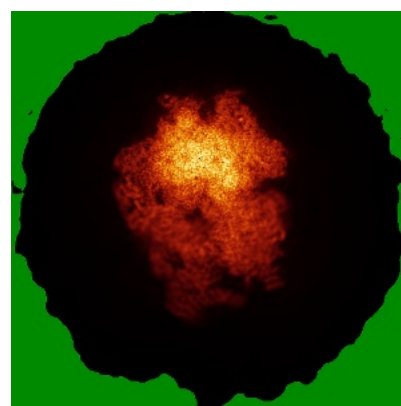
6.4.1 Primary map



X



Y

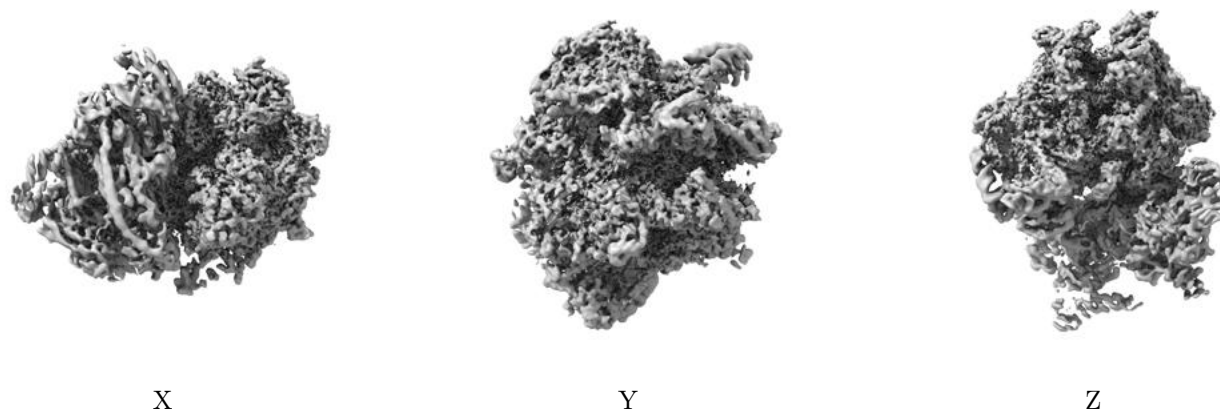


Z

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.

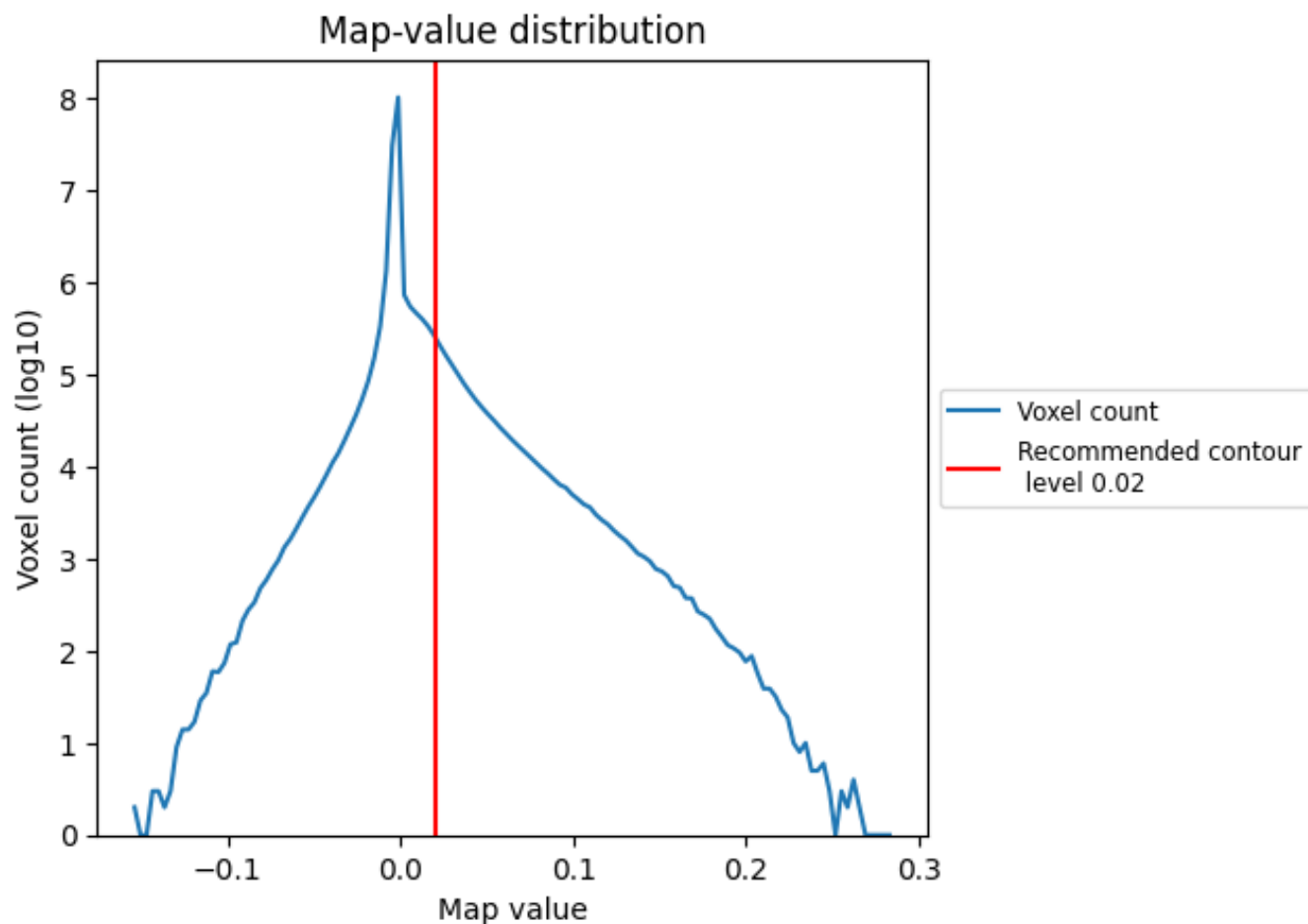
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

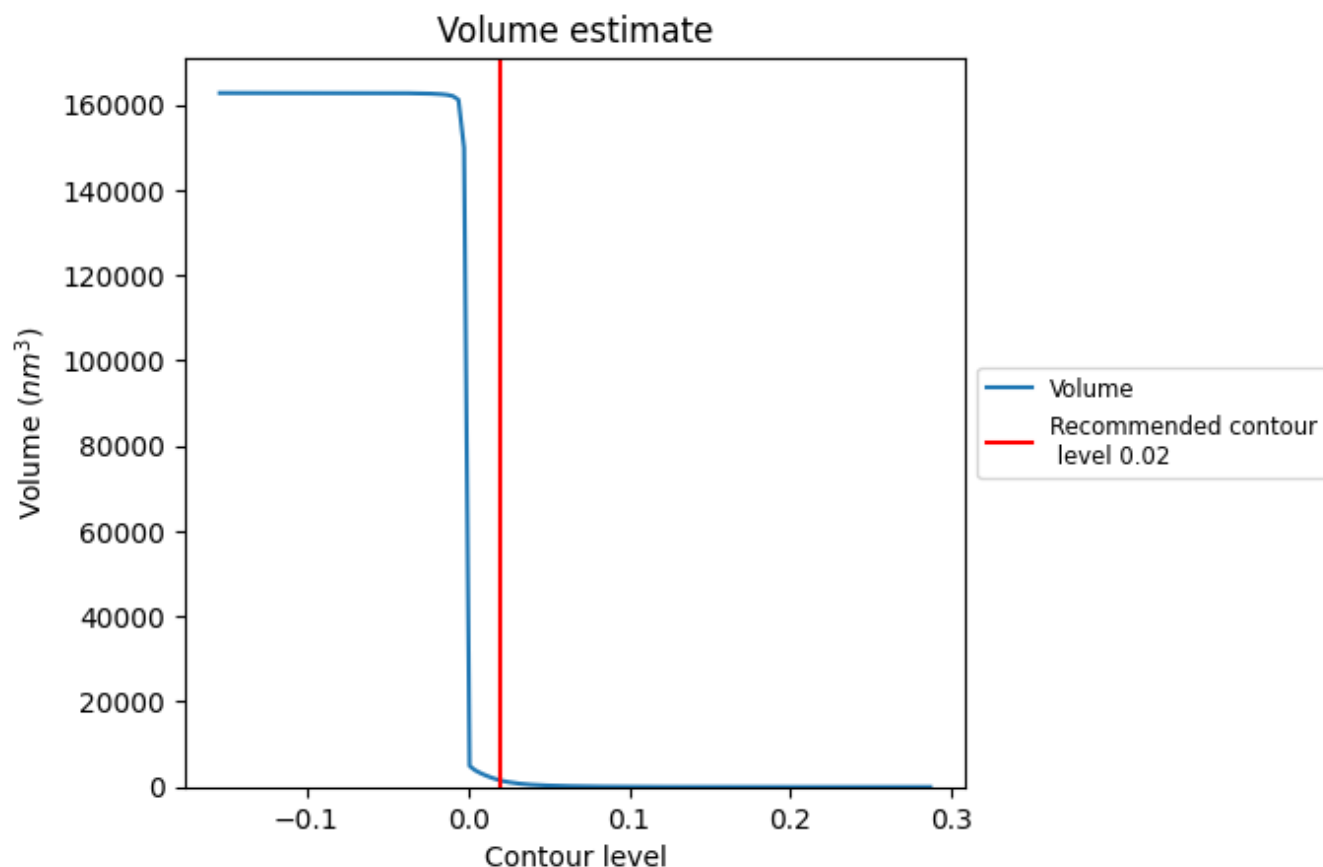
This section contains the results of statistical analysis of the map.

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.

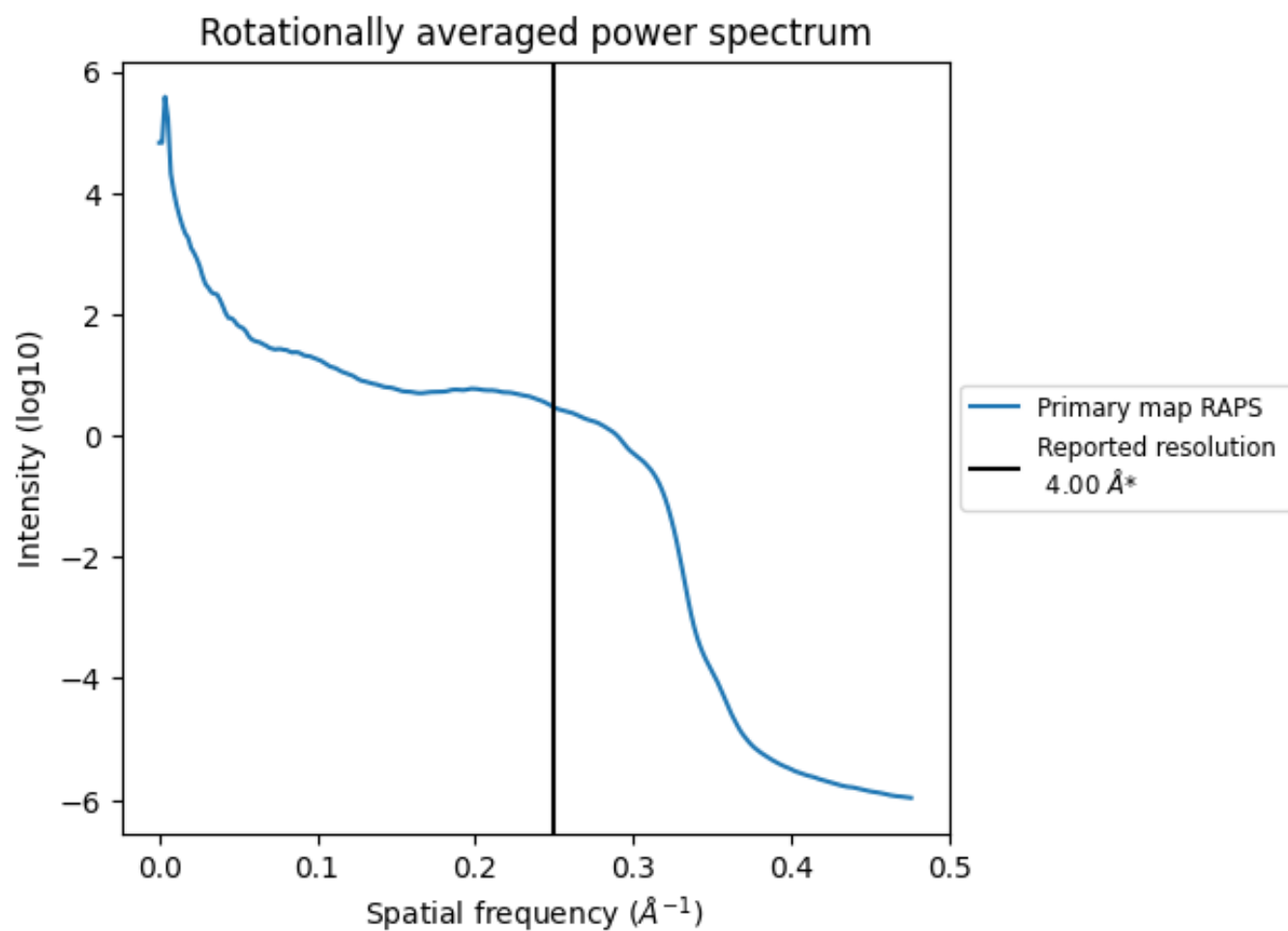
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1563 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

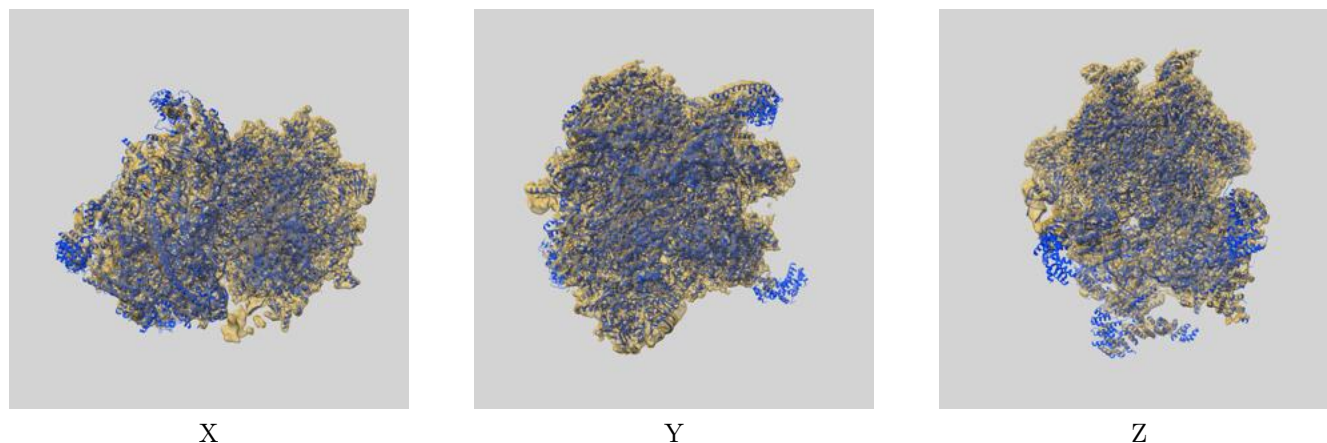
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

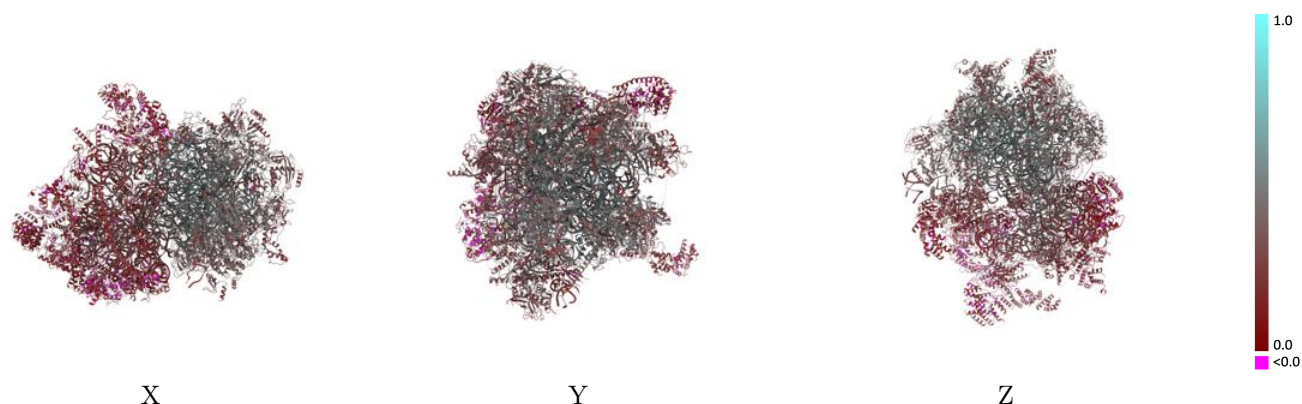
This section contains information regarding the fit between EMDB map EMD-11390 and PDB model 6ZS9. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



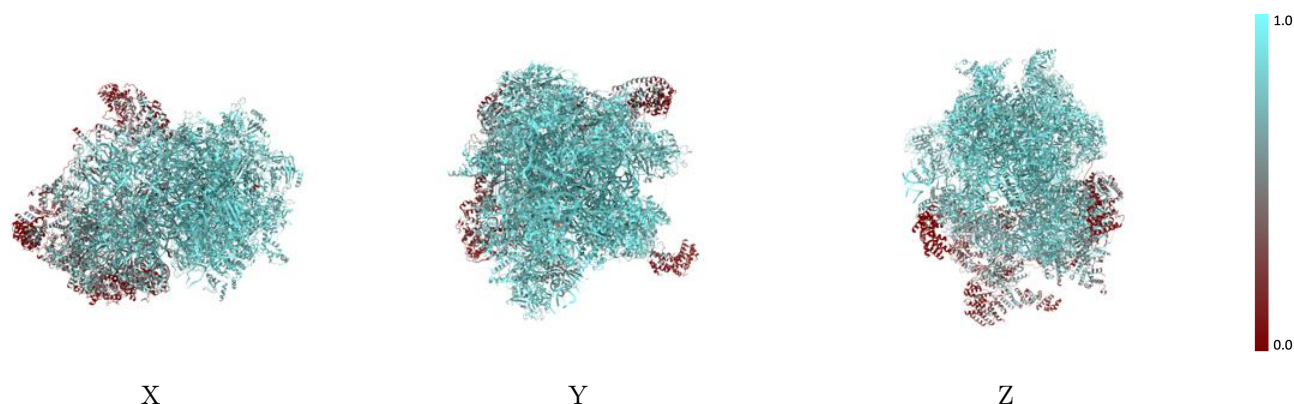
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



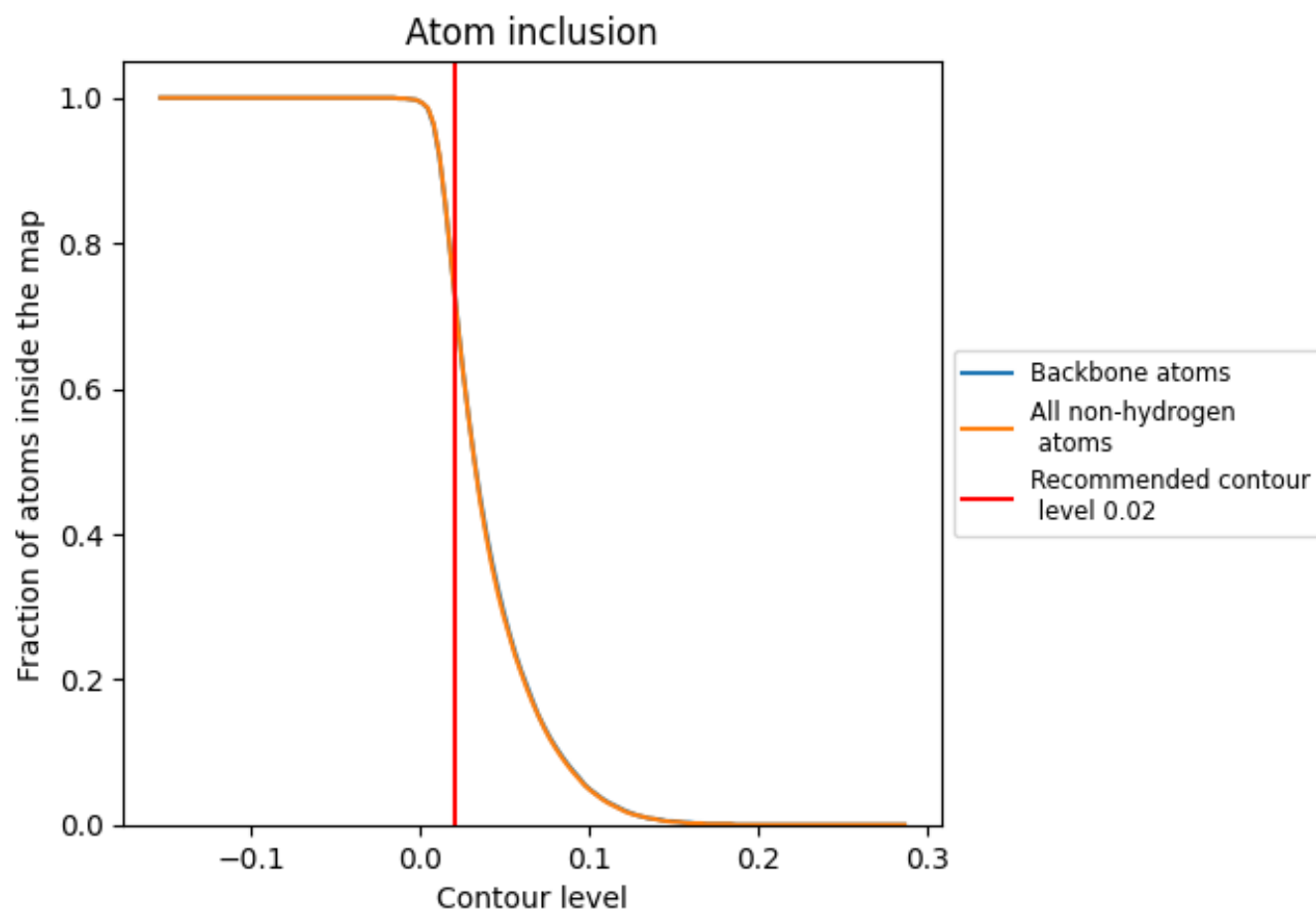
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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