Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 06:24 am GMT

PDB ID	:	7OG4
EMDB ID	:	EMD-12877
Title	:	Human mitochondrial ribosome in complex with P/E-tRNA
Authors	:	Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.
Deposited on	:	2021-05-06
Resolution	:	3.80 Å(reported)

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

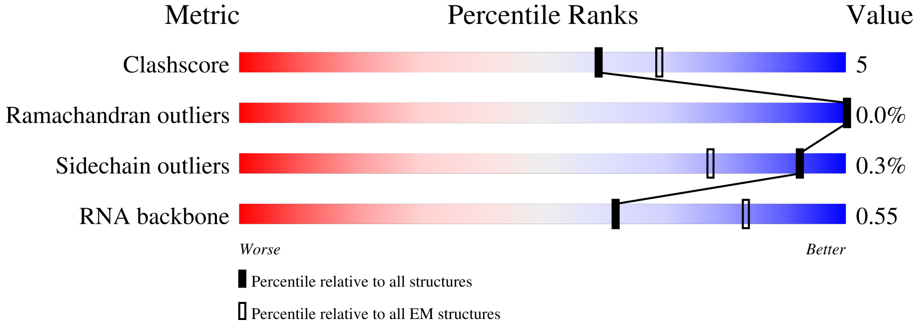
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

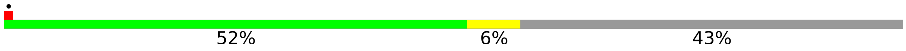
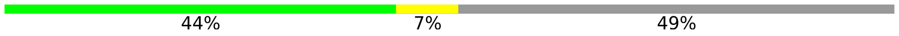
The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	0	188	
2	1	65	
3	2	92	
4	3	188	
5	4	103	
6	5	423	
7	6	380	

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Mol	Chain	Length	Quality of chain
8	7	338	75% 11% 14%
9	8	206	9% 59% 5% 35%
10	9	137	• 80% 11% 9%
11	XA	1561	64% 28% • •
12	A0	218	44% 82% 11% 8%
13	A1	323	34% 74% 11% 15%
14	A2	118	19% 82% 16% •
15	A3	199	• 28% 7% 65%
16	A4	689	56% 70% 10% 20%
17	AA	954	• 65% 26% 5% •
18	AB	296	6% 67% 7% 26%
19	AC	167	21% 72% 7% 21%
20	AD	430	20% 71% 9% 20%
21	AE	125	18% 82% 16% •
22	AF	242	18% 72% 11% 17%
23	AG	396	20% 67% 10% 23%
24	AH	201	29% 57% 10% 33%
25	AI	194	13% 61% 9% 30%
26	AJ	138	8% 70% 8% 22%
27	AK	128	34% 70% 9% 21%
28	AL	257	9% 55% 9% 36%
29	AM	137	31% 74% 10% 15%
30	AN	130	15% 71% 12% 18%
31	AO	258	24% 61% 10% 28%
32	AP	142	• 61% 6% 33%

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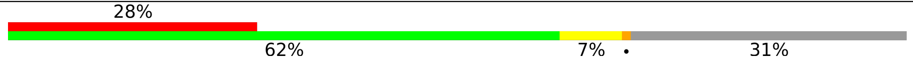
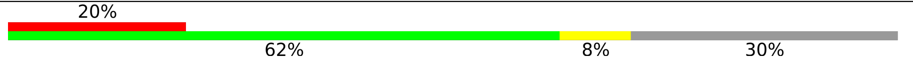
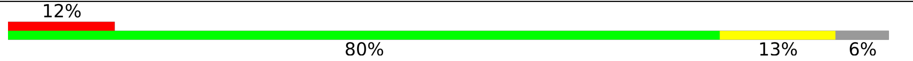
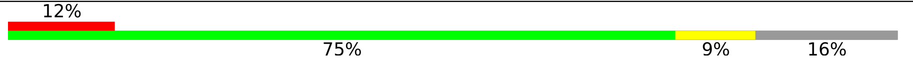
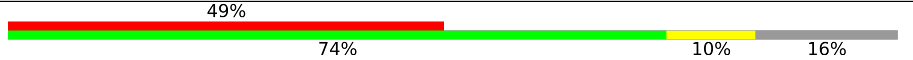
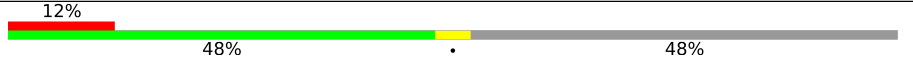
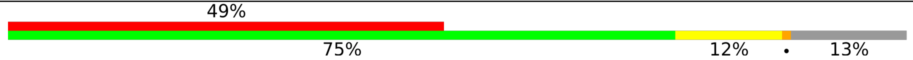
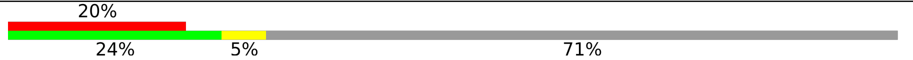
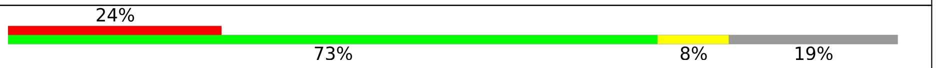
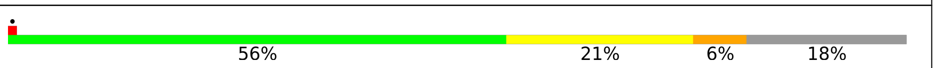
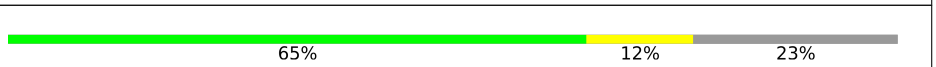
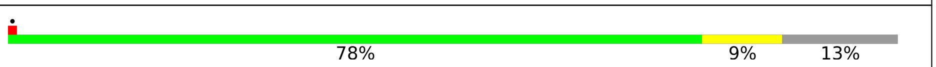
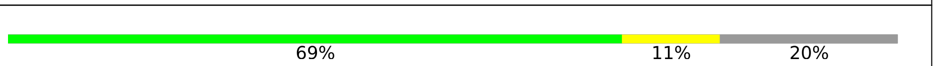
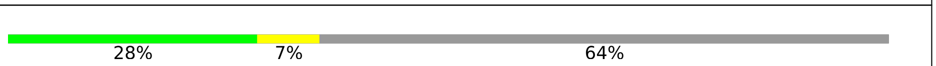
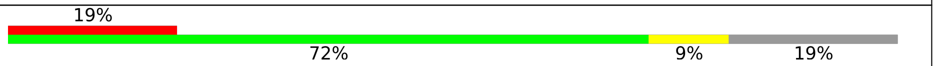
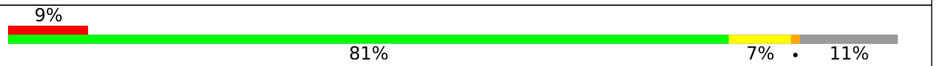
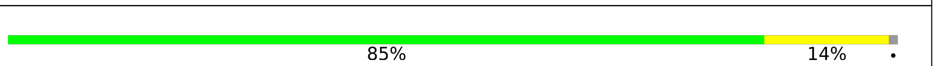
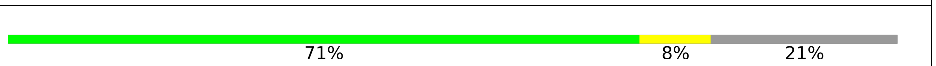
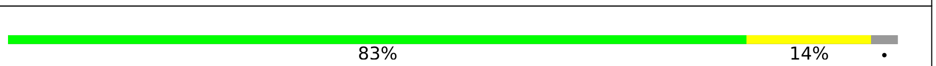
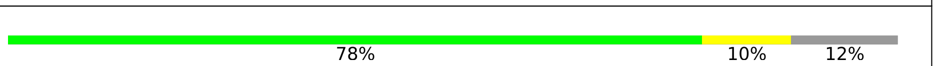
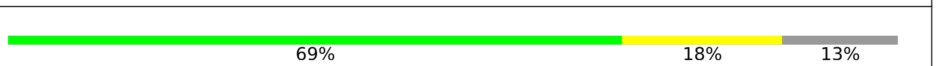
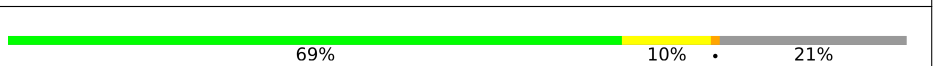
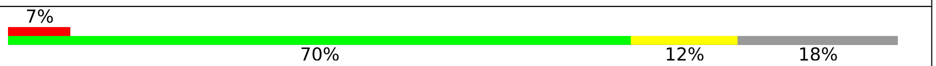
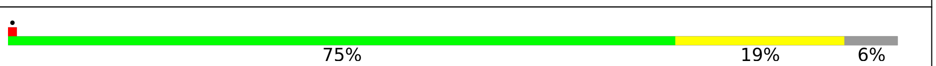
Mol	Chain	Length	Quality of chain
33	AQ	87	
34	AR	360	
35	AS	190	
36	AT	173	
37	AU	205	
38	AV	414	
39	AW	187	
40	AX	398	
41	AY	395	
42	AZ	106	
43	XB	72	
44	XD	305	
45	XE	348	
46	XF	311	
47	XH	267	
48	XI	261	
49	XJ	192	
50	XK	178	
51	XL	145	
52	XM	296	
53	XN	251	
54	XO	175	
55	XP	180	
56	XQ	292	
57	XR	149	

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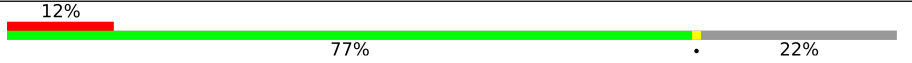
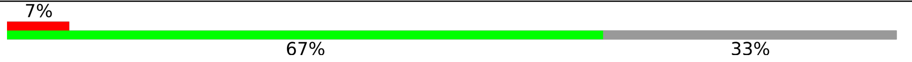
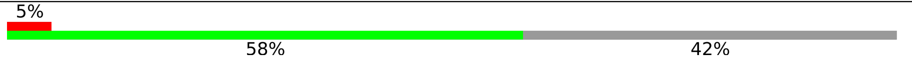
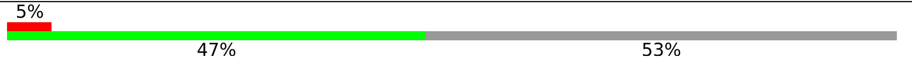
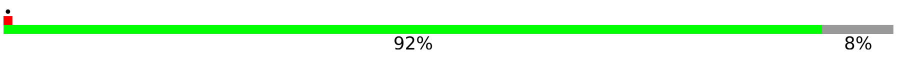
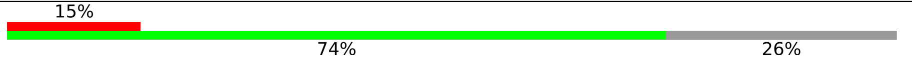
Mol	Chain	Length	Quality of chain
58	XS	205	
59	XT	206	
60	XU	153	
61	XV	216	
62	XW	148	
63	XX	256	
64	XY	250	
65	XZ	161	
66	a	142	
67	b	215	
68	c	332	
69	d	306	
70	e	279	
71	f	212	
72	g	166	
73	h	158	
74	i	128	
75	j	123	
76	k	112	
77	l	138	
78	m	128	
79	o	102	
80	p	206	
81	q	222	
82	r	196	

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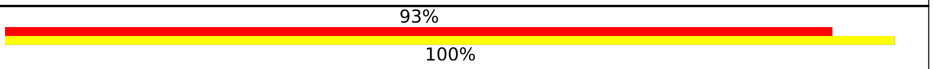
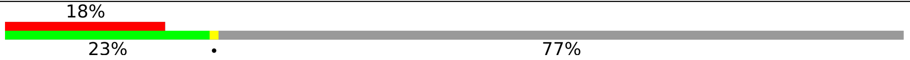
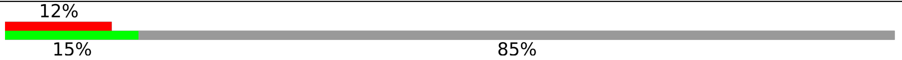
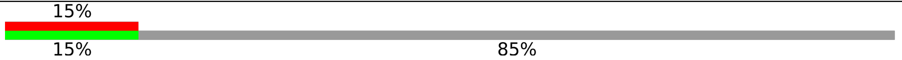
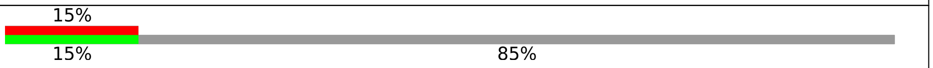
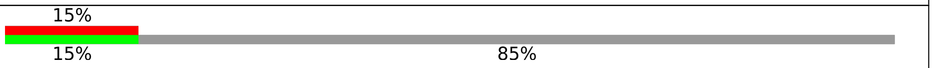
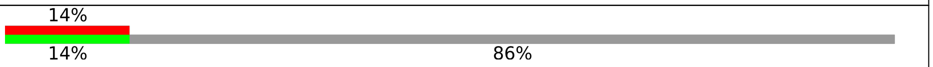
Mol	Chain	Length	Quality of chain
83	r3	75	
84	s	439	
85	t1	198	
85	t2	198	
85	t3	198	
85	t4	198	
85	t5	198	
85	t6	198	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 311905 atoms, of which 143004 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	0	108	1783	545	903	172	157	6	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	5	393	6404	2070	3200	559	564	11	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	8	134	Total 2301	C 724	H 1166	N 201	O 208	S 2	0	0

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	XA	1498	Total 47973	C 14274	H 16160	N 5751	O 10290	P 1498	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	A4	552	8955	2866	4485	756	820	28	0	0

- Molecule 17 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
17	AA	924	29598	8800	9970	3540	6364	924	0	0

- Molecule 18 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 19 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 20 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 21 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 22 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	AF	201	3382	1069	1714	305	283	11	0	0

- Molecule 23 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 24 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 26 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 27 is a protein called 28S ribosomal protein S14, mitochondrial.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	AL	164	2854	883	1472	257	235	7	0	0

- Molecule 29 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 30 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 31 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 32 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 33 is a protein called 28S ribosomal protein S21, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 34 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 35 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 36 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	AT	162	Total	C	H	N	O	S	0	0
			2672	850	1342	231	238	11		

- Molecule 37 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 38 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	AV	349	Total	C	H	N	O	S	0	0
			5730	1841	2863	478	536	12		

- Molecule 39 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 40 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	AX	348	Total	C	H	N	O	S	0	0
			5619	1802	2805	491	510	11		

- Molecule 41 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	AY	113	1867	621	911	157	176	2	0	0

- Molecule 42 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 43 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
43	XB	59	1895	563	640	227	406	59	0	0

- Molecule 44 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 46 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 48 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 50 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 52 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 53 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 54 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 55 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 56 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 57 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 58 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 59 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 60 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 61 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 62 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 63 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 64 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 65 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 66 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 67 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 68 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 69 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
69	d	216	3501	1125	1743	305	315	13	0	0

- Molecule 70 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 71 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 72 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 73 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
73	h	108	1748	560	866	154	165	3	0	0

- Molecule 74 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 75 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 76 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 77 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 78 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 79 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 80 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 81 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 82 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 83 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
83	r3	75	1468	714	228	451	75	0	0

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

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

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

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

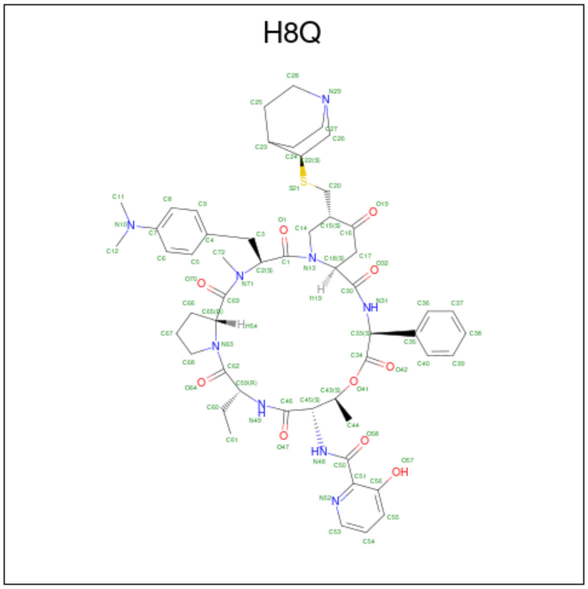
- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
86	0	1	1	1	0
86	4	1	1	1	0
86	AB	1	1	1	0
86	AO	1	1	1	0
86	AP	1	1	1	0
86	AT	1	1	1	0
86	r	1	1	1	0

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

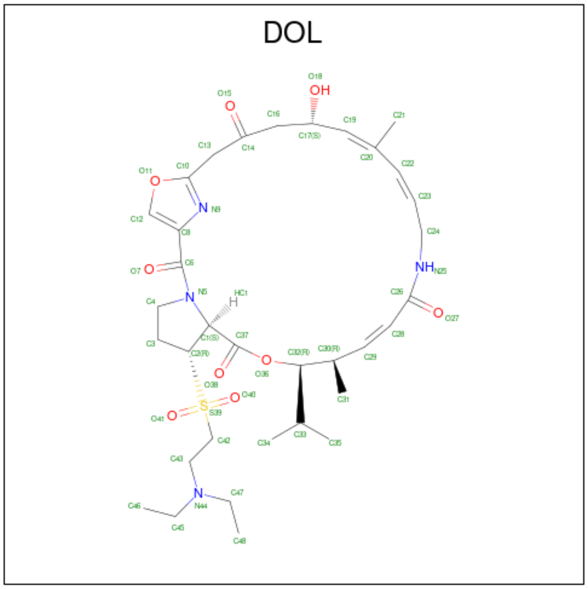
Mol	Chain	Residues	Atoms	AltConf
87	9	1	Total Mg 1 1	0
87	XA	143	Total Mg 143 143	0
87	AA	46	Total Mg 46 46	0
87	XD	1	Total Mg 1 1	0
87	XI	1	Total Mg 1 1	0
87	XM	1	Total Mg 1 1	0
87	XW	1	Total Mg 1 1	0
87	g	1	Total Mg 1 1	0

- Molecule 88 is {N}-[(3 {S},6 {R},12 {R},15 {S},16 {S},19 {S},22 {S},25 {S})-25-[[(3 {S})-1-azabicyclo[2.2.2]octan-3-yl]sulfanylmethyl]-3-[[4-(dimethylamino)phenyl]methyl]-12-ethyl-4,16-dimethyl-2,5,11,14,18,21,24-heptakis(oxidanylidene)-19-phenyl-17-oxa-1,4,10,13,20-pentazatricyclo[20.4.0.0^{6,10}]hexacosan-15-yl]-3-oxidanyl-pyridine-2-carboxamide (three-letter code: H8Q) (formula: $C_{53}H_{67}N_9O_{10}S$).



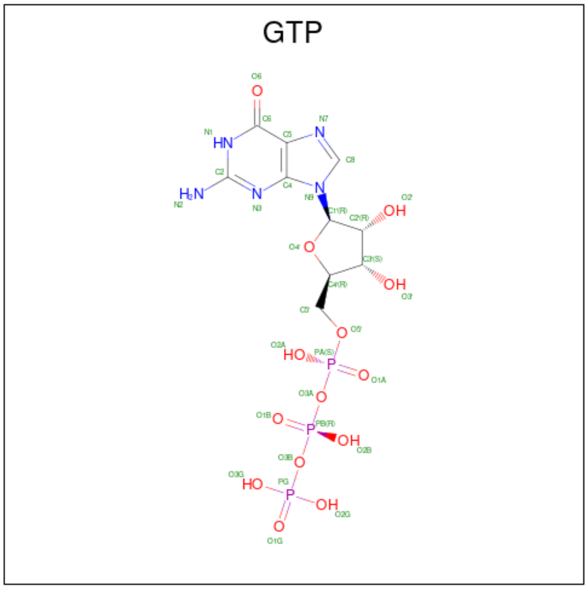
Mol	Chain	Residues	Atoms	AltConf
88	XA	1	Total C H N O S 140 53 67 9 10 1	0

- Molecule 89 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: $C_{34}H_{50}N_4O_9S$).



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

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

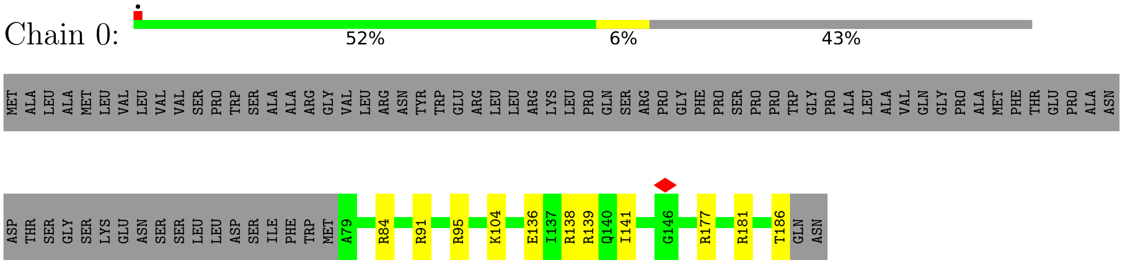


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
90	AX	1	42	10	10	5	14	3	0

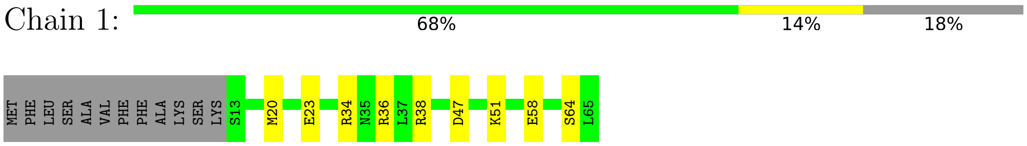
3 Residue-property plots

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

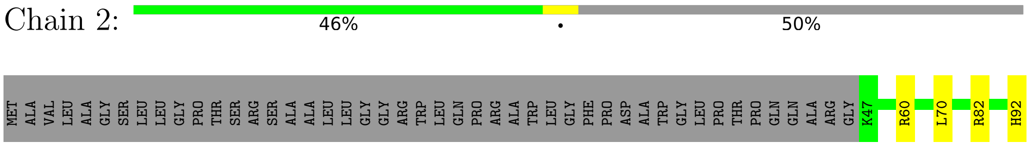
- Molecule 1: 39S ribosomal protein L32, mitochondrial



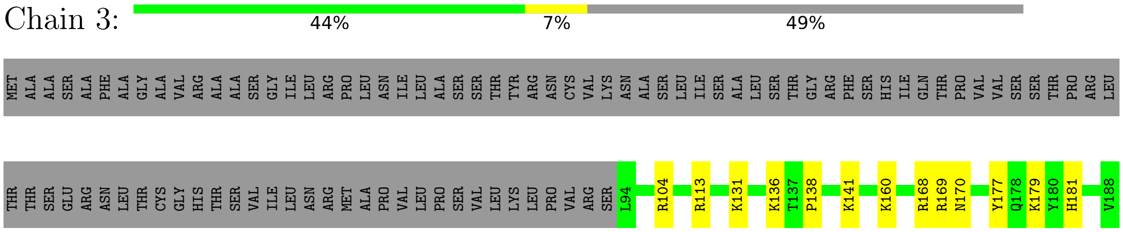
- Molecule 2: 39S ribosomal protein L33, mitochondrial



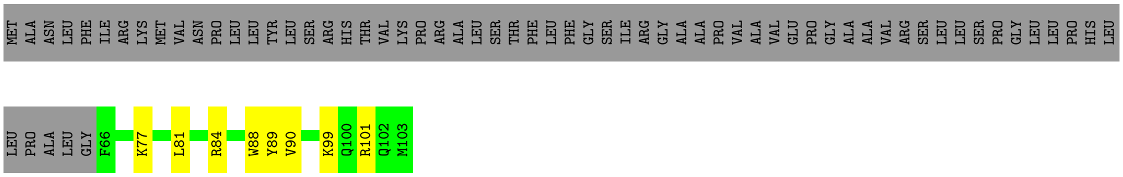
- Molecule 3: 39S ribosomal protein L34, mitochondrial



- Molecule 4: 39S ribosomal protein L35, mitochondrial

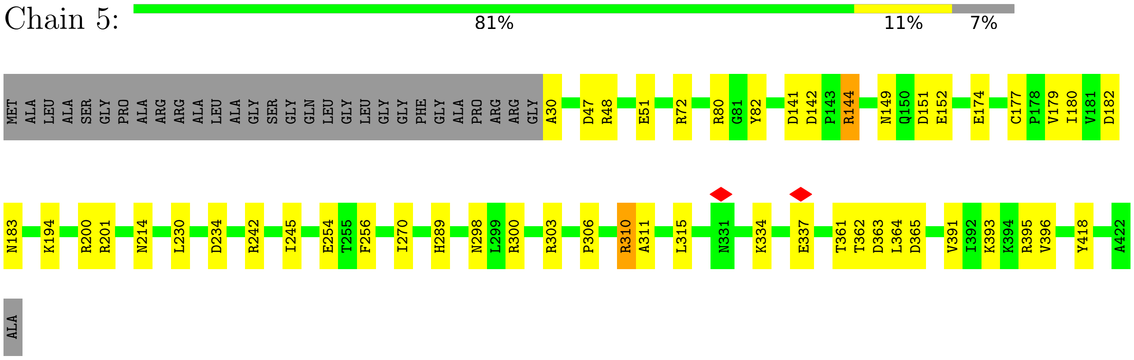


- Molecule 5: 39S ribosomal protein L36, mitochondrial



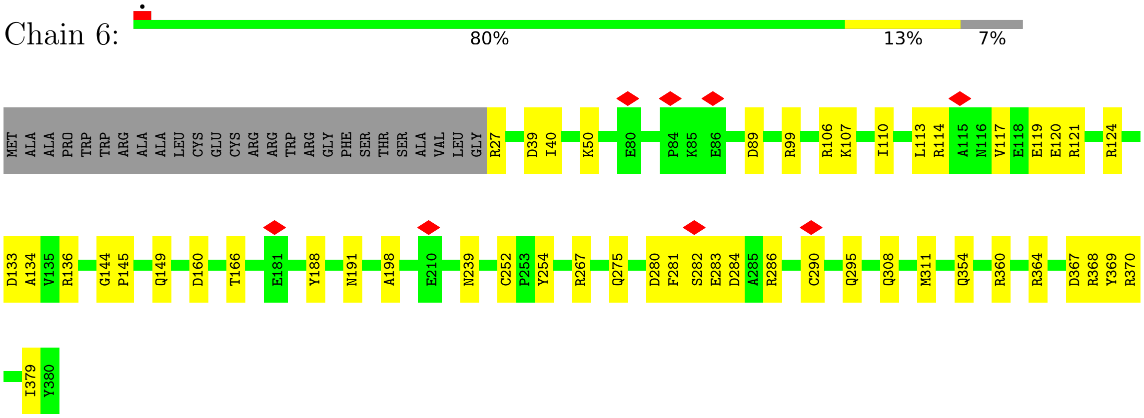
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:



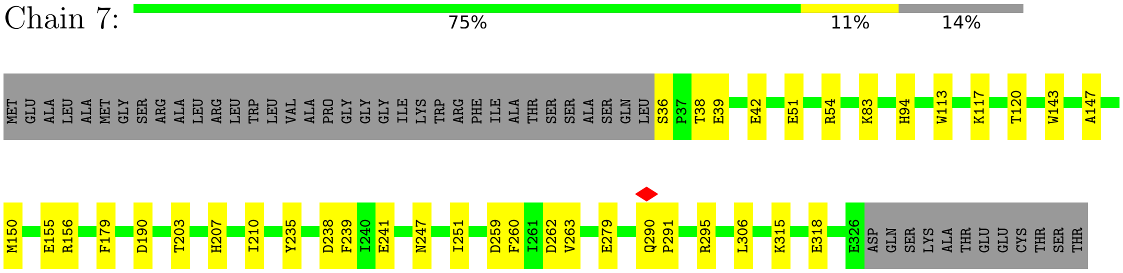
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:



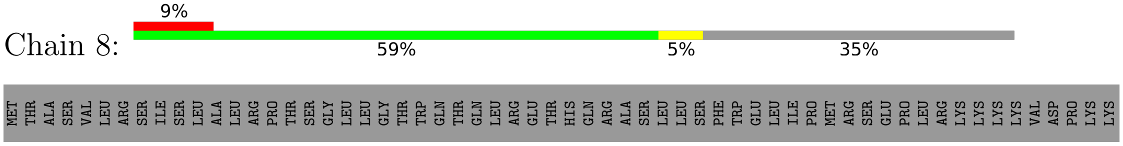
- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:



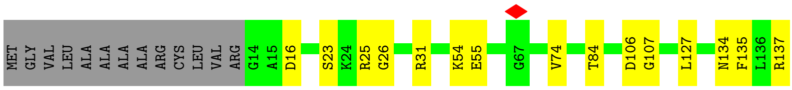
- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:



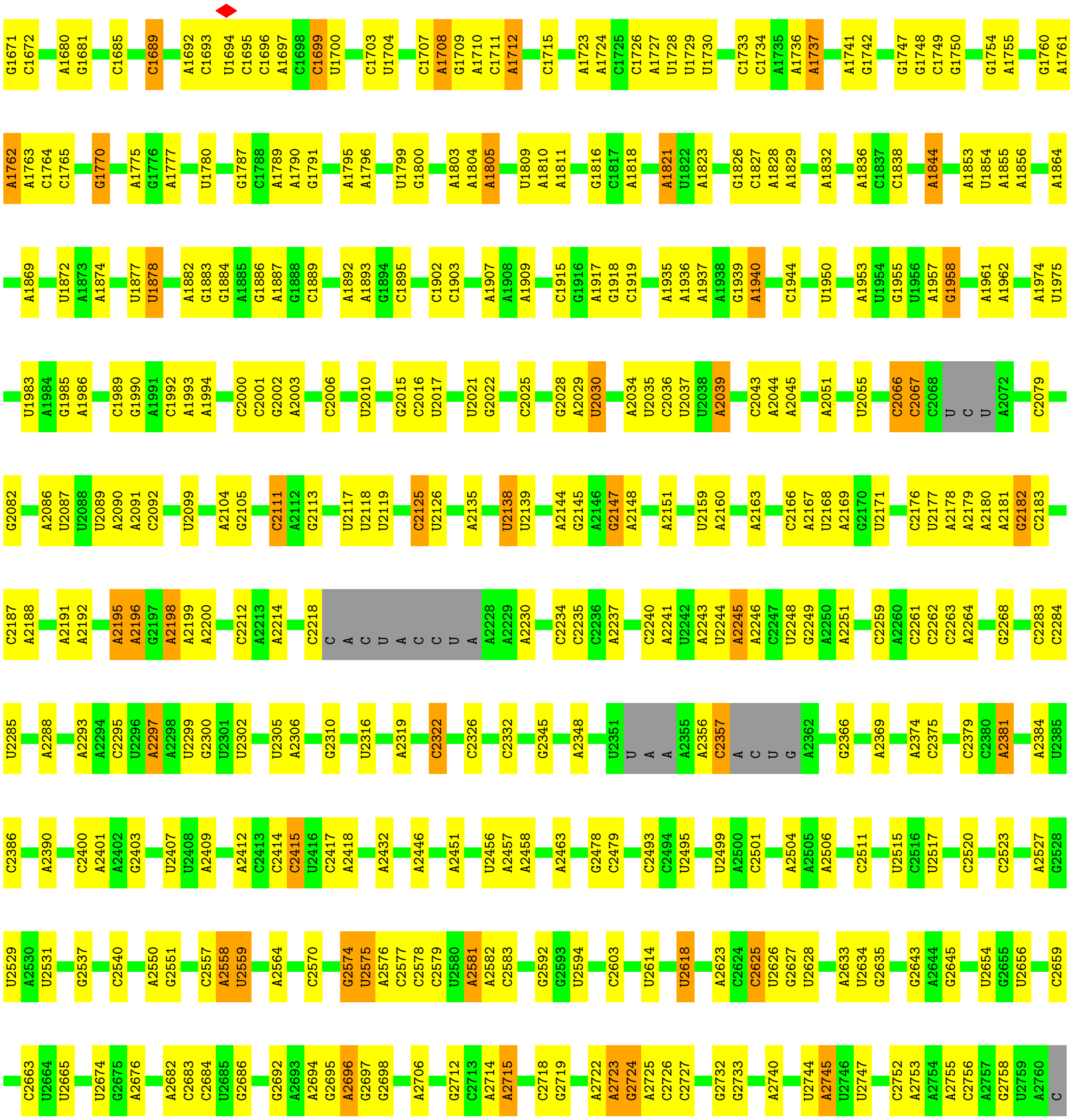
- Molecule 10: 39S ribosomal protein L41, mitochondrial

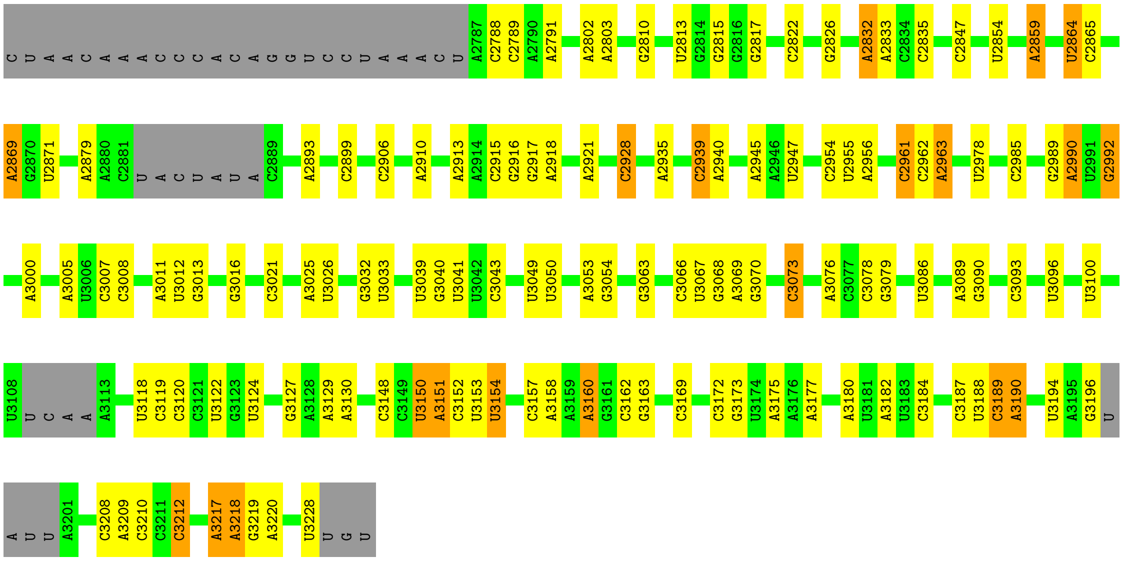
Chain 9:



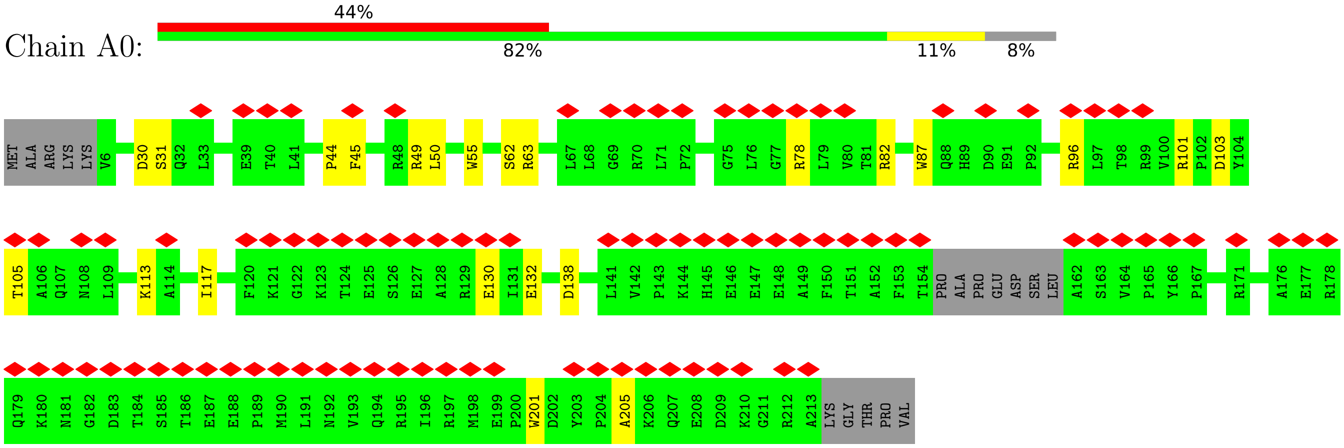
- Molecule 11: 16S mitochondrial rRNA

Chain XA:

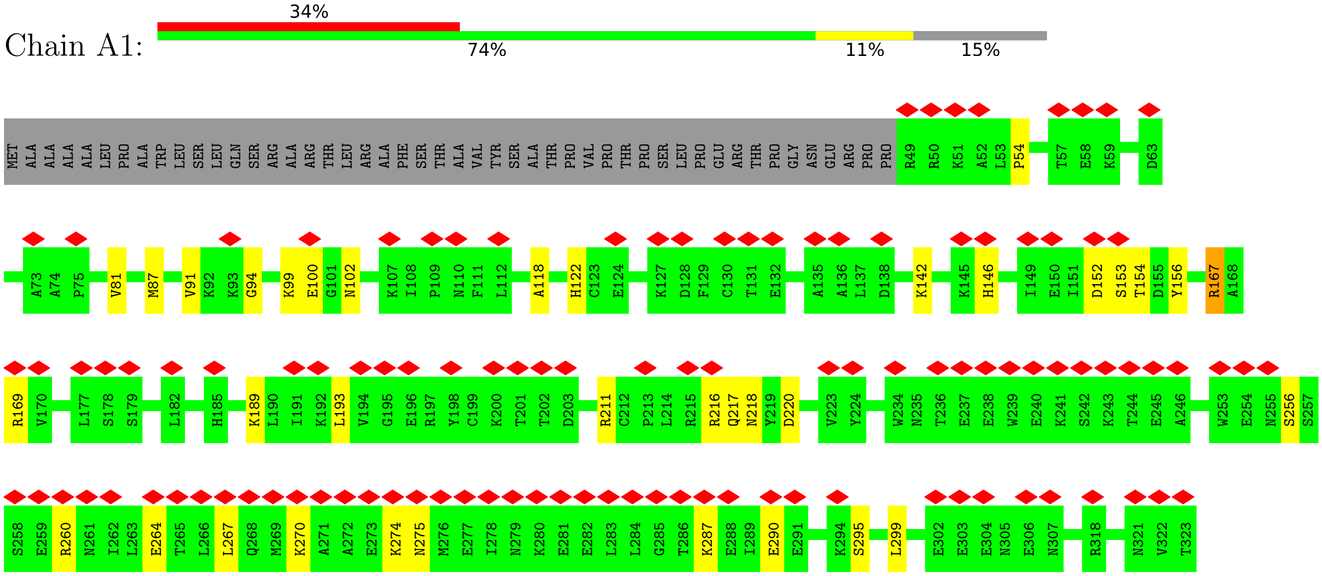




- Molecule 12: 28S ribosomal protein S34, mitochondrial

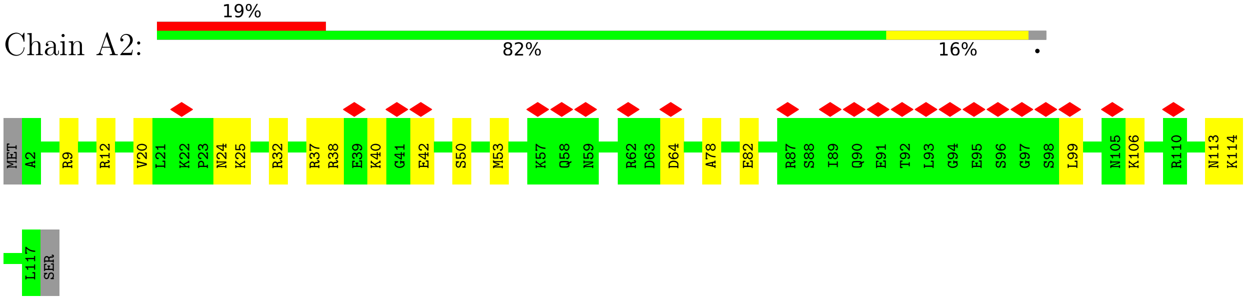


- Molecule 13: 28S ribosomal protein S35, mitochondrial



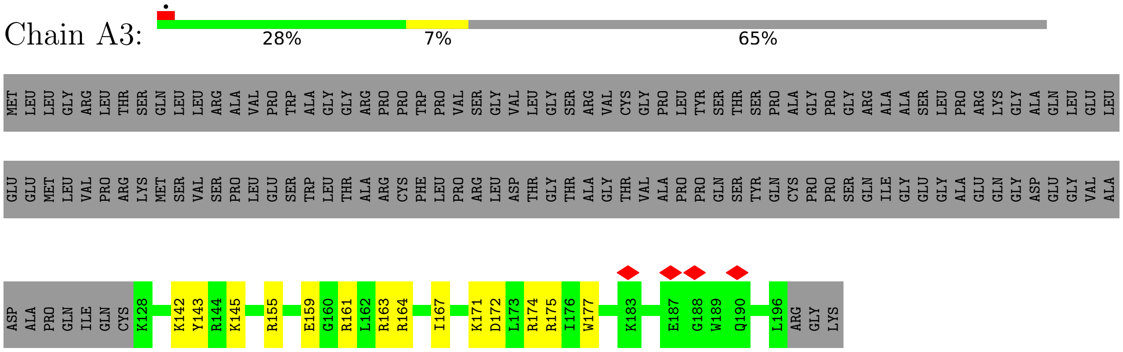
- Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2:



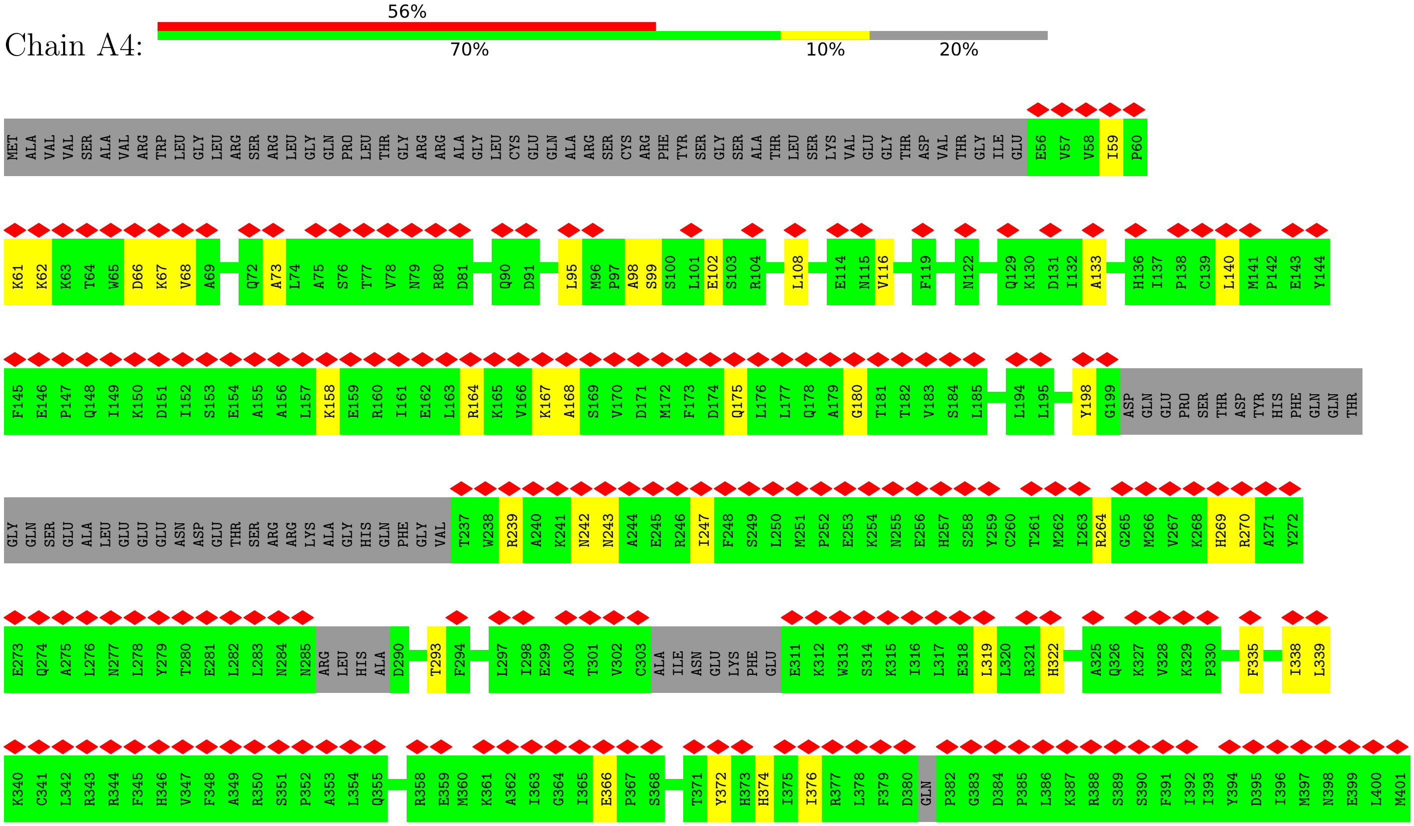
- Molecule 15: Aurora kinase A-interacting protein

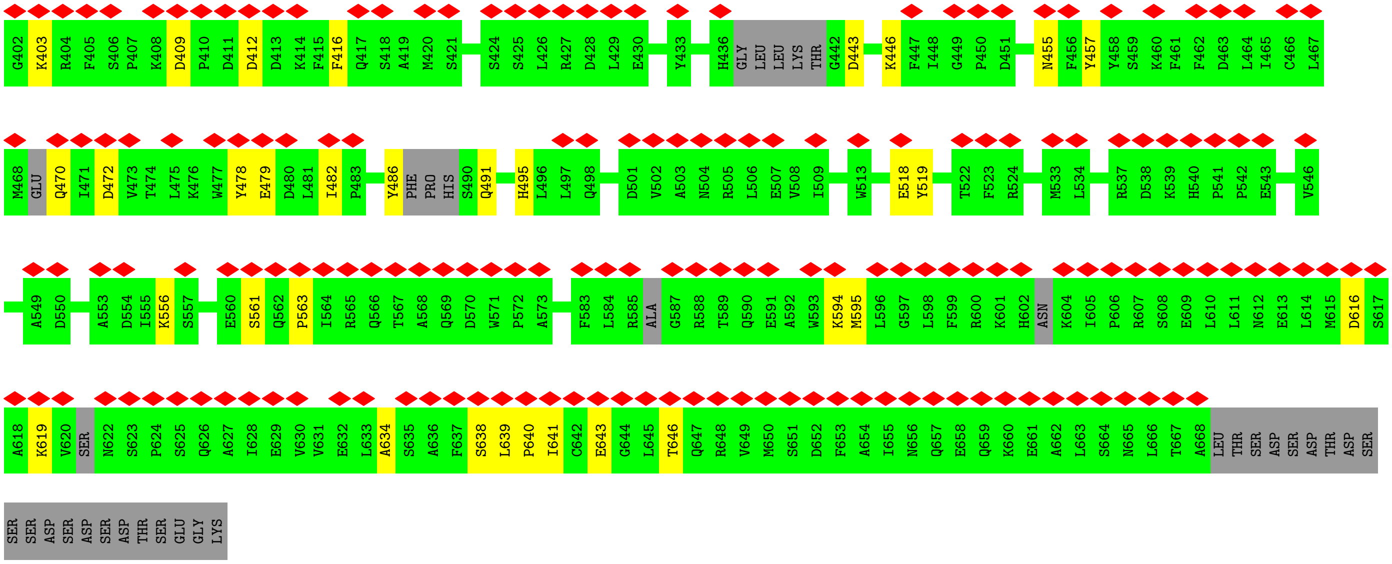
Chain A3:



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

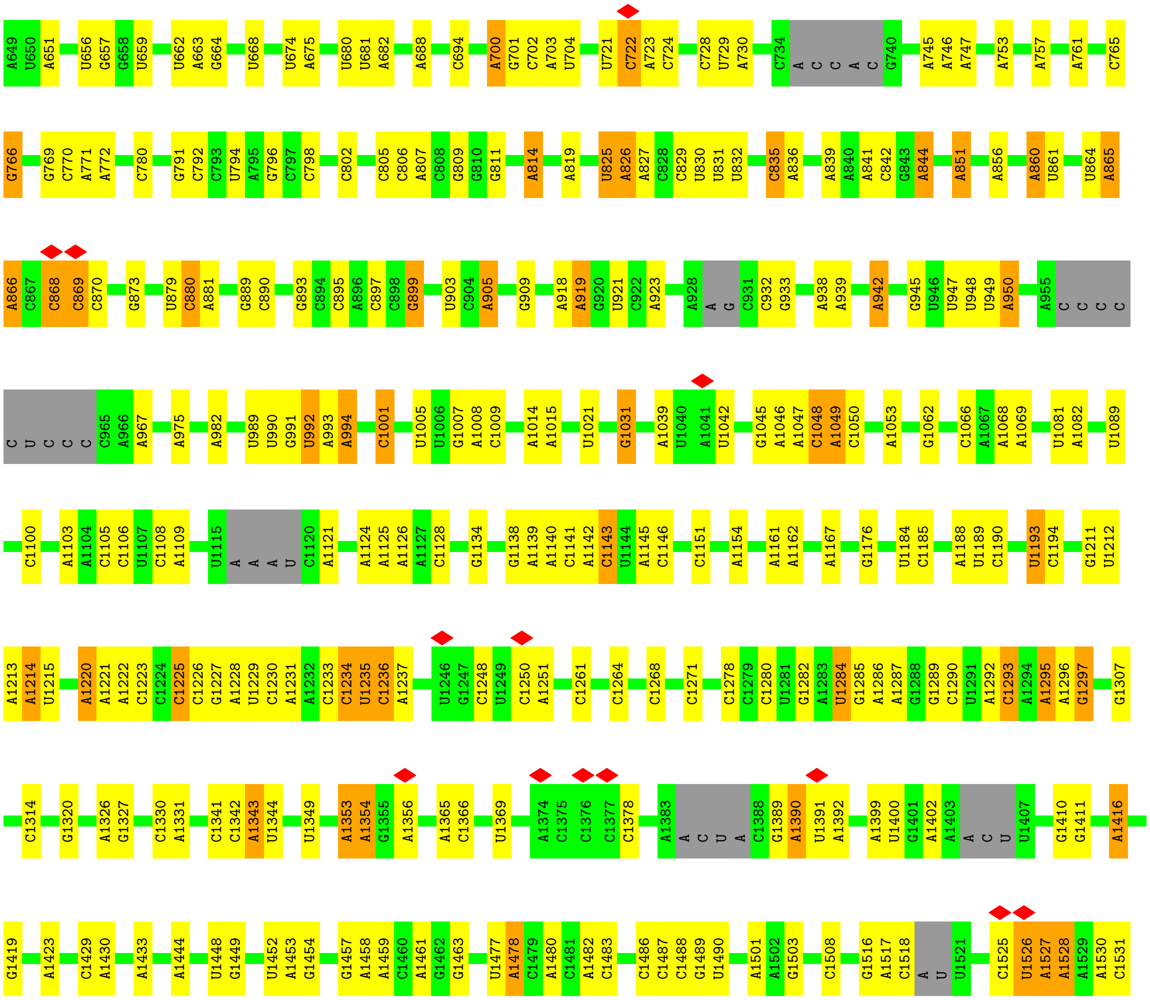
Chain A4:

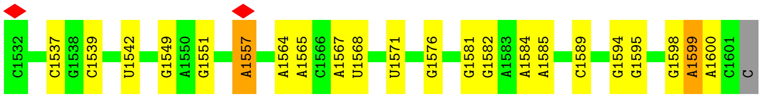




- Molecule 17: 12S mitochondrial rRNA

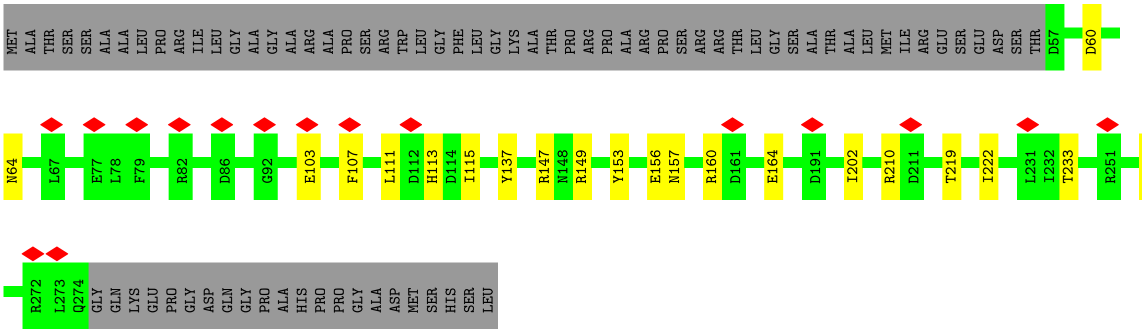
Chain AA:





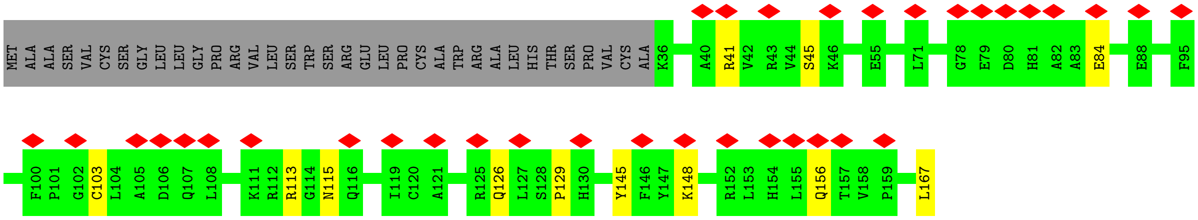
- Molecule 18: 28S ribosomal protein S2, mitochondrial

Chain AB:



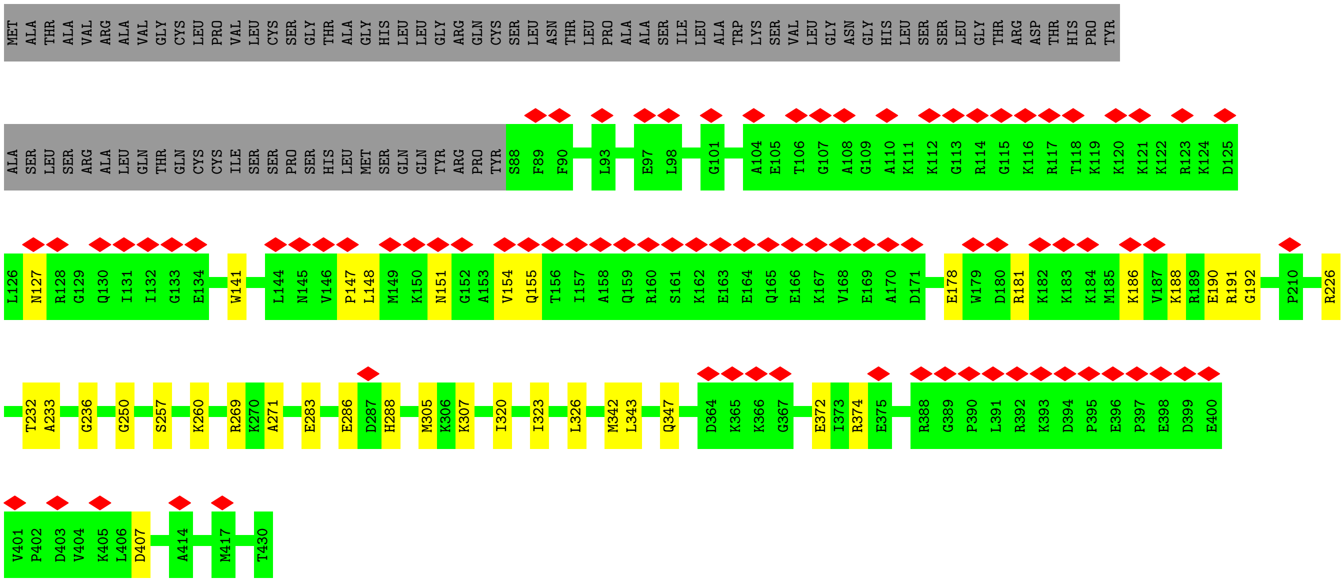
- Molecule 19: 28S ribosomal protein S24, mitochondrial

Chain AC:



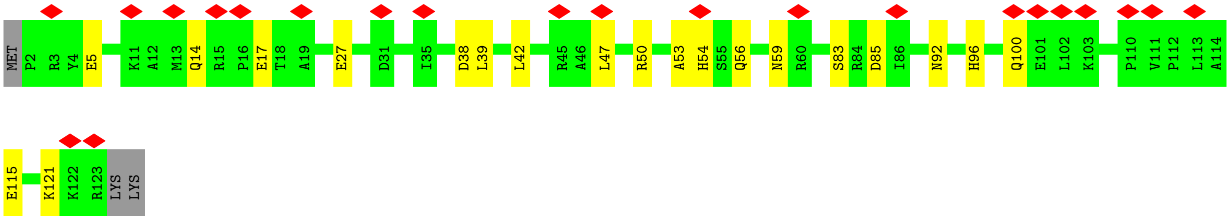
- Molecule 20: 28S ribosomal protein S5, mitochondrial

Chain AD:



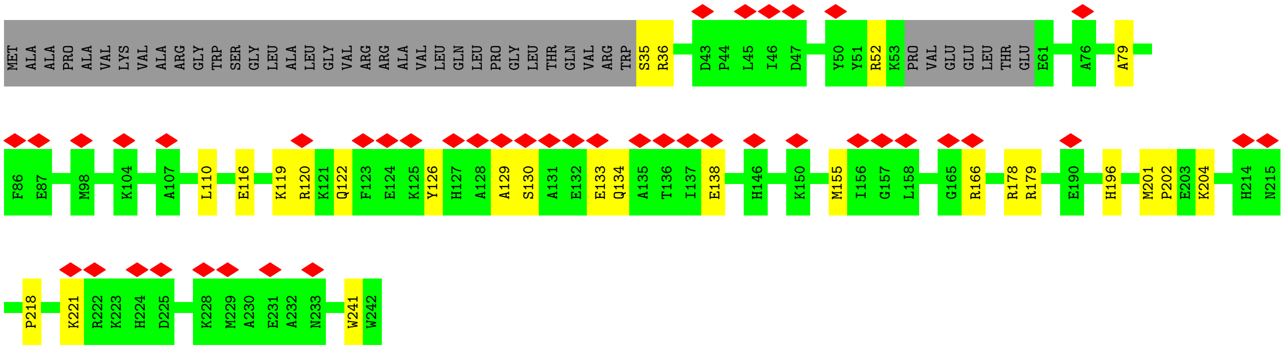
- Molecule 21: 28S ribosomal protein S6, mitochondrial

Chain AE:



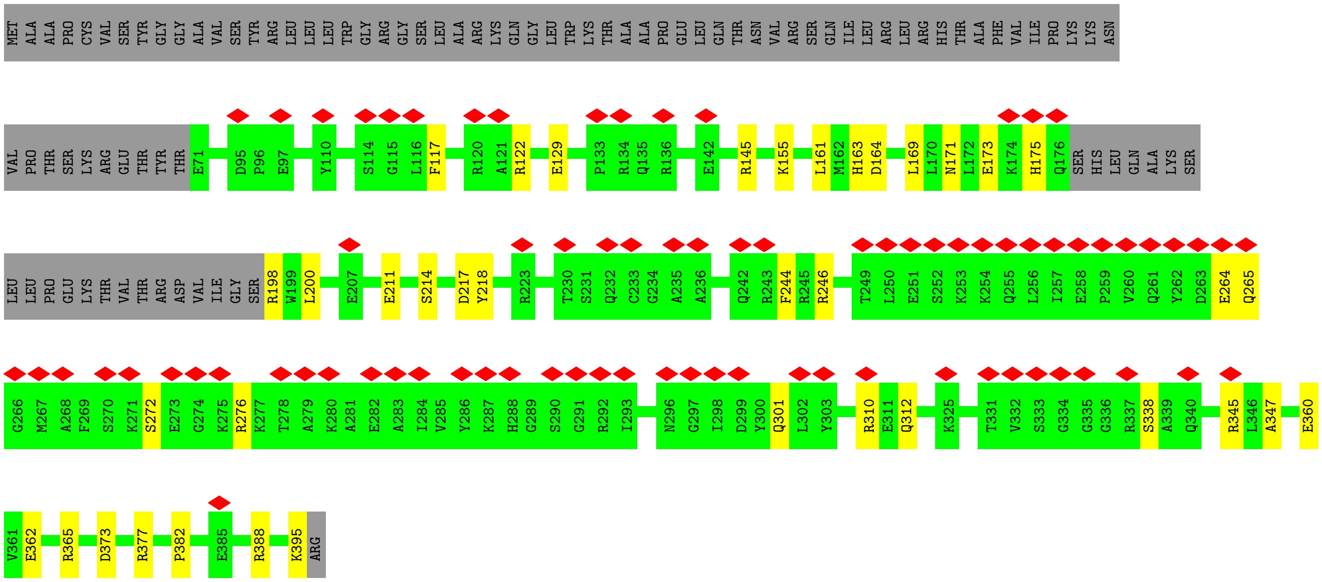
- Molecule 22: 28S ribosomal protein S7, mitochondrial

Chain AF:



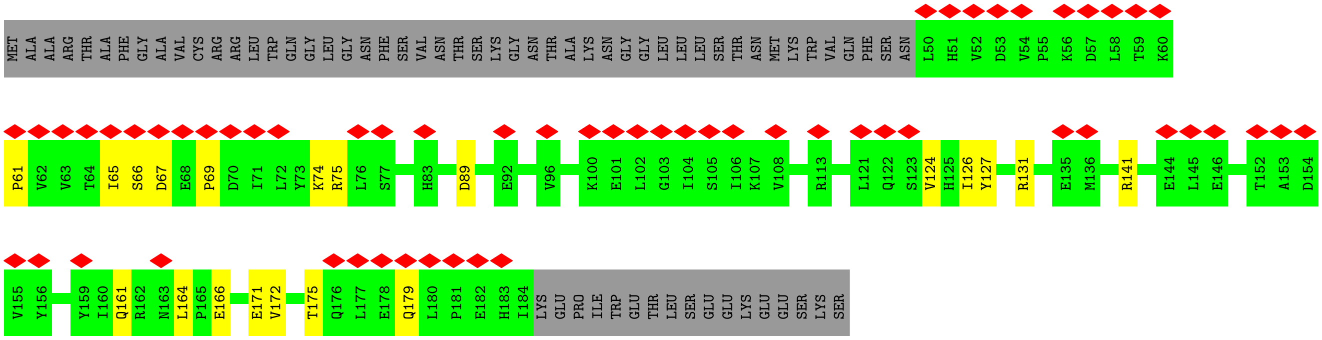
- Molecule 23: 28S ribosomal protein S9, mitochondrial

Chain AG:



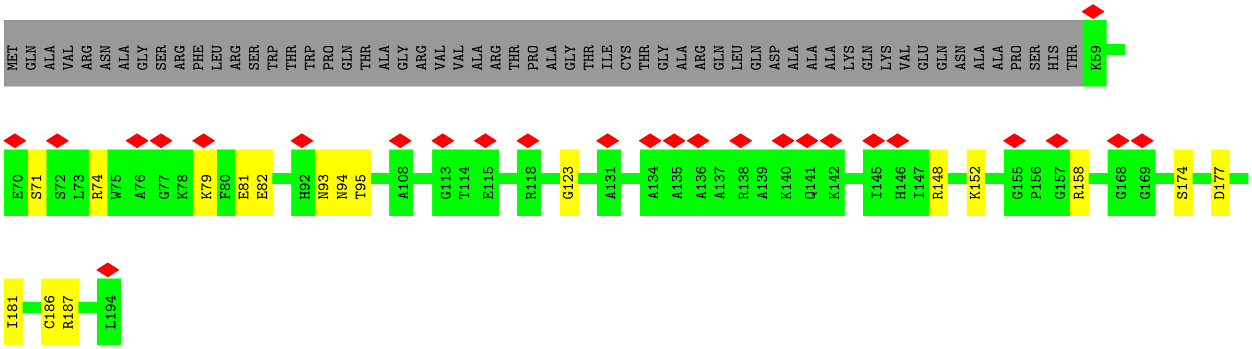
- Molecule 24: 28S ribosomal protein S10, mitochondrial

Chain AH:



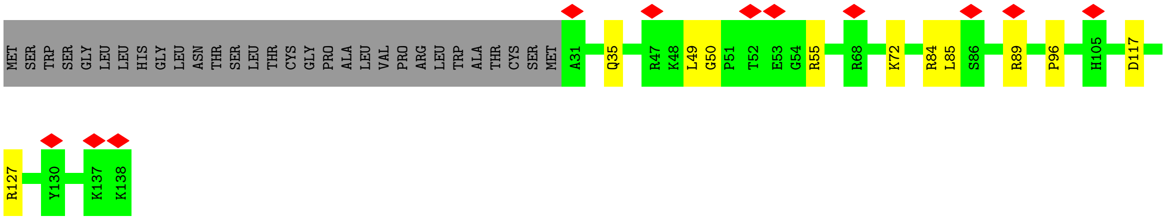
- Molecule 25: 28S ribosomal protein S11, mitochondrial

Chain AI:



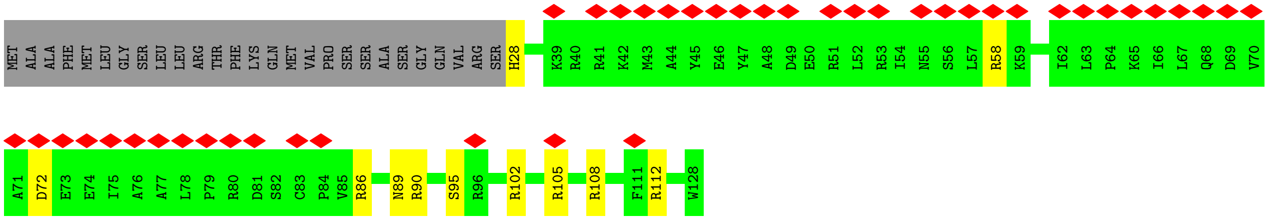
- Molecule 26: 28S ribosomal protein S12, mitochondrial

Chain AJ:

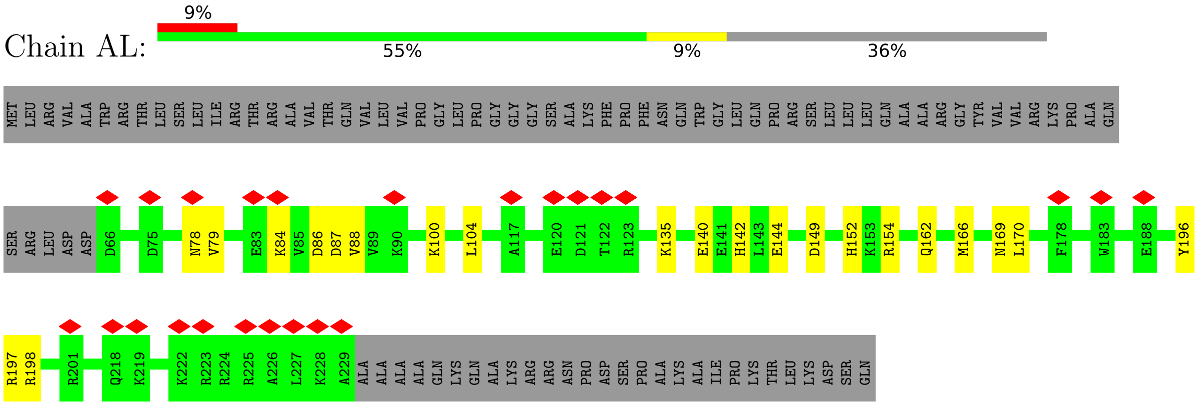


- Molecule 27: 28S ribosomal protein S14, mitochondrial

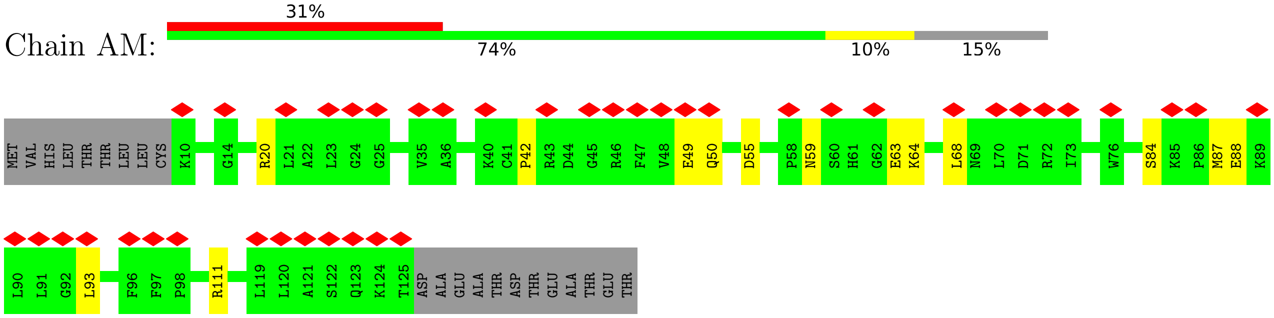
Chain AK:



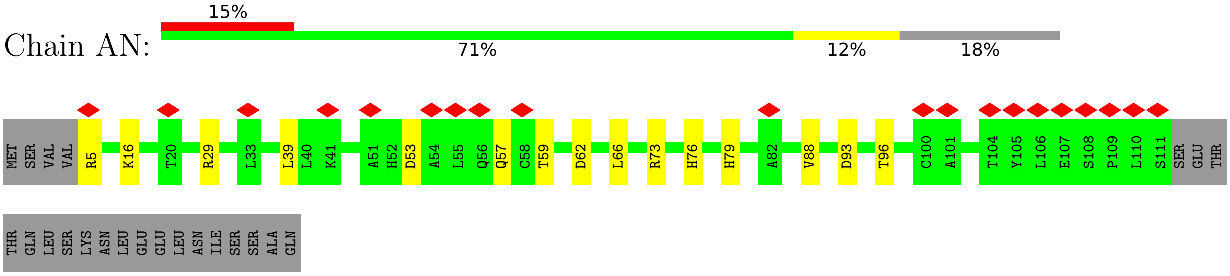
- Molecule 28: 28S ribosomal protein S15, mitochondrial



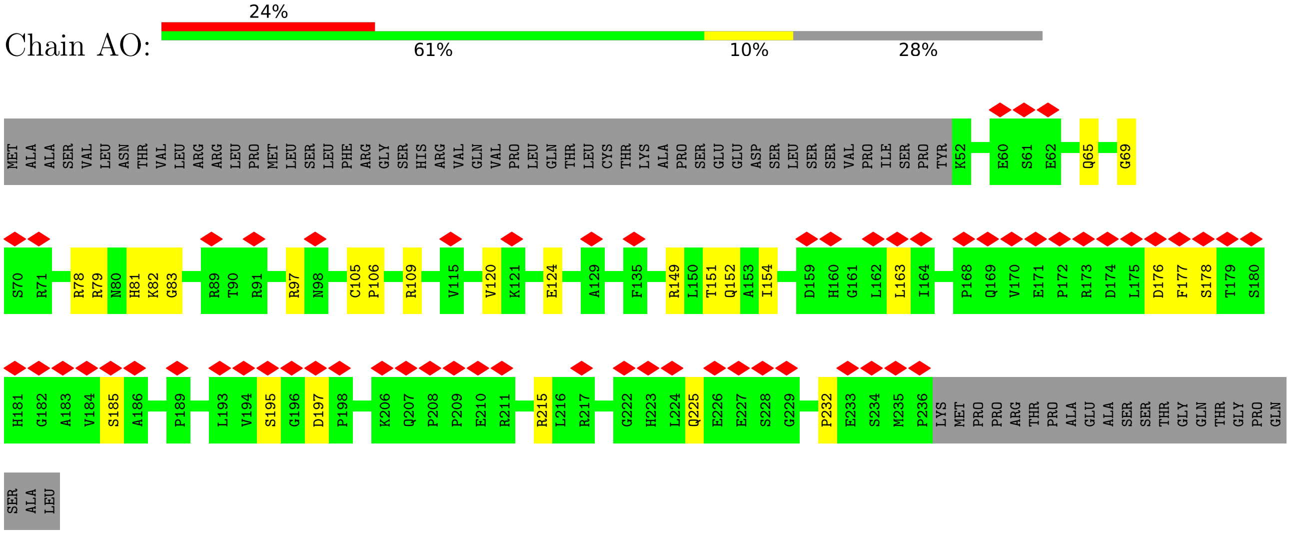
- Molecule 29: 28S ribosomal protein S16, mitochondrial



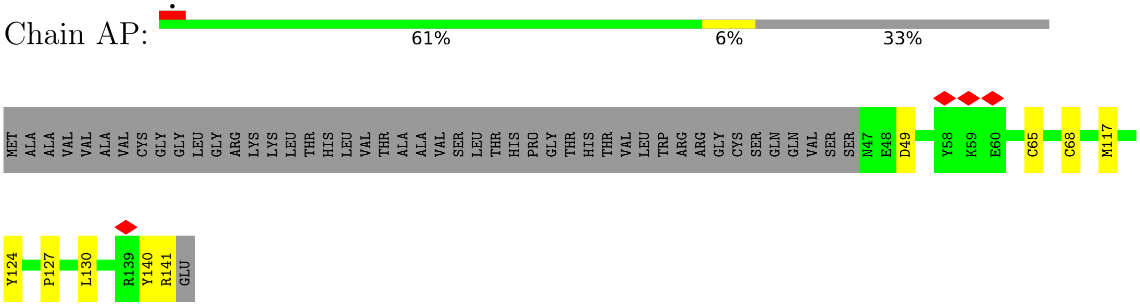
- Molecule 30: 28S ribosomal protein S17, mitochondrial



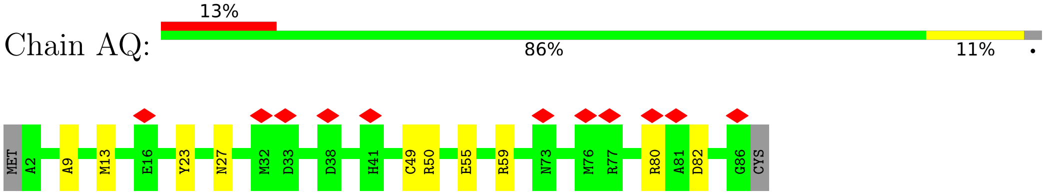
- Molecule 31: 28S ribosomal protein S18b, mitochondrial



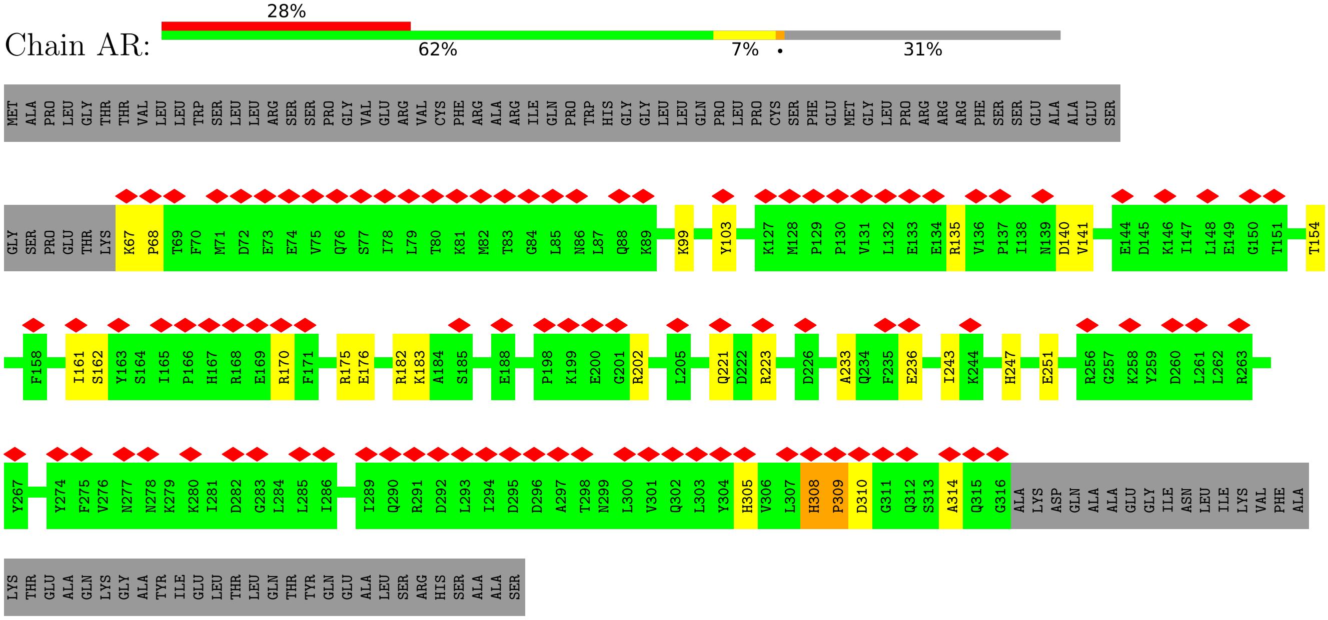
- Molecule 32: 28S ribosomal protein S18c, mitochondrial



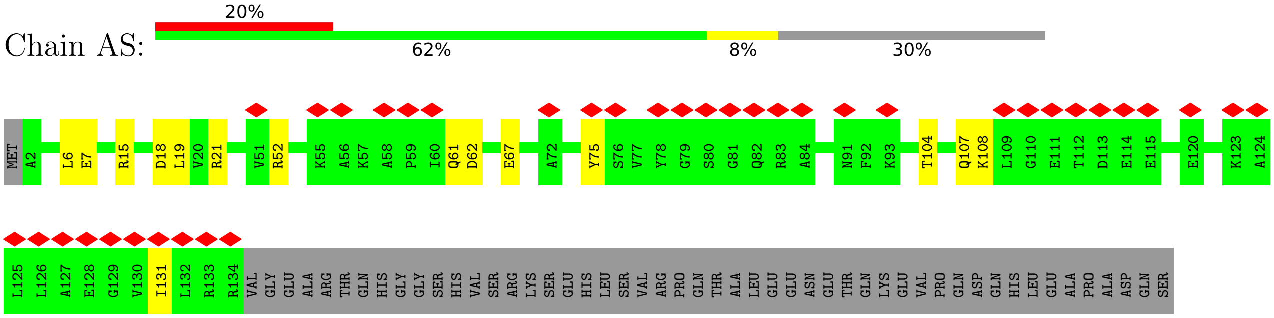
- Molecule 33: 28S ribosomal protein S21, mitochondrial



- Molecule 34: 28S ribosomal protein S22, mitochondrial

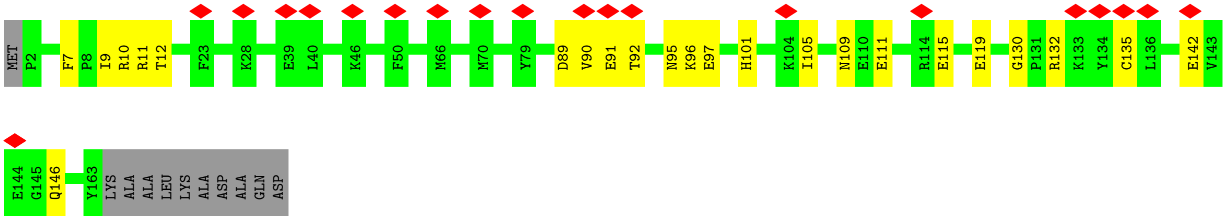


- Molecule 35: 28S ribosomal protein S23, mitochondrial



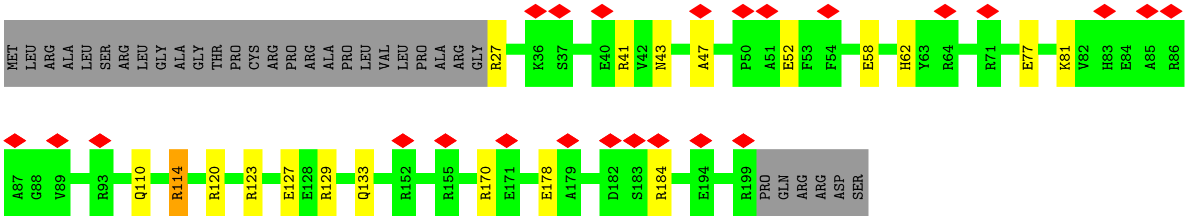
- Molecule 36: 28S ribosomal protein S25, mitochondrial

Chain AT:



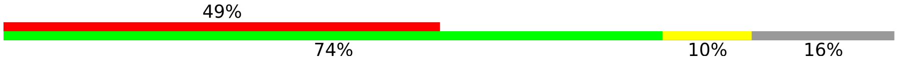
- Molecule 37: 28S ribosomal protein S26, mitochondrial

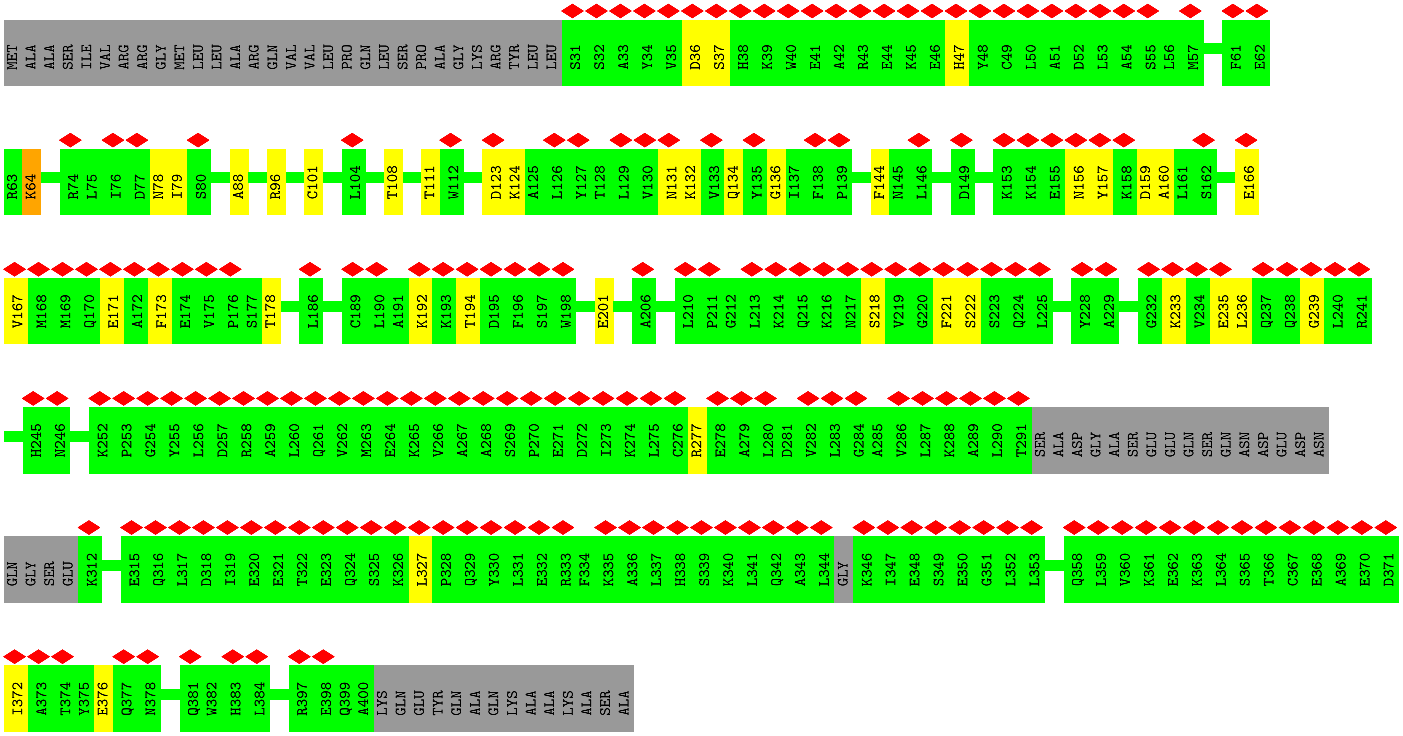
Chain AU:



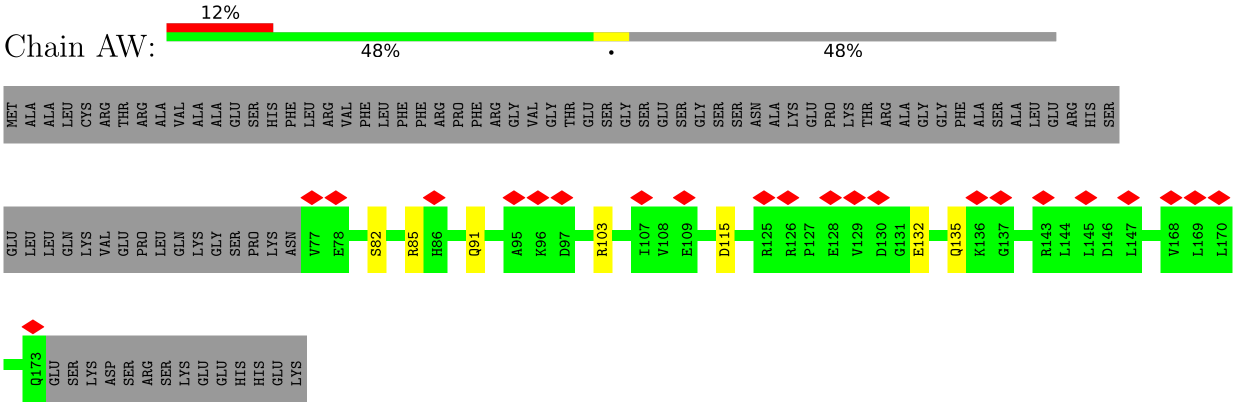
- Molecule 38: 28S ribosomal protein S27, mitochondrial

Chain AV:

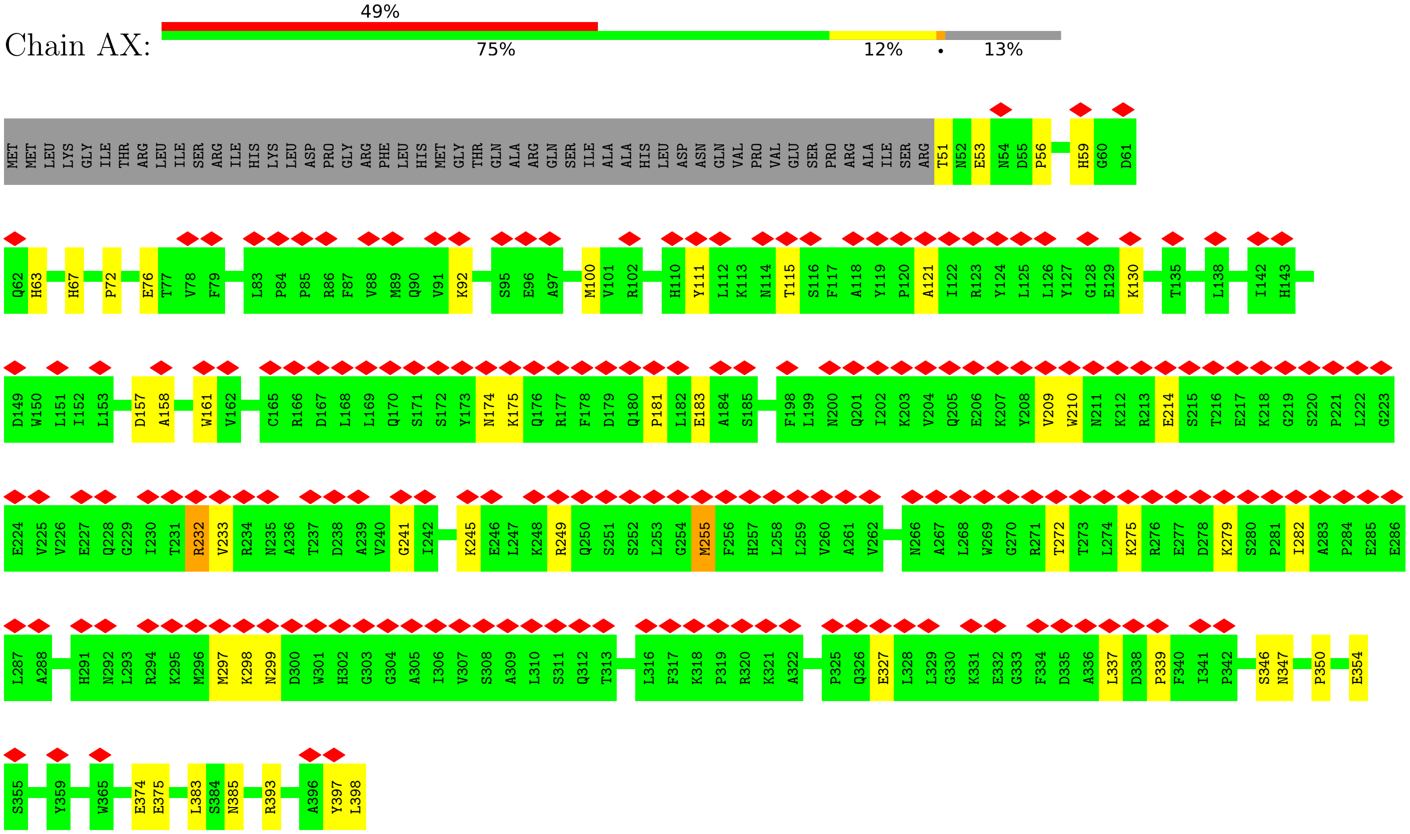




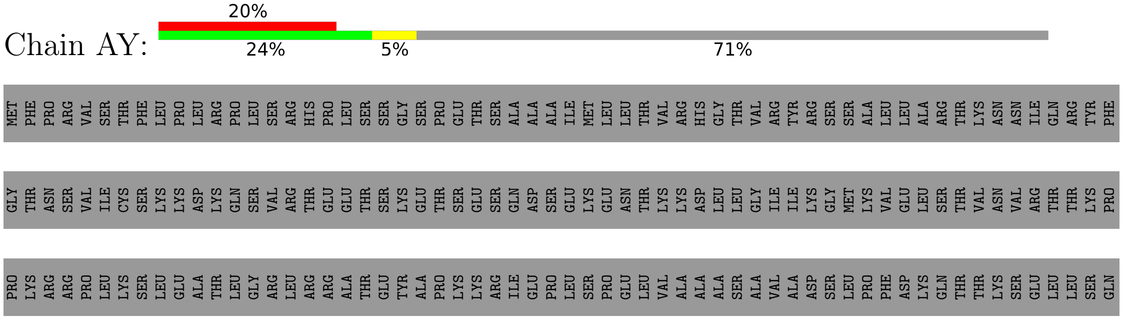
- Molecule 39: 28S ribosomal protein S28, mitochondrial

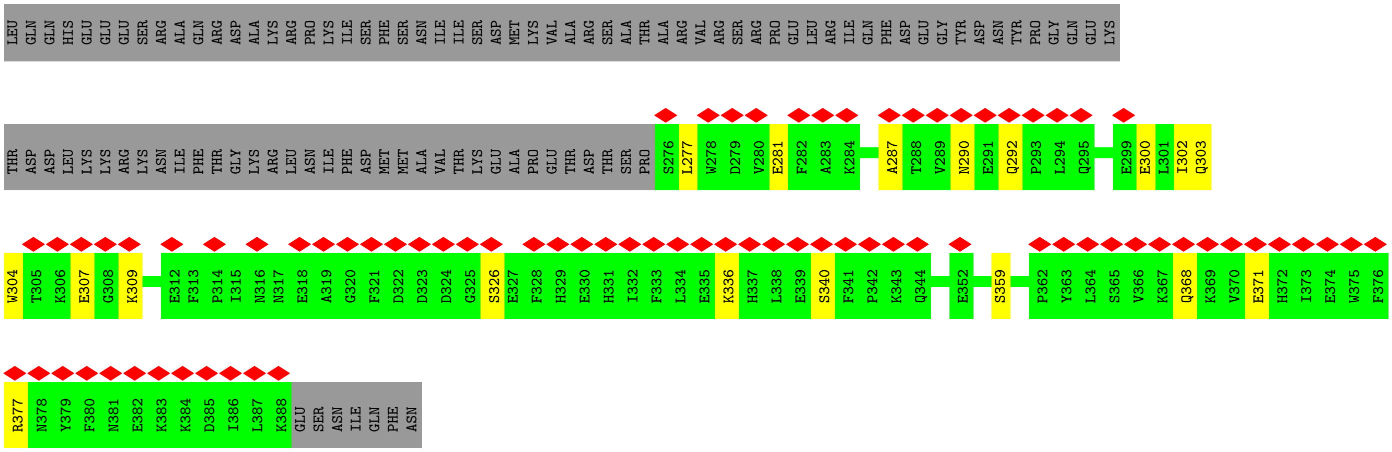


- Molecule 40: 28S ribosomal protein S29, mitochondrial



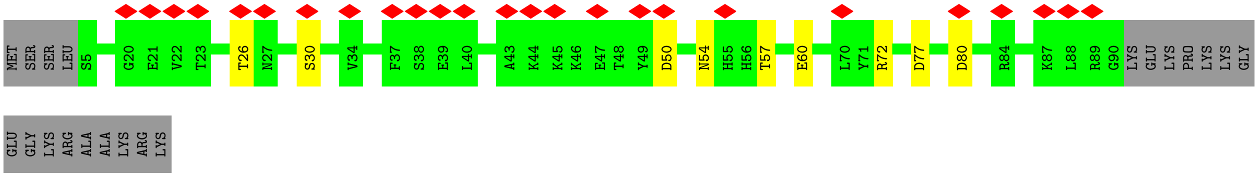
- Molecule 41: 28S ribosomal protein S31, mitochondrial





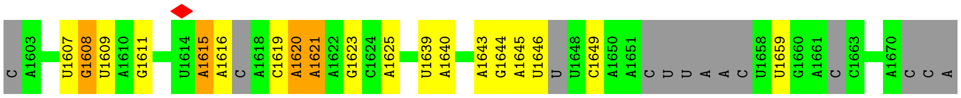
- Molecule 42: 28S ribosomal protein S33, mitochondrial

Chain AZ:



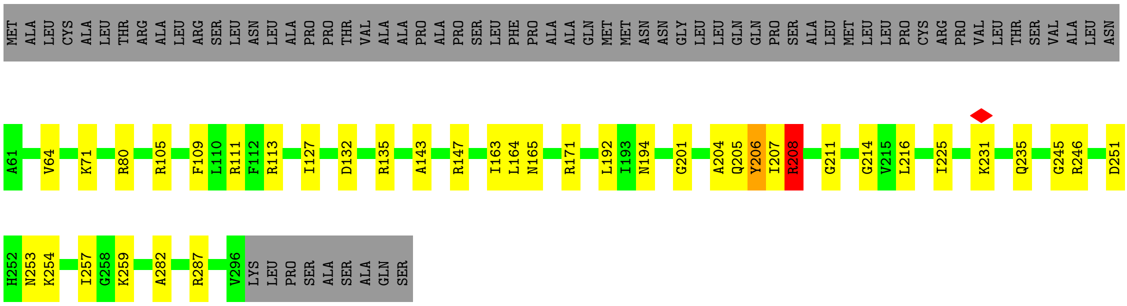
- Molecule 43: mitochondrial tRNAVal

Chain XB:



- Molecule 44: 39S ribosomal protein L2, mitochondrial

Chain XD:

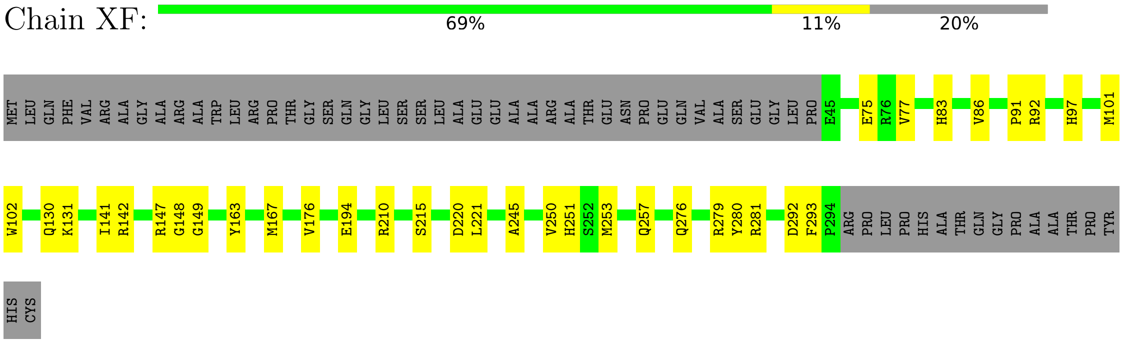


- Molecule 45: 39S ribosomal protein L3, mitochondrial

Chain XE:

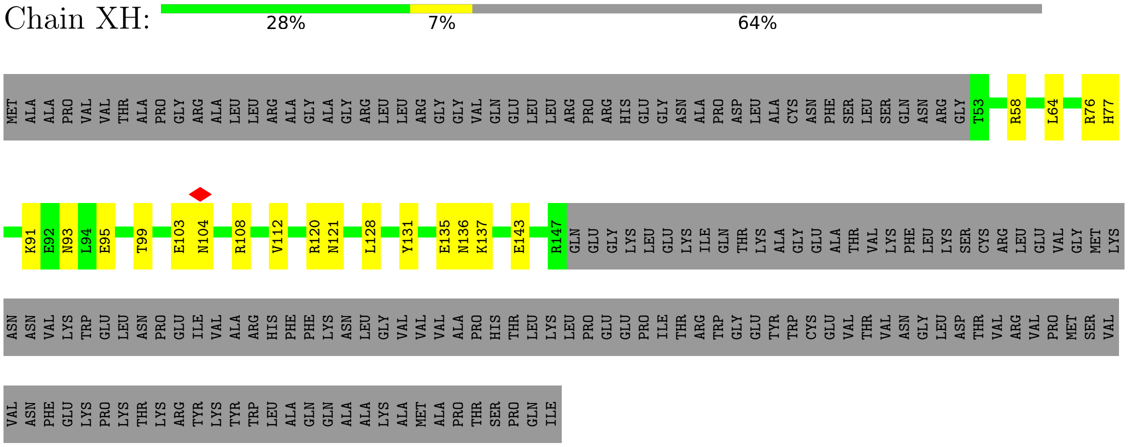
- Molecule 46: 39S ribosomal protein L4, mitochondrial

Chain XF:



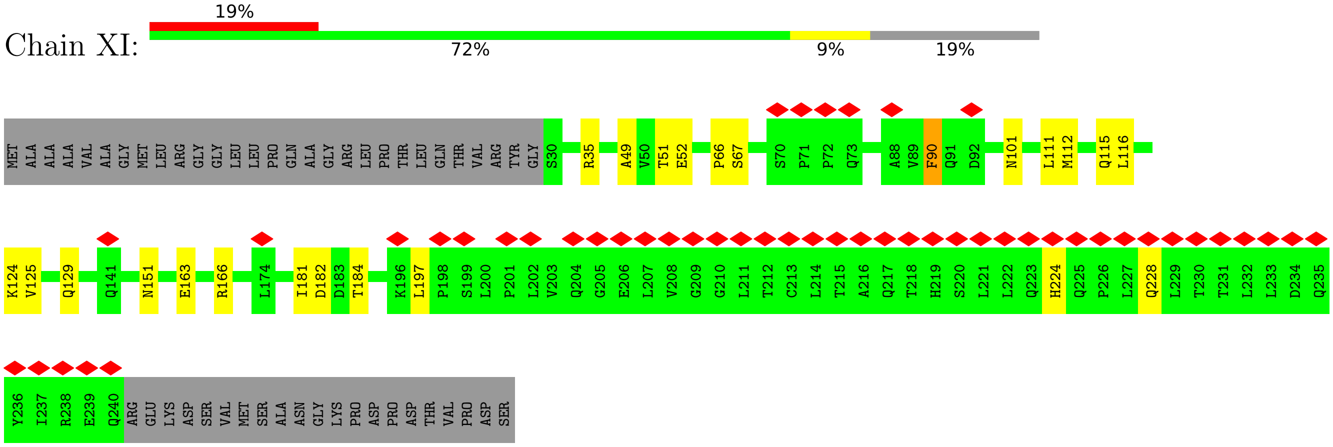
- Molecule 47: 39S ribosomal protein L9, mitochondrial

Chain XH:



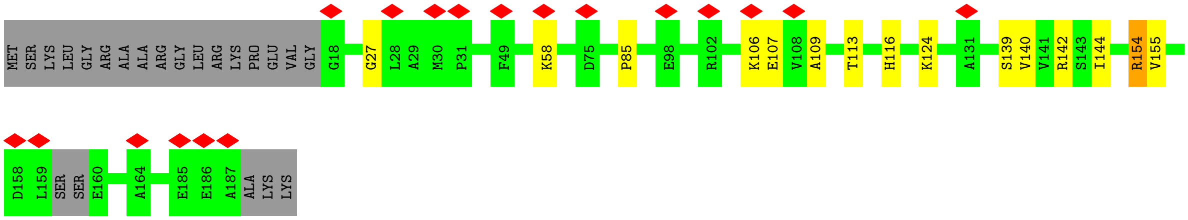
- Molecule 48: 39S ribosomal protein L10, mitochondrial

Chain XI:



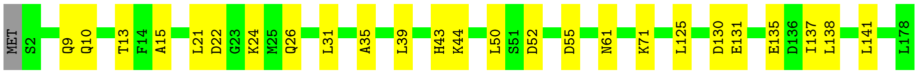
- Molecule 49: 39S ribosomal protein L11, mitochondrial

Chain XJ:



- Molecule 50: 39S ribosomal protein L13, mitochondrial

Chain XK:

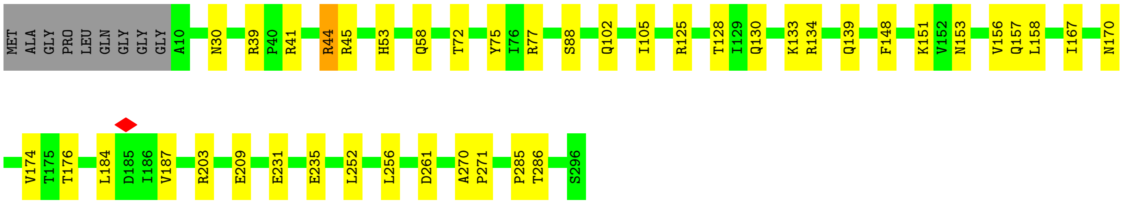


- Molecule 51: 39S ribosomal protein L14, mitochondrial

Chain XL:

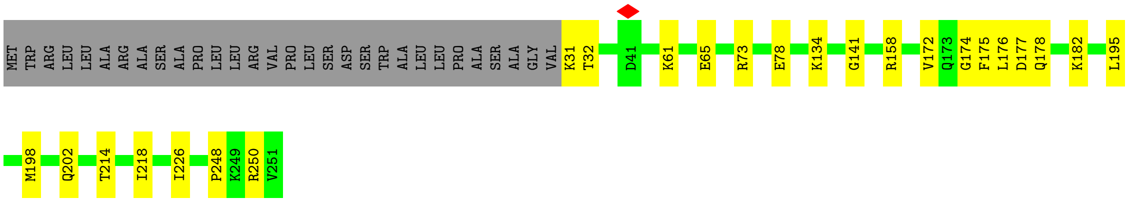
- Molecule 52: 39S ribosomal protein L15, mitochondrial

Chain XM:



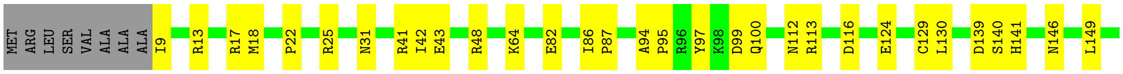
- Molecule 53: 39S ribosomal protein L16, mitochondrial

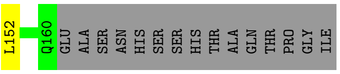
Chain XN:



- Molecule 54: 39S ribosomal protein L17, mitochondrial

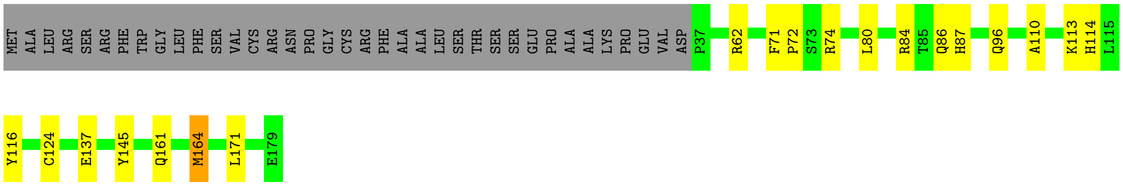
Chain XO:





- Molecule 55: 39S ribosomal protein L18, mitochondrial

Chain XP:

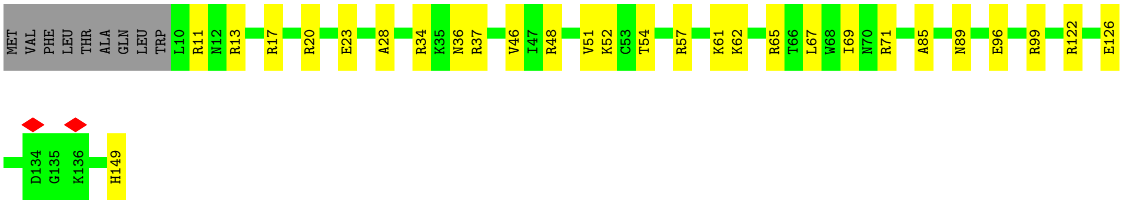


- Molecule 56: 39S ribosomal protein L19, mitochondrial

Chain XQ:

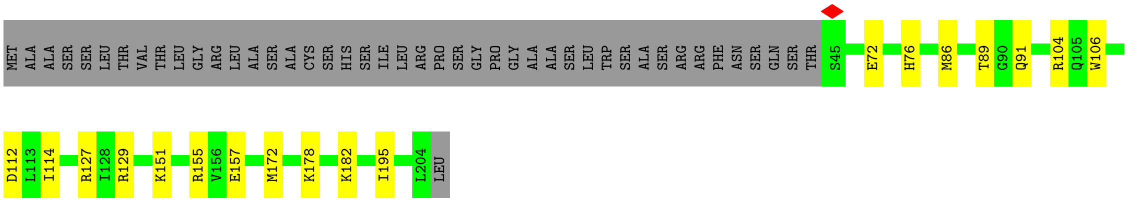
- Molecule 57: 39S ribosomal protein L20, mitochondrial

Chain XR:



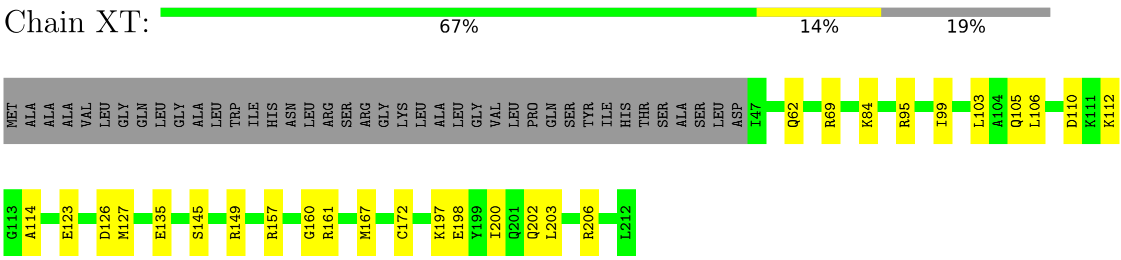
- Molecule 58: 39S ribosomal protein L21, mitochondrial

Chain XS:



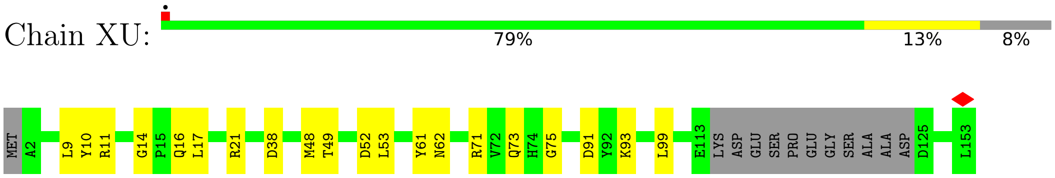
- Molecule 59: 39S ribosomal protein L22, mitochondrial

Chain XT:



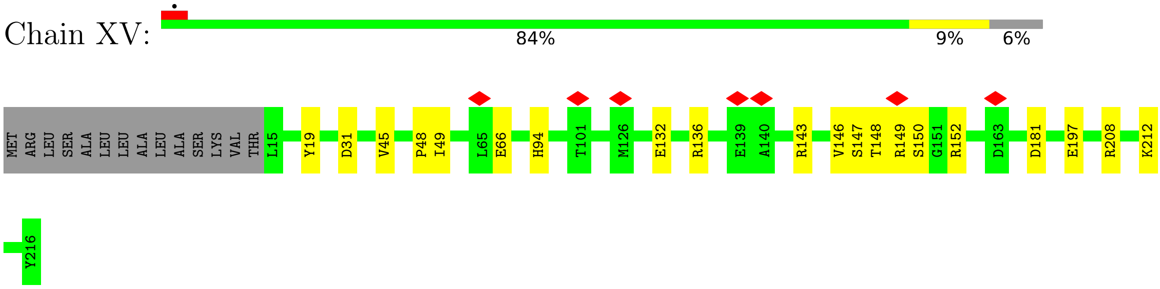
- Molecule 60: 39S ribosomal protein L23, mitochondrial

Chain XU:



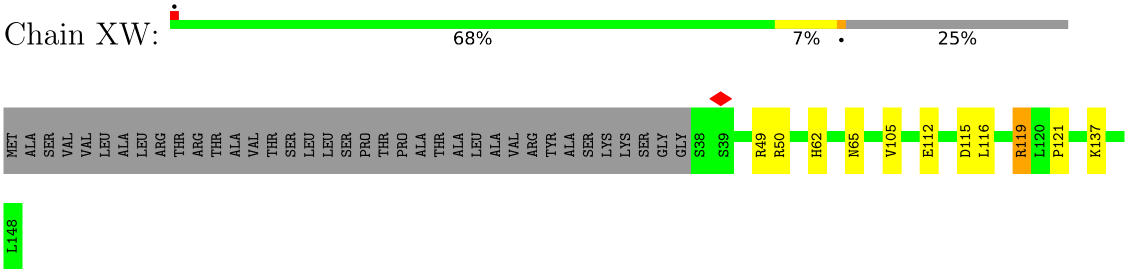
- Molecule 61: 39S ribosomal protein L24, mitochondrial

Chain XV:



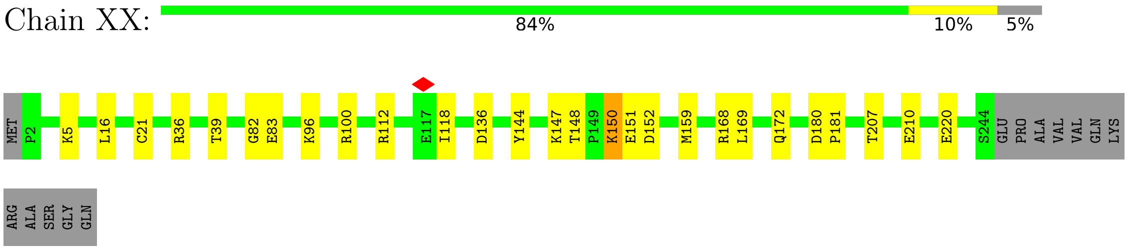
- Molecule 62: 39S ribosomal protein L27, mitochondrial

Chain XW:



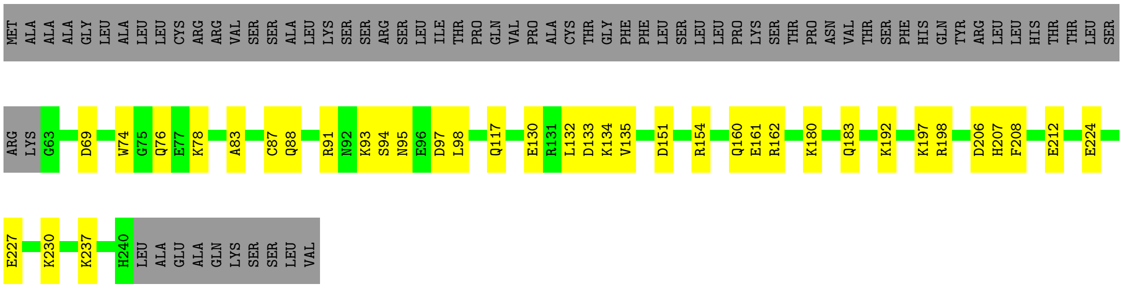
- Molecule 63: 39S ribosomal protein L28, mitochondrial

Chain XX:



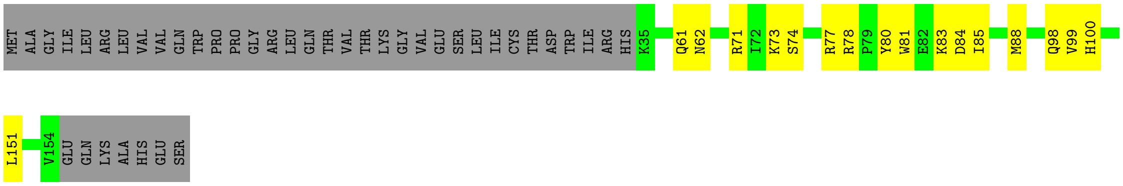
- Molecule 64: 39S ribosomal protein L47, mitochondrial

Chain XY:



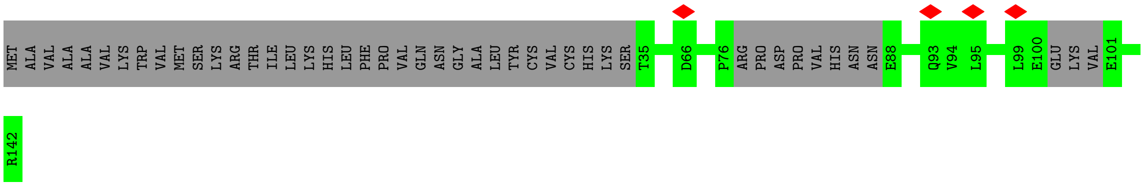
- Molecule 65: 39S ribosomal protein L30, mitochondrial

Chain XZ:



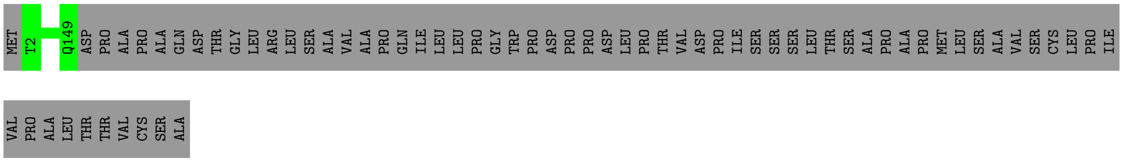
- Molecule 66: 39S ribosomal protein L42, mitochondrial

Chain a:



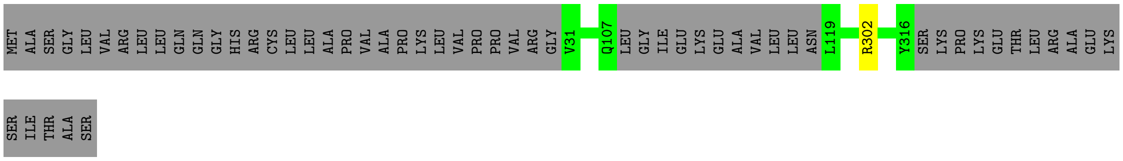
- Molecule 67: 39S ribosomal protein L43, mitochondrial

Chain b:



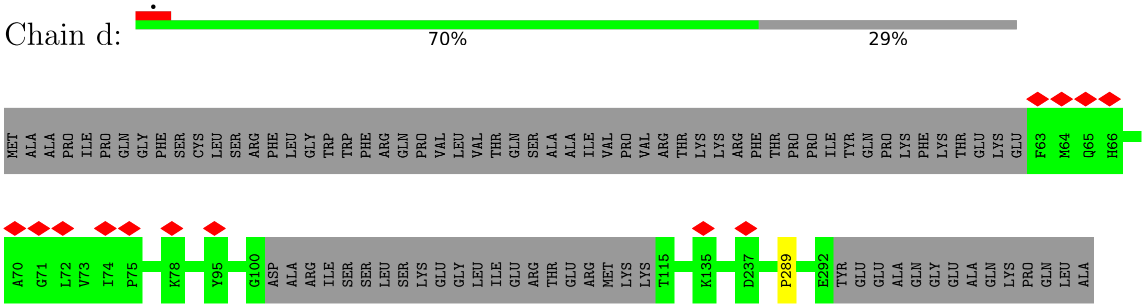
- Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c:



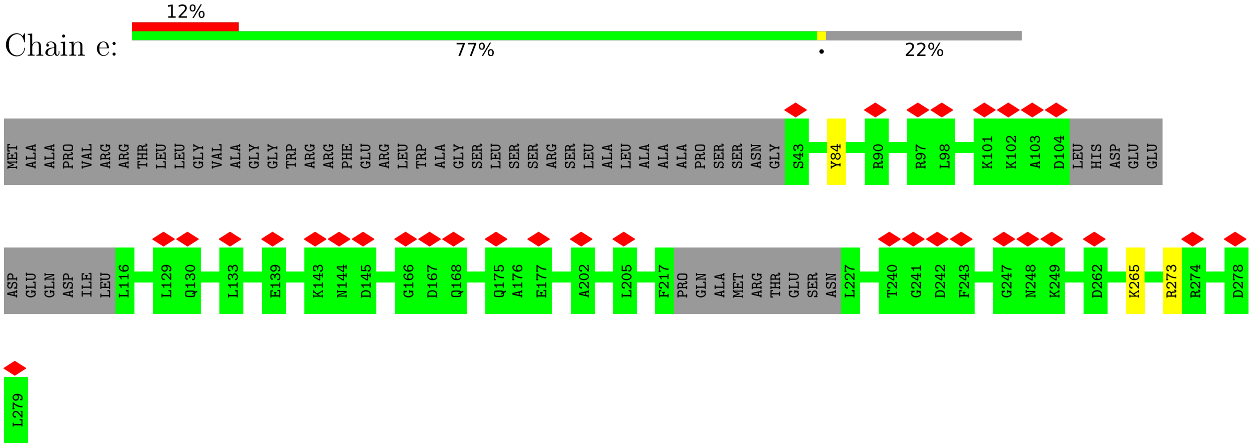
- Molecule 69: 39S ribosomal protein L45, mitochondrial

Chain d:



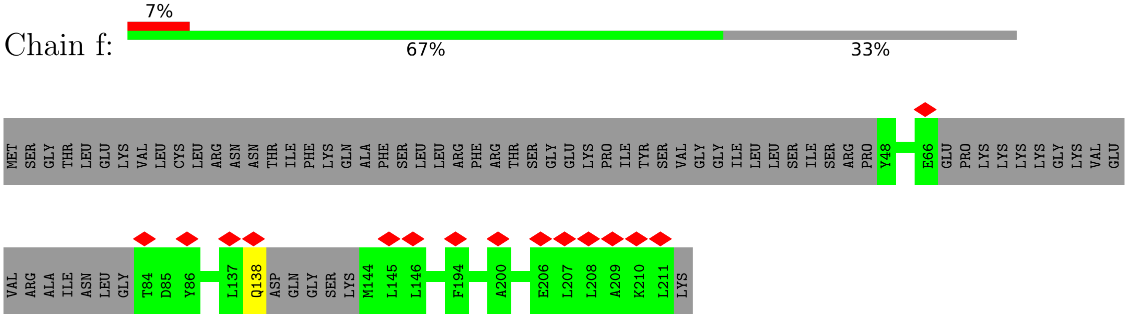
- Molecule 70: 39S ribosomal protein L46, mitochondrial

Chain e:



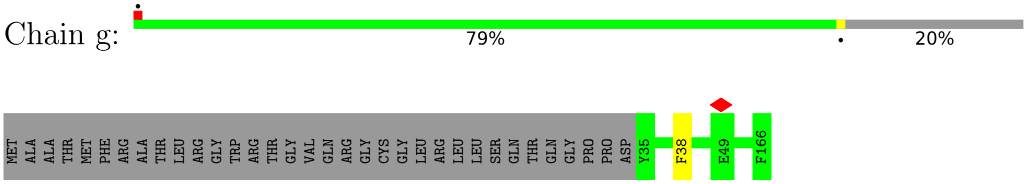
- Molecule 71: 39S ribosomal protein L48, mitochondrial

Chain f:



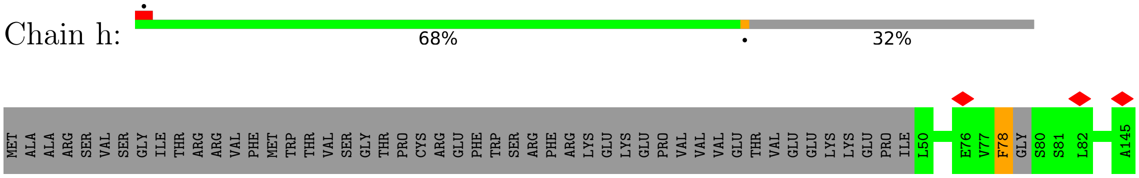
- Molecule 72: 39S ribosomal protein L49, mitochondrial

Chain g:

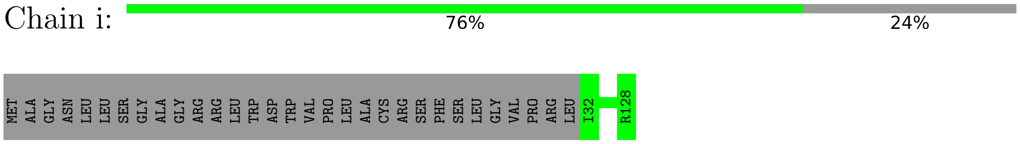


- Molecule 73: 39S ribosomal protein L50, mitochondrial

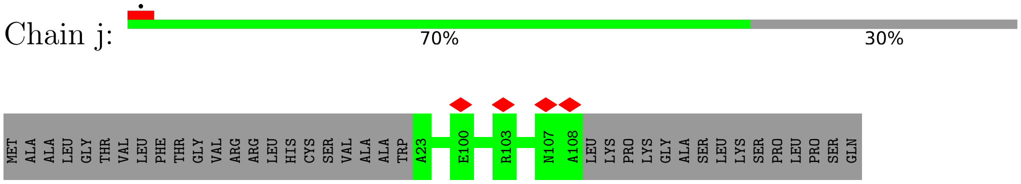
Chain h:



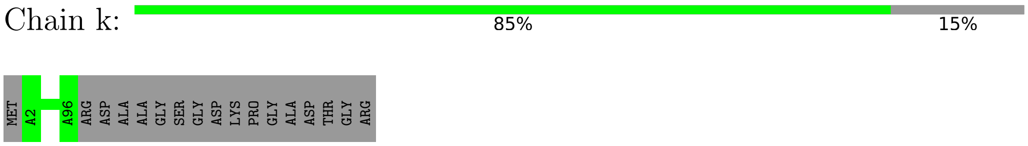
- Molecule 74: 39S ribosomal protein L51, mitochondrial



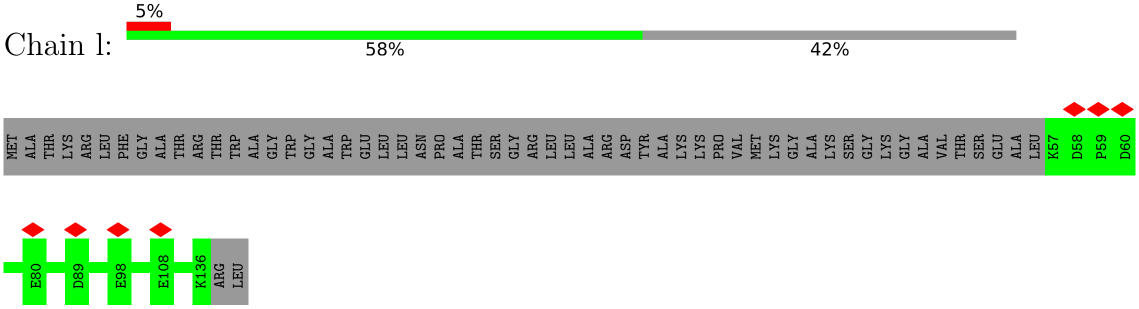
- Molecule 75: 39S ribosomal protein L52, mitochondrial



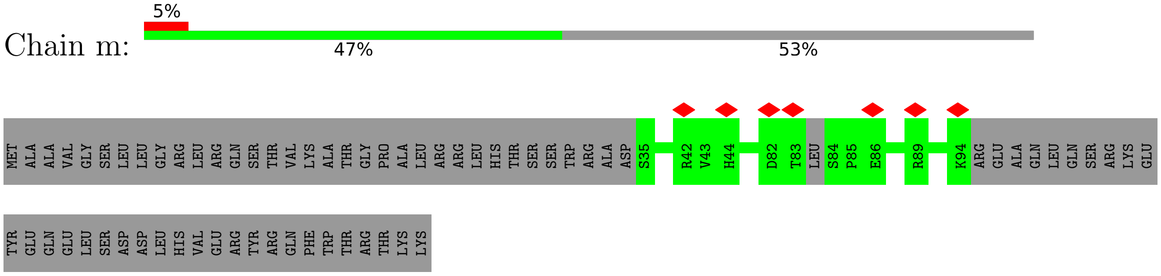
- Molecule 76: 39S ribosomal protein L53, mitochondrial



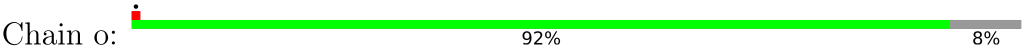
- Molecule 77: 39S ribosomal protein L54, mitochondrial

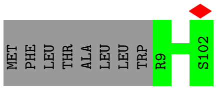


- Molecule 78: 39S ribosomal protein L55, mitochondrial



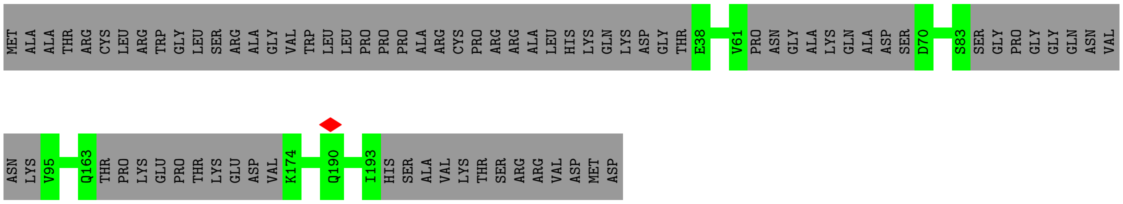
- Molecule 79: Ribosomal protein 63, mitochondrial





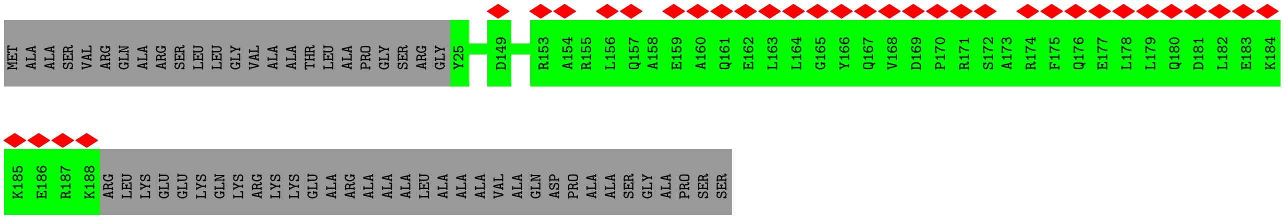
- Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:



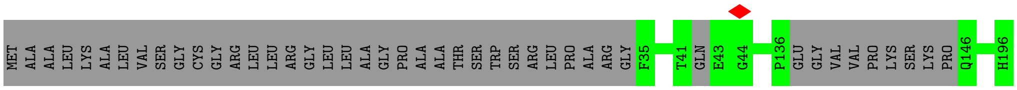
- Molecule 81: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



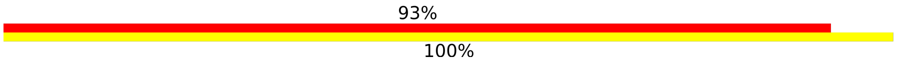
- Molecule 82: 39S ribosomal protein S18a, mitochondrial

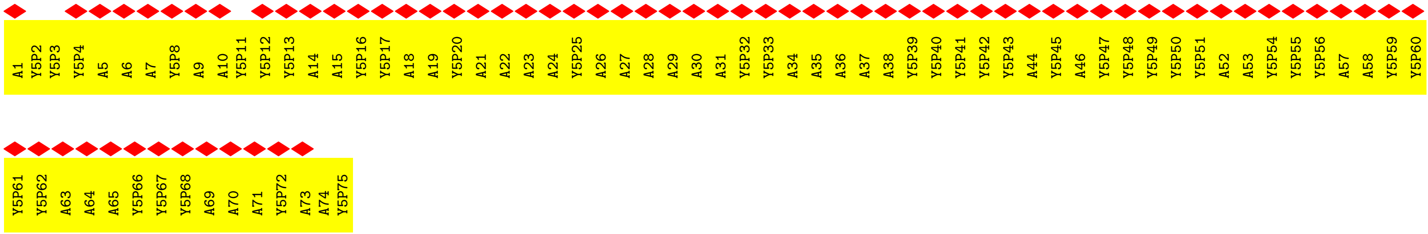
Chain r:



- Molecule 83: P/E-tRNA

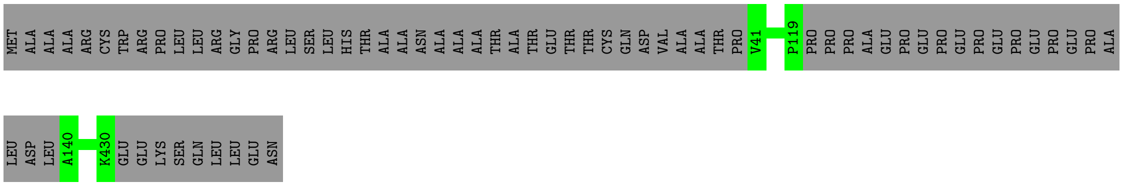
Chain r3:





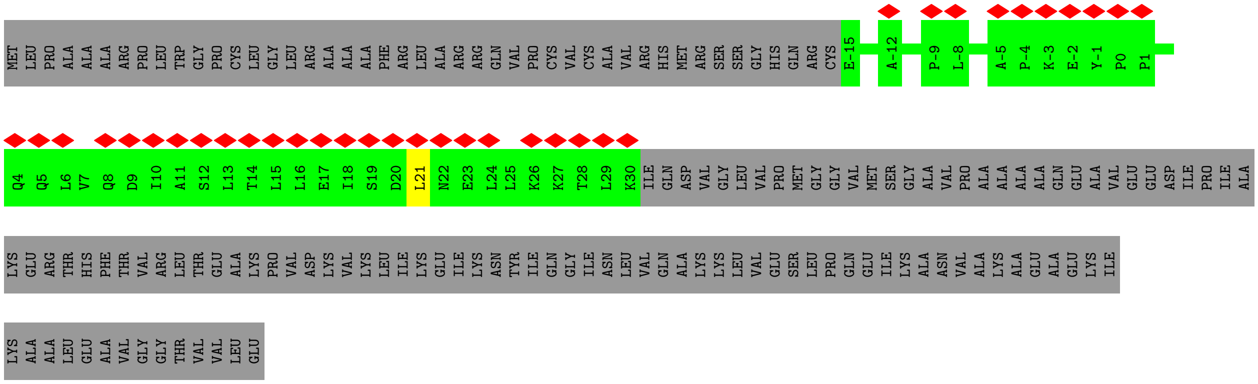
- Molecule 84: 39S ribosomal protein S30, mitochondrial

Chain s:



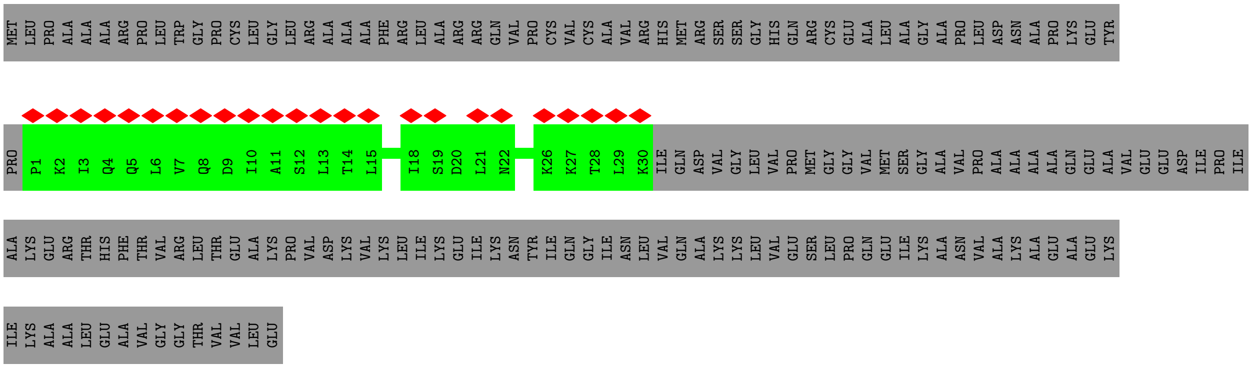
- Molecule 85: 39S ribosomal protein L12, mitochondrial

Chain t1:



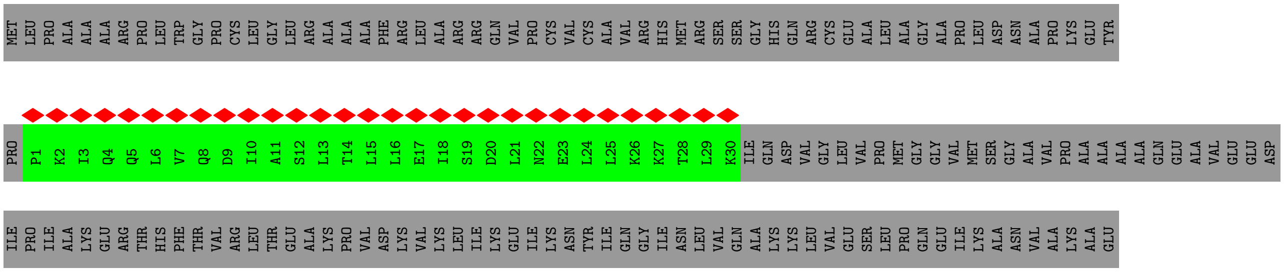
- Molecule 85: 39S ribosomal protein L12, mitochondrial

Chain t2:

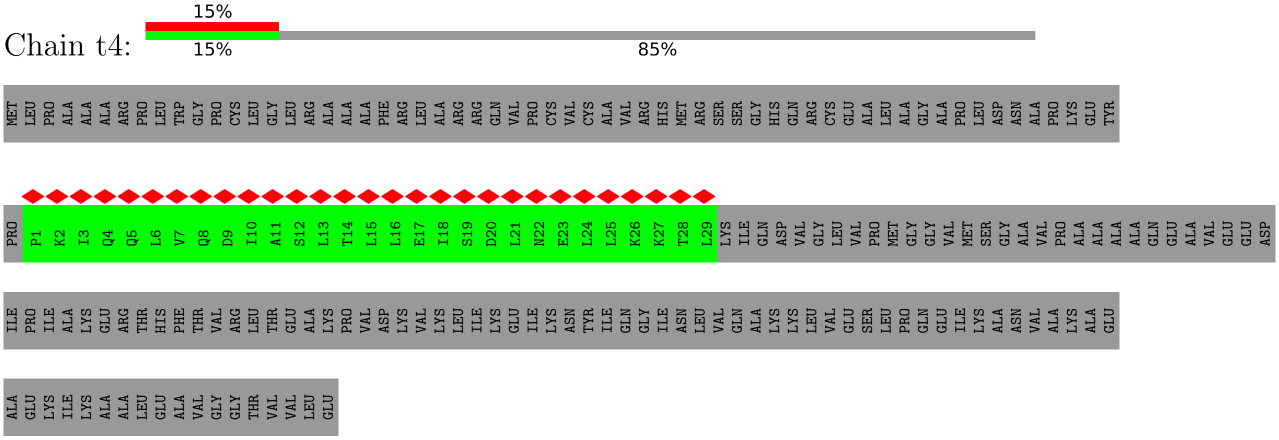


- Molecule 85: 39S ribosomal protein L12, mitochondrial

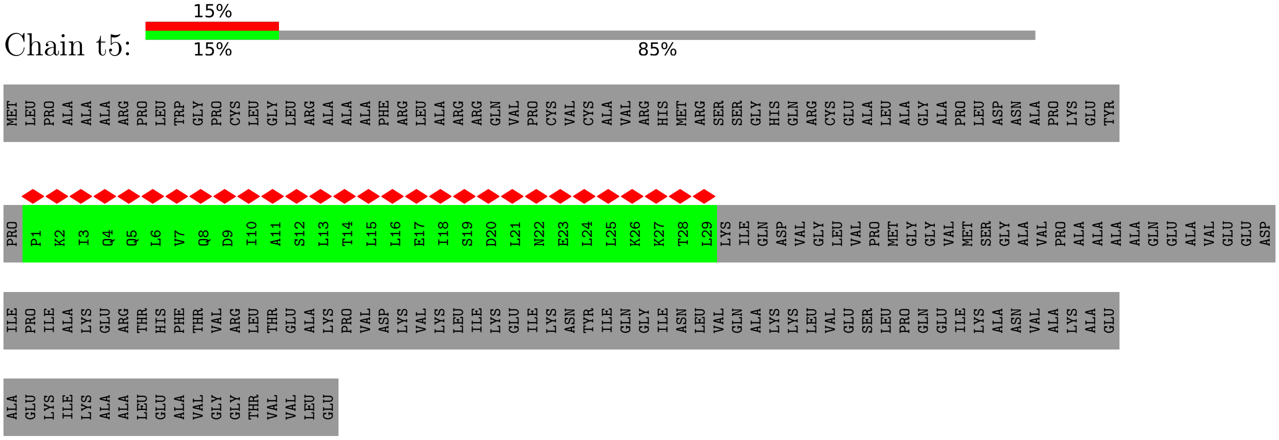
Chain t3:



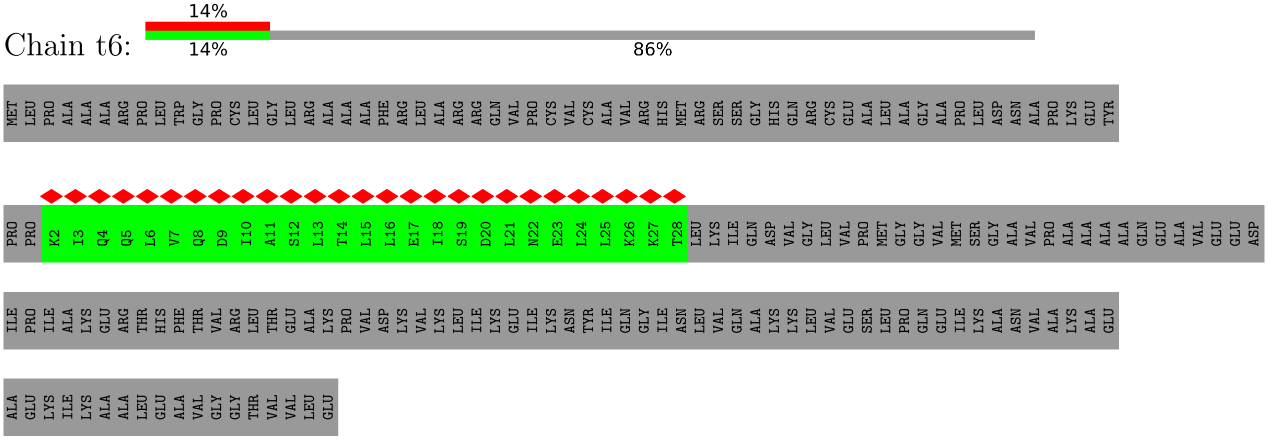
- Molecule 85: 39S ribosomal protein L12, mitochondrial



- Molecule 85: 39S ribosomal protein L12, mitochondrial



- Molecule 85: 39S ribosomal protein L12, mitochondrial



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19968	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	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	0.244	Depositor
Minimum map value	-0.124	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DOL, H8Q, P5P, Y5P, GTP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.31	0/895	0.46	0/1201
2	1	0.28	0/444	0.49	0/591
3	2	0.34	0/382	0.45	0/507
4	3	0.35	0/852	0.45	0/1136
5	4	0.32	0/349	0.45	0/461
6	5	0.28	0/3298	0.42	0/4492
7	6	0.28	0/3040	0.42	0/4134
8	7	0.27	0/2420	0.43	0/3270
9	8	1.84	1/1159 (0.1%)	0.46	2/1559 (0.1%)
10	9	0.29	0/1024	0.42	0/1379
11	XA	0.40	2/35592 (0.0%)	0.78	0/55390
12	A0	0.23	0/1727	0.43	0/2338
13	A1	0.24	0/2276	0.40	0/3079
14	A2	0.25	0/939	0.42	0/1256
15	A3	0.27	0/621	0.44	0/820
16	A4	0.25	0/4559	0.41	0/6149
17	AA	0.21	0/21952	0.75	1/34164 (0.0%)
18	AB	0.24	0/1819	0.40	0/2462
19	AC	0.24	0/1112	0.41	0/1505
20	AD	0.24	0/2768	0.44	0/3707
21	AE	0.24	0/989	0.44	0/1335
22	AF	0.24	0/1708	0.39	0/2291
23	AG	0.25	0/2559	0.41	0/3429
24	AH	0.24	0/1128	0.43	0/1529
25	AI	0.25	0/1031	0.43	0/1390
26	AJ	0.25	0/854	0.45	0/1148
27	AK	0.22	0/879	0.40	0/1182
28	AL	0.25	0/1406	0.40	0/1878
29	AM	0.24	0/941	0.42	0/1265
30	AN	0.25	0/864	0.43	0/1169
31	AO	0.24	0/1580	0.39	0/2150
32	AP	0.25	0/782	0.38	0/1050

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
33	AQ	0.24	0/746	0.42	0/993
34	AR	0.68	1/2103 (0.0%)	0.52	3/2842 (0.1%)
35	AS	0.25	0/1127	0.40	0/1518
36	AT	0.26	0/1361	0.42	0/1829
37	AU	0.23	0/1482	0.41	0/1987
38	AV	0.24	0/2925	0.40	0/3948
39	AW	0.25	0/778	0.44	0/1048
40	AX	0.25	0/2886	0.44	0/3909
41	AY	0.25	0/985	0.39	0/1329
42	AZ	0.24	0/748	0.38	0/1000
43	XB	0.21	0/1400	0.73	0/2168
44	XD	0.30	0/1879	0.48	0/2527
45	XE	0.31	0/2465	0.45	0/3344
46	XF	0.34	0/2071	0.47	0/2817
47	XH	0.27	0/798	0.46	0/1073
48	XI	0.26	0/1727	0.45	0/2340
49	XJ	0.24	0/1309	0.40	0/1764
50	XK	0.33	0/1495	0.44	0/2029
51	XL	0.30	0/904	0.46	0/1218
52	XM	0.32	0/2359	0.45	0/3185
53	XN	0.31	0/1825	0.45	0/2458
54	XO	0.28	0/1269	0.46	0/1708
55	XP	0.27	0/1190	0.46	0/1611
56	XQ	0.27	0/2026	0.44	0/2734
57	XR	0.36	0/1174	0.48	0/1572
58	XS	0.33	0/1311	0.47	0/1778
59	XT	0.35	0/1402	0.45	0/1886
60	XU	0.32	0/1200	0.43	0/1623
61	XV	0.29	0/1693	0.45	0/2297
62	XW	0.33	0/893	0.45	0/1204
63	XX	0.37	2/2090 (0.1%)	0.56	4/2825 (0.1%)
64	XY	0.29	0/1571	0.41	0/2106
65	XZ	0.32	0/1003	0.44	0/1354
66	a	0.30	0/838	0.46	0/1138
67	b	0.33	0/1202	0.45	0/1626
68	c	0.28	0/2264	0.44	0/3059
69	d	0.27	0/1807	0.42	0/2450
70	e	1.43	6/1797 (0.3%)	0.43	0/2422
71	f	0.27	0/1159	0.42	0/1565
72	g	0.33	0/1134	0.49	0/1547
73	h	0.26	0/905	0.45	0/1233
74	i	0.34	0/849	0.48	0/1135
75	j	0.29	0/703	0.44	0/947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	k	0.24	0/743	0.45	0/1003
77	l	0.24	0/692	0.37	0/939
78	m	0.23	0/508	0.45	0/682
79	o	0.32	0/818	0.45	0/1097
80	p	0.24	0/1071	0.43	0/1433
81	q	0.26	0/1413	0.42	0/1906
82	r	0.29	0/1282	0.43	0/1734
84	s	0.29	0/3114	0.44	0/4225
85	t1	0.24	0/366	0.36	0/497
85	t2	0.22	0/238	0.38	0/319
85	t3	0.23	0/238	0.37	0/319
85	t4	0.22	0/229	0.36	0/308
85	t5	0.23	0/229	0.40	0/308
85	t6	0.25	0/213	0.42	0/286
All	All	0.37	12/175956 (0.0%)	0.58	10/249618 (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
44	XD	0	1
48	XI	0	2
70	e	0	1
71	f	0	1
73	h	0	1
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	99	ARG	CG-CD	61.76	3.06	1.51
70	e	84	TYR	CD2-CE2	31.77	1.87	1.39
70	e	84	TYR	CD1-CE1	31.12	1.86	1.39
34	AR	308	HIS	C-N	28.79	1.89	1.34
70	e	84	TYR	CE2-CZ	21.80	1.66	1.38
70	e	84	TYR	CE1-CZ	21.18	1.66	1.38
70	e	84	TYR	CG-CD1	18.69	1.63	1.39
70	e	84	TYR	CG-CD2	17.15	1.61	1.39
11	XA	2625	C	OP3-P	-11.29	1.47	1.61
11	XA	3039	U	OP3-P	-11.25	1.47	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	XX	147	LYS	C-N	8.23	1.52	1.34
63	XX	150	LYS	C-N	7.75	1.51	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	XX	147	LYS	O-C-N	13.68	144.58	122.70
34	AR	309	PRO	O-C-N	11.64	141.32	122.70
63	XX	147	LYS	CA-C-N	-9.85	95.52	117.20
34	AR	309	PRO	CA-C-N	-8.79	97.86	117.20
63	XX	150	LYS	O-C-N	-6.82	111.78	122.70
34	AR	309	PRO	C-N-CA	-5.93	106.88	121.70
9	8	99	ARG	CG-CD-NE	5.85	124.08	111.80
9	8	99	ARG	CB-CG-CD	5.73	126.51	111.60
63	XX	150	LYS	CA-C-N	5.73	129.80	117.20
17	AA	765	C	C2-N1-C1'	5.21	124.53	118.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	XD	206	TYR	Peptide
48	XI	197	LEU	Peptide
48	XI	90	PHE	Peptide
70	e	265	LYS	Peptide
71	f	138	GLN	Peptide
73	h	78	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	880	903	903	9	0
2	1	439	480	480	5	0
3	2	376	406	406	3	0
4	3	831	883	883	10	0
5	4	341	361	361	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	5	3204	3200	3200	31	0
7	6	2947	2839	2839	36	0
8	7	2365	2373	2372	22	0
9	8	1135	1166	1166	7	0
10	9	996	987	987	11	0
11	XA	31813	16160	16160	230	0
12	A0	1684	1685	1685	15	0
13	A1	2230	2261	2261	25	0
14	A2	925	964	964	13	0
15	A3	610	682	682	11	0
16	A4	4470	4485	4486	64	0
17	AA	19628	9970	9971	144	0
18	AB	1776	1769	1769	15	0
19	AC	1082	1088	1088	12	0
20	AD	2716	2785	2785	36	0
21	AE	972	1001	1001	14	0
22	AF	1668	1714	1716	18	0
23	AG	2505	2492	2490	27	0
24	AH	1105	1136	1136	23	0
25	AI	1011	1052	1052	13	0
26	AJ	838	887	887	10	0
27	AK	861	885	885	10	0
28	AL	1382	1472	1472	15	0
29	AM	920	951	951	11	0
30	AN	846	908	908	12	0
31	AO	1528	1490	1490	19	0
32	AP	765	796	796	6	0
33	AQ	734	749	749	7	0
34	AR	2060	2074	2074	20	0
35	AS	1100	1103	1103	12	0
36	AT	1330	1342	1342	15	0
37	AU	1461	1471	1471	14	0
38	AV	2867	2863	2862	22	0
39	AW	766	785	785	5	0
40	AX	2814	2805	2804	32	0
41	AY	956	911	911	12	0
42	AZ	731	734	734	6	0
43	XB	1255	640	640	9	0
44	XD	1842	1896	1896	27	0
45	XE	2396	2402	2402	23	0
46	XF	2013	2045	2044	26	0
47	XH	784	832	832	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	XI	1691	1783	1783	16	0
49	XJ	1291	1367	1364	11	0
50	XK	1451	1448	1448	15	0
51	XL	889	941	941	8	0
52	XM	2305	2378	2378	30	0
53	XN	1778	1808	1808	16	0
54	XO	1245	1283	1283	23	0
55	XP	1164	1162	1162	18	0
56	XQ	1978	2022	2022	23	0
57	XR	1153	1214	1214	25	0
58	XS	1284	1354	1354	13	0
59	XT	1368	1410	1410	20	0
60	XU	1171	1164	1164	13	0
61	XV	1648	1656	1654	14	0
62	XW	871	898	898	10	0
63	XX	2035	2054	2054	26	0
64	XY	1534	1575	1575	27	0
65	XZ	978	1030	1030	12	0
66	a	813	777	777	0	0
67	b	1178	1180	1180	0	0
68	c	2217	2220	2220	0	0
69	d	1758	1743	1742	0	0
70	e	1762	1767	1767	0	0
71	f	1139	1152	1152	0	0
72	g	1097	1086	1085	0	0
73	h	882	866	867	0	0
74	i	827	857	857	0	0
75	j	689	678	678	0	0
76	k	732	745	745	0	0
77	l	673	654	653	0	0
78	m	500	525	525	0	0
79	o	797	804	804	0	0
80	p	1058	1083	1083	0	0
81	q	1379	1359	1359	0	0
82	r	1247	1267	1267	0	0
83	r3	1468	0	823	0	0
84	s	3036	3023	3022	0	0
85	t1	354	379	374	0	0
85	t2	238	268	270	0	0
85	t3	238	268	270	0	0
85	t4	229	255	257	0	0
85	t5	229	255	257	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	t6	214	236	236	0	0
86	0	1	0	0	0	0
86	4	1	0	0	0	0
86	AB	1	0	0	0	0
86	AO	1	0	0	0	0
86	AP	1	0	0	0	0
86	AT	1	0	0	0	0
86	r	1	0	0	0	0
87	9	1	0	0	0	0
87	AA	46	0	0	0	0
87	XA	143	0	0	0	0
87	XD	1	0	0	0	0
87	XI	1	0	0	0	0
87	XM	1	0	0	0	0
87	XW	1	0	0	0	0
87	g	1	0	0	0	0
88	XA	73	67	0	2	0
89	XA	48	50	50	0	0
90	AX	32	10	12	1	0
All	All	168901	143004	143755	1148	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 (1148) 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)
34:AR:308:HIS:C	34:AR:309:PRO:N	1.88	1.27
63:XX:144:TYR:O	63:XX:148:THR:HB	1.64	0.98
42:AZ:26:THR:HG1	42:AZ:30:SER:HG	1.04	0.97
16:A4:108:LEU:HD21	20:AD:154:VAL:CG1	1.98	0.92
11:XA:2954:C:O2	53:XN:182:LYS:NZ	2.03	0.92
47:XH:91:LYS:NZ	47:XH:93:ASN:OD1	2.05	0.90
23:AG:198:ARG:N	23:AG:246:ARG:O	2.06	0.89
53:XN:134:LYS:NZ	53:XN:141:GLY:O	2.06	0.89
11:XA:1962:A:OP2	11:XA:2501:C:N4	2.07	0.88
11:XA:1777:A:N6	11:XA:1780:U:OP2	2.07	0.88
60:XU:16:GLN:NE2	60:XU:17:LEU:O	2.08	0.87
11:XA:2166:C:O2	11:XA:2214:A:N6	2.07	0.87
22:AF:79:ALA:O	23:AG:312:GLN:NE2	2.08	0.87
6:5:72:ARG:NH2	11:XA:1712:A:OP2	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:160:ASP:OD2	7:6:267:ARG:NH1	2.08	0.86
11:XA:2864:U:O5'	62:XW:50:ARG:NH1	2.07	0.86
11:XA:1680:A:OP1	64:XY:230:LYS:NZ	2.09	0.86
1:0:95:ARG:NH1	11:XA:1821:A:OP2	2.09	0.86
17:AA:1005:U:OP1	25:AI:152:LYS:NZ	2.09	0.85
50:XK:52:ASP:OD1	59:XT:206:ARG:NH1	2.08	0.85
4:3:104:ARG:NH1	4:3:160:LYS:O	2.09	0.85
16:A4:108:LEU:CD2	20:AD:154:VAL:HG12	2.06	0.85
29:AM:93:LEU:O	34:AR:175:ARG:NH2	2.09	0.85
26:AJ:84:ARG:NH1	26:AJ:85:LEU:O	2.10	0.84
63:XX:144:TYR:O	63:XX:148:THR:CB	2.24	0.84
11:XA:1689:C:OP2	63:XX:5:LYS:NZ	2.11	0.84
17:AA:1557:A:O2'	26:AJ:72:LYS:NZ	2.11	0.84
23:AG:310:ARG:NH1	40:AX:383:LEU:O	2.11	0.84
14:A2:38:ARG:NH2	17:AA:1184:U:OP1	2.10	0.84
25:AI:71:SER:O	25:AI:74:ARG:NH1	2.11	0.84
11:XA:3068:G:N2	11:XA:3068:G:OP2	2.12	0.83
18:AB:103:GLU:OE2	35:AS:52:ARG:NH2	2.11	0.83
17:AA:1530:A:OP1	38:AV:64:LYS:NZ	2.11	0.83
6:5:141:ASP:O	6:5:142:ASP:N	2.12	0.83
11:XA:2517:U:OP1	44:XD:287:ARG:NH2	2.12	0.83
17:AA:826:A:OP1	26:AJ:55:ARG:NH1	2.12	0.83
21:AE:92:ASN:ND2	32:AP:117:MET:SD	2.52	0.82
11:XA:3063:G:O2'	11:XA:3066:C:OP2	1.98	0.82
31:AO:185:SER:O	34:AR:183:LYS:NZ	2.13	0.82
29:AM:20:ARG:NH1	29:AM:42:PRO:O	2.13	0.81
11:XA:2822:C:O2'	11:XA:2915:C:OP2	1.97	0.81
30:AN:59:THR:OG1	30:AN:62:ASP:OD2	1.97	0.81
16:A4:133:ALA:HB2	19:AC:148:LYS:HB2	1.61	0.81
13:A1:154:THR:OG1	24:AH:171:GLU:OE2	1.99	0.81
17:AA:728:C:OP1	30:AN:5:ARG:NH2	2.14	0.80
11:XA:2369:A:OP1	64:XY:117:GLN:NE2	2.15	0.80
16:A4:108:LEU:CD2	20:AD:154:VAL:CG1	2.60	0.80
51:XL:31:ALA:N	51:XL:91:MET:SD	2.54	0.80
1:0:84:ARG:NH2	11:XA:2306:A:O2'	2.15	0.79
17:AA:701:G:N2	17:AA:841:A:O2'	2.14	0.79
5:4:84:ARG:NE	11:XA:3188:U:OP2	2.16	0.79
12:A0:49:ARG:NH2	37:AU:41:ARG:O	2.15	0.79
17:AA:860:A:N7	17:AA:919:A:O2'	2.15	0.79
34:AR:176:GLU:OE2	34:AR:182:ARG:NE	2.16	0.79
6:5:30:ALA:N	44:XD:201:GLY:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2499:U:OP2	11:XA:2504:A:N6	2.15	0.78
11:XA:1696:C:OP2	64:XY:180:LYS:NZ	2.15	0.78
16:A4:59:ILE:HG21	24:AH:69:PRO:HB2	1.65	0.78
11:XA:1958:G:OP2	59:XT:160:GLY:N	2.16	0.78
17:AA:825:U:N3	17:AA:827:A:OP1	2.17	0.78
1:0:139:ARG:NH2	11:XA:2322:C:OP1	2.17	0.77
17:AA:1487:C:O2	17:AA:1564:A:N6	2.17	0.77
7:6:114:ARG:NH1	43:XB:1643:A:OP1	2.17	0.77
14:A2:106:LYS:NZ	17:AA:1292:A:OP1	2.17	0.77
7:6:27:ARG:N	11:XA:2832:A:N1	2.32	0.77
11:XA:3050:U:O3'	51:XL:63:LYS:NZ	2.17	0.77
61:XV:181:ASP:O	64:XY:93:LYS:NZ	2.18	0.77
40:AX:111:TYR:O	40:AX:115:THR:OG1	2.02	0.77
17:AA:1233:C:OP1	17:AA:1353:A:N6	2.18	0.77
29:AM:59:ASN:ND2	29:AM:63:GLU:OE2	2.16	0.76
17:AA:868:C:OP2	17:AA:870:C:N4	2.18	0.76
32:AP:140:TYR:O	32:AP:141:ARG:NE	2.18	0.76
55:XP:74:ARG:O	55:XP:96:GLN:NE2	2.19	0.76
17:AA:1411:G:O3'	40:AX:279:LYS:NZ	2.19	0.76
12:A0:78:ARG:NH1	38:AV:171:GLU:OE1	2.18	0.76
38:AV:192:LYS:NZ	38:AV:194:THR:O	2.19	0.76
40:AX:121:ALA:N	40:AX:299:ASN:OD1	2.18	0.76
20:AD:127:ASN:O	42:AZ:72:ARG:NH1	2.18	0.76
31:AO:195:SER:OG	31:AO:197:ASP:OD1	2.04	0.76
11:XA:1800:G:N1	11:XA:1803:A:OP2	2.18	0.76
27:AK:90:ARG:NH2	27:AK:95:SER:O	2.19	0.76
58:XS:72:GLU:O	58:XS:76:HIS:ND1	2.19	0.76
9:8:110:GLU:OE2	9:8:114:ARG:NE	2.19	0.76
11:XA:2167:A:N6	11:XA:2212:C:OP2	2.19	0.76
11:XA:2187:C:O3'	49:XJ:106:LYS:NZ	2.19	0.75
17:AA:869:C:OP2	31:AO:97:ARG:NH2	2.19	0.75
40:AX:53:GLU:N	40:AX:67:HIS:O	2.20	0.75
17:AA:945:G:O2'	28:AL:154:ARG:NH2	2.18	0.75
63:XX:118:ILE:O	63:XX:168:ARG:NH1	2.19	0.75
23:AG:276:ARG:NH1	23:AG:373:ASP:OD2	2.20	0.75
41:AY:340:SER:OG	41:AY:377:ARG:NH2	2.19	0.75
44:XD:132:ASP:OD2	44:XD:135:ARG:NH1	2.20	0.75
56:XQ:165:GLU:OE2	56:XQ:170:ARG:NH2	2.20	0.75
11:XA:2537:G:O2'	11:XA:2634:U:OP2	2.04	0.75
15:A3:155:ARG:NH2	17:AA:1154:A:OP2	2.19	0.75
17:AA:1141:C:O2	17:AA:1162:A:N6	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:XR:122:ARG:NH2	57:XR:126:GLU:OE2	2.20	0.75
11:XA:1883:G:N7	46:XF:281:ARG:NH1	2.35	0.75
17:AA:947:U:OP1	28:AL:162:GLN:NE2	2.19	0.74
44:XD:111:ARG:NE	44:XD:165:ASN:OD1	2.19	0.74
46:XF:97:HIS:NE2	46:XF:101:MET:SD	2.61	0.74
20:AD:307:LYS:NZ	34:AR:103:TYR:OH	2.20	0.74
16:A4:269:HIS:O	16:A4:270:ARG:NE	2.20	0.74
52:XM:72:THR:OG1	52:XM:77:ARG:NH2	2.20	0.74
11:XA:2240:C:OP2	50:XK:71:LYS:NZ	2.20	0.74
47:XH:103:GLU:OE1	47:XH:104:ASN:ND2	2.21	0.74
1:0:181:ARG:NH1	1:0:186:THR:O	2.20	0.73
52:XM:53:HIS:O	52:XM:58:GLN:NE2	2.20	0.73
64:XY:76:GLN:NE2	64:XY:78:LYS:O	2.21	0.73
17:AA:942:A:N6	17:AA:1047:A:OP1	2.20	0.73
56:XQ:71:PRO:O	56:XQ:73:ARG:NH1	2.21	0.73
7:6:282:SER:OG	7:6:283:GLU:OE1	2.06	0.73
11:XA:3078:C:N4	11:XA:3079:G:O6	2.20	0.73
17:AA:1220:A:O2'	23:AG:395:LYS:O	2.07	0.73
20:AD:188:LYS:NZ	20:AD:190:GLU:OE2	2.21	0.73
7:6:117:VAL:O	7:6:121:ARG:NH2	2.21	0.73
53:XN:61:LYS:NZ	53:XN:65:GLU:OE2	2.22	0.73
17:AA:949:U:O3'	30:AN:29:ARG:NH1	2.22	0.73
23:AG:312:GLN:OE1	23:AG:345:ARG:NH2	2.21	0.73
38:AV:132:LYS:NZ	38:AV:166:GLU:OE1	2.21	0.73
4:3:168:ARG:NH2	4:3:170:ASN:OD1	2.20	0.73
11:XA:2248:U:OP1	57:XR:99:ARG:NH2	2.22	0.73
61:XV:150:SER:O	61:XV:152:ARG:NH1	2.22	0.73
25:AI:81:GLU:O	25:AI:148:ARG:NH1	2.22	0.73
49:XJ:154:ARG:NH1	49:XJ:155:VAL:O	2.22	0.73
11:XA:2191:A:N6	11:XA:2198:A:OP2	2.21	0.73
56:XQ:118:ARG:NH2	56:XQ:202:VAL:O	2.22	0.73
14:A2:32:ARG:NH1	17:AA:1599:A:OP2	2.22	0.73
16:A4:108:LEU:HD21	20:AD:154:VAL:HG12	1.68	0.72
17:AA:1014:A:O2'	17:AA:1031:G:O4'	2.07	0.72
10:9:74:VAL:O	64:XY:83:ALA:N	2.22	0.72
14:A2:12:ARG:NH2	17:AA:1125:A:O4'	2.22	0.72
4:3:169:ARG:NH2	11:XA:1892:A:OP1	2.21	0.72
23:AG:155:LYS:NZ	23:AG:217:ASP:OD2	2.22	0.72
11:XA:3220:A:OP1	45:XE:260:LYS:NZ	2.23	0.72
15:A3:145:LYS:NZ	17:AA:1581:G:O6	2.22	0.72
17:AA:1429:C:OP1	23:AG:388:ARG:NH2	2.23	0.72

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
6:5:149:ASN:ND2	6:5:152:GLU:OE2	2.22	0.71
16:A4:479:GLU:HA	16:A4:482:ILE:HD12	1.71	0.71
17:AA:1314:C:N3	22:AF:36:ARG:NH2	2.38	0.71
23:AG:117:PHE:O	23:AG:122:ARG:NH1	2.23	0.71
1:0:136:GLU:OE1	1:0:177:ARG:NH2	2.23	0.71
24:AH:74:LYS:N	24:AH:175:THR:O	2.23	0.71
15:A3:172:ASP:OD1	15:A3:175:ARG:NH1	2.23	0.71
52:XM:203:ARG:NH2	52:XM:261:ASP:O	2.23	0.71
11:XA:2458:A:OP2	54:XO:9:ILE:N	2.24	0.71
11:XA:2145:G:N3	58:XS:104:ARG:NH2	2.39	0.70
17:AA:668:U:O2'	31:AO:83:GLY:O	2.08	0.70
37:AU:77:GLU:OE1	37:AU:81:LYS:NZ	2.23	0.70
8:7:190:ASP:O	8:7:295:ARG:NH1	2.25	0.70
13:A1:81:VAL:O	13:A1:99:LYS:NZ	2.23	0.70
23:AG:200:LEU:O	23:AG:218:TYR:OH	2.10	0.70
11:XA:2558:A:O5'	17:AA:1001:C:N4	2.25	0.70
14:A2:9:ARG:NH2	17:AA:1021:U:OP2	2.25	0.70
33:AQ:55:GLU:OE2	33:AQ:59:ARG:NE	2.24	0.70
21:AE:54:HIS:NE2	21:AE:83:SER:O	2.24	0.70
11:XA:3151:A:N6	11:XA:3163:G:O2'	2.24	0.70
16:A4:470:GLN:OE1	16:A4:472:ASP:N	2.25	0.70
34:AR:305:HIS:HD2	34:AR:314:ALA:HB2	1.57	0.70
45:XE:54:SER:OG	45:XE:57:ASN:OD1	2.09	0.70
22:AF:52:ARG:NH2	23:AG:360:GLU:OE1	2.25	0.69
22:AF:119:LYS:NZ	40:AX:398:LEU:O	2.25	0.69
59:XT:157:ARG:NH1	59:XT:167:MET:SD	2.63	0.69
7:6:198:ALA:O	7:6:254:TYR:OH	2.08	0.69
17:AA:1454:G:OP2	23:AG:377:ARG:NH2	2.25	0.69
11:XA:2755:A:O2'	63:XX:112:ARG:NH2	2.25	0.69
11:XA:2643:G:O2'	11:XA:2645:G:OP2	2.10	0.69
38:AV:132:LYS:O	38:AV:136:GLY:N	2.25	0.69
59:XT:126:ASP:OD1	59:XT:127:MET:N	2.26	0.69
17:AA:1225:C:O2'	17:AA:1449:G:O2'	2.10	0.69
62:XW:62:HIS:N	62:XW:65:ASN:OD1	2.26	0.69
38:AV:173:PHE:O	38:AV:178:THR:OG1	2.11	0.69
16:A4:61:LYS:HE3	24:AH:67:ASP:HA	1.75	0.68
4:3:113:ARG:NH1	52:XM:75:TYR:O	2.27	0.68
11:XA:1755:A:O2'	47:XH:64:LEU:O	2.12	0.68
46:XF:220:ASP:O	46:XF:245:ALA:N	2.27	0.68
17:AA:1280:C:O3'	18:AB:210:ARG:NH2	2.27	0.68
48:XI:101:ASN:OD1	48:XI:151:ASN:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:XR:149:HIS:O	65:XZ:151:LEU:N	2.26	0.68
8:7:279:GLU:N	8:7:279:GLU:OE1	2.27	0.68
10:9:127:LEU:O	10:9:134:ASN:ND2	2.25	0.68
11:XA:2457:A:N3	54:XO:17:ARG:NH2	2.41	0.68
40:AX:56:PRO:O	40:AX:59:HIS:NE2	2.27	0.68
30:AN:62:ASP:OD1	30:AN:88:VAL:N	2.27	0.67
39:AW:132:GLU:O	39:AW:135:GLN:NE2	2.28	0.67
10:9:54:LYS:NZ	11:XA:2415:C:O3'	2.28	0.67
11:XA:1672:C:O2'	59:XT:149:ARG:O	2.13	0.67
11:XA:1889:C:OP1	52:XM:133:LYS:NZ	2.28	0.67
26:AJ:96:PRO:O	26:AJ:127:ARG:NH2	2.28	0.67
17:AA:703:A:OP2	37:AU:43:ASN:ND2	2.27	0.67
22:AF:126:TYR:O	22:AF:134:GLN:NE2	2.27	0.67
35:AS:61:GLN:NE2	35:AS:62:ASP:O	2.28	0.67
52:XM:148:PHE:O	52:XM:170:ASN:ND2	2.28	0.67
63:XX:150:LYS:HG3	63:XX:159:MET:CE	2.25	0.67
17:AA:1066:C:O2'	25:AI:187:ARG:O	2.11	0.67
41:AY:300:GLU:OE2	41:AY:304:TRP:NE1	2.28	0.67
49:XJ:27:GLY:O	49:XJ:58:LYS:NZ	2.28	0.67
4:3:179:LYS:O	7:6:370:ARG:NH2	2.28	0.66
11:XA:1742:G:O2'	11:XA:1754:G:O6	2.13	0.66
63:XX:220:GLU:N	63:XX:220:GLU:OE1	2.28	0.66
10:9:26:GLY:O	10:9:31:ARG:NH1	2.29	0.66
11:XA:2682:A:OP1	57:XR:34:ARG:NH2	2.29	0.66
63:XX:144:TYR:O	63:XX:148:THR:CG2	2.43	0.66
11:XA:2144:A:OP1	57:XR:57:ARG:NH1	2.28	0.66
64:XY:151:ASP:OD1	64:XY:154:ARG:NH2	2.27	0.66
51:XL:35:MET:N	51:XL:57:CYS:O	2.28	0.66
7:6:239:ASN:OD1	7:6:275:GLN:NE2	2.29	0.66
11:XA:1953:A:O2'	11:XA:2463:A:OP1	2.12	0.66
6:5:174:GLU:OE1	6:5:298:ASN:ND2	2.28	0.66
16:A4:478:TYR:CE2	16:A4:482:ILE:HD11	2.31	0.66
8:7:155:GLU:OE1	8:7:156:ARG:NH1	2.29	0.65
34:AR:135:ARG:NH2	34:AR:236:GLU:OE2	2.29	0.65
16:A4:62:LYS:O	24:AH:66:SER:N	2.29	0.65
11:XA:1749:C:OP2	11:XA:2899:C:O2'	2.13	0.65
17:AA:780:C:N3	28:AL:197:ARG:NH2	2.45	0.65
11:XA:1864:A:O3'	57:XR:13:ARG:NH1	2.29	0.65
11:XA:2531:U:O4	44:XD:246:ARG:NH2	2.29	0.65
21:AE:5:GLU:OE2	21:AE:96:HIS:ND1	2.29	0.65
16:A4:198:TYR:O	16:A4:239:ARG:NH1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:1231:A:O2'	17:AA:1236:C:N4	2.30	0.65
7:6:191:ASN:ND2	55:XP:137:GLU:O	2.30	0.65
11:XA:1730:U:OP1	47:XH:76:ARG:NH2	2.31	0.64
43:XB:1625:A:N7	55:XP:86:GLN:NE2	2.45	0.64
41:AY:303:GLN:NE2	41:AY:307:GLU:OE1	2.30	0.64
11:XA:2302:U:O2'	46:XF:147:ARG:NH1	2.31	0.64
11:XA:2192:A:OP1	49:XJ:142:ARG:NE	2.28	0.64
13:A1:169:ARG:O	13:A1:218:ASN:ND2	2.30	0.64
17:AA:1053:A:N1	17:AA:1100:C:O2'	2.30	0.64
17:AA:1389:G:N1	17:AA:1416:A:OP2	2.31	0.64
11:XA:2214:A:OP1	53:XN:31:LYS:NZ	2.30	0.64
16:A4:478:TYR:CD2	16:A4:482:ILE:HD11	2.32	0.64
17:AA:1287:A:OP2	20:AD:260:LYS:NZ	2.31	0.64
11:XA:2326:C:O2	54:XO:31:ASN:ND2	2.29	0.64
36:AT:109:ASN:ND2	36:AT:111:GLU:OE2	2.30	0.64
27:AK:28:HIS:NE2	42:AZ:60:GLU:OE2	2.30	0.63
17:AA:659:U:OP1	20:AD:226:ARG:NH2	2.30	0.63
23:AG:272:SER:OG	23:AG:347:ALA:O	2.15	0.63
18:AB:137:TYR:O	18:AB:264:ARG:NH2	2.31	0.63
17:AA:1143:C:N4	17:AA:1576:G:OP1	2.31	0.63
38:AV:47:HIS:N	38:AV:78:ASN:OD1	2.31	0.63
4:3:177:TYR:O	4:3:181:HIS:ND1	2.31	0.63
7:6:308:GLN:NE2	7:6:311:MET:SD	2.72	0.63
25:AI:79:LYS:N	25:AI:82:GLU:OE2	2.31	0.63
6:5:334:LYS:N	6:5:362:THR:OG1	2.31	0.63
38:AV:96:ARG:NH1	38:AV:101:CYS:SG	2.72	0.63
13:A1:154:THR:OG1	24:AH:172:VAL:O	2.13	0.62
17:AA:1366:C:O2'	17:AA:1419:G:O4'	2.14	0.62
60:XU:48:MET:O	60:XU:93:LYS:NZ	2.32	0.62
16:A4:455:ASN:O	16:A4:486:TYR:OH	2.17	0.62
11:XA:1747:G:OP2	11:XA:1749:C:N4	2.31	0.62
11:XA:3127:G:O2'	11:XA:3130:A:N6	2.32	0.62
48:XI:224:HIS:O	48:XI:228:GLN:N	2.27	0.62
11:XA:1805:A:OP2	61:XV:94:HIS:NE2	2.32	0.62
11:XA:2692:G:N1	11:XA:2696:A:OP2	2.29	0.62
16:A4:133:ALA:HB2	19:AC:148:LYS:CB	2.29	0.62
61:XV:147:SER:OG	61:XV:152:ARG:N	2.31	0.62
28:AL:149:ASP:OD2	28:AL:152:HIS:ND1	2.33	0.62
52:XM:153:ASN:ND2	52:XM:256:LEU:O	2.33	0.62
63:XX:144:TYR:O	63:XX:148:THR:HG22	2.00	0.62
11:XA:1694:U:O4'	64:XY:162:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:826:A:N7	26:AJ:55:ARG:NE	2.48	0.62
37:AU:110:GLN:O	37:AU:114:ARG:NE	2.31	0.62
50:XK:10:GLN:NE2	59:XT:203:LEU:O	2.32	0.62
8:7:238:ASP:OD1	8:7:239:PHE:N	2.33	0.61
17:AA:819:A:O2'	17:AA:831:U:O2'	2.14	0.61
40:AX:272:THR:OG1	40:AX:282:ILE:O	2.16	0.61
7:6:136:ARG:NH1	55:XP:137:GLU:OE2	2.32	0.61
36:AT:89:ASP:OD2	37:AU:120:ARG:NH2	2.32	0.61
54:XO:64:LYS:NZ	54:XO:97:TYR:O	2.31	0.61
10:9:106:ASP:OD1	10:9:107:GLY:N	2.32	0.61
12:A0:103:ASP:OD2	12:A0:105:THR:OG1	2.18	0.61
17:AA:1008:A:OP1	21:AE:50:ARG:NE	2.34	0.61
7:6:368:ARG:NH2	11:XA:2859:A:OP2	2.33	0.61
32:AP:49:ASP:OD2	39:AW:82:SER:N	2.33	0.61
44:XD:113:ARG:O	44:XD:147:ARG:NH1	2.34	0.61
7:6:282:SER:O	7:6:283:GLU:N	2.34	0.61
20:AD:178:GLU:OE2	20:AD:181:ARG:NH2	2.33	0.61
56:XQ:227:LYS:O	56:XQ:229:TRP:N	2.34	0.61
11:XA:2581:A:O2'	11:XA:2583:C:N4	2.34	0.61
58:XS:91:GLN:N	58:XS:91:GLN:OE1	2.33	0.61
6:5:200:ARG:NH1	6:5:234:ASP:OD2	2.33	0.61
10:9:134:ASN:OD1	10:9:135:PHE:N	2.34	0.61
11:XA:2195:A:O2'	11:XA:2196:A:O5'	2.17	0.61
12:A0:132:GLU:OE1	12:A0:205:ALA:N	2.34	0.61
17:AA:656:U:N3	17:AA:659:U:OP2	2.34	0.61
11:XA:2928:C:OP2	11:XA:3073:C:O2'	2.18	0.60
17:AA:950:A:OP2	30:AN:16:LYS:NZ	2.34	0.60
32:AP:65:CYS:SG	32:AP:68:CYS:N	2.74	0.60
11:XA:1761:A:O2'	11:XA:1762:A:O5'	2.20	0.60
13:A1:156:TYR:O	13:A1:167:ARG:NH1	2.35	0.60
47:XH:136:ASN:OD1	47:XH:137:LYS:N	2.35	0.60
46:XF:281:ARG:NH2	52:XM:128:THR:OG1	2.33	0.60
48:XI:51:THR:O	53:XN:250:ARG:NH1	2.35	0.60
63:XX:207:THR:N	63:XX:210:GLU:OE2	2.31	0.60
29:AM:64:LYS:NZ	34:AR:154:THR:OG1	2.35	0.60
6:5:361:THR:OG1	6:5:363:ASP:OD1	2.18	0.60
45:XE:69:ASP:OD1	45:XE:154:ARG:NH1	2.34	0.60
17:AA:1108:C:N4	17:AA:1125:A:N7	2.50	0.59
17:AA:1124:A:OP2	21:AE:121:LYS:NZ	2.35	0.59
56:XQ:103:ARG:NH2	56:XQ:167:TYR:OH	2.33	0.59
16:A4:99:SER:N	16:A4:102:GLU:OE2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2082:G:N2	65:XZ:88:MET:SD	2.72	0.59
61:XV:19:TYR:OH	61:XV:31:ASP:OD2	2.21	0.59
16:A4:339:LEU:O	16:A4:374:HIS:NE2	2.36	0.59
16:A4:443:ASP:O	16:A4:446:LYS:NZ	2.35	0.59
11:XA:1737:A:N6	11:XA:1760:G:O2'	2.36	0.59
38:AV:222:SER:OG	38:AV:277:ARG:NH1	2.35	0.59
20:AD:192:GLY:O	31:AO:78:ARG:NH2	2.36	0.58
10:9:16:ASP:OD1	10:9:25:ARG:NH1	2.36	0.58
11:XA:1699:C:OP1	64:XY:197:LYS:NZ	2.36	0.58
11:XA:2990:A:O2'	11:XA:2992:G:OP2	2.19	0.58
7:6:106:ARG:NH1	43:XB:1621:A:OP2	2.36	0.58
11:XA:1936:A:O5'	11:XA:1937:A:N6	2.37	0.58
7:6:124:ARG:NH2	9:8:112:GLU:OE1	2.33	0.58
11:XA:2104:A:OP1	53:XN:73:ARG:NH1	2.36	0.58
13:A1:256:SER:O	13:A1:260:ARG:NH1	2.36	0.58
17:AA:700:A:OP2	37:AU:27:ARG:NH1	2.36	0.58
20:AD:250:GLY:N	20:AD:326:LEU:O	2.36	0.58
11:XA:2182:G:N2	11:XA:2199:A:N3	2.52	0.58
15:A3:142:LYS:NZ	17:AA:1490:U:OP1	2.30	0.58
20:AD:286:GLU:O	20:AD:288:HIS:ND1	2.34	0.58
17:AA:1320:G:OP1	19:AC:41:ARG:NH1	2.34	0.58
9:8:134:ASP:OD1	9:8:137:ARG:NH1	2.37	0.58
11:XA:2506:A:N6	11:XA:3093:C:O4'	2.35	0.58
17:AA:819:A:HO2'	17:AA:831:U:HO2'	1.49	0.58
6:5:80:ARG:NH2	6:5:82:TYR:OH	2.36	0.57
16:A4:61:LYS:HB2	24:AH:65:ILE:CG2	2.33	0.57
11:XA:2727:C:O2'	11:XA:2815:G:N2	2.36	0.57
18:AB:153:TYR:O	18:AB:157:ASN:ND2	2.37	0.57
37:AU:58:GLU:OE2	37:AU:62:HIS:NE2	2.37	0.57
46:XF:75:GLU:OE2	46:XF:210:ARG:NE	2.34	0.57
22:AF:130:SER:OG	22:AF:133:GLU:OE1	2.22	0.57
60:XU:11:ARG:NH2	61:XV:212:LYS:O	2.37	0.57
60:XU:75:GLY:N	60:XU:91:ASP:OD1	2.34	0.57
56:XQ:260:TRP:O	56:XQ:262:GLN:NE2	2.37	0.57
2:1:23:GLU:N	2:1:23:GLU:OE1	2.35	0.57
61:XV:136:ARG:O	61:XV:143:ARG:NH2	2.38	0.57
36:AT:95:ASN:OD1	36:AT:96:LYS:N	2.37	0.57
17:AA:1483:C:N3	17:AA:1567:A:N1	2.53	0.57
37:AU:178:GLU:N	37:AU:178:GLU:OE1	2.37	0.57
16:A4:61:LYS:HE2	24:AH:66:SER:O	2.05	0.57
16:A4:108:LEU:HD21	20:AD:154:VAL:HG11	1.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:XX:83:GLU:N	63:XX:83:GLU:OE1	2.38	0.57
12:A0:50:LEU:O	12:A0:55:TRP:NE1	2.38	0.56
16:A4:59:ILE:HG21	24:AH:69:PRO:CB	2.34	0.56
17:AA:1508:C:N3	17:AA:1542:U:O4	2.38	0.56
11:XA:1787:G:N2	11:XA:1790:A:OP2	2.30	0.56
11:XA:3175:A:OP2	11:XA:3187:C:N4	2.39	0.56
49:XJ:85:PRO:O	49:XJ:124:LYS:NZ	2.38	0.56
55:XP:84:ARG:NH1	55:XP:124:CYS:SG	2.78	0.56
53:XN:78:GLU:OE2	53:XN:158:ARG:NE	2.37	0.56
11:XA:1728:U:O2	63:XX:96:LYS:NZ	2.39	0.56
11:XA:2663:C:OP1	54:XO:13:ARG:NH1	2.36	0.56
14:A2:24:ASN:OD1	14:A2:25:LYS:N	2.38	0.56
64:XY:206:ASP:OD1	64:XY:207:HIS:N	2.39	0.56
23:AG:362:GLU:OE2	23:AG:365:ARG:NH1	2.38	0.56
12:A0:96:ARG:N	12:A0:117:ILE:O	2.39	0.56
17:AA:1039:A:O3'	28:AL:135:LYS:NZ	2.39	0.56
2:1:47:ASP:O	2:1:51:LYS:N	2.39	0.56
11:XA:2016:C:OP1	11:XA:2039:A:O2'	2.22	0.56
13:A1:118:ALA:O	13:A1:122:HIS:ND1	2.39	0.56
17:AA:1293:C:N4	33:AQ:80:ARG:O	2.39	0.55
23:AG:129:GLU:N	23:AG:129:GLU:OE1	2.39	0.55
46:XF:167:MET:SD	46:XF:276:GLN:NE2	2.77	0.55
12:A0:101:ARG:NH1	17:AA:1528:A:OP1	2.39	0.55
17:AA:1176:G:O6	17:AA:1477:U:O2	2.25	0.55
47:XH:108:ARG:NH1	47:XH:143:GLU:OE2	2.39	0.55
41:AY:292:GLN:OE1	41:AY:292:GLN:N	2.39	0.55
11:XA:1770:G:OP2	57:XR:11:ARG:NH1	2.38	0.55
16:A4:175:GLN:O	16:A4:180:GLY:N	2.40	0.55
56:XQ:84:ARG:NH1	56:XQ:271:ARG:O	2.39	0.55
16:A4:264:ARG:HE	16:A4:293:THR:HG22	1.72	0.55
11:XA:1864:A:OP1	57:XR:17:ARG:NH1	2.39	0.55
44:XD:64:VAL:O	44:XD:80:ARG:NH2	2.40	0.55
60:XU:38:ASP:OD1	60:XU:99:LEU:N	2.40	0.55
17:AA:949:U:O2'	30:AN:29:ARG:NH1	2.40	0.54
36:AT:9:ILE:O	36:AT:12:THR:OG1	2.24	0.54
2:1:36:ARG:NH2	2:1:64:SER:OG	2.39	0.54
59:XT:84:LYS:N	59:XT:172:CYS:SG	2.80	0.54
7:6:283:GLU:OE1	7:6:283:GLU:N	2.40	0.54
11:XA:2400:C:O2'	11:XA:2401:A:O5'	2.23	0.54
17:AA:769:G:OP2	30:AN:73:ARG:NH2	2.40	0.54
22:AF:129:ALA:O	22:AF:134:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AD:257:SER:OG	20:AD:271:ALA:O	2.26	0.54
11:XA:1955:G:O2'	11:XA:1958:G:O2'	2.21	0.54
25:AI:158:ARG:NH2	25:AI:177:ASP:OD2	2.41	0.54
47:XH:95:GLU:OE2	47:XH:112:VAL:N	2.41	0.54
58:XS:127:ARG:NH2	58:XS:157:GLU:OE1	2.36	0.54
59:XT:95:ARG:NH2	59:XT:145:SER:O	2.40	0.54
1:0:91:ARG:HG3	1:0:95:ARG:HE	1.72	0.54
17:AA:1289:G:O2'	17:AA:1297:G:OP2	2.23	0.54
6:5:51:GLU:OE1	6:5:51:GLU:N	2.41	0.54
39:AW:103:ARG:O	39:AW:115:ASP:N	2.40	0.54
17:AA:1284:U:O2'	20:AD:347:GLN:NE2	2.40	0.53
31:AO:149:ARG:O	31:AO:152:GLN:NE2	2.41	0.53
34:AR:247:HIS:O	34:AR:251:GLU:OE1	2.26	0.53
11:XA:2139:U:O4	65:XZ:77:ARG:NH1	2.41	0.53
11:XA:2151:A:OP2	11:XA:2249:G:N1	2.33	0.53
40:AX:327:GLU:N	40:AX:327:GLU:OE1	2.41	0.53
63:XX:144:TYR:O	63:XX:148:THR:N	2.40	0.53
12:A0:130:GLU:OE1	12:A0:130:GLU:N	2.36	0.53
17:AA:702:C:O2'	17:AA:842:C:O2	2.24	0.53
53:XN:218:ILE:HG22	53:XN:226:ILE:HD11	1.91	0.53
31:AO:176:ASP:OD1	31:AO:177:PHE:N	2.41	0.53
16:A4:116:VAL:HG11	20:AD:141:TRP:HZ3	1.74	0.53
65:XZ:98:GLN:OE1	65:XZ:100:HIS:NE2	2.41	0.53
11:XA:1878:U:O3'	46:XF:92:ARG:NH2	2.42	0.53
13:A1:87:MET:O	13:A1:102:ASN:ND2	2.42	0.53
21:AE:85:ASP:OD1	44:XD:171:ARG:NH1	2.38	0.53
28:AL:169:ASN:OD1	28:AL:170:LEU:N	2.42	0.53
40:AX:255:MET:SD	40:AX:255:MET:N	2.81	0.53
54:XO:18:MET:HE1	54:XO:48:ARG:HE	1.72	0.53
11:XA:2125:C:OP2	58:XS:178:LYS:NZ	2.28	0.53
24:AH:161:GLN:HA	24:AH:164:LEU:CD1	2.38	0.53
38:AV:159:ASP:OD1	38:AV:160:ALA:N	2.40	0.53
48:XI:181:ILE:O	48:XI:184:THR:N	2.40	0.53
7:6:360:ARG:NH2	11:XA:2869:A:N7	2.57	0.53
38:AV:131:ASN:ND2	38:AV:134:GLN:OE1	2.42	0.53
11:XA:2529:U:O2'	44:XD:206:TYR:O	2.27	0.53
12:A0:82:ARG:NH2	12:A0:138:ASP:O	2.38	0.53
21:AE:14:GLN:N	21:AE:17:GLU:OE2	2.37	0.53
38:AV:108:THR:O	38:AV:111:THR:OG1	2.23	0.53
57:XR:51:VAL:O	57:XR:54:THR:OG1	2.26	0.53
11:XA:1884:G:N3	11:XA:1895:C:O2'	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:994:A:O2'	22:AF:166:ARG:NH2	2.40	0.52
8:7:36:SER:N	8:7:39:GLU:OE2	2.42	0.52
11:XA:2515:U:O2'	44:XD:282:ALA:O	2.27	0.52
54:XO:113:ARG:NH1	54:XO:116:ASP:OD2	2.43	0.52
11:XA:2305:U:OP1	59:XT:149:ARG:NH1	2.41	0.52
17:AA:766:G:OP2	30:AN:76:HIS:NE2	2.33	0.52
13:A1:146:HIS:O	24:AH:179:GLN:NE2	2.43	0.52
16:A4:61:LYS:CE	24:AH:67:ASP:HA	2.39	0.52
17:AA:1285:G:O2'	17:AA:1286:A:O4'	2.24	0.52
11:XA:2029:A:N6	11:XA:2125:C:OP1	2.41	0.52
11:XA:3011:A:O2'	11:XA:3173:G:N2	2.42	0.52
13:A1:54:PRO:HD2	16:A4:518:GLU:OE2	2.10	0.52
22:AF:122:GLN:NE2	22:AF:138:GLU:O	2.43	0.52
14:A2:9:ARG:O	14:A2:20:VAL:N	2.36	0.52
17:AA:722:C:N3	17:AA:798:C:O2'	2.40	0.52
8:7:262:ASP:OD1	8:7:263:VAL:N	2.43	0.52
12:A0:30:ASP:OD1	12:A0:31:SER:N	2.42	0.52
45:XE:316:PHE:HB3	45:XE:317:PRO:HD3	1.92	0.52
54:XO:129:CYS:SG	54:XO:130:LEU:N	2.83	0.52
7:6:367:ASP:OD1	7:6:370:ARG:NH1	2.43	0.51
56:XQ:268:ASP:OD1	56:XQ:269:MET:N	2.43	0.51
16:A4:108:LEU:CD2	20:AD:154:VAL:HG11	2.37	0.51
36:AT:130:GLY:N	36:AT:135:CYS:SG	2.83	0.51
53:XN:177:ASP:OD1	53:XN:178:GLN:N	2.43	0.51
11:XA:2218:C:OP2	48:XI:129:GLN:NE2	2.38	0.51
3:2:82:ARG:NH2	11:XA:1790:A:OP1	2.44	0.51
16:A4:478:TYR:O	16:A4:482:ILE:HG13	2.11	0.51
50:XK:9:GLN:NE2	50:XK:13:THR:OG1	2.43	0.51
50:XK:15:ALA:O	50:XK:44:LYS:NZ	2.43	0.51
54:XO:18:MET:CE	54:XO:48:ARG:HE	2.23	0.51
17:AA:723:A:OP1	17:AA:724:C:N4	2.38	0.51
19:AC:113:ARG:NE	24:AH:164:LEU:O	2.44	0.51
29:AM:49:GLU:OE1	29:AM:50:GLN:N	2.44	0.51
47:XH:120:ARG:NH2	63:XX:136:ASP:OD2	2.44	0.51
54:XO:112:ASN:ND2	59:XT:110:ASP:OD2	2.43	0.51
16:A4:98:ALA:N	16:A4:102:GLU:OE2	2.44	0.51
28:AL:142:HIS:NE2	28:AL:149:ASP:OD2	2.40	0.51
11:XA:2614:U:O3'	51:XL:53:ARG:NH1	2.44	0.51
1:0:104:LYS:O	59:XT:105:GLN:NE2	2.39	0.51
54:XO:82:GLU:OE1	54:XO:82:GLU:N	2.33	0.51
63:XX:36:ARG:NE	63:XX:151:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2182:G:O2'	11:XA:2183:C:O4'	2.22	0.51
25:AI:94:ASN:OD1	25:AI:95:THR:N	2.44	0.51
30:AN:53:ASP:OD2	30:AN:57:GLN:N	2.44	0.51
34:AR:140:ASP:OD1	34:AR:141:VAL:N	2.44	0.51
46:XF:102:TRP:NE1	46:XF:163:TYR:O	2.44	0.51
40:AX:161:TRP:NE1	40:AX:183:GLU:OE2	2.44	0.50
6:5:337:GLU:N	6:5:337:GLU:OE1	2.44	0.50
11:XA:1907:A:O2'	46:XF:130:GLN:OE1	2.23	0.50
17:AA:1048:C:O2'	17:AA:1049:A:OP1	2.22	0.50
40:AX:175:LYS:HE3	40:AX:175:LYS:HA	1.93	0.50
52:XM:88:SER:O	52:XM:134:ARG:NE	2.44	0.50
62:XW:115:ASP:OD1	62:XW:116:LEU:N	2.44	0.50
11:XA:3160:A:OP1	45:XE:213:LYS:NZ	2.36	0.50
47:XH:120:ARG:NE	63:XX:136:ASP:OD2	2.43	0.50
61:XV:66:GLU:N	61:XV:66:GLU:OE1	2.44	0.50
8:7:290:GLN:N	8:7:291:PRO:HD2	2.26	0.50
11:XA:1816:G:OP2	57:XR:37:ARG:NE	2.43	0.50
17:AA:1433:A:N3	17:AA:1458:A:N6	2.60	0.50
40:AX:157:ASP:OD1	40:AX:158:ALA:N	2.45	0.50
45:XE:334:ASP:OD1	45:XE:335:GLU:N	2.44	0.50
11:XA:2166:C:N4	11:XA:2212:C:OP2	2.45	0.50
17:AA:982:A:N6	17:AA:1007:G:O6	2.45	0.50
29:AM:55:ASP:OD2	36:AT:146:GLN:NE2	2.45	0.50
33:AQ:23:TYR:O	33:AQ:27:ASN:ND2	2.44	0.50
46:XF:250:VAL:HA	46:XF:253:MET:HG2	1.94	0.50
6:5:300:ARG:HA	6:5:303:ARG:HE	1.77	0.50
6:5:306:PRO:O	6:5:310:ARG:NE	2.44	0.50
11:XA:3218:A:OP2	45:XE:212:GLY:N	2.44	0.50
20:AD:320:ILE:HA	20:AD:323:ILE:HG12	1.94	0.50
46:XF:292:ASP:OD1	46:XF:293:PHE:N	2.45	0.50
12:A0:62:SER:OG	12:A0:63:ARG:N	2.45	0.49
17:AA:1278:C:OP2	20:AD:269:ARG:NH1	2.44	0.49
11:XA:2813:U:N3	11:XA:2817:G:OP2	2.42	0.49
11:XA:3148:C:OP1	45:XE:211:ILE:HD12	2.12	0.49
53:XN:202:GLN:NE2	53:XN:248:PRO:O	2.42	0.49
1:0:138:ARG:HA	1:0:141:ILE:HG12	1.94	0.49
47:XH:131:TYR:O	47:XH:136:ASN:ND2	2.41	0.49
57:XR:17:ARG:HA	57:XR:20:ARG:HG2	1.94	0.49
11:XA:2187:C:O2'	49:XJ:106:LYS:NZ	2.44	0.49
20:AD:343:LEU:O	20:AD:347:GLN:OE1	2.31	0.49
3:2:70:LEU:O	64:XY:198:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:1855:A:N6	11:XA:2697:G:OP1	2.45	0.49
11:XA:2295:C:O2'	11:XA:2297:A:OP1	2.25	0.49
14:A2:113:ASN:OD1	14:A2:114:LYS:N	2.44	0.49
36:AT:97:GLU:OE1	36:AT:97:GLU:N	2.44	0.49
11:XA:2384:A:N1	11:XA:2409:A:N6	2.59	0.49
17:AA:1046:A:O2'	17:AA:1048:C:OP1	2.30	0.49
42:AZ:54:ASN:ND2	42:AZ:57:THR:OG1	2.45	0.49
51:XL:32:ILE:O	51:XL:67:GLY:N	2.44	0.49
63:XX:150:LYS:HG3	63:XX:159:MET:HE2	1.93	0.49
13:A1:142:LYS:O	13:A1:146:HIS:ND1	2.41	0.49
31:AO:176:ASP:OD1	31:AO:178:SER:N	2.45	0.49
17:AA:1050:C:OP2	28:AL:198:ARG:NH1	2.42	0.49
23:AG:171:ASN:O	23:AG:175:HIS:ND1	2.45	0.49
6:5:144:ARG:NH2	6:5:194:LYS:O	2.46	0.49
18:AB:202:ILE:O	18:AB:202:ILE:HG22	2.12	0.49
36:AT:111:GLU:O	36:AT:115:GLU:OE1	2.31	0.49
38:AV:123:ASP:OD1	38:AV:124:LYS:N	2.44	0.49
45:XE:63:GLN:NE2	45:XE:67:ASP:OD2	2.46	0.49
63:XX:148:THR:HG23	63:XX:148:THR:O	2.12	0.49
11:XA:2288:A:O2'	46:XF:101:MET:SD	2.71	0.48
58:XS:86:MET:O	58:XS:89:THR:OG1	2.26	0.48
64:XY:97:ASP:OD1	64:XY:98:LEU:N	2.46	0.48
11:XA:2386:C:OP2	44:XD:71:LYS:NZ	2.41	0.48
11:XA:2674:U:OP1	59:XT:112:LYS:NZ	2.45	0.48
19:AC:45:SER:N	19:AC:167:LEU:O	2.43	0.48
45:XE:119:VAL:HG21	45:XE:284:TYR:HB3	1.95	0.48
57:XR:36:ASN:OD1	57:XR:37:ARG:N	2.46	0.48
61:XV:132:GLU:O	61:XV:148:THR:OG1	2.30	0.48
8:7:94:HIS:NE2	59:XT:135:GLU:OE2	2.46	0.48
11:XA:1940:A:OP1	11:XA:2495:U:O2'	2.21	0.48
11:XA:1957:A:OP2	88:XA:5144:H8Q:C28	2.61	0.48
11:XA:2025:C:OP2	58:XS:182:LYS:NZ	2.46	0.48
17:AA:1234:C:O2'	17:AA:1235:U:OP1	2.27	0.48
55:XP:161:GLN:HA	55:XP:164:MET:SD	2.53	0.48
6:5:270:ILE:HG22	6:5:270:ILE:O	2.13	0.48
43:XB:1644:G:O6	55:XP:87:HIS:NE2	2.36	0.48
46:XF:194:GLU:OE1	46:XF:194:GLU:N	2.46	0.48
60:XU:14:GLY:O	61:XV:208:ARG:NE	2.47	0.48
19:AC:84:GLU:OE2	27:AK:105:ARG:NH1	2.46	0.48
38:AV:79:ILE:HD11	38:AV:88:ALA:HB2	1.95	0.48
56:XQ:108:ILE:O	56:XQ:108:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:84:THR:OG1	64:XY:88:GLN:NE2	2.43	0.48
17:AA:918:A:O2'	17:AA:919:A:O4'	2.30	0.48
18:AB:156:GLU:OE1	23:AG:163:HIS:ND1	2.47	0.48
19:AC:113:ARG:NH2	24:AH:166:GLU:OE2	2.47	0.48
55:XP:71:PHE:HB3	55:XP:72:PRO:HD3	1.96	0.48
6:5:151:ASP:OD1	6:5:152:GLU:N	2.46	0.48
6:5:182:ASP:OD1	6:5:183:ASN:N	2.47	0.48
11:XA:1708:A:O5'	64:XY:192:LYS:NZ	2.45	0.48
11:XA:1939:G:O4'	44:XD:259:LYS:NZ	2.43	0.48
57:XR:57:ARG:O	57:XR:61:LYS:HG2	2.13	0.48
63:XX:207:THR:OG1	63:XX:210:GLU:OE1	2.32	0.48
64:XY:94:SER:OG	64:XY:95:ASN:N	2.47	0.48
11:XA:2029:A:O2'	11:XA:2030:U:OP1	2.29	0.48
17:AA:1478:A:N6	17:AA:1565:A:O2'	2.47	0.48
34:AR:162:SER:O	34:AR:170:ARG:NH2	2.45	0.48
64:XY:154:ARG:NH1	64:XY:160:GLN:O	2.47	0.48
35:AS:7:GLU:N	35:AS:7:GLU:OE1	2.45	0.48
65:XZ:98:GLN:NE2	65:XZ:99:VAL:O	2.47	0.48
7:6:39:ASP:OD1	7:6:40:ILE:N	2.47	0.47
8:7:143:TRP:HE3	8:7:179:PHE:HB3	1.79	0.47
13:A1:216:ARG:NH2	41:AY:326:SER:O	2.39	0.47
34:AR:221:GLN:OE1	34:AR:223:ARG:NH2	2.47	0.47
16:A4:59:ILE:CG2	24:AH:69:PRO:HB2	2.41	0.47
17:AA:1483:C:C4	17:AA:1567:A:N1	2.82	0.47
38:AV:235:GLU:O	38:AV:239:GLY:N	2.44	0.47
48:XI:181:ILE:O	48:XI:184:THR:OG1	2.32	0.47
55:XP:110:ALA:O	55:XP:113:LYS:NZ	2.43	0.47
56:XQ:283:TRP:O	56:XQ:287:GLU:OE1	2.32	0.47
17:AA:1282:G:N2	17:AA:1286:A:OP2	2.38	0.47
22:AF:155:MET:SD	22:AF:179:ARG:NH1	2.87	0.47
49:XJ:113:THR:OG1	49:XJ:116:HIS:ND1	2.38	0.47
6:5:214:ASN:ND2	6:5:365:ASP:OD2	2.47	0.47
9:8:186:GLN:N	9:8:186:GLN:OE1	2.47	0.47
17:AA:1526:U:O2'	17:AA:1527:A:O4'	2.32	0.47
34:AR:308:HIS:C	34:AR:310:ASP:H	2.18	0.47
35:AS:104:THR:O	35:AS:108:LYS:HG2	2.15	0.47
38:AV:144:PHE:CZ	38:AV:167:VAL:HG21	2.49	0.47
62:XW:115:ASP:O	62:XW:119:ARG:NE	2.45	0.47
11:XA:1877:U:O3'	52:XM:30:ASN:ND2	2.48	0.47
17:AA:1221:A:OP2	17:AA:1222:A:O2'	2.25	0.47
29:AM:111:ARG:NH2	31:AO:232:PRO:O	2.47	0.47

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
35:AS:6:LEU:O	35:AS:15:ARG:NH1	2.48	0.47
40:AX:174:ASN:O	40:AX:175:LYS:HD2	2.14	0.47
11:XA:1844:A:OP2	57:XR:48:ARG:NH2	2.36	0.47
11:XA:2195:A:HO2'	11:XA:2196:A:P	2.37	0.47
11:XA:2714:A:OP2	45:XE:239:ARG:NH1	2.46	0.47
40:AX:297:MET:O	40:AX:297:MET:HG2	2.14	0.47
44:XD:194:ASN:ND2	44:XD:245:GLY:O	2.48	0.47
54:XO:41:ARG:NE	54:XO:124:GLU:OE1	2.42	0.47
54:XO:140:SER:O	54:XO:146:ASN:ND2	2.48	0.47
64:XY:87:CYS:SG	64:XY:91:ARG:NH2	2.88	0.47
2:1:34:ARG:NH2	2:1:38:ARG:O	2.47	0.47
8:7:83:LYS:NZ	8:7:120:THR:O	2.46	0.47
15:A3:143:TYR:OH	17:AA:1145:A:OP1	2.33	0.47
16:A4:61:LYS:HB3	24:AH:66:SER:O	2.14	0.47
16:A4:366:GLU:OE1	16:A4:366:GLU:N	2.42	0.47
17:AA:806:C:OP2	17:AA:807:A:N6	2.34	0.47
18:AB:164:GLU:OE1	23:AG:145:ARG:NH2	2.48	0.47
34:AR:305:HIS:HD2	34:AR:314:ALA:CB	2.25	0.47
45:XE:145:LEU:HD13	45:XE:181:ILE:HG21	1.96	0.47
50:XK:130:ASP:OD1	50:XK:131:GLU:N	2.44	0.47
63:XX:82:GLY:N	63:XX:83:GLU:OE1	2.48	0.47
11:XA:2028:G:N1	11:XA:2264:A:OP2	2.37	0.47
23:AG:382:PRO:O	24:AH:131:ARG:NH1	2.47	0.47
62:XW:112:GLU:O	62:XW:115:ASP:OD1	2.33	0.47
19:AC:103:CYS:SG	19:AC:126:GLN:NE2	2.88	0.47
40:AX:346:SER:OG	40:AX:347:ASN:N	2.47	0.47
46:XF:167:MET:SD	46:XF:279:ARG:NH1	2.88	0.47
7:6:133:ASP:OD1	7:6:134:ALA:N	2.48	0.47
8:7:259:ASP:OD1	8:7:260:PHE:N	2.48	0.47
8:7:306:LEU:O	8:7:306:LEU:HG	2.15	0.47
16:A4:95:LEU:HD13	19:AC:129:PRO:HB3	1.97	0.47
17:AA:864:U:O4	17:AA:865:A:N6	2.48	0.47
38:AV:201:GLU:OE1	38:AV:233:LYS:NZ	2.48	0.47
6:5:201:ARG:NH1	6:5:418:TYR:O	2.45	0.46
6:5:47:ASP:OD1	6:5:48:ARG:N	2.48	0.46
10:9:23:SER:O	10:9:31:ARG:HG2	2.15	0.46
11:XA:2234:C:O2'	11:XA:2235:C:OP2	2.33	0.46
17:AA:989:U:OP1	25:AI:94:ASN:ND2	2.48	0.46
21:AE:47:LEU:N	21:AE:59:ASN:O	2.44	0.46
27:AK:58:ARG:NE	27:AK:72:ASP:OD1	2.46	0.46
11:XA:1791:G:HO2'	11:XA:2006:C:HO2'	1.62	0.46

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
22:AF:35:SER:OG	22:AF:36:ARG:N	2.49	0.46
22:AF:201:MET:N	22:AF:202:PRO:HD2	2.30	0.46
31:AO:81:HIS:ND1	31:AO:82:LYS:O	2.49	0.46
46:XF:215:SER:OG	46:XF:257:GLN:N	2.40	0.46
47:XH:135:GLU:OE1	47:XH:135:GLU:N	2.48	0.46
60:XU:49:THR:O	60:XU:52:ASP:OD1	2.34	0.46
11:XA:2575:U:O2	11:XA:2582:A:N6	2.48	0.46
16:A4:68:VAL:HG13	41:AY:302:ILE:HG23	1.96	0.46
24:AH:75:ARG:N	24:AH:175:THR:OG1	2.49	0.46
30:AN:93:ASP:OD1	30:AN:96:THR:OG1	2.33	0.46
48:XI:182:ASP:OD1	48:XI:184:THR:OG1	2.31	0.46
5:4:89:TYR:CE1	5:4:101:ARG:HG3	2.50	0.46
7:6:280:ASP:OD1	7:6:281:PHE:N	2.49	0.46
21:AE:115:GLU:N	21:AE:115:GLU:OE1	2.48	0.46
26:AJ:50:GLY:O	26:AJ:89:ARG:NH1	2.48	0.46
44:XD:253:ASN:OD1	44:XD:254:LYS:N	2.47	0.46
45:XE:103:LYS:O	45:XE:294:ASN:N	2.47	0.46
6:5:393:LYS:O	6:5:396:VAL:HG12	2.16	0.46
11:XA:3119:C:C2	11:XA:3120:C:C5	3.03	0.46
17:AA:835:C:N4	17:AA:851:A:OP2	2.45	0.46
17:AA:1193:U:O2’	22:AF:178:ARG:NH1	2.49	0.46
18:AB:219:THR:O	18:AB:233:THR:OG1	2.32	0.46
21:AE:38:ASP:OD1	21:AE:39:LEU:N	2.46	0.46
21:AE:53:ALA:N	21:AE:56:GLN:O	2.47	0.46
41:AY:368:GLN:O	41:AY:371:GLU:HG2	2.16	0.46
49:XJ:107:GLU:OE1	49:XJ:109:ALA:N	2.48	0.46
60:XU:9:LEU:N	64:XY:183:GLN:OE1	2.48	0.46
11:XA:3076:A:N1	11:XA:3093:C:N4	2.62	0.46
17:AA:1589:C:OP1	25:AI:187:ARG:NH1	2.49	0.46
40:AX:130:LYS:O	40:AX:130:LYS:HG3	2.16	0.46
40:AX:393:ARG:O	40:AX:397:TYR:CD2	2.69	0.46
11:XA:2310:G:N2	11:XA:2676:A:OP2	2.40	0.46
11:XA:2665:U:OP2	54:XO:17:ARG:HD2	2.16	0.46
17:AA:745:A:C4	17:AA:746:A:C8	3.04	0.46
24:AH:89:ASP:OD1	24:AH:141:ARG:NH1	2.49	0.46
43:XB:1620:A:N3	43:XB:1620:A:H2’	2.31	0.46
56:XQ:226:PRO:O	56:XQ:229:TRP:NE1	2.49	0.46
64:XY:130:GLU:O	64:XY:133:ASP:OD1	2.34	0.46
11:XA:2139:U:OP2	65:XZ:74:SER:N	2.38	0.46
11:XA:2017:U:O2’	11:XA:2723:A:N1	2.47	0.45
11:XA:2171:U:N3	11:XA:2198:A:N7	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:3040:G:N3	11:XA:3070:G:H1'	2.30	0.45
18:AB:160:ARG:NE	18:AB:160:ARG:HA	2.31	0.45
34:AR:202:ARG:NE	34:AR:233:ALA:O	2.41	0.45
60:XU:61:TYR:O	60:XU:62:ASN:OD1	2.34	0.45
7:6:120:GLU:OE2	55:XP:116:TYR:OH	2.32	0.45
13:A1:152:ASP:N	13:A1:152:ASP:OD1	2.47	0.45
16:A4:66:ASP:OD1	16:A4:67:LYS:N	2.49	0.45
16:A4:556:LYS:HD3	16:A4:595:MET:HE1	1.98	0.45
29:AM:87:MET:SD	29:AM:88:GLU:N	2.89	0.45
36:AT:7:PHE:HB2	36:AT:10:ARG:HE	1.80	0.45
3:2:60:ARG:HD2	3:2:92:HIS:CE1	2.52	0.45
11:XA:2802:A:H2'	11:XA:2803:A:O4'	2.16	0.45
11:XA:2826:G:OP1	62:XW:49:ARG:NH1	2.43	0.45
11:XA:2939:C:H2'	11:XA:2940:A:O4'	2.16	0.45
11:XA:3025:A:C2	11:XA:3026:U:C5	3.04	0.45
16:A4:164:ARG:H	16:A4:167:LYS:HE3	1.82	0.45
17:AA:682:A:N6	17:AA:865:A:H61	2.14	0.45
17:AA:889:G:N1	17:AA:905:A:OP2	2.40	0.45
11:XA:2623:A:HO2'	17:AA:1549:G:HO2'	1.61	0.45
11:XA:2724:G:OP1	46:XF:131:LYS:NZ	2.37	0.45
14:A2:42:GLU:N	22:AF:241:TRP:O	2.49	0.45
17:AA:663:A:H2'	17:AA:664:G:H8	1.82	0.45
23:AG:264:GLU:O	23:AG:265:GLN:HG2	2.15	0.45
63:XX:39:THR:N	63:XX:152:ASP:OD1	2.38	0.45
1:0:91:ARG:NH2	11:XA:1818:A:OP2	2.41	0.45
8:7:51:GLU:OE2	8:7:54:ARG:NH2	2.42	0.45
11:XA:3012:U:O4'	11:XA:3173:G:N2	2.46	0.45
26:AJ:49:LEU:HD23	26:AJ:50:GLY:H	1.82	0.45
37:AU:129:ARG:O	37:AU:133:GLN:OE1	2.35	0.45
55:XP:113:LYS:HG3	55:XP:114:HIS:N	2.31	0.45
11:XA:1723:A:N6	11:XA:1726:C:OP2	2.49	0.45
11:XA:3152:C:OP1	56:XQ:141:SER:OG	2.30	0.45
17:AA:1234:C:H2'	17:AA:1234:C:O2	2.15	0.45
21:AE:42:LEU:O	37:AU:184:ARG:NE	2.50	0.45
35:AS:75:TYR:OH	39:AW:91:GLN:O	2.35	0.45
36:AT:91:GLU:O	36:AT:92:THR:HG22	2.16	0.45
6:5:391:VAL:O	6:5:391:VAL:HG13	2.17	0.45
7:6:149:GLN:NE2	7:6:166:THR:OG1	2.45	0.45
11:XA:2118:U:C2	11:XA:2119:U:C5	3.05	0.45
88:XA:5144:H8Q:O57	88:XA:5144:H8Q:O58	2.33	0.45
40:AX:214:GLU:OE2	40:AX:232:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:XF:91:PRO:O	46:XF:176:VAL:HG21	2.15	0.45
48:XI:112:MET:O	48:XI:116:LEU:HD23	2.17	0.45
49:XJ:139:SER:OG	49:XJ:142:ARG:NH2	2.49	0.45
50:XK:43:HIS:NE2	50:XK:55:ASP:OD2	2.49	0.45
11:XA:2148:A:OP2	57:XR:65:ARG:NH1	2.49	0.45
11:XA:2356:A:C2	11:XA:2357:C:H1'	2.51	0.45
11:XA:2744:U:O2	11:XA:2745:A:N6	2.49	0.45
11:XA:3150:U:N3	11:XA:3151:A:C2	2.85	0.45
14:A2:99:LEU:O	17:AA:1600:A:N6	2.50	0.45
35:AS:67:GLU:OE2	39:AW:85:ARG:NE	2.50	0.45
56:XQ:237:ASN:OD1	56:XQ:238:PHE:N	2.49	0.45
65:XZ:61:GLN:O	65:XZ:62:ASN:OD1	2.35	0.45
65:XZ:81:TRP:O	65:XZ:84:ASP:OD1	2.35	0.45
16:A4:116:VAL:HG11	20:AD:141:TRP:CZ3	2.51	0.45
17:AA:948:U:OP2	17:AA:1045:G:N1	2.43	0.45
49:XJ:140:VAL:O	49:XJ:144:ILE:HD12	2.16	0.45
5:4:77:LYS:NZ	11:XA:2163:A:OP1	2.50	0.45
7:6:119:GLU:OE1	7:6:119:GLU:N	2.44	0.45
8:7:38:THR:O	8:7:42:GLU:OE1	2.35	0.45
11:XA:1939:G:O5'	44:XD:259:LYS:NZ	2.45	0.45
11:XA:2111:C:OP1	48:XI:35:ARG:NH1	2.50	0.45
13:A1:267:LEU:O	13:A1:270:LYS:NZ	2.42	0.45
53:XN:172:VAL:HG13	53:XN:175:PHE:CZ	2.52	0.45
6:5:393:LYS:HE2	11:XA:1936:A:C6	2.52	0.44
11:XA:2379:C:O2	11:XA:2379:C:O4'	2.35	0.44
17:AA:873:G:O2'	17:AA:921:U:O2	2.33	0.44
17:AA:1233:C:O2'	27:AK:86:ARG:NH1	2.48	0.44
31:AO:106:PRO:HA	31:AO:109:ARG:HG2	2.00	0.44
40:AX:51:THR:O	40:AX:67:HIS:N	2.48	0.44
48:XI:181:ILE:O	48:XI:182:ASP:OD1	2.35	0.44
51:XL:99:ARG:HH12	56:XQ:191:ARG:HE	1.65	0.44
56:XQ:225:LYS:HG2	56:XQ:226:PRO:HD2	1.99	0.44
11:XA:1799:U:H2'	11:XA:1800:G:O4'	2.17	0.44
11:XA:2021:U:O4	52:XM:41:ARG:NH2	2.50	0.44
11:XA:2182:G:H2'	11:XA:2183:C:C6	2.53	0.44
11:XA:2403:G:OP2	44:XD:105:ARG:NH2	2.37	0.44
11:XA:3212:C:O4'	11:XA:3212:C:O2	2.35	0.44
11:XA:3217:A:O4'	56:XQ:86:ARG:NH2	2.50	0.44
16:A4:73:ALA:HB2	24:AH:61:PRO:CG	2.47	0.44
16:A4:482:ILE:CG2	16:A4:519:TYR:HE2	2.30	0.44
17:AA:746:A:C4	17:AA:747:A:C8	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:1483:C:N4	17:AA:1567:A:C2	2.85	0.44
21:AE:96:HIS:O	21:AE:100:GLN:NE2	2.48	0.44
46:XF:141:ILE:O	46:XF:142:ARG:HB2	2.18	0.44
52:XM:285:PRO:O	52:XM:286:THR:OG1	2.33	0.44
54:XO:86:ILE:HB	54:XO:87:PRO:HD3	1.99	0.44
57:XR:54:THR:HG21	58:XS:172:MET:H	1.82	0.44
61:XV:48:PRO:O	61:XV:49:ILE:HD13	2.17	0.44
56:XQ:107:HIS:O	56:XQ:108:ILE:HG13	2.17	0.44
7:6:113:LEU:CD1	55:XP:113:LYS:O	2.65	0.44
11:XA:1829:A:N3	57:XR:52:LYS:NZ	2.62	0.44
11:XA:2043:C:C2	11:XA:2044:A:C8	3.06	0.44
11:XA:2319:A:O3’	54:XO:42:ILE:HD11	2.18	0.44
11:XA:2712:G:N2	45:XE:257:MET:SD	2.91	0.44
16:A4:73:ALA:HB2	24:AH:61:PRO:HG2	1.99	0.44
16:A4:108:LEU:HD23	20:AD:148:LEU:HD21	2.00	0.44
17:AA:807:A:O2’	17:AA:809:G:O6	2.32	0.44
17:AA:1068:A:N6	17:AA:1089:U:OP2	2.46	0.44
17:AA:1444:A:OP2	27:AK:102:ARG:NH1	2.45	0.44
40:AX:337:LEU:HG	40:AX:337:LEU:O	2.16	0.44
56:XQ:278:ILE:O	56:XQ:282:ILE:HD12	2.17	0.44
11:XA:2192:A:H4’	49:XJ:139:SER:HB3	1.99	0.44
12:A0:87:TRP:O	31:AO:215:ARG:NH2	2.50	0.44
14:A2:64:ASP:N	14:A2:64:ASP:OD1	2.51	0.44
17:AA:657:G:O4’	17:AA:1480:A:O2’	2.27	0.44
17:AA:1211:G:N1	17:AA:1354:A:C6	2.85	0.44
25:AI:93:ASN:O	25:AI:123:GLY:N	2.50	0.44
31:AO:65:GLN:O	31:AO:69:GLY:N	2.51	0.44
31:AO:120:VAL:HG12	31:AO:124:GLU:OE1	2.17	0.44
33:AQ:49:CYS:SG	33:AQ:50:ARG:N	2.91	0.44
57:XR:96:GLU:OE1	57:XR:96:GLU:N	2.50	0.44
64:XY:208:PHE:O	64:XY:212:GLU:OE1	2.35	0.44
10:9:137:ARG:NE	60:XU:21:ARG:O	2.47	0.44
40:AX:209:VAL:HG12	40:AX:210:TRP:N	2.32	0.44
44:XD:216:LEU:HD23	44:XD:216:LEU:H	1.82	0.44
64:XY:69:ASP:OD1	64:XY:74:TRP:NE1	2.50	0.44
11:XA:1874:A:O2’	11:XA:2090:A:O2’	2.36	0.44
11:XA:2756:C:OP1	47:XH:121:ASN:ND2	2.48	0.44
17:AA:1212:U:O2’	17:AA:1214:A:N6	2.51	0.44
17:AA:1433:A:C4	17:AA:1458:A:N6	2.86	0.44
18:AB:149:ARG:NH2	33:AQ:82:ASP:OD2	2.50	0.44
23:AG:161:LEU:O	23:AG:164:ASP:OD1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:XN:174:GLY:O	53:XN:177:ASP:OD1	2.36	0.44
53:XN:195:LEU:O	53:XN:198:MET:HG3	2.18	0.44
57:XR:65:ARG:O	57:XR:69:ILE:HG12	2.17	0.44
58:XS:106:TRP:CD2	58:XS:114:ILE:HD11	2.53	0.44
11:XA:2147:G:OP1	58:XS:104:ARG:NE	2.51	0.44
11:XA:2245:A:H1'	11:XA:2246:A:C8	2.53	0.44
11:XA:3013:G:O6	11:XA:3025:A:C6	2.71	0.44
17:AA:1517:A:O2'	17:AA:1518:C:O4'	2.36	0.44
27:AK:89:ASN:OD1	27:AK:102:ARG:NH1	2.51	0.44
48:XI:111:LEU:O	48:XI:115:GLN:OE1	2.36	0.44
52:XM:139:GLN:HB3	52:XM:158:LEU:HB2	1.99	0.44
52:XM:252:LEU:HD23	52:XM:252:LEU:H	1.83	0.44
52:XM:270:ALA:HB1	52:XM:271:PRO:HD2	2.00	0.44
60:XU:71:ARG:NH2	60:XU:73:GLN:OE1	2.47	0.44
61:XV:197:GLU:OE1	64:XY:95:ASN:ND2	2.51	0.44
6:5:177:CYS:O	6:5:180:ILE:HG22	2.17	0.44
11:XA:1697:A:N3	11:XA:1703:C:O2'	2.48	0.44
11:XA:3220:A:P	45:XE:260:LYS:NZ	2.91	0.44
20:AD:407:ASP:OD1	20:AD:407:ASP:N	2.44	0.44
46:XF:250:VAL:HG23	46:XF:251:HIS:N	2.32	0.44
46:XF:280:TYR:CE2	52:XM:125:ARG:HD3	2.53	0.44
58:XS:155:ARG:NE	58:XS:157:GLU:OE2	2.50	0.44
11:XA:2259:C:O2'	11:XA:2261:C:OP2	2.32	0.43
11:XA:2268:G:N7	52:XM:44:ARG:NH1	2.53	0.43
13:A1:270:LYS:O	13:A1:275:ASN:ND2	2.51	0.43
13:A1:290:GLU:HA	13:A1:290:GLU:OE1	2.17	0.43
17:AA:769:G:N2	17:AA:772:A:OP2	2.42	0.43
28:AL:140:GLU:O	28:AL:144:GLU:OE1	2.36	0.43
37:AU:52:GLU:OE1	37:AU:52:GLU:N	2.48	0.43
50:XK:135:GLU:HA	50:XK:138:LEU:CD2	2.48	0.43
54:XO:99:ASP:OD1	54:XO:100:GLN:N	2.51	0.43
6:5:242:ARG:HA	6:5:245:ILE:HG12	1.99	0.43
11:XA:1826:G:OP1	11:XA:2684:C:O2	2.36	0.43
11:XA:2955:U:OP2	11:XA:2963:A:N6	2.51	0.43
13:A1:264:GLU:OE1	40:AX:339:PRO:HG3	2.18	0.43
13:A1:274:LYS:HE3	13:A1:274:LYS:HA	2.00	0.43
14:A2:50:SER:O	14:A2:53:MET:HG2	2.17	0.43
16:A4:108:LEU:HD22	20:AD:154:VAL:CG1	2.46	0.43
20:AD:342:MET:SD	20:AD:342:MET:N	2.87	0.43
48:XI:163:GLU:O	48:XI:166:ARG:HG3	2.18	0.43
11:XA:2511:C:O2'	44:XD:257:ILE:O	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:3118:U:C2	11:XA:3119:C:C5	3.07	0.43
15:A3:159:GLU:OE2	15:A3:163:ARG:NH2	2.51	0.43
15:A3:164:ARG:NH2	17:AA:1501:A:OP1	2.44	0.43
18:AB:107:PHE:N	18:AB:115:ILE:O	2.51	0.43
22:AF:110:LEU:HD13	22:AF:201:MET:HE3	2.00	0.43
37:AU:123:ARG:O	37:AU:127:GLU:OE1	2.36	0.43
47:XH:99:THR:OG1	47:XH:128:LEU:O	2.31	0.43
52:XM:156:VAL:HG22	52:XM:157:GLN:H	1.83	0.43
59:XT:62:GLN:OE1	59:XT:69:ARG:NH2	2.51	0.43
11:XA:2044:A:C4	11:XA:2045:A:C8	3.06	0.43
11:XA:2714:A:P	45:XE:239:ARG:HH11	2.41	0.43
13:A1:295:SER:O	13:A1:299:LEU:HD23	2.18	0.43
17:AA:1457:G:OP2	23:AG:338:SER:OG	2.31	0.43
23:AG:211:GLU:OE1	23:AG:211:GLU:N	2.52	0.43
23:AG:214:SER:O	23:AG:217:ASP:OD1	2.36	0.43
48:XI:66:PRO:O	48:XI:67:SER:OG	2.34	0.43
52:XM:231:GLU:O	52:XM:235:GLU:OE1	2.35	0.43
59:XT:99:ILE:O	59:XT:103:LEU:HD23	2.18	0.43
5:4:90:VAL:O	5:4:99:LYS:HA	2.18	0.43
18:AB:60:ASP:OD2	18:AB:64:ASN:ND2	2.51	0.43
31:AO:225:GLN:NE2	37:AU:47:ALA:O	2.51	0.43
44:XD:211:GLY:O	44:XD:246:ARG:NH2	2.49	0.43
45:XE:142:MET:HG2	45:XE:181:ILE:O	2.19	0.43
52:XM:167:ILE:HG21	52:XM:174:VAL:CG2	2.49	0.43
58:XS:129:ARG:NH2	58:XS:151:LYS:O	2.50	0.43
59:XT:197:LYS:HA	59:XT:200:ILE:HG12	2.00	0.43
63:XX:36:ARG:NH2	63:XX:151:GLU:OE1	2.52	0.43
30:AN:66:LEU:HD13	30:AN:79:HIS:HB3	2.01	0.43
41:AY:277:LEU:O	41:AY:281:GLU:OE1	2.37	0.43
50:XK:137:ILE:O	50:XK:141:LEU:CD1	2.67	0.43
54:XO:139:ASP:OD1	54:XO:140:SER:N	2.52	0.43
11:XA:1961:A:O4'	59:XT:161:ARG:HA	2.19	0.43
11:XA:2529:U:OP2	44:XD:208:ARG:NH1	2.52	0.43
13:A1:100:GLU:O	19:AC:156:GLN:NE2	2.47	0.43
16:A4:634:ALA:HB3	16:A4:641:ILE:HG21	2.01	0.43
20:AD:283:GLU:OE1	35:AS:21:ARG:NH2	2.49	0.43
35:AS:18:ASP:OD1	35:AS:19:LEU:N	2.52	0.43
52:XM:133:LYS:C	52:XM:134:ARG:HG2	2.39	0.43
53:XN:214:THR:O	53:XN:218:ILE:HD12	2.18	0.43
8:7:235:TYR:O	8:7:238:ASP:OD1	2.36	0.43
8:7:247:ASN:ND2	8:7:251:ILE:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:1838:C:C4	50:XK:50:LEU:HD12	2.54	0.43
11:XA:2529:U:N3	44:XD:205:GLN:OE1	2.43	0.43
13:A1:91:VAL:O	13:A1:94:GLY:N	2.52	0.43
17:AA:1235:U:H5”	17:AA:1236:C:OP2	2.17	0.43
19:AC:115:ASN:ND2	41:AY:309:LYS:O	2.52	0.43
36:AT:101:HIS:O	36:AT:105:ILE:HD12	2.18	0.43
56:XQ:201:ASP:OD1	56:XQ:202:VAL:N	2.52	0.43
59:XT:106:LEU:O	59:XT:114:ALA:HB1	2.18	0.43
7:6:144:GLY:N	7:6:145:PRO:CD	2.82	0.43
20:AD:232:THR:N	20:AD:236:GLY:O	2.52	0.43
25:AI:181:ILE:O	25:AI:181:ILE:HG13	2.19	0.43
31:AO:163:LEU:HD23	31:AO:163:LEU:H	1.82	0.43
40:AX:297:MET:O	40:AX:298:LYS:HD2	2.19	0.43
40:AX:350:PRO:O	40:AX:354:GLU:OE1	2.37	0.43
50:XK:22:ASP:OD1	50:XK:61:ASN:ND2	2.52	0.43
11:XA:1917:A:C8	11:XA:1983:U:C4	3.07	0.43
11:XA:3153:U:C2’	11:XA:3154:U:H5’	2.49	0.43
17:AA:805:C:O2	17:AA:805:C:O4’	2.35	0.43
23:AG:169:LEU:O	23:AG:173:GLU:OE1	2.37	0.43
28:AL:87:ASP:OD1	28:AL:88:VAL:N	2.52	0.43
6:5:362:THR:O	6:5:364:LEU:N	2.51	0.42
8:7:315:LYS:O	8:7:318:GLU:HG3	2.19	0.42
11:XA:2835:C:H4’	62:XW:50:ARG:HE	1.83	0.42
22:AF:116:GLU:O	22:AF:120:ARG:HG2	2.19	0.42
35:AS:15:ARG:O	35:AS:18:ASP:OD1	2.36	0.42
43:XB:1639:U:O4	43:XB:1640:A:N6	2.51	0.42
50:XK:24:LYS:O	50:XK:26:GLN:NE2	2.52	0.42
57:XR:67:LEU:HD21	57:XR:71:ARG:CZ	2.48	0.42
59:XT:123:GLU:O	59:XT:126:ASP:OD1	2.37	0.42
9:8:165:ASP:OD1	9:8:165:ASP:N	2.49	0.42
11:XA:2574:G:O2’	11:XA:2575:U:P	2.76	0.42
16:A4:243:ASN:O	16:A4:247:ILE:HG12	2.19	0.42
16:A4:372:TYR:O	16:A4:376:ILE:HG12	2.19	0.42
17:AA:1134:G:N7	26:AJ:35:GLN:NE2	2.67	0.42
55:XP:62:ARG:NH1	62:XW:137:LYS:O	2.50	0.42
8:7:207:HIS:HA	8:7:210:ILE:HG12	2.00	0.42
11:XA:2034:A:H2’	11:XA:2035:U:O4’	2.20	0.42
11:XA:2138:U:O2’	11:XA:2151:A:N3	2.43	0.42
11:XA:2249:G:O3’	57:XR:62:LYS:NZ	2.52	0.42
15:A3:161:ARG:NH2	17:AA:1146:C:OP1	2.44	0.42
17:AA:662:U:H2’	17:AA:663:A:O4’	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:865:A:H2'	17:AA:866:A:N9	2.35	0.42
21:AE:27:GLU:OE2	37:AU:170:ARG:NH1	2.50	0.42
36:AT:115:GLU:O	36:AT:119:GLU:OE1	2.36	0.42
6:5:230:LEU:O	6:5:289:HIS:N	2.50	0.42
11:XA:2249:G:P	57:XR:65:ARG:HE	2.42	0.42
11:XA:3008:C:C2	11:XA:3032:G:N2	2.87	0.42
11:XA:3189:C:C2'	11:XA:3190:A:OP2	2.67	0.42
16:A4:108:LEU:HD22	20:AD:154:VAL:HG12	1.98	0.42
17:AA:1390:A:H1'	17:AA:1392:A:N7	2.34	0.42
24:AH:124:VAL:O	27:AK:108:ARG:NH1	2.45	0.42
38:AV:36:ASP:OD1	38:AV:37:SER:N	2.52	0.42
44:XD:163:ILE:HG22	44:XD:164:LEU:N	2.34	0.42
45:XE:310:LEU:HG	45:XE:310:LEU:O	2.19	0.42
65:XZ:84:ASP:OD1	65:XZ:85:ILE:N	2.53	0.42
11:XA:1789:A:H1'	11:XA:1915:C:O2'	2.19	0.42
11:XA:1989:C:H2'	11:XA:1990:G:O4'	2.19	0.42
17:AA:681:U:H2'	17:AA:682:A:C8	2.55	0.42
17:AA:839:A:P	29:AM:84:SER:HG	2.42	0.42
34:AR:221:GLN:OE1	34:AR:223:ARG:NE	2.51	0.42
60:XU:52:ASP:OD1	60:XU:53:LEU:N	2.51	0.42
61:XV:45:VAL:HG21	64:XY:237:LYS:HE2	2.01	0.42
2:1:20:MET:HA	2:1:58:GLU:HA	2.02	0.42
4:3:113:ARG:NH2	11:XA:1750:G:OP2	2.53	0.42
4:3:131:LYS:O	4:3:136:LYS:NZ	2.50	0.42
8:7:238:ASP:O	8:7:241:GLU:HG3	2.20	0.42
11:XA:2747:U:C2	11:XA:2802:A:C2	3.08	0.42
14:A2:78:ALA:O	14:A2:82:GLU:OE1	2.38	0.42
16:A4:638:SER:OG	16:A4:640:PRO:HD2	2.20	0.42
20:AD:372:GLU:OE2	20:AD:374:ARG:NE	2.41	0.42
26:AJ:49:LEU:HD23	26:AJ:50:GLY:N	2.34	0.42
40:AX:63:HIS:O	40:AX:63:HIS:ND1	2.52	0.42
40:AX:100:MET:HB3	90:AX:500:GTP:HN1	1.84	0.42
43:XB:1615:A:O2'	43:XB:1616:A:O4'	2.28	0.42
45:XE:342:ALA:HB1	45:XE:343:PRO:HD2	2.01	0.42
6:5:214:ASN:OD1	6:5:214:ASN:N	2.53	0.42
11:XA:2550:A:C2	11:XA:2551:G:C8	3.08	0.42
11:XA:3032:G:H2'	11:XA:3033:U:O4'	2.20	0.42
16:A4:319:LEU:HA	16:A4:322:HIS:CD2	2.55	0.42
16:A4:643:GLU:O	16:A4:646:THR:OG1	2.34	0.42
57:XR:20:ARG:HA	57:XR:23:GLU:OE1	2.19	0.42
7:6:50:LYS:HA	62:XW:121:PRO:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2091:A:H2’	11:XA:2092:C:O4’	2.20	0.42
11:XA:2752:C:C2	11:XA:2753:A:C8	3.08	0.42
17:AA:1452:U:H2’	17:AA:1453:A:C8	2.54	0.42
52:XM:44:ARG:HD3	52:XM:45:ARG:HG3	2.02	0.42
55:XP:171:LEU:O	55:XP:171:LEU:HG	2.20	0.42
7:6:364:ARG:NE	11:XA:2859:A:OP2	2.35	0.42
16:A4:335:PHE:HA	16:A4:338:ILE:HG22	2.01	0.42
17:AA:802:C:O4’	17:AA:814:A:O2’	2.38	0.42
17:AA:990:U:H2’	17:AA:991:G:O4’	2.20	0.42
50:XK:21:LEU:HD21	50:XK:31:LEU:HD22	2.02	0.42
54:XO:94:ALA:HB3	54:XO:95:PRO:HD3	2.02	0.42
54:XO:149:LEU:HA	54:XO:152:LEU:CD2	2.49	0.42
64:XY:161:GLU:OE1	64:XY:161:GLU:N	2.52	0.42
6:5:311:ALA:O	6:5:315:LEU:HD23	2.20	0.42
11:XA:2558:A:C4’	11:XA:2559:U:OP2	2.68	0.42
11:XA:2954:C:H2’	11:XA:2955:U:O4’	2.19	0.42
16:A4:640:PRO:O	16:A4:643:GLU:HG2	2.20	0.42
17:AA:895:C:N4	17:AA:899:G:O6	2.52	0.42
17:AA:1399:A:H2’	17:AA:1400:U:C6	2.55	0.42
38:AV:372:ILE:O	38:AV:376:GLU:OE1	2.38	0.42
9:8:116:LEU:O	9:8:119:LYS:HG3	2.20	0.41
11:XA:2066:C:O2’	11:XA:2067:C:OP1	2.33	0.41
38:AV:236:LEU:CD2	38:AV:327:LEU:HD11	2.49	0.41
40:AX:181:PRO:HB2	40:AX:233:VAL:HG22	2.02	0.41
44:XD:251:ASP:OD1	44:XD:251:ASP:C	2.59	0.41
45:XE:56:GLU:OE2	54:XO:141:HIS:ND1	2.53	0.41
50:XK:39:LEU:HD21	50:XK:125:LEU:HB2	2.02	0.41
51:XL:70:GLY:O	51:XL:130:ARG:NH1	2.53	0.41
56:XQ:231:LYS:HB3	56:XQ:233:TRP:CE2	2.55	0.41
57:XR:85:ALA:O	57:XR:89:ASN:OD1	2.38	0.41
7:6:107:LYS:HA	7:6:110:ILE:HG12	2.01	0.41
10:9:55:GLU:HG3	60:XU:10:TYR:CZ	2.55	0.41
12:A0:201:TRP:CD2	17:AA:844:A:C2	3.08	0.41
13:A1:153:SER:OG	13:A1:154:THR:N	2.53	0.41
18:AB:111:LEU:O	18:AB:113:HIS:ND1	2.53	0.41
31:AO:151:THR:O	31:AO:154:ILE:HG22	2.19	0.41
42:AZ:77:ASP:O	42:AZ:80:ASP:OD1	2.38	0.41
46:XF:220:ASP:OD1	46:XF:221:LEU:N	2.50	0.41
50:XK:35:ALA:O	50:XK:39:LEU:HD13	2.19	0.41
6:5:254:GLU:OE2	6:5:256:PHE:N	2.52	0.41
11:XA:1729:U:OP2	63:XX:100:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2086:A:H2'	11:XA:2087:U:C6	2.55	0.41
11:XA:2293:A:C6	52:XM:39:ARG:HD2	2.55	0.41
11:XA:2348:A:N6	11:XA:2366:G:O6	2.53	0.41
11:XA:2945:A:O2'	11:XA:2947:U:O4	2.35	0.41
15:A3:174:ARG:HA	15:A3:177:TRP:CE2	2.56	0.41
16:A4:455:ASN:HA	16:A4:486:TYR:CE1	2.55	0.41
17:AA:991:G:C6	17:AA:992:U:O4	2.73	0.41
25:AI:174:SER:OG	33:AQ:13:MET:SD	2.78	0.41
25:AI:186:CYS:SG	25:AI:187:ARG:N	2.93	0.41
64:XY:132:LEU:O	64:XY:135:VAL:HG22	2.20	0.41
65:XZ:71:ARG:NH1	65:XZ:73:LYS:O	2.51	0.41
4:3:168:ARG:NH1	52:XM:130:GLN:OE1	2.51	0.41
9:8:138:ALA:O	9:8:141:GLU:HG3	2.19	0.41
17:AA:1161:A:C2	17:AA:1162:A:C8	3.09	0.41
17:AA:1410:G:H2'	17:AA:1411:G:H8	1.86	0.41
29:AM:68:LEU:O	34:AR:161:ILE:N	2.53	0.41
34:AR:176:GLU:N	34:AR:176:GLU:OE1	2.53	0.41
36:AT:90:VAL:HG22	36:AT:90:VAL:O	2.20	0.41
38:AV:156:ASN:OD1	38:AV:157:TYR:N	2.54	0.41
46:XF:77:VAL:O	46:XF:77:VAL:HG13	2.20	0.41
51:XL:96:MET:SD	56:XQ:170:ARG:NE	2.92	0.41
52:XM:102:GLN:HA	52:XM:105:ILE:HG12	2.01	0.41
54:XO:43:GLU:OE1	54:XO:43:GLU:N	2.53	0.41
4:3:138:PRO:HA	4:3:141:LYS:HG2	2.02	0.41
11:XA:2089:U:O4	11:XA:2090:A:N6	2.52	0.41
11:XA:2479:C:O2	45:XE:230:THR:HB	2.21	0.41
11:XA:2955:U:C5	11:XA:2963:A:N1	2.88	0.41
17:AA:1295:A:OP2	18:AB:147:ARG:NH1	2.52	0.41
28:AL:78:ASN:OD1	28:AL:79:VAL:N	2.53	0.41
48:XI:49:ALA:HA	48:XI:52:GLU:OE2	2.21	0.41
61:XV:146:VAL:HG12	61:XV:147:SER:N	2.36	0.41
7:6:252:CYS:SG	7:6:286:ARG:NH2	2.94	0.41
11:XA:1935:A:N7	11:XA:1936:A:C4	2.88	0.41
16:A4:561:SER:O	16:A4:563:PRO:HD3	2.21	0.41
16:A4:616:ASP:HA	16:A4:619:LYS:HG2	2.01	0.41
16:A4:639:LEU:N	16:A4:640:PRO:CD	2.83	0.41
17:AA:1516:G:C6	17:AA:1517:A:N6	2.89	0.41
22:AF:218:PRO:HA	22:AF:221:LYS:HG2	2.02	0.41
30:AN:39:LEU:O	36:AT:11:ARG:NH1	2.53	0.41
44:XD:127:ILE:HD11	44:XD:143:ALA:HB3	2.02	0.41
52:XM:184:LEU:HA	52:XM:187:VAL:HG12	2.03	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
7:6:188:TYR:CG	55:XP:137:GLU:OE2	2.74	0.41
8:7:147:ALA:O	8:7:150:MET:HG2	2.19	0.41
11:XA:2696:A:H1’	11:XA:2698:G:OP2	2.21	0.41
11:XA:2961:C:O2	11:XA:2961:C:H2’	2.21	0.41
13:A1:217:GLN:O	13:A1:220:ASP:OD1	2.39	0.41
18:AB:222:ILE:O	18:AB:222:ILE:HG13	2.21	0.41
27:AK:105:ARG:NH1	42:AZ:50:ASP:O	2.53	0.41
34:AR:67:LYS:N	34:AR:68:PRO:CD	2.84	0.41
36:AT:132:ARG:NH2	36:AT:142:GLU:OE2	2.53	0.41
11:XA:2618:U:O4	11:XA:3043:C:N4	2.53	0.41
13:A1:211:ARG:NH2	41:AY:359:SER:OG	2.54	0.41
34:AR:243:ILE:HG22	34:AR:247:HIS:CD2	2.56	0.41
35:AS:131:ILE:HD12	35:AS:131:ILE:H	1.84	0.41
65:XZ:80:TYR:HA	65:XZ:83:LYS:HG2	2.02	0.41
11:XA:1671:G:O2’	11:XA:1672:C:O5’	2.27	0.41
11:XA:2715:A:O2’	45:XE:245:THR:O	2.35	0.41
11:XA:3180:A:C4	11:XA:3190:A:C6	3.09	0.41
12:A0:44:PRO:O	12:A0:45:PHE:HB3	2.21	0.41
15:A3:164:ARG:HA	15:A3:167:ILE:HG12	2.02	0.41
16:A4:116:VAL:CG1	20:AD:141:TRP:HZ3	2.34	0.41
16:A4:416:PHE:CE2	16:A4:457:TYR:CG	3.09	0.41
16:A4:491:GLN:O	16:A4:495:HIS:ND1	2.45	0.41
17:AA:895:C:N4	26:AJ:117:ASP:OD1	2.54	0.41
17:AA:1139:A:C6	17:AA:1140:A:C6	3.08	0.41
28:AL:86:ASP:OD1	28:AL:87:ASP:N	2.53	0.41
28:AL:166:MET:O	28:AL:169:ASN:OD1	2.39	0.41
40:AX:374:GLU:HG2	40:AX:375:GLU:N	2.35	0.41
45:XE:73:LEU:O	45:XE:77:LEU:HG	2.21	0.41
48:XI:124:LYS:HG3	48:XI:125:VAL:N	2.36	0.41
52:XM:209:GLU:N	52:XM:209:GLU:OE1	2.54	0.41
53:XN:172:VAL:HG12	53:XN:176:LEU:HG	2.02	0.41
55:XP:80:LEU:HB3	55:XP:145:TYR:HB3	2.03	0.41
56:XQ:246:ASP:OD1	56:XQ:247:LEU:N	2.54	0.41
57:XR:28:ALA:HB2	57:XR:46:VAL:CG2	2.51	0.41
64:XY:224:GLU:O	64:XY:227:GLU:HG2	2.21	0.41
8:7:113:TRP:NE1	8:7:117:LYS:O	2.41	0.41
17:AA:1486:C:O2	17:AA:1486:C:O4’	2.38	0.41
28:AL:100:LYS:O	28:AL:104:LEU:HG	2.20	0.41
31:AO:105:CYS:HB2	31:AO:106:PRO:HD2	2.03	0.41
32:AP:124:TYR:HB3	33:AQ:9:ALA:HB2	2.03	0.41
44:XD:225:ILE:HD13	44:XD:235:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:XM:133:LYS:O	52:XM:134:ARG:HG2	2.20	0.41
54:XO:22:PRO:HA	54:XO:25:ARG:HG2	2.03	0.41
59:XT:198:GLU:OE2	59:XT:202:GLN:NE2	2.54	0.41
62:XW:105:VAL:HG23	62:XW:105:VAL:O	2.21	0.41
65:XZ:78:ARG:O	65:XZ:83:LYS:NZ	2.54	0.41
20:AD:191:ARG:NH1	31:AO:79:ARG:O	2.55	0.40
20:AD:283:GLU:OE2	20:AD:283:GLU:HA	2.21	0.40
32:AP:127:PRO:HA	32:AP:130:LEU:HD23	2.03	0.40
41:AY:287:ALA:O	41:AY:290:ASN:N	2.53	0.40
44:XD:192:LEU:HA	44:XD:214:GLY:O	2.19	0.40
46:XF:83:HIS:HB3	46:XF:86:VAL:HG12	2.03	0.40
52:XM:151:LYS:O	52:XM:151:LYS:HG2	2.21	0.40
56:XQ:225:LYS:CG	56:XQ:226:PRO:HD2	2.51	0.40
5:4:88:TRP:NE1	11:XA:2160:A:OP2	2.41	0.40
7:6:379:ILE:O	7:6:379:ILE:HG13	2.21	0.40
11:XA:1795:A:H2'	11:XA:1796:A:O4'	2.21	0.40
11:XA:2117:U:N3	11:XA:2118:U:C5	2.90	0.40
11:XA:2381:A:N6	11:XA:2412:A:C6	2.89	0.40
11:XA:2550:A:C6	11:XA:2551:G:N7	2.90	0.40
17:AA:879:U:OP2	17:AA:880:C:H2'	2.21	0.40
17:AA:1343:A:H2'	17:AA:1343:A:N3	2.36	0.40
23:AG:244:PHE:O	23:AG:246:ARG:NH1	2.54	0.40
44:XD:109:PHE:HB3	44:XD:204:ALA:HB3	2.03	0.40
46:XF:142:ARG:HA	46:XF:149:GLY:HA2	2.03	0.40
58:XS:112:ASP:OD1	58:XS:195:ILE:HB	2.21	0.40
5:4:81:LEU:HD23	5:4:81:LEU:H	1.87	0.40
6:5:179:VAL:O	6:5:182:ASP:OD1	2.38	0.40
7:6:89:ASP:OD1	7:6:89:ASP:N	2.54	0.40
7:6:282:SER:O	7:6:284:ASP:N	2.54	0.40
7:6:354:GLN:HE21	7:6:369:TYR:CB	2.35	0.40
8:7:203:THR:O	8:7:207:HIS:ND1	2.51	0.40
22:AF:196:HIS:HB3	22:AF:204:LYS:HD3	2.03	0.40
23:AG:301:GLN:OE1	40:AX:385:ASN:HB3	2.22	0.40
29:AM:84:SER:O	29:AM:87:MET:HG3	2.21	0.40
35:AS:104:THR:O	35:AS:107:GLN:HG3	2.21	0.40
40:AX:241:GLY:O	40:AX:245:LYS:HG3	2.21	0.40
43:XB:1623:G:OP2	55:XP:87:HIS:HB2	2.22	0.40
47:XH:58:ARG:NH1	47:XH:77:HIS:O	2.54	0.40
48:XI:90:PHE:CD2	48:XI:90:PHE:O	2.74	0.40
7:6:290:CYS:SG	7:6:295:GLN:NE2	2.95	0.40
11:XA:1775:A:OP1	46:XF:148:GLY:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2456:U:H2'	11:XA:2457:A:O4'	2.21	0.40
15:A3:171:LYS:HA	15:A3:174:ARG:HG2	2.02	0.40
16:A4:140:LEU:CD1	19:AC:145:TYR:HD1	2.35	0.40
16:A4:167:LYS:HG3	16:A4:168:ALA:N	2.37	0.40
16:A4:409:ASP:O	16:A4:412:ASP:OD2	2.40	0.40
17:AA:729:U:O2'	17:AA:745:A:N6	2.55	0.40
20:AD:147:PRO:O	20:AD:155:GLN:NE2	2.55	0.40
20:AD:151:ASN:O	20:AD:151:ASN:ND2	2.54	0.40
20:AD:232:THR:HG22	20:AD:233:ALA:N	2.36	0.40
38:AV:218:SER:HA	38:AV:221:PHE:CE2	2.56	0.40
52:XM:156:VAL:O	52:XM:176:THR:HA	2.22	0.40
55:XP:171:LEU:HD23	55:XP:171:LEU:H	1.87	0.40
63:XX:169:LEU:O	63:XX:172:GLN:NE2	2.52	0.40
11:XA:2726:C:H2'	11:XA:2726:C:O2	2.21	0.40
12:A0:201:TRP:CG	17:AA:844:A:C2	3.10	0.40
13:A1:189:LYS:O	13:A1:193:LEU:HD23	2.20	0.40
17:AA:674:U:N3	17:AA:675:A:N7	2.69	0.40
17:AA:1048:C:O2'	28:AL:196:TYR:O	2.39	0.40
17:AA:1264:C:O3'	27:AK:112:ARG:NH2	2.54	0.40
24:AH:126:ILE:O	24:AH:127:TYR:CG	2.74	0.40
40:AX:72:PRO:O	40:AX:76:GLU:OE1	2.40	0.40
41:AY:336:LYS:HD3	41:AY:336:LYS:N	2.37	0.40
43:XB:1607:U:O2'	43:XB:1608:G:H5'	2.22	0.40
53:XN:32:THR:HG23	53:XN:32:THR:O	2.21	0.40
63:XX:16:LEU:HA	63:XX:21:CYS:SG	2.62	0.40
63:XX:180:ASP:N	63:XX:181:PRO:HD3	2.36	0.40
64:XY:133:ASP:OD1	64:XY:134:LYS:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
2	1	51/65 (78%)	50 (98%)	1 (2%)	0	100	100
3	2	44/92 (48%)	44 (100%)	0	0	100	100
4	3	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
5	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
6	5	389/423 (92%)	366 (94%)	23 (6%)	0	100	100
7	6	348/380 (92%)	321 (92%)	27 (8%)	0	100	100
8	7	285/338 (84%)	262 (92%)	23 (8%)	0	100	100
9	8	132/206 (64%)	126 (96%)	6 (4%)	0	100	100
10	9	122/137 (89%)	116 (95%)	6 (5%)	0	100	100
12	A0	197/218 (90%)	188 (95%)	9 (5%)	0	100	100
13	A1	273/323 (84%)	255 (93%)	18 (7%)	0	100	100
14	A2	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
15	A3	67/199 (34%)	67 (100%)	0	0	100	100
16	A4	526/689 (76%)	493 (94%)	33 (6%)	0	100	100
18	AB	216/296 (73%)	214 (99%)	2 (1%)	0	100	100
19	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
20	AD	341/430 (79%)	324 (95%)	17 (5%)	0	100	100
21	AE	120/125 (96%)	115 (96%)	5 (4%)	0	100	100
22	AF	197/242 (81%)	192 (98%)	5 (2%)	0	100	100
23	AG	300/396 (76%)	288 (96%)	12 (4%)	0	100	100
24	AH	133/201 (66%)	124 (93%)	9 (7%)	0	100	100
25	AI	134/194 (69%)	130 (97%)	4 (3%)	0	100	100
26	AJ	106/138 (77%)	99 (93%)	7 (7%)	0	100	100
27	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
28	AL	162/257 (63%)	157 (97%)	5 (3%)	0	100	100
29	AM	114/137 (83%)	113 (99%)	1 (1%)	0	100	100
30	AN	105/130 (81%)	101 (96%)	4 (4%)	0	100	100
31	AO	183/258 (71%)	179 (98%)	4 (2%)	0	100	100
32	AP	93/142 (66%)	87 (94%)	6 (6%)	0	100	100
33	AQ	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
34	AR	248/360 (69%)	238 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	AS	131/190 (69%)	123 (94%)	8 (6%)	0	100	100
36	AT	160/173 (92%)	147 (92%)	13 (8%)	0	100	100
37	AU	171/205 (83%)	169 (99%)	2 (1%)	0	100	100
38	AV	341/414 (82%)	322 (94%)	19 (6%)	0	100	100
39	AW	95/187 (51%)	90 (95%)	5 (5%)	0	100	100
40	AX	346/398 (87%)	329 (95%)	17 (5%)	0	100	100
41	AY	111/395 (28%)	104 (94%)	7 (6%)	0	100	100
42	AZ	84/106 (79%)	83 (99%)	1 (1%)	0	100	100
44	XD	234/305 (77%)	219 (94%)	13 (6%)	2 (1%)	17	54
45	XE	302/348 (87%)	288 (95%)	14 (5%)	0	100	100
46	XF	248/311 (80%)	239 (96%)	9 (4%)	0	100	100
47	XH	93/267 (35%)	87 (94%)	6 (6%)	0	100	100
48	XI	209/261 (80%)	193 (92%)	16 (8%)	0	100	100
49	XJ	168/192 (88%)	156 (93%)	12 (7%)	0	100	100
50	XK	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
51	XL	113/145 (78%)	106 (94%)	7 (6%)	0	100	100
52	XM	285/296 (96%)	277 (97%)	8 (3%)	0	100	100
53	XN	219/251 (87%)	208 (95%)	11 (5%)	0	100	100
54	XO	150/175 (86%)	145 (97%)	5 (3%)	0	100	100
55	XP	141/180 (78%)	130 (92%)	11 (8%)	0	100	100
56	XQ	236/292 (81%)	226 (96%)	10 (4%)	0	100	100
57	XR	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
58	XS	158/205 (77%)	153 (97%)	5 (3%)	0	100	100
59	XT	164/206 (80%)	161 (98%)	3 (2%)	0	100	100
60	XU	137/153 (90%)	130 (95%)	7 (5%)	0	100	100
61	XV	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
62	XW	109/148 (74%)	105 (96%)	4 (4%)	0	100	100
63	XX	241/256 (94%)	234 (97%)	7 (3%)	0	100	100
64	XY	176/250 (70%)	173 (98%)	3 (2%)	0	100	100
65	XZ	118/161 (73%)	114 (97%)	4 (3%)	0	100	100
66	a	93/142 (66%)	87 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	b	146/215 (68%)	135 (92%)	11 (8%)	0	100	100
68	c	271/332 (82%)	260 (96%)	11 (4%)	0	100	100
69	d	212/306 (69%)	201 (95%)	10 (5%)	1 (0%)	29	66
70	e	211/279 (76%)	202 (96%)	9 (4%)	0	100	100
71	f	138/212 (65%)	132 (96%)	6 (4%)	0	100	100
72	g	130/166 (78%)	122 (94%)	7 (5%)	1 (1%)	19	57
73	h	106/158 (67%)	103 (97%)	2 (2%)	1 (1%)	17	54
74	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
75	j	84/123 (68%)	83 (99%)	1 (1%)	0	100	100
76	k	93/112 (83%)	90 (97%)	3 (3%)	0	100	100
77	l	78/138 (56%)	73 (94%)	5 (6%)	0	100	100
78	m	58/128 (45%)	53 (91%)	5 (9%)	0	100	100
79	o	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
80	p	119/206 (58%)	113 (95%)	6 (5%)	0	100	100
81	q	162/222 (73%)	157 (97%)	5 (3%)	0	100	100
82	r	144/196 (74%)	137 (95%)	7 (5%)	0	100	100
84	s	366/439 (83%)	351 (96%)	15 (4%)	0	100	100
85	t1	45/198 (23%)	40 (89%)	5 (11%)	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%)	26 (96%)	1 (4%)	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
All	All	13778/19160 (72%)	13145 (95%)	628 (5%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
72	g	38	PHE
44	XD	207	ILE
44	XD	208	ARG
73	h	78	PHE
69	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
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%)	350 (99%)	3 (1%)	81	89
7	6	313/332 (94%)	312 (100%)	1 (0%)	92	96
8	7	267/303 (88%)	267 (100%)	0	100	100
9	8	124/190 (65%)	123 (99%)	1 (1%)	81	89
10	9	104/112 (93%)	104 (100%)	0	100	100
12	A0	176/190 (93%)	175 (99%)	1 (1%)	86	92
13	A1	253/291 (87%)	251 (99%)	2 (1%)	81	89
14	A2	99/101 (98%)	97 (98%)	2 (2%)	55	75
15	A3	63/166 (38%)	63 (100%)	0	100	100
16	A4	494/609 (81%)	490 (99%)	4 (1%)	81	89
18	AB	192/249 (77%)	192 (100%)	0	100	100
19	AC	115/143 (80%)	115 (100%)	0	100	100
20	AD	283/357 (79%)	281 (99%)	2 (1%)	84	91
21	AE	104/107 (97%)	104 (100%)	0	100	100
22	AF	178/209 (85%)	178 (100%)	0	100	100
23	AG	264/342 (77%)	264 (100%)	0	100	100
24	AH	125/180 (69%)	125 (100%)	0	100	100
25	AI	104/147 (71%)	104 (100%)	0	100	100
26	AJ	93/118 (79%)	93 (100%)	0	100	100
27	AK	91/113 (80%)	91 (100%)	0	100	100
28	AL	152/226 (67%)	151 (99%)	1 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	AM	95/113 (84%)	95 (100%)	0	100	100
30	AN	93/115 (81%)	93 (100%)	0	100	100
31	AO	166/230 (72%)	166 (100%)	0	100	100
32	AP	86/123 (70%)	86 (100%)	0	100	100
33	AQ	77/79 (98%)	77 (100%)	0	100	100
34	AR	229/318 (72%)	228 (100%)	1 (0%)	91	95
35	AS	115/164 (70%)	115 (100%)	0	100	100
36	AT	150/157 (96%)	150 (100%)	0	100	100
37	AU	149/174 (86%)	148 (99%)	1 (1%)	84	91
38	AV	315/364 (86%)	314 (100%)	1 (0%)	92	96
39	AW	84/158 (53%)	84 (100%)	0	100	100
40	AX	307/351 (88%)	302 (98%)	5 (2%)	62	79
41	AY	104/357 (29%)	104 (100%)	0	100	100
42	AZ	79/95 (83%)	79 (100%)	0	100	100
44	XD	190/245 (78%)	188 (99%)	2 (1%)	73	85
45	XE	259/290 (89%)	259 (100%)	0	100	100
46	XF	217/262 (83%)	217 (100%)	0	100	100
47	XH	86/228 (38%)	86 (100%)	0	100	100
48	XI	194/232 (84%)	194 (100%)	0	100	100
49	XJ	133/150 (89%)	132 (99%)	1 (1%)	81	89
50	XK	155/156 (99%)	155 (100%)	0	100	100
51	XL	98/124 (79%)	98 (100%)	0	100	100
52	XM	245/249 (98%)	244 (100%)	1 (0%)	91	95
53	XN	188/211 (89%)	188 (100%)	0	100	100
54	XO	133/150 (89%)	133 (100%)	0	100	100
55	XP	125/155 (81%)	124 (99%)	1 (1%)	81	89
56	XQ	220/256 (86%)	220 (100%)	0	100	100
57	XR	118/126 (94%)	118 (100%)	0	100	100
58	XS	145/180 (81%)	145 (100%)	0	100	100
59	XT	146/176 (83%)	146 (100%)	0	100	100
60	XU	126/135 (93%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	XV	179/191 (94%)	178 (99%)	1 (1%)	86	92
62	XW	91/119 (76%)	90 (99%)	1 (1%)	73	85
63	XX	219/229 (96%)	219 (100%)	0	100	100
64	XY	161/223 (72%)	161 (100%)	0	100	100
65	XZ	111/147 (76%)	111 (100%)	0	100	100
66	a	93/133 (70%)	93 (100%)	0	100	100
67	b	130/186 (70%)	130 (100%)	0	100	100
68	c	241/288 (84%)	240 (100%)	1 (0%)	91	95
69	d	196/274 (72%)	196 (100%)	0	100	100
70	e	188/236 (80%)	187 (100%)	1 (0%)	88	94
71	f	127/188 (68%)	127 (100%)	0	100	100
72	g	122/148 (82%)	122 (100%)	0	100	100
73	h	103/148 (70%)	103 (100%)	0	100	100
74	i	86/110 (78%)	86 (100%)	0	100	100
75	j	68/97 (70%)	68 (100%)	0	100	100
76	k	80/90 (89%)	80 (100%)	0	100	100
77	l	74/116 (64%)	74 (100%)	0	100	100
78	m	54/113 (48%)	54 (100%)	0	100	100
79	o	80/87 (92%)	80 (100%)	0	100	100
80	p	117/181 (65%)	117 (100%)	0	100	100
81	q	141/178 (79%)	141 (100%)	0	100	100
82	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%)	49	71
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
All	All	12392/16507 (75%)	12357 (100%)	35 (0%)	92	96

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	5	144	ARG
6	5	310	ARG
6	5	395	ARG
7	6	99	ARG
9	8	119	LYS
12	A0	113	LYS
13	A1	167	ARG
13	A1	287	LYS
14	A2	37	ARG
14	A2	40	LYS
16	A4	158	LYS
16	A4	242	ASN
16	A4	403	LYS
16	A4	594	LYS
20	AD	186	LYS
20	AD	305	MET
28	AL	84	LYS
34	AR	99	LYS
37	AU	114	ARG
38	AV	64	LYS
40	AX	92	LYS
40	AX	232	ARG
40	AX	249	ARG
40	AX	255	MET
40	AX	275	LYS
44	XD	208	ARG
44	XD	231	LYS
49	XJ	154	ARG
52	XM	44	ARG
55	XP	164	MET
61	XV	149	ARG
62	XW	119	ARG
68	c	302	ARG
70	e	273	ARG
85	t1	21[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	106	ASN
7	6	102	GLN
7	6	249	GLN
13	A1	275	ASN

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Mol	Chain	Res	Type
13	A1	279	ASN
16	A4	242	ASN
16	A4	566	GLN
16	A4	590	GLN
16	A4	656	ASN
20	AD	151	ASN
20	AD	347	GLN
22	AF	122	GLN
23	AG	77	GLN
24	AH	163	ASN
25	AI	104	ASN
25	AI	129	GLN
27	AK	55	ASN
27	AK	60	ASN
29	AM	50	GLN
33	AQ	79	ASN
34	AR	278	ASN
38	AV	215	GLN
38	AV	238	GLN
38	AV	316	GLN
40	AX	159	HIS
40	AX	176	GLN
40	AX	291	HIS
40	AX	292	ASN
40	AX	347	ASN
41	AY	378	ASN
50	XK	9	GLN
55	XP	54	ASN
56	XQ	158	GLN
62	XW	41	ASN
70	e	144	ASN
76	k	15	GLN
77	l	76	ASN
77	l	135	ASN
84	s	343	GLN
85	t6	8	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	XA	1489/1561 (95%)	262 (17%)	7 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	AA	916/954 (96%)	161 (17%)	3 (0%)
43	XB	54/72 (75%)	11 (20%)	0
83	r3	0/75	-	-
All	All	2459/2662 (92%)	434 (17%)	10 (0%)

All (434) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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	1804	A
11	XA	1805	A
11	XA	1809	U
11	XA	1810	A
11	XA	1811	A

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Mol	Chain	Res	Type
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	1886	G
11	XA	1887	A
11	XA	1893	A
11	XA	1902	C
11	XA	1903	C
11	XA	1909	A
11	XA	1918	G
11	XA	1919	C
11	XA	1940	A
11	XA	1944	C
11	XA	1950	U
11	XA	1958	G
11	XA	1974	A
11	XA	1975	U
11	XA	1985	G
11	XA	1986	A
11	XA	1992	C
11	XA	1993	A
11	XA	1994	A
11	XA	2000	C
11	XA	2001	C
11	XA	2002	G
11	XA	2003	A
11	XA	2010	U
11	XA	2015	G
11	XA	2022	G
11	XA	2030	U
11	XA	2036	C

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Mol	Chain	Res	Type
11	XA	2037	U
11	XA	2039	A
11	XA	2051	A
11	XA	2055	U
11	XA	2067	C
11	XA	2079	C
11	XA	2099	U
11	XA	2105	G
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	2230	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	2262	C
11	XA	2263	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	2357	C
11	XA	2374	A
11	XA	2375	C
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	2478	G
11	XA	2493	C
11	XA	2520	C
11	XA	2523	C
11	XA	2527	A
11	XA	2540	C
11	XA	2557	C
11	XA	2558	A
11	XA	2559	U
11	XA	2564	A
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	2603	C
11	XA	2618	U
11	XA	2625	C
11	XA	2626	U

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Mol	Chain	Res	Type
11	XA	2627	G
11	XA	2628	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	2722	A
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	2791	A
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	2893	A
11	XA	2906	C
11	XA	2910	A

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Mol	Chain	Res	Type
11	XA	2913	A
11	XA	2916	G
11	XA	2917	G
11	XA	2918	A
11	XA	2921	A
11	XA	2928	C
11	XA	2935	A
11	XA	2939	C
11	XA	2956	A
11	XA	2962	C
11	XA	2963	A
11	XA	2978	U
11	XA	2985	C
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	3067	U
11	XA	3069	A
11	XA	3073	C
11	XA	3086	U
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

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Mol	Chain	Res	Type
11	XA	3162	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
17	AA	651	A
17	AA	680	U
17	AA	688	A
17	AA	694	C
17	AA	700	A
17	AA	704	U
17	AA	721	U
17	AA	722	C
17	AA	730	A
17	AA	753	A
17	AA	757	A
17	AA	761	A
17	AA	766	G
17	AA	771	A
17	AA	791	G
17	AA	792	C
17	AA	794	U
17	AA	796	G
17	AA	811	G
17	AA	814	A
17	AA	825	U
17	AA	826	A
17	AA	829	C
17	AA	830	U

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Mol	Chain	Res	Type
17	AA	832	U
17	AA	835	C
17	AA	836	A
17	AA	844	A
17	AA	851	A
17	AA	856	A
17	AA	860	A
17	AA	861	U
17	AA	865	A
17	AA	866	A
17	AA	868	C
17	AA	869	C
17	AA	880	C
17	AA	881	A
17	AA	890	C
17	AA	893	G
17	AA	897	C
17	AA	899	G
17	AA	903	U
17	AA	905	A
17	AA	909	G
17	AA	919	A
17	AA	923	A
17	AA	932	C
17	AA	933	G
17	AA	938	A
17	AA	939	A
17	AA	942	A
17	AA	950	A
17	AA	967	A
17	AA	975	A
17	AA	992	U
17	AA	993	A
17	AA	994	A
17	AA	1001	C
17	AA	1009	C
17	AA	1015	A
17	AA	1031	G
17	AA	1042	U
17	AA	1049	A
17	AA	1062	G
17	AA	1069	A

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Mol	Chain	Res	Type
17	AA	1081	U
17	AA	1082	A
17	AA	1103	A
17	AA	1105	C
17	AA	1106	C
17	AA	1109	A
17	AA	1121	A
17	AA	1126	A
17	AA	1128	C
17	AA	1138	G
17	AA	1142	A
17	AA	1143	C
17	AA	1151	C
17	AA	1167	A
17	AA	1185	C
17	AA	1188	A
17	AA	1189	U
17	AA	1190	C
17	AA	1193	U
17	AA	1194	C
17	AA	1213	A
17	AA	1214	A
17	AA	1215	U
17	AA	1220	A
17	AA	1223	C
17	AA	1225	C
17	AA	1226	C
17	AA	1227	G
17	AA	1228	A
17	AA	1229	U
17	AA	1230	C
17	AA	1235	U
17	AA	1236	C
17	AA	1237	A
17	AA	1248	C
17	AA	1250	C
17	AA	1251	A
17	AA	1261	C
17	AA	1268	C
17	AA	1271	C
17	AA	1284	U
17	AA	1290	C

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Mol	Chain	Res	Type
17	AA	1293	C
17	AA	1295	A
17	AA	1296	A
17	AA	1297	G
17	AA	1307	G
17	AA	1326	A
17	AA	1327	G
17	AA	1330	C
17	AA	1331	A
17	AA	1341	C
17	AA	1342	C
17	AA	1343	A
17	AA	1344	U
17	AA	1349	U
17	AA	1353	A
17	AA	1354	A
17	AA	1356	A
17	AA	1365	A
17	AA	1369	U
17	AA	1378	C
17	AA	1390	A
17	AA	1391	U
17	AA	1402	A
17	AA	1416	A
17	AA	1423	A
17	AA	1430	A
17	AA	1448	U
17	AA	1459	A
17	AA	1461	A
17	AA	1463	G
17	AA	1478	A
17	AA	1482	A
17	AA	1488	C
17	AA	1489	G
17	AA	1503	G
17	AA	1525	C
17	AA	1526	U
17	AA	1527	A
17	AA	1528	A
17	AA	1531	C
17	AA	1537	C
17	AA	1539	C

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Mol	Chain	Res	Type
17	AA	1551	G
17	AA	1557	A
17	AA	1568	U
17	AA	1571	U
17	AA	1582	G
17	AA	1584	A
17	AA	1585	A
17	AA	1594	G
17	AA	1595	G
17	AA	1598	G
17	AA	1599	A
43	XB	1608	G
43	XB	1609	U
43	XB	1611	G
43	XB	1615	A
43	XB	1619	C
43	XB	1620	A
43	XB	1621	A
43	XB	1645	A
43	XB	1646	U
43	XB	1649	C
43	XB	1659	U

All (10) RNA pucker outliers are listed below:

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

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

75 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	$\#\|Z\| > 2$
83	P5P	r3	65	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	3	83	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
83	P5P	r3	5	83	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	14	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	41	83	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
83	P5P	r3	27	83	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	60	83	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
83	P5P	r3	69	83	16,23,24	0.94	1 (6%)	14,33,36	1.97	3 (21%)
83	Y5P	r3	12	83	14,19,20	3.15	3 (21%)	18,26,29	0.56	0
83	Y5P	r3	17	83	14,19,20	3.15	3 (21%)	18,26,29	0.57	0
83	P5P	r3	28	83	16,23,24	0.94	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	39	83	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
83	Y5P	r3	2	83	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
83	Y5P	r3	20	83	14,19,20	3.14	4 (28%)	18,26,29	0.59	0
83	P5P	r3	18	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	52	83	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	24	83	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
83	P5P	r3	19	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	48	83	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
83	P5P	r3	21	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	74	11,83	16,23,24	0.96	1 (6%)	14,33,36	2.11	3 (21%)
83	P5P	r3	7	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	32	83	14,19,20	3.14	3 (21%)	18,26,29	0.61	0
83	P5P	r3	44	83	16,23,24	0.94	1 (6%)	14,33,36	2.00	3 (21%)
83	P5P	r3	10	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	50	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	75	83	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
83	Y5P	r3	67	83	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
83	P5P	r3	23	83	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
83	P5P	r3	73	83	16,23,24	0.97	1 (6%)	14,33,36	2.00	3 (21%)
83	Y5P	r3	43	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	P5P	r3	71	83	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	68	83	14,19,20	3.16	3 (21%)	18,26,29	0.58	0
83	P5P	r3	26	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	38	83	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	66	83	14,19,20	3.15	3 (21%)	18,26,29	0.54	0
83	P5P	r3	1	83	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
83	Y5P	r3	51	83	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
83	Y5P	r3	62	83	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
83	Y5P	r3	55	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	45	83	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
83	P5P	r3	46	83	16,23,24	0.95	1 (6%)	14,33,36	1.96	3 (21%)
83	Y5P	r3	8	83	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
83	P5P	r3	57	83	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	16	83	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
83	P5P	r3	34	83	16,23,24	0.96	1 (6%)	14,33,36	2.02	3 (21%)
83	P5P	r3	64	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	9	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	36	83	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	61	83	14,19,20	3.15	3 (21%)	18,26,29	0.54	0
83	P5P	r3	6	83	16,23,24	0.95	1 (6%)	14,33,36	2.01	3 (21%)
83	Y5P	r3	72	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	40	83	14,19,20	3.15	3 (21%)	18,26,29	0.57	0
83	P5P	r3	53	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	11	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	13	83	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
83	Y5P	r3	4	83	14,19,20	3.12	3 (21%)	18,26,29	0.60	0
83	P5P	r3	30	83	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	22	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	42	83	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
83	Y5P	r3	47	83	14,19,20	3.13	3 (21%)	18,26,29	0.61	0
83	Y5P	r3	56	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	P5P	r3	70	83	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	25	83	14,19,20	3.15	3 (21%)	18,26,29	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
83	P5P	r3	31	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	54	83	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
83	P5P	r3	63	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	49	83	14,19,20	3.15	3 (21%)	18,26,29	0.57	0
83	P5P	r3	35	83	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
83	P5P	r3	15	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	58	83	16,23,24	0.94	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	33	83	14,19,20	3.14	3 (21%)	18,26,29	0.53	0
83	Y5P	r3	59	83	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
83	P5P	r3	37	83	20,24,24	0.87	1 (5%)	21,36,36	4.65	9 (42%)
83	P5P	r3	29	83	16,23,24	0.94	1 (6%)	14,33,36	2.01	3 (21%)

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
83	P5P	r3	65	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	3	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	5	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	14	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	41	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	27	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	60	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	69	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	12	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	17	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	28	83	-	2/3/25/26	0/3/3/3
83	Y5P	r3	39	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	2	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	20	83	-	2/7/33/34	0/2/2/2
83	P5P	r3	18	83	-	2/3/25/26	0/3/3/3
83	P5P	r3	52	83	-	3/3/25/26	0/3/3/3
83	P5P	r3	24	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	19	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	48	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	21	83	-	1/3/25/26	0/3/3/3
83	P5P	r3	74	11,83	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	P5P	r3	7	83	-	2/3/25/26	0/3/3/3
83	Y5P	r3	32	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	44	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	10	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	50	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	75	83	-	6/7/33/34	0/2/2/2
83	Y5P	r3	67	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	23	83	-	3/3/25/26	0/3/3/3
83	P5P	r3	73	83	-	2/3/25/26	0/3/3/3
83	Y5P	r3	43	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	71	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	68	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	26	83	-	2/3/25/26	0/3/3/3
83	P5P	r3	38	83	-	1/3/25/26	0/3/3/3
83	Y5P	r3	66	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	1	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	51	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	62	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	55	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	45	83	-	4/7/33/34	0/2/2/2
83	P5P	r3	46	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	8	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	57	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	16	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	34	83	-	1/3/25/26	0/3/3/3
83	P5P	r3	64	83	-	2/3/25/26	0/3/3/3
83	P5P	r3	9	83	-	2/3/25/26	0/3/3/3
83	P5P	r3	36	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	61	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	6	83	-	2/3/25/26	0/3/3/3
83	Y5P	r3	72	83	-	3/7/33/34	0/2/2/2
83	Y5P	r3	40	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	53	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	11	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	13	83	-	3/7/33/34	0/2/2/2
83	Y5P	r3	4	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	30	83	-	1/3/25/26	0/3/3/3
83	P5P	r3	22	83	-	3/3/25/26	0/3/3/3
83	Y5P	r3	42	83	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	Y5P	r3	47	83	-	4/7/33/34	0/2/2/2
83	Y5P	r3	56	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	70	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	25	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	31	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	54	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	63	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	49	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	35	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	15	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	58	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	33	83	-	2/7/33/34	0/2/2/2
83	Y5P	r3	59	83	-	2/7/33/34	0/2/2/2
83	P5P	r3	37	83	-	2/6/26/26	0/3/3/3
83	P5P	r3	29	83	-	2/3/25/26	0/3/3/3

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r3	68	Y5P	C6-C5	10.61	1.52	1.33
83	r3	17	Y5P	C6-C5	10.58	1.52	1.33
83	r3	39	Y5P	C6-C5	10.58	1.52	1.33
83	r3	66	Y5P	C6-C5	10.58	1.52	1.33
83	r3	3	Y5P	C6-C5	10.58	1.52	1.33
83	r3	50	Y5P	C6-C5	10.57	1.52	1.33
83	r3	49	Y5P	C6-C5	10.56	1.52	1.33
83	r3	25	Y5P	C6-C5	10.56	1.52	1.33
83	r3	12	Y5P	C6-C5	10.56	1.52	1.33
83	r3	40	Y5P	C6-C5	10.55	1.52	1.33
83	r3	8	Y5P	C6-C5	10.55	1.52	1.33
83	r3	61	Y5P	C6-C5	10.55	1.52	1.33
83	r3	72	Y5P	C6-C5	10.54	1.52	1.33
83	r3	33	Y5P	C6-C5	10.54	1.52	1.33
83	r3	11	Y5P	C6-C5	10.53	1.52	1.33
83	r3	41	Y5P	C6-C5	10.53	1.52	1.33
83	r3	2	Y5P	C6-C5	10.53	1.52	1.33
83	r3	42	Y5P	C6-C5	10.53	1.52	1.33
83	r3	45	Y5P	C6-C5	10.52	1.52	1.33
83	r3	59	Y5P	C6-C5	10.52	1.52	1.33
83	r3	43	Y5P	C6-C5	10.51	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r3	48	Y5P	C6-C5	10.51	1.52	1.33
83	r3	55	Y5P	C6-C5	10.51	1.52	1.33
83	r3	62	Y5P	C6-C5	10.51	1.52	1.33
83	r3	20	Y5P	C6-C5	10.51	1.52	1.33
83	r3	54	Y5P	C6-C5	10.51	1.52	1.33
83	r3	60	Y5P	C6-C5	10.51	1.52	1.33
83	r3	32	Y5P	C6-C5	10.50	1.52	1.33
83	r3	67	Y5P	C6-C5	10.50	1.52	1.33
83	r3	75	Y5P	C6-C5	10.50	1.52	1.33
83	r3	56	Y5P	C6-C5	10.49	1.52	1.33
83	r3	16	Y5P	C6-C5	10.49	1.52	1.33
83	r3	51	Y5P	C6-C5	10.49	1.52	1.33
83	r3	13	Y5P	C6-C5	10.48	1.52	1.33
83	r3	47	Y5P	C6-C5	10.46	1.52	1.33
83	r3	4	Y5P	C6-C5	10.45	1.52	1.33
83	r3	56	Y5P	C2-N1	3.90	1.45	1.36
83	r3	43	Y5P	C2-N1	3.89	1.45	1.36
83	r3	16	Y5P	C2-N1	3.89	1.45	1.36
83	r3	20	Y5P	C2-N1	3.88	1.45	1.36
83	r3	47	Y5P	C2-N1	3.87	1.45	1.36
83	r3	72	Y5P	C2-N1	3.86	1.45	1.36
83	r3	48	Y5P	C2-N1	3.86	1.45	1.36
83	r3	11	Y5P	C2-N1	3.86	1.45	1.36
83	r3	41	Y5P	C2-N1	3.85	1.45	1.36
83	r3	12	Y5P	C2-N1	3.85	1.45	1.36
83	r3	59	Y5P	C2-N1	3.85	1.45	1.36
83	r3	60	Y5P	C2-N1	3.85	1.45	1.36
83	r3	32	Y5P	C2-N1	3.84	1.45	1.36
83	r3	62	Y5P	C2-N1	3.84	1.45	1.36
83	r3	4	Y5P	C2-N1	3.84	1.45	1.36
83	r3	8	Y5P	C2-N1	3.84	1.45	1.36
83	r3	25	Y5P	C2-N1	3.84	1.45	1.36
83	r3	17	Y5P	C2-N1	3.83	1.45	1.36
83	r3	54	Y5P	C2-N1	3.83	1.45	1.36
83	r3	67	Y5P	C2-N1	3.83	1.45	1.36
83	r3	55	Y5P	C2-N1	3.83	1.45	1.36
83	r3	61	Y5P	C2-N1	3.83	1.45	1.36
83	r3	33	Y5P	C2-N1	3.83	1.45	1.36
83	r3	45	Y5P	C2-N1	3.82	1.45	1.36
83	r3	3	Y5P	C2-N1	3.82	1.45	1.36
83	r3	66	Y5P	C2-N1	3.82	1.45	1.36
83	r3	51	Y5P	C2-N1	3.82	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r3	49	Y5P	C2-N1	3.81	1.45	1.36
83	r3	13	Y5P	C2-N1	3.81	1.45	1.36
83	r3	42	Y5P	C2-N1	3.81	1.45	1.36
83	r3	40	Y5P	C2-N1	3.81	1.45	1.36
83	r3	68	Y5P	C2-N1	3.81	1.45	1.36
83	r3	39	Y5P	C2-N1	3.80	1.45	1.36
83	r3	75	Y5P	C2-N1	3.80	1.45	1.36
83	r3	2	Y5P	C2-N1	3.80	1.45	1.36
83	r3	50	Y5P	C2-N1	3.78	1.45	1.36
83	r3	55	Y5P	C6-N1	2.70	1.44	1.37
83	r3	62	Y5P	C6-N1	2.69	1.44	1.37
83	r3	75	Y5P	C6-N1	2.69	1.44	1.37
83	r3	56	Y5P	C6-N1	2.68	1.44	1.37
83	r3	48	Y5P	C6-N1	2.68	1.44	1.37
83	r3	8	Y5P	C6-N1	2.68	1.44	1.37
83	r3	42	Y5P	C6-N1	2.68	1.44	1.37
83	r3	43	Y5P	C6-N1	2.68	1.44	1.37
83	r3	40	Y5P	C6-N1	2.68	1.44	1.37
83	r3	12	Y5P	C6-N1	2.68	1.44	1.37
83	r3	51	Y5P	C6-N1	2.68	1.44	1.37
83	r3	72	Y5P	C6-N1	2.67	1.44	1.37
83	r3	11	Y5P	C6-N1	2.67	1.44	1.37
83	r3	13	Y5P	C6-N1	2.67	1.44	1.37
83	r3	33	Y5P	C6-N1	2.67	1.44	1.37
83	r3	16	Y5P	C6-N1	2.67	1.43	1.37
83	r3	20	Y5P	C6-N1	2.66	1.43	1.37
83	r3	61	Y5P	C6-N1	2.66	1.43	1.37
83	r3	66	Y5P	C6-N1	2.66	1.43	1.37
83	r3	54	Y5P	C6-N1	2.66	1.43	1.37
83	r3	60	Y5P	C6-N1	2.66	1.43	1.37
83	r3	25	Y5P	C6-N1	2.66	1.43	1.37
83	r3	39	Y5P	C6-N1	2.66	1.43	1.37
83	r3	49	Y5P	C6-N1	2.66	1.43	1.37
83	r3	17	Y5P	C6-N1	2.65	1.43	1.37
83	r3	47	Y5P	C6-N1	2.65	1.43	1.37
83	r3	50	Y5P	C6-N1	2.65	1.43	1.37
83	r3	59	Y5P	C6-N1	2.65	1.43	1.37
83	r3	45	Y5P	C6-N1	2.65	1.43	1.37
83	r3	68	Y5P	C6-N1	2.64	1.43	1.37
83	r3	32	Y5P	C6-N1	2.64	1.43	1.37
83	r3	2	Y5P	C6-N1	2.64	1.43	1.37
83	r3	3	Y5P	C6-N1	2.64	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r3	41	Y5P	C6-N1	2.64	1.43	1.37
83	r3	67	Y5P	C6-N1	2.63	1.43	1.37
83	r3	4	Y5P	C6-N1	2.60	1.43	1.37
83	r3	73	P5P	C5-C4	-2.22	1.35	1.40
83	r3	36	P5P	C5-C4	-2.21	1.35	1.40
83	r3	53	P5P	C5-C4	-2.21	1.35	1.40
83	r3	1	P5P	C5-C4	-2.20	1.35	1.40
83	r3	7	P5P	C5-C4	-2.20	1.35	1.40
83	r3	21	P5P	C5-C4	-2.20	1.35	1.40
83	r3	74	P5P	C5-C4	-2.20	1.35	1.40
83	r3	31	P5P	C5-C4	-2.20	1.35	1.40
83	r3	9	P5P	C5-C4	-2.19	1.35	1.40
83	r3	35	P5P	C5-C4	-2.19	1.35	1.40
83	r3	30	P5P	C5-C4	-2.19	1.35	1.40
83	r3	52	P5P	C5-C4	-2.19	1.35	1.40
83	r3	57	P5P	C5-C4	-2.19	1.35	1.40
83	r3	22	P5P	C5-C4	-2.19	1.35	1.40
83	r3	6	P5P	C5-C4	-2.18	1.35	1.40
83	r3	24	P5P	C5-C4	-2.18	1.35	1.40
83	r3	23	P5P	C5-C4	-2.18	1.35	1.40
83	r3	19	P5P	C5-C4	-2.18	1.35	1.40
83	r3	34	P5P	C5-C4	-2.18	1.35	1.40
83	r3	58	P5P	C5-C4	-2.18	1.35	1.40
83	r3	71	P5P	C5-C4	-2.18	1.35	1.40
83	r3	46	P5P	C5-C4	-2.18	1.35	1.40
83	r3	26	P5P	C5-C4	-2.18	1.35	1.40
83	r3	65	P5P	C5-C4	-2.18	1.35	1.40
83	r3	15	P5P	C5-C4	-2.17	1.35	1.40
83	r3	27	P5P	C5-C4	-2.17	1.35	1.40
83	r3	37	P5P	C5-C4	-2.17	1.35	1.40
83	r3	5	P5P	C5-C4	-2.17	1.35	1.40
83	r3	38	P5P	C5-C4	-2.17	1.35	1.40
83	r3	70	P5P	C5-C4	-2.17	1.35	1.40
83	r3	63	P5P	C5-C4	-2.17	1.35	1.40
83	r3	64	P5P	C5-C4	-2.17	1.35	1.40
83	r3	44	P5P	C5-C4	-2.16	1.35	1.40
83	r3	14	P5P	C5-C4	-2.16	1.35	1.40
83	r3	69	P5P	C5-C4	-2.16	1.35	1.40
83	r3	28	P5P	C5-C4	-2.16	1.35	1.40
83	r3	18	P5P	C5-C4	-2.15	1.35	1.40
83	r3	10	P5P	C5-C4	-2.13	1.35	1.40
83	r3	29	P5P	C5-C4	-2.12	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r3	20	Y5P	C4-N3	2.03	1.48	1.46

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r3	37	P5P	OP2-P-O5’	-10.25	79.46	106.73
83	r3	37	P5P	O5’-P-OP1	-9.37	80.20	106.47
83	r3	37	P5P	OP2-P-OP1	8.11	142.42	110.68
83	r3	37	P5P	OP3-P-O5’	7.05	125.48	106.73
83	r3	37	P5P	OP3-P-OP1	-6.90	83.67	110.68
83	r3	37	P5P	OP3-P-OP2	-6.47	82.91	107.64
83	r3	74	P5P	N1-C2-N3	-6.02	119.94	127.65
83	r3	6	P5P	N1-C2-N3	-6.01	119.96	127.65
83	r3	1	P5P	N1-C2-N3	-5.98	120.00	127.65
83	r3	73	P5P	N1-C2-N3	-5.97	120.00	127.65
83	r3	34	P5P	N1-C2-N3	-5.95	120.03	127.65
83	r3	31	P5P	N1-C2-N3	-5.95	120.04	127.65
83	r3	71	P5P	N1-C2-N3	-5.95	120.04	127.65
83	r3	15	P5P	N1-C2-N3	-5.94	120.05	127.65
83	r3	38	P5P	N1-C2-N3	-5.94	120.05	127.65
83	r3	18	P5P	N1-C2-N3	-5.93	120.06	127.65
83	r3	46	P5P	N1-C2-N3	-5.93	120.06	127.65
83	r3	21	P5P	N1-C2-N3	-5.93	120.06	127.65
83	r3	52	P5P	N1-C2-N3	-5.93	120.06	127.65
83	r3	57	P5P	N1-C2-N3	-5.93	120.06	127.65
83	r3	70	P5P	N1-C2-N3	-5.93	120.06	127.65
83	r3	53	P5P	N1-C2-N3	-5.93	120.06	127.65
83	r3	35	P5P	N1-C2-N3	-5.92	120.07	127.65
83	r3	28	P5P	N1-C2-N3	-5.92	120.07	127.65
83	r3	58	P5P	N1-C2-N3	-5.92	120.08	127.65
83	r3	5	P5P	N1-C2-N3	-5.92	120.08	127.65
83	r3	24	P5P	N1-C2-N3	-5.91	120.08	127.65
83	r3	19	P5P	N1-C2-N3	-5.91	120.08	127.65
83	r3	14	P5P	N1-C2-N3	-5.91	120.08	127.65
83	r3	9	P5P	N1-C2-N3	-5.91	120.08	127.65
83	r3	23	P5P	N1-C2-N3	-5.91	120.09	127.65
83	r3	30	P5P	N1-C2-N3	-5.91	120.09	127.65
83	r3	22	P5P	N1-C2-N3	-5.91	120.09	127.65
83	r3	37	P5P	N1-C2-N3	-5.91	120.09	127.65
83	r3	63	P5P	N1-C2-N3	-5.91	120.09	127.65
83	r3	27	P5P	N1-C2-N3	-5.91	120.09	127.65
83	r3	29	P5P	N1-C2-N3	-5.91	120.09	127.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	r3	26	P5P	N1-C2-N3	-5.90	120.09	127.65
83	r3	7	P5P	N1-C2-N3	-5.90	120.10	127.65
83	r3	64	P5P	N1-C2-N3	-5.89	120.11	127.65
83	r3	44	P5P	N1-C2-N3	-5.89	120.12	127.65
83	r3	36	P5P	N1-C2-N3	-5.88	120.12	127.65
83	r3	65	P5P	N1-C2-N3	-5.88	120.12	127.65
83	r3	69	P5P	N1-C2-N3	-5.88	120.12	127.65
83	r3	10	P5P	N1-C2-N3	-5.87	120.13	127.65
83	r3	74	P5P	C1'-N9-C4	3.26	132.36	126.64
83	r3	29	P5P	C1'-N9-C4	3.18	132.23	126.64
83	r3	6	P5P	C6-N1-C2	3.17	120.38	115.84
83	r3	74	P5P	C6-N1-C2	3.13	120.33	115.84
83	r3	1	P5P	C6-N1-C2	3.09	120.26	115.84
83	r3	10	P5P	C1'-N9-C4	3.08	132.06	126.64
83	r3	31	P5P	C6-N1-C2	3.08	120.25	115.84
83	r3	28	P5P	C6-N1-C2	3.07	120.23	115.84
83	r3	21	P5P	C6-N1-C2	3.07	120.23	115.84
83	r3	52	P5P	C6-N1-C2	3.06	120.22	115.84
83	r3	30	P5P	C6-N1-C2	3.06	120.22	115.84
83	r3	18	P5P	C6-N1-C2	3.06	120.22	115.84
83	r3	15	P5P	C6-N1-C2	3.06	120.22	115.84
83	r3	70	P5P	C6-N1-C2	3.06	120.22	115.84
83	r3	14	P5P	C6-N1-C2	3.05	120.21	115.84
83	r3	5	P5P	C6-N1-C2	3.05	120.21	115.84
83	r3	38	P5P	C6-N1-C2	3.05	120.21	115.84
83	r3	44	P5P	C6-N1-C2	3.05	120.21	115.84
83	r3	35	P5P	C6-N1-C2	3.05	120.20	115.84
83	r3	53	P5P	C6-N1-C2	3.05	120.20	115.84
83	r3	63	P5P	C6-N1-C2	3.05	120.20	115.84
83	r3	9	P5P	C6-N1-C2	3.05	120.20	115.84
83	r3	37	P5P	C6-N1-C2	3.05	120.20	115.84
83	r3	58	P5P	C6-N1-C2	3.04	120.20	115.84
83	r3	22	P5P	C6-N1-C2	3.04	120.20	115.84
83	r3	46	P5P	C6-N1-C2	3.04	120.20	115.84
83	r3	57	P5P	C6-N1-C2	3.04	120.20	115.84
83	r3	71	P5P	C6-N1-C2	3.04	120.20	115.84
83	r3	7	P5P	C6-N1-C2	3.04	120.19	115.84
83	r3	24	P5P	C6-N1-C2	3.04	120.19	115.84
83	r3	26	P5P	C6-N1-C2	3.04	120.19	115.84
83	r3	34	P5P	C6-N1-C2	3.04	120.19	115.84
83	r3	36	P5P	C6-N1-C2	3.04	120.19	115.84
83	r3	29	P5P	C6-N1-C2	3.03	120.19	115.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r3	69	P5P	C6-N1-C2	3.03	120.19	115.84
83	r3	19	P5P	C6-N1-C2	3.03	120.18	115.84
83	r3	23	P5P	C6-N1-C2	3.03	120.17	115.84
83	r3	27	P5P	C6-N1-C2	3.03	120.17	115.84
83	r3	64	P5P	C6-N1-C2	3.02	120.17	115.84
83	r3	65	P5P	C6-N1-C2	3.02	120.16	115.84
83	r3	73	P5P	C1'-N9-C4	3.02	131.94	126.64
83	r3	10	P5P	C6-N1-C2	3.00	120.14	115.84
83	r3	73	P5P	C6-N1-C2	3.00	120.13	115.84
83	r3	23	P5P	C1'-N9-C4	2.99	131.90	126.64
83	r3	44	P5P	C1'-N9-C4	2.97	131.86	126.64
83	r3	5	P5P	C1'-N9-C4	2.89	131.71	126.64
83	r3	64	P5P	C1'-N9-C4	2.88	131.71	126.64
83	r3	22	P5P	C1'-N9-C4	2.88	131.70	126.64
83	r3	35	P5P	C1'-N9-C4	2.87	131.69	126.64
83	r3	14	P5P	C1'-N9-C4	2.87	131.68	126.64
83	r3	18	P5P	C1'-N9-C4	2.85	131.64	126.64
83	r3	30	P5P	C1'-N9-C4	2.84	131.64	126.64
83	r3	63	P5P	C1'-N9-C4	2.82	131.59	126.64
83	r3	19	P5P	C1'-N9-C4	2.82	131.59	126.64
83	r3	26	P5P	C1'-N9-C4	2.81	131.58	126.64
83	r3	15	P5P	C1'-N9-C4	2.81	131.58	126.64
83	r3	65	P5P	C1'-N9-C4	2.80	131.56	126.64
83	r3	34	P5P	C1'-N9-C4	2.79	131.55	126.64
83	r3	37	P5P	C1'-N9-C4	2.79	131.55	126.64
83	r3	28	P5P	C1'-N9-C4	2.79	131.55	126.64
83	r3	9	P5P	C1'-N9-C4	2.79	131.54	126.64
83	r3	27	P5P	C1'-N9-C4	2.78	131.52	126.64
83	r3	36	P5P	C1'-N9-C4	2.77	131.51	126.64
83	r3	7	P5P	C1'-N9-C4	2.77	131.51	126.64
83	r3	1	P5P	C1'-N9-C4	2.77	131.50	126.64
83	r3	21	P5P	C1'-N9-C4	2.76	131.49	126.64
83	r3	53	P5P	C1'-N9-C4	2.75	131.47	126.64
83	r3	6	P5P	C1'-N9-C4	2.75	131.47	126.64
83	r3	70	P5P	C1'-N9-C4	2.74	131.46	126.64
83	r3	69	P5P	C1'-N9-C4	2.74	131.45	126.64
83	r3	24	P5P	C1'-N9-C4	2.73	131.44	126.64
83	r3	71	P5P	C1'-N9-C4	2.72	131.42	126.64
83	r3	38	P5P	C1'-N9-C4	2.70	131.39	126.64
83	r3	58	P5P	C1'-N9-C4	2.69	131.38	126.64
83	r3	57	P5P	C1'-N9-C4	2.69	131.37	126.64
83	r3	52	P5P	C1'-N9-C4	2.67	131.33	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r3	46	P5P	C1'-N9-C4	2.63	131.26	126.64
83	r3	31	P5P	C1'-N9-C4	2.56	131.14	126.64

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	r3	9	P5P	O4'-C4'-C5'-O5'
83	r3	13	Y5P	C3'-C4'-C5'-O5'
83	r3	13	Y5P	O4'-C1'-N1-C2
83	r3	16	Y5P	O4'-C1'-N1-C2
83	r3	17	Y5P	O4'-C4'-C5'-O5'
83	r3	20	Y5P	O4'-C1'-N1-C2
83	r3	21	P5P	C4'-C5'-O5'-P
83	r3	22	P5P	C3'-C4'-C5'-O5'
83	r3	22	P5P	O4'-C4'-C5'-O5'
83	r3	26	P5P	C3'-C4'-C5'-O5'
83	r3	29	P5P	C3'-C4'-C5'-O5'
83	r3	29	P5P	O4'-C4'-C5'-O5'
83	r3	37	P5P	C5'-O5'-P-OP2
83	r3	37	P5P	C5'-O5'-P-OP3
83	r3	39	Y5P	O4'-C1'-N1-C2
83	r3	41	Y5P	C3'-C4'-C5'-O5'
83	r3	47	Y5P	O4'-C1'-N1-C2
83	r3	54	Y5P	O4'-C1'-N1-C2
83	r3	55	Y5P	O4'-C1'-N1-C2
83	r3	56	Y5P	O4'-C4'-C5'-O5'
83	r3	59	Y5P	O4'-C1'-N1-C2
83	r3	64	P5P	C3'-C4'-C5'-O5'
83	r3	64	P5P	O4'-C4'-C5'-O5'
83	r3	67	Y5P	O4'-C1'-N1-C2
83	r3	68	Y5P	O4'-C1'-N1-C2
83	r3	72	Y5P	C3'-C4'-C5'-O5'
83	r3	73	P5P	C4'-C5'-O5'-P
83	r3	75	Y5P	C2'-C1'-N1-C6
83	r3	2	Y5P	O4'-C1'-N1-C2
83	r3	4	Y5P	O4'-C1'-N1-C2
83	r3	8	Y5P	O4'-C1'-N1-C2
83	r3	12	Y5P	O4'-C1'-N1-C2
83	r3	17	Y5P	O4'-C1'-N1-C2
83	r3	25	Y5P	O4'-C1'-N1-C2
83	r3	32	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
83	r3	40	Y5P	O4'-C1'-N1-C2
83	r3	41	Y5P	O4'-C1'-N1-C2
83	r3	42	Y5P	O4'-C1'-N1-C2
83	r3	43	Y5P	O4'-C1'-N1-C2
83	r3	48	Y5P	O4'-C1'-N1-C2
83	r3	49	Y5P	O4'-C1'-N1-C2
83	r3	50	Y5P	O4'-C1'-N1-C2
83	r3	51	Y5P	O4'-C1'-N1-C2
83	r3	56	Y5P	O4'-C1'-N1-C2
83	r3	60	Y5P	O4'-C1'-N1-C2
83	r3	61	Y5P	O4'-C1'-N1-C2
83	r3	62	Y5P	O4'-C1'-N1-C2
83	r3	66	Y5P	O4'-C1'-N1-C2
83	r3	75	Y5P	C2'-C1'-N1-C2
83	r3	6	P5P	O4'-C4'-C5'-O5'
83	r3	9	P5P	C3'-C4'-C5'-O5'
83	r3	26	P5P	O4'-C4'-C5'-O5'
83	r3	28	P5P	O4'-C4'-C5'-O5'
83	r3	45	Y5P	O4'-C4'-C5'-O5'
83	r3	45	Y5P	C3'-C4'-C5'-O5'
83	r3	56	Y5P	C3'-C4'-C5'-O5'
83	r3	66	Y5P	O4'-C4'-C5'-O5'
83	r3	66	Y5P	C3'-C4'-C5'-O5'
83	r3	75	Y5P	O4'-C4'-C5'-O5'
83	r3	75	Y5P	C3'-C4'-C5'-O5'
83	r3	20	Y5P	C4'-C5'-O5'-P
83	r3	13	Y5P	O4'-C4'-C5'-O5'
83	r3	41	Y5P	O4'-C4'-C5'-O5'
83	r3	47	Y5P	O4'-C4'-C5'-O5'
83	r3	47	Y5P	C3'-C4'-C5'-O5'
83	r3	72	Y5P	O4'-C4'-C5'-O5'
83	r3	3	Y5P	O4'-C1'-N1-C2
83	r3	11	Y5P	O4'-C1'-N1-C2
83	r3	23	P5P	C4'-C5'-O5'-P
83	r3	6	P5P	C3'-C4'-C5'-O5'
83	r3	25	Y5P	C3'-C4'-C5'-O5'
83	r3	45	Y5P	O4'-C1'-N1-C2
83	r3	49	Y5P	O4'-C4'-C5'-O5'
83	r3	72	Y5P	O4'-C1'-N1-C2
83	r3	22	P5P	C4'-C5'-O5'-P
83	r3	49	Y5P	C3'-C4'-C5'-O5'
83	r3	25	Y5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
83	r3	28	P5P	C3'-C4'-C5'-O5'
83	r3	52	P5P	C3'-C4'-C5'-O5'
83	r3	30	P5P	C4'-C5'-O5'-P
83	r3	45	Y5P	C4'-C5'-O5'-P
83	r3	47	Y5P	C4'-C5'-O5'-P
83	r3	75	Y5P	C4'-C5'-O5'-P
83	r3	23	P5P	C3'-C4'-C5'-O5'
83	r3	18	P5P	C4'-C5'-O5'-P
83	r3	33	Y5P	O4'-C1'-N1-C2
83	r3	7	P5P	O4'-C4'-C5'-O5'
83	r3	67	Y5P	C2'-C1'-N1-C6
83	r3	75	Y5P	O4'-C1'-N1-C6
83	r3	74	P5P	O4'-C4'-C5'-O5'
83	r3	38	P5P	O4'-C4'-C5'-O5'
83	r3	52	P5P	O4'-C4'-C5'-O5'
83	r3	33	Y5P	C2'-C1'-N1-C2
83	r3	17	Y5P	C3'-C4'-C5'-O5'
83	r3	23	P5P	O4'-C4'-C5'-O5'
83	r3	52	P5P	C4'-C5'-O5'-P
83	r3	7	P5P	C3'-C4'-C5'-O5'
83	r3	34	P5P	O4'-C4'-C5'-O5'
83	r3	67	Y5P	C2'-C1'-N1-C2
83	r3	18	P5P	O4'-C4'-C5'-O5'
83	r3	59	Y5P	O4'-C4'-C5'-O5'
83	r3	73	P5P	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 205 ligands modelled in this entry, 202 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
88	H8Q	XA	5144	-	77,80,80	1.08	5 (6%)	103,115,115	1.34	15 (14%)
90	GTP	AX	500	-	26,34,34	1.12	2 (7%)	32,54,54	1.51	6 (18%)
89	DOL	XA	5145	-	43,50,50	3.50	17 (39%)	51,70,70	2.67	9 (17%)

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
88	H8Q	XA	5144	-	-	31/83/127/127	0/8/8/8
90	GTP	AX	500	-	-	8/18/38/38	0/3/3/3
89	DOL	XA	5145	-	-	14/58/77/77	0/2/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	XA	5145	DOL	C28-C29	10.06	1.56	1.32
89	XA	5145	DOL	C22-C23	9.59	1.57	1.32
89	XA	5145	DOL	C19-C20	7.17	1.57	1.34
89	XA	5145	DOL	C6-N5	6.56	1.49	1.34
89	XA	5145	DOL	C26-N25	6.40	1.48	1.34
89	XA	5145	DOL	C22-C20	5.54	1.57	1.45
89	XA	5145	DOL	O36-C37	5.28	1.46	1.34
88	XA	5144	H8Q	C20-S21	-5.24	1.76	1.82
89	XA	5145	DOL	C42-S39	5.10	1.86	1.78
88	XA	5144	H8Q	O41-C34	4.98	1.45	1.34
89	XA	5145	DOL	C13-C10	4.64	1.57	1.50
90	AX	500	GTP	C5-C6	-3.98	1.39	1.47
89	XA	5145	DOL	C16-C14	3.96	1.56	1.51
89	XA	5145	DOL	C28-C26	3.62	1.55	1.48
88	XA	5144	H8Q	C22-S21	-3.48	1.76	1.82
89	XA	5145	DOL	C8-C6	3.08	1.56	1.50
89	XA	5145	DOL	O27-C26	-2.86	1.18	1.24
89	XA	5145	DOL	O18-C17	-2.54	1.39	1.43
88	XA	5144	H8Q	O41-C43	-2.33	1.42	1.46
89	XA	5145	DOL	C13-C14	2.30	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	AX	500	GTP	C2-N3	2.20	1.38	1.33
89	XA	5145	DOL	O36-C32	-2.10	1.41	1.44
88	XA	5144	H8Q	C35-C33	-2.07	1.49	1.52
89	XA	5145	DOL	C24-C23	2.06	1.57	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	XA	5145	DOL	O40-S39-O41	-15.14	100.93	118.19
89	XA	5145	DOL	C24-N25-C26	-5.45	113.21	122.03
89	XA	5145	DOL	C23-C22-C20	-3.87	120.04	125.89
88	XA	5144	H8Q	O41-C34-C33	3.84	122.03	110.83
90	AX	500	GTP	PA-O3A-PB	-3.70	120.14	132.83
89	XA	5145	DOL	C32-O36-C37	-3.63	111.55	117.78
90	AX	500	GTP	C5-C6-N1	3.29	119.77	113.95
89	XA	5145	DOL	C4-N5-C1	-3.29	108.40	112.45
88	XA	5144	H8Q	C43-O41-C34	-3.29	112.74	117.51
88	XA	5144	H8Q	C3-C2-N71	-3.26	107.38	112.69
88	XA	5144	H8Q	C40-C35-C33	-3.24	115.48	120.80
88	XA	5144	H8Q	C50-C51-N52	3.14	121.92	115.78
90	AX	500	GTP	C8-N7-C5	3.08	108.86	102.99
90	AX	500	GTP	C2-N1-C6	-3.06	119.47	125.10
90	AX	500	GTP	PB-O3B-PG	-3.05	122.37	132.83
88	XA	5144	H8Q	C17-C16-C15	2.99	119.86	115.43
88	XA	5144	H8Q	O41-C34-O42	-2.97	118.38	123.94
88	XA	5144	H8Q	C36-C35-C33	2.93	125.62	120.80
89	XA	5145	DOL	C30-C29-C28	-2.89	118.54	126.44
88	XA	5144	H8Q	C35-C33-N31	-2.85	105.49	112.89
89	XA	5145	DOL	C3-C4-N5	2.77	106.19	103.33
89	XA	5145	DOL	O36-C32-C30	2.70	111.59	107.09
88	XA	5144	H8Q	O58-C50-C51	-2.67	116.60	120.59
88	XA	5144	H8Q	C14-C15-C16	2.57	111.23	107.65
88	XA	5144	H8Q	C17-C18-N13	-2.47	107.50	109.92
88	XA	5144	H8Q	C34-C33-N31	2.36	114.46	109.54
88	XA	5144	H8Q	C53-N52-C51	2.34	121.26	116.83
89	XA	5145	DOL	O15-C14-C13	2.17	124.01	120.77
90	AX	500	GTP	O6-C6-C5	-2.15	120.17	124.37
88	XA	5144	H8Q	C2-C1-N13	2.05	122.76	117.72

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	XA	5144	H8Q	C2-C1-N13-C14
88	XA	5144	H8Q	C2-C1-N13-C18
88	XA	5144	H8Q	O1-C1-N13-C14
88	XA	5144	H8Q	O1-C1-N13-C18
88	XA	5144	H8Q	C33-C34-O41-C43
88	XA	5144	H8Q	O42-C34-O41-C43
88	XA	5144	H8Q	C59-C62-N63-C65
88	XA	5144	H8Q	C59-C62-N63-C68
88	XA	5144	H8Q	O64-C62-N63-C65
88	XA	5144	H8Q	O64-C62-N63-C68
88	XA	5144	H8Q	C66-C65-C69-N71
88	XA	5144	H8Q	C66-C65-C69-O70
88	XA	5144	H8Q	C65-C69-N71-C2
88	XA	5144	H8Q	C65-C69-N71-C72
88	XA	5144	H8Q	O70-C69-N71-C2
88	XA	5144	H8Q	O70-C69-N71-C72
89	XA	5145	DOL	C1-C2-S39-O41
89	XA	5145	DOL	C1-C2-S39-O40
89	XA	5145	DOL	C43-C42-S39-C2
89	XA	5145	DOL	C43-C42-S39-O41
89	XA	5145	DOL	C29-C30-C32-C33
89	XA	5145	DOL	C29-C30-C32-O36
89	XA	5145	DOL	C31-C30-C32-C33
90	AX	500	GTP	PB-O3B-PG-O3G
90	AX	500	GTP	C5'-O5'-PA-O3A
88	XA	5144	H8Q	C6-C7-N10-C12
88	XA	5144	H8Q	C8-C7-N10-C11
88	XA	5144	H8Q	C6-C7-N10-C11
88	XA	5144	H8Q	C8-C7-N10-C12
88	XA	5144	H8Q	C43-C45-C46-O47
88	XA	5144	H8Q	C43-C45-C46-N49
89	XA	5145	DOL	C3-C2-S39-C42
88	XA	5144	H8Q	N48-C45-C46-O47
89	XA	5145	DOL	O18-C17-C19-C20
90	AX	500	GTP	O4'-C4'-C5'-O5'
88	XA	5144	H8Q	N48-C45-C46-N49
89	XA	5145	DOL	C28-C29-C30-C31
89	XA	5145	DOL	C3-C2-S39-O40
89	XA	5145	DOL	C31-C30-C32-O36
90	AX	500	GTP	C5'-O5'-PA-O2A
90	AX	500	GTP	C3'-C4'-C5'-O5'
89	XA	5145	DOL	C3-C2-S39-O41
88	XA	5144	H8Q	N13-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
89	XA	5145	DOL	C16-C17-C19-C20
88	XA	5144	H8Q	N13-C18-C30-N31
88	XA	5144	H8Q	N13-C18-C30-O32
88	XA	5144	H8Q	N31-C33-C34-O42
88	XA	5144	H8Q	C34-C33-C35-C40
88	XA	5144	H8Q	N31-C33-C34-O41
88	XA	5144	H8Q	C34-C33-C35-C36
90	AX	500	GTP	PB-O3B-PG-O1G
90	AX	500	GTP	PB-O3B-PG-O2G
90	AX	500	GTP	C5'-O5'-PA-O1A

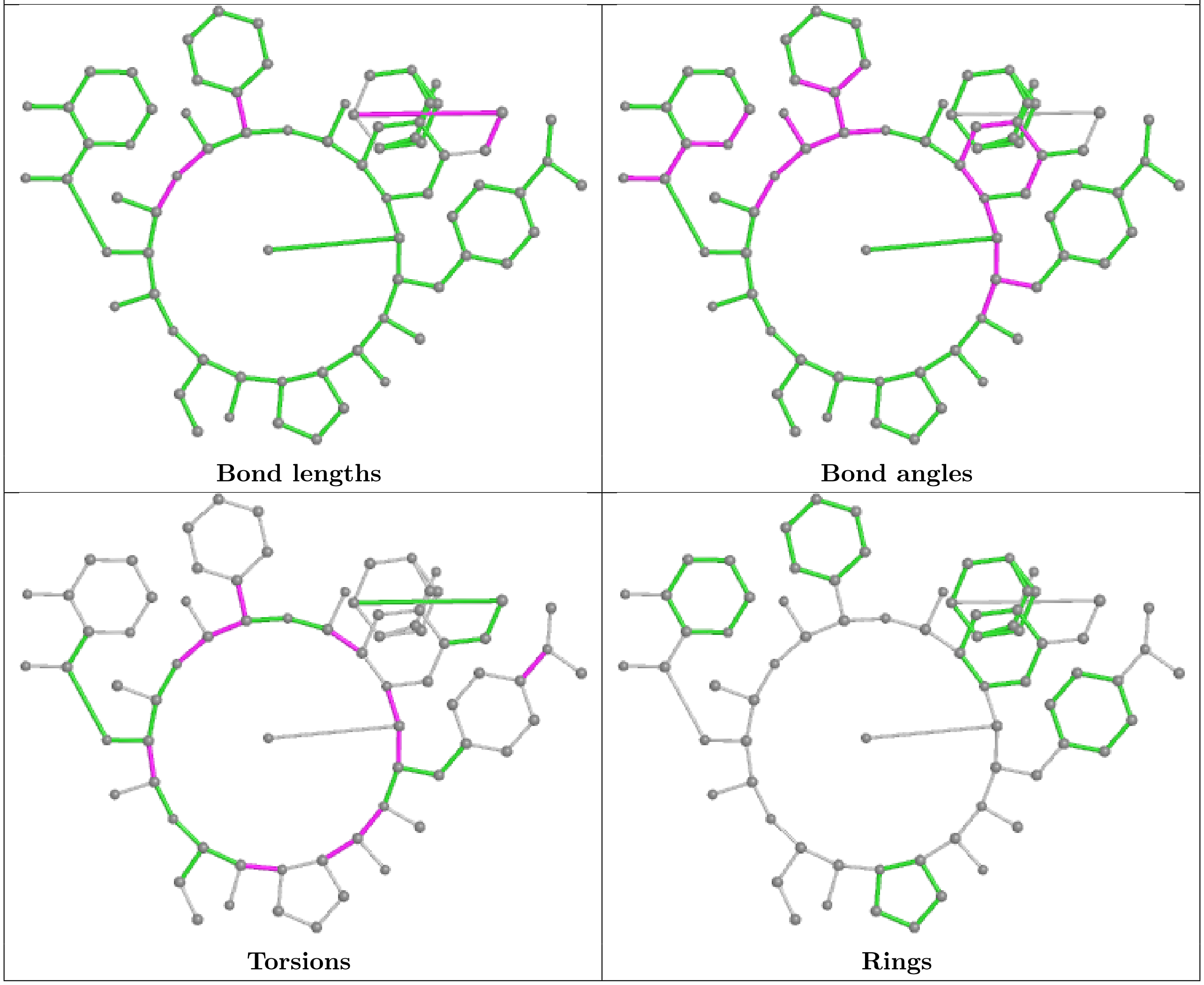
There are no ring outliers.

2 monomers are involved in 3 short contacts:

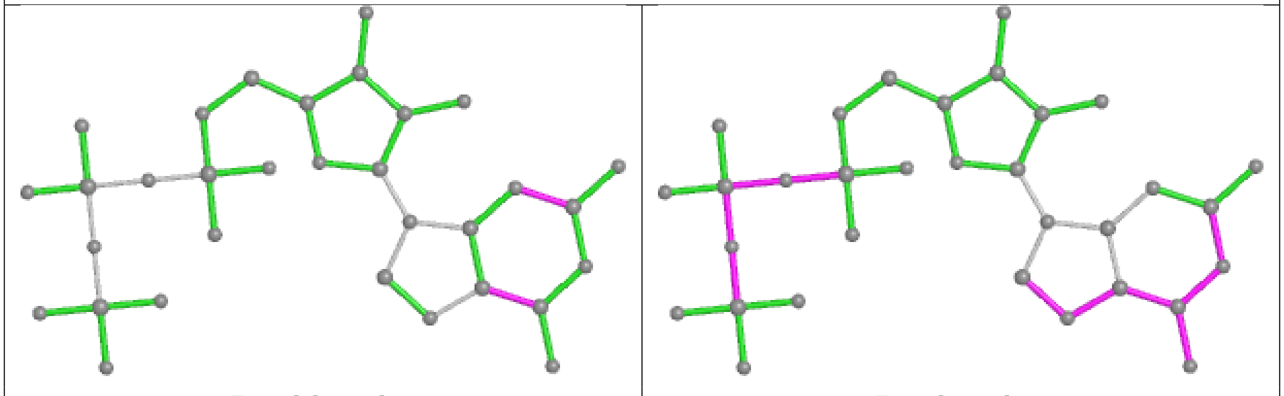
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	XA	5144	H8Q	2	0
90	AX	500	GTP	1	0

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

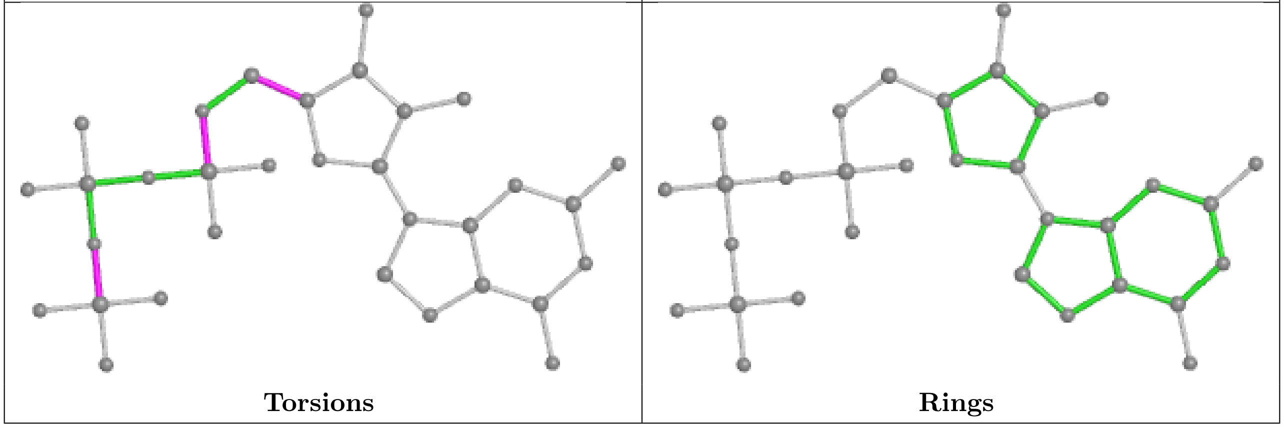
Ligand H8Q XA 5144



Ligand GTP AX 500

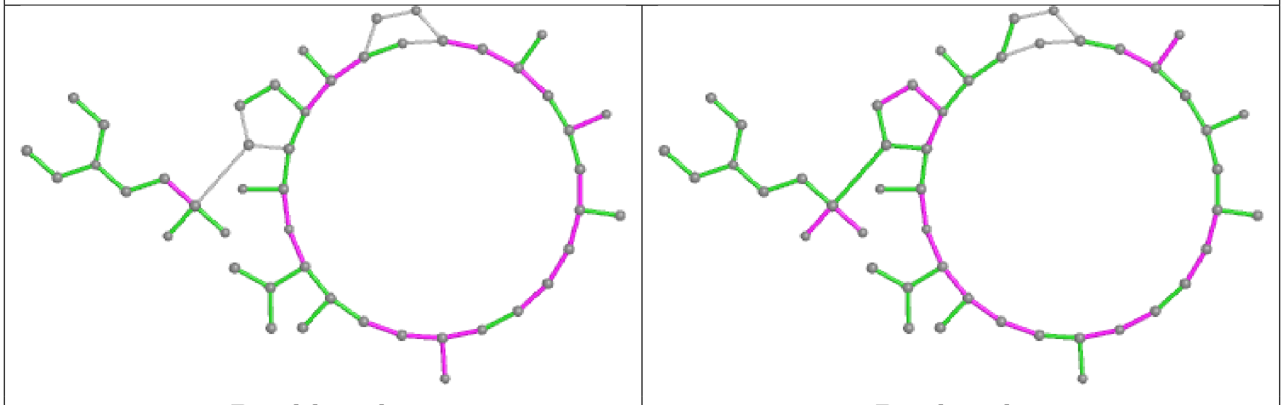


Bond lengths **Bond angles**

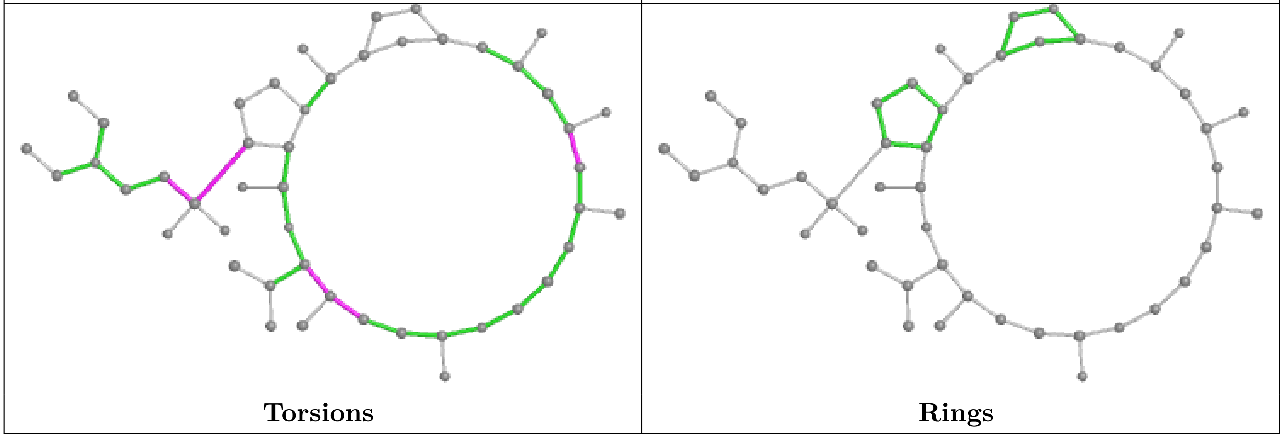


Torsions **Rings**

Ligand DOL XA 5145



Bond lengths **Bond angles**



Torsions **Rings**

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	A4	2
8	7	2
7	6	2
82	r	1
38	AV	1
6	5	1
34	AR	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A4	537:ARG	C	538:ASP	N	6.17
1	7	285:ASN	C	286:LEU	N	5.98
1	r	134:ARG	C	135:LEU	N	5.26
1	AV	269:SER	C	270:PRO	N	4.49
1	7	185:LEU	C	186:ASP	N	3.31
1	6	79:GLY	C	80:GLU	N	3.20
1	5	141:ASP	C	142:ASP	N	3.13
1	A4	143:GLU	C	144:TYR	N	3.07
1	6	282:SER	C	283:GLU	N	3.00
1	AR	308:HIS	C	309:PRO	N	1.88

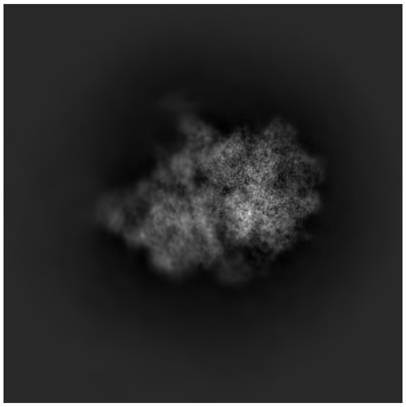
6 Map visualisation

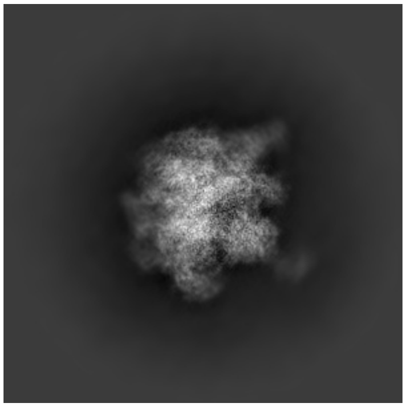
This section contains visualisations of the EMDB entry EMD-12877. These allow visual inspection of the internal detail of the map and identification of artifacts.

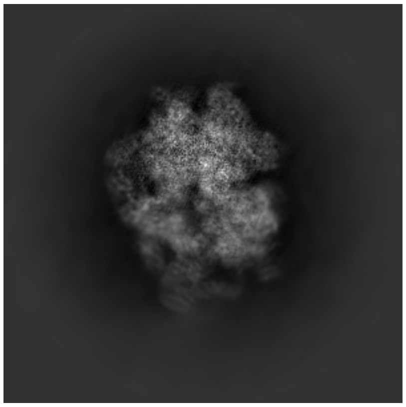
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

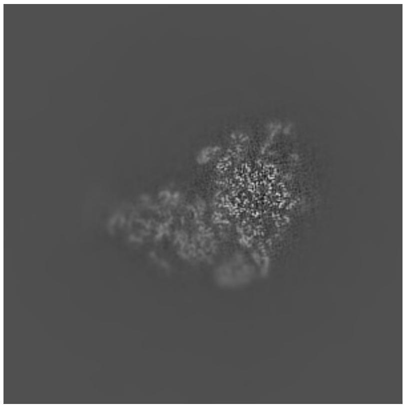

Y

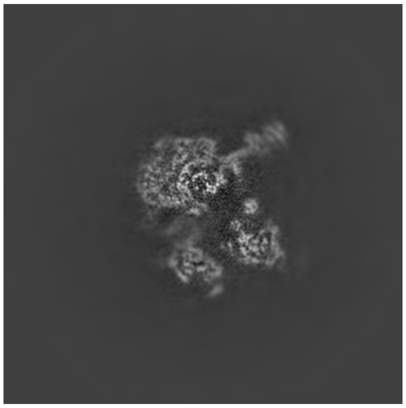

Z

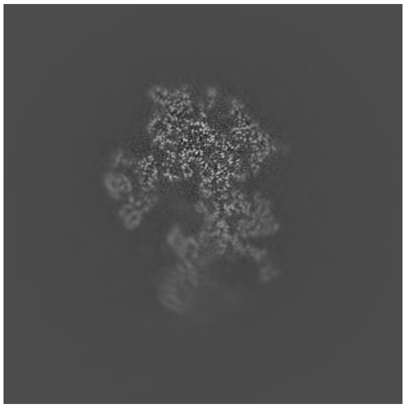
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 260

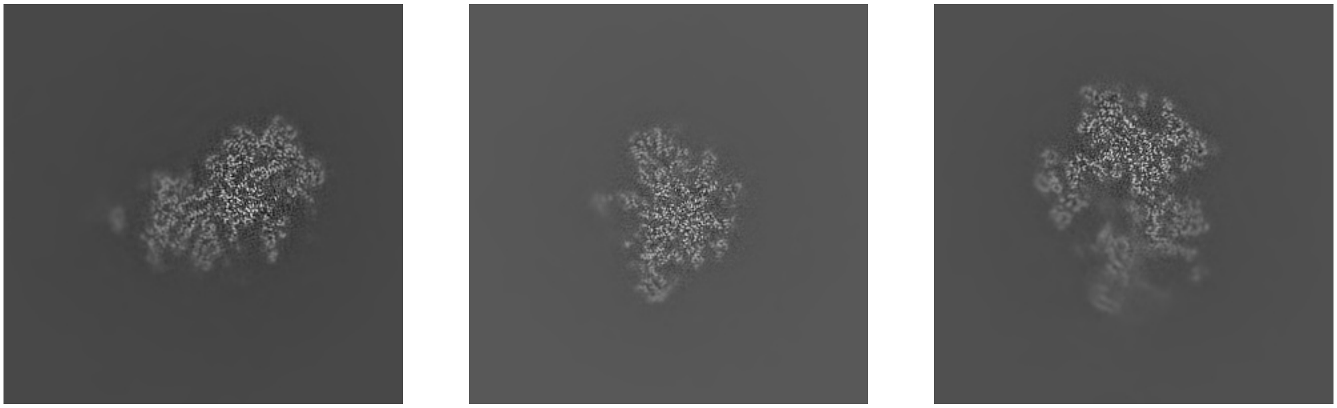

Y Index: 260


Z Index: 260

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

6.3 Largest variance slices

6.3.1 Primary map

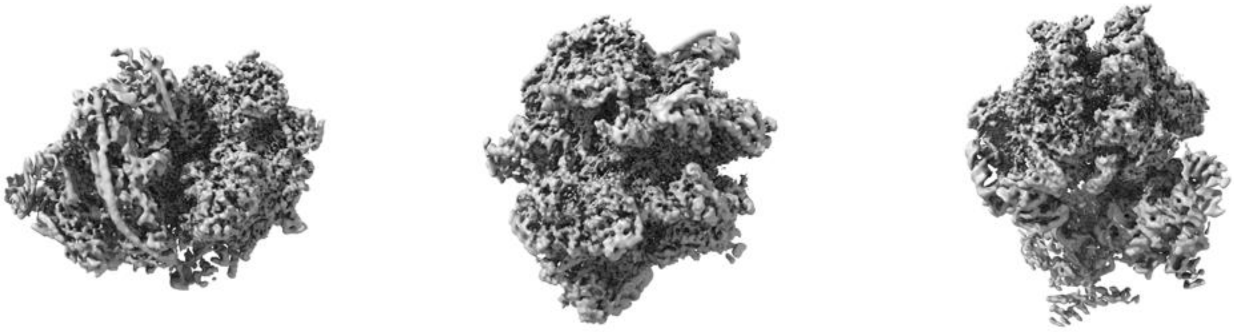


X Index: 282 Y Index: 321 Z Index: 257

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

6.4 Orthogonal surface views

6.4.1 Primary map



X Y Z

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.

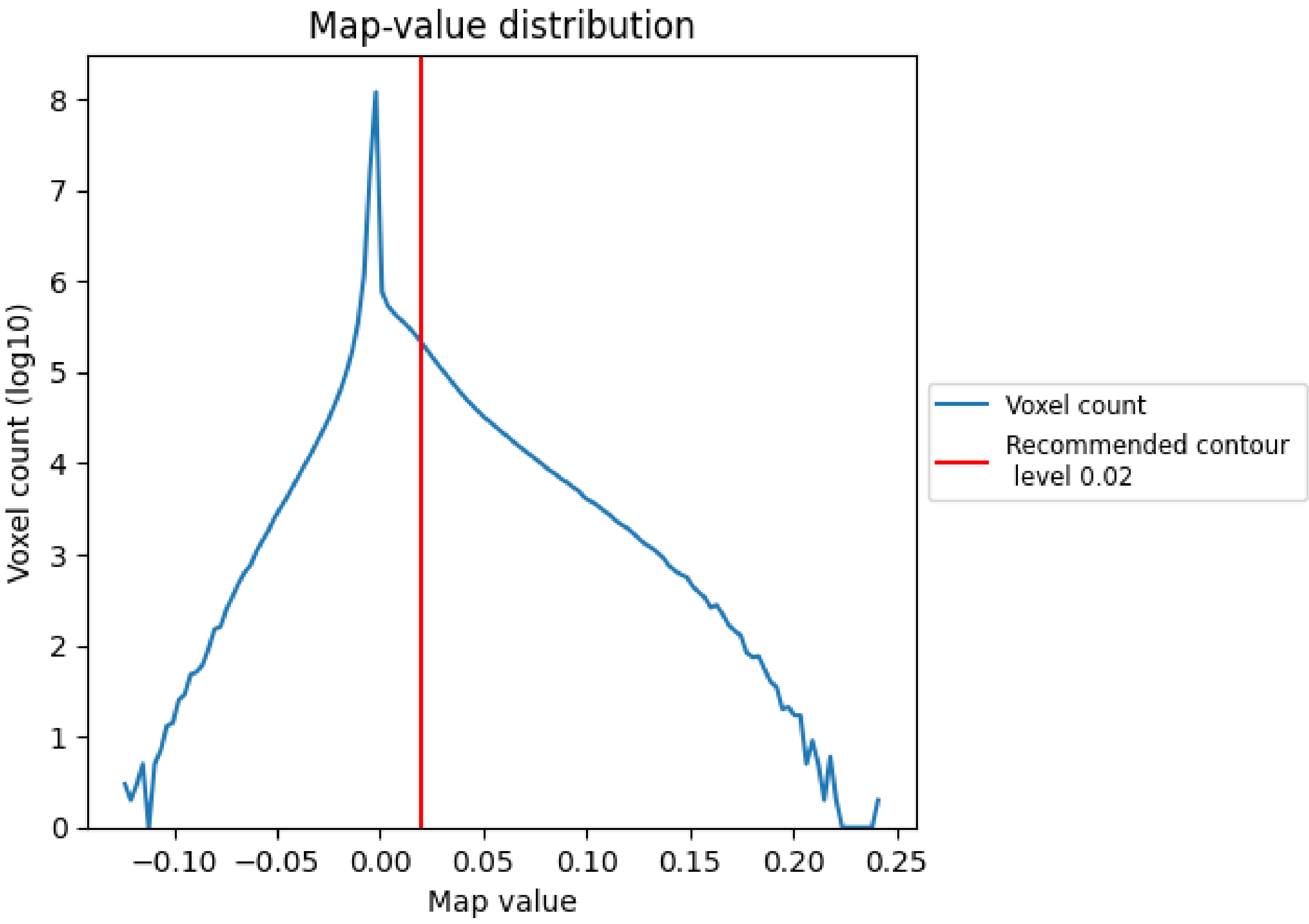
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

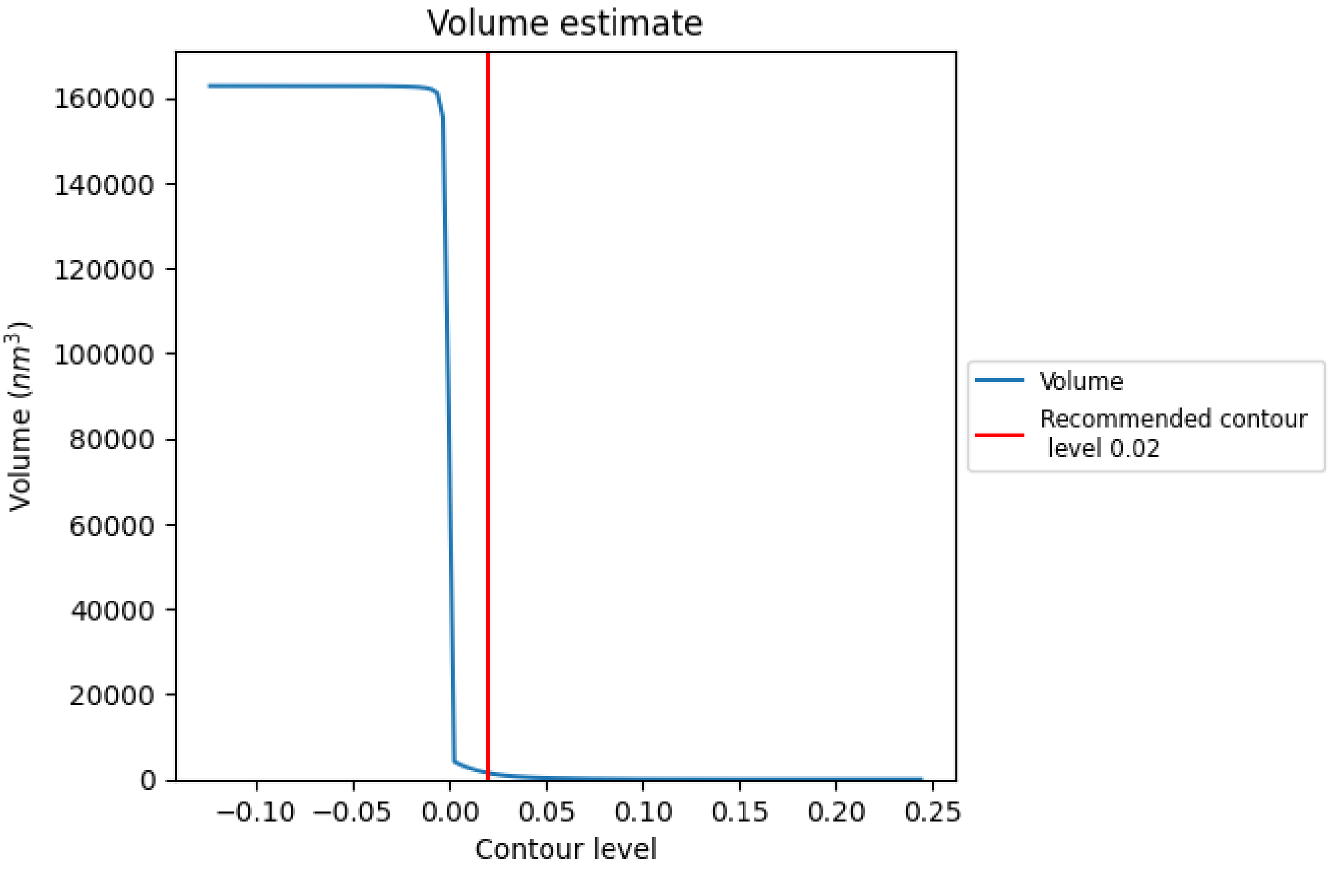
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

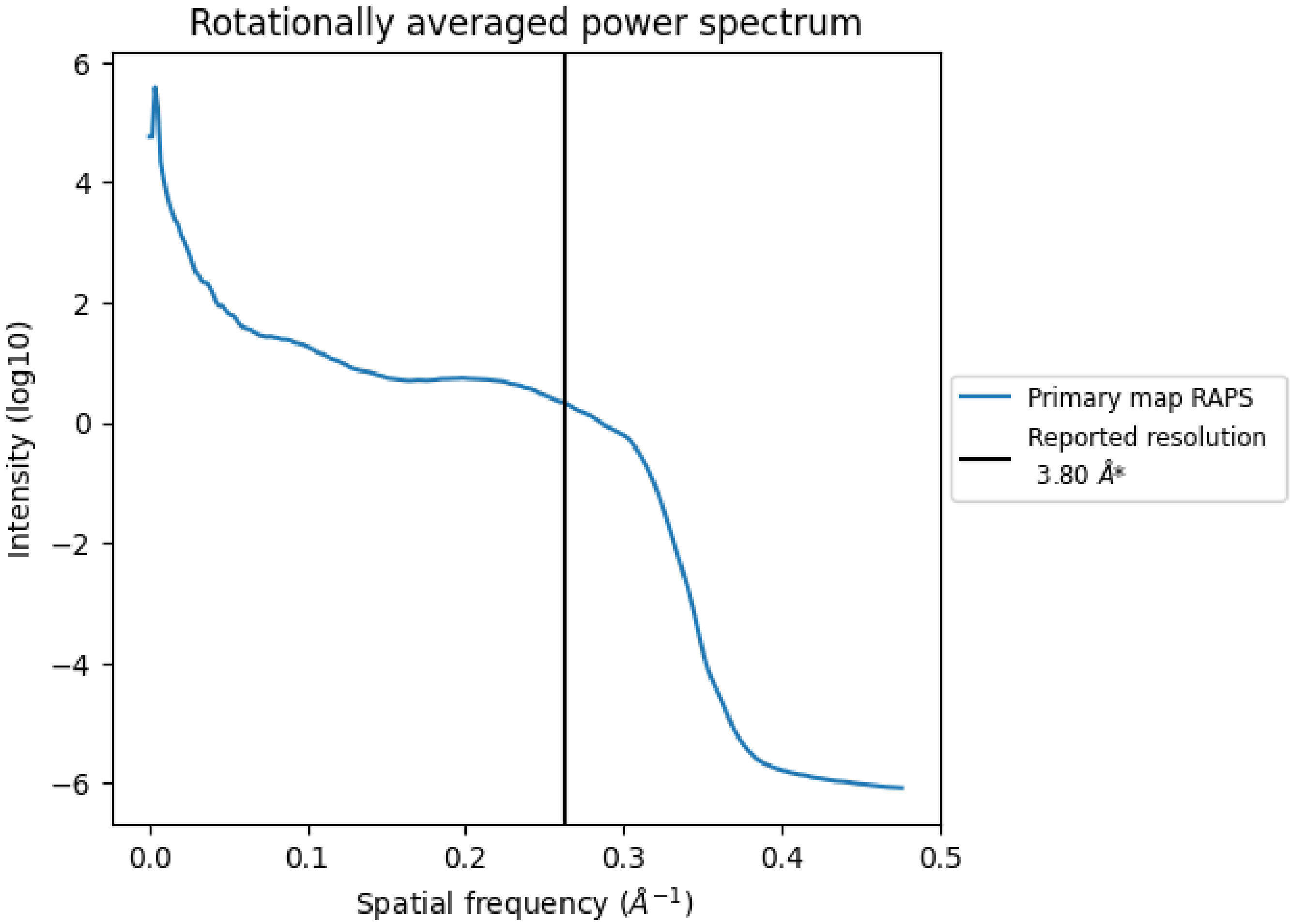
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1527 nm^3; this corresponds to an approximate mass of 1379 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 0.263 Å^{-1}

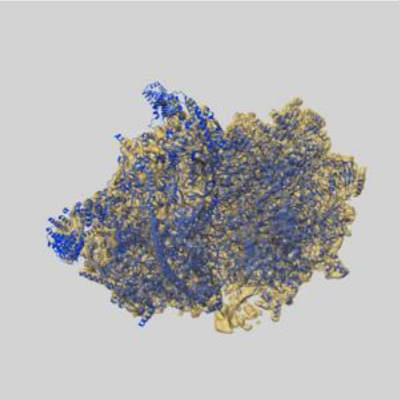
8 Fourier-Shell correlation

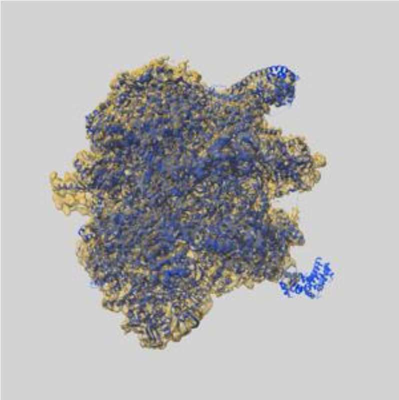
This section was not generated. No FSC curve or half-maps provided.

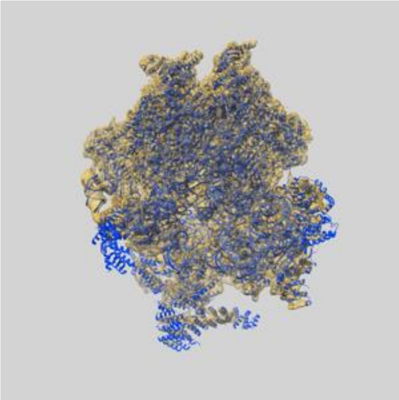
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12877 and PDB model 7OG4. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay

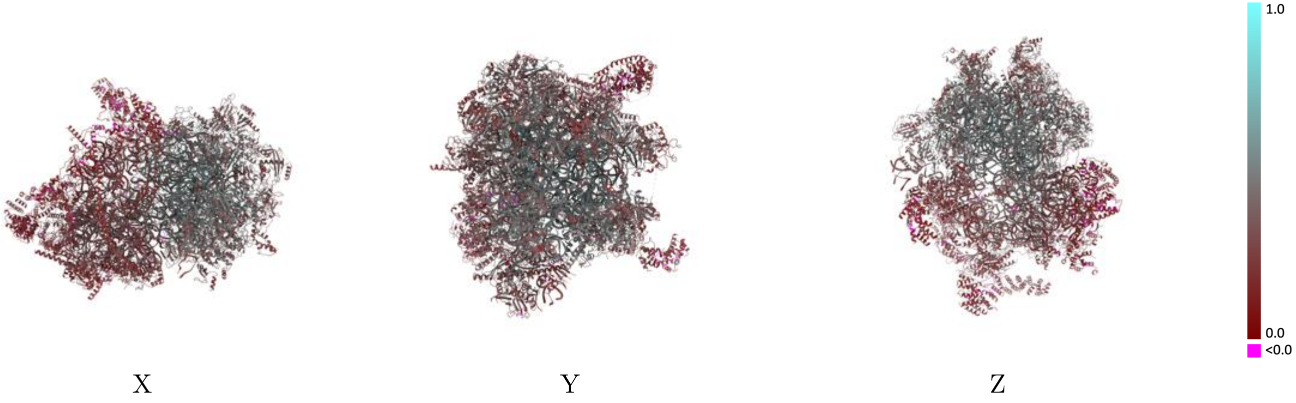

X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

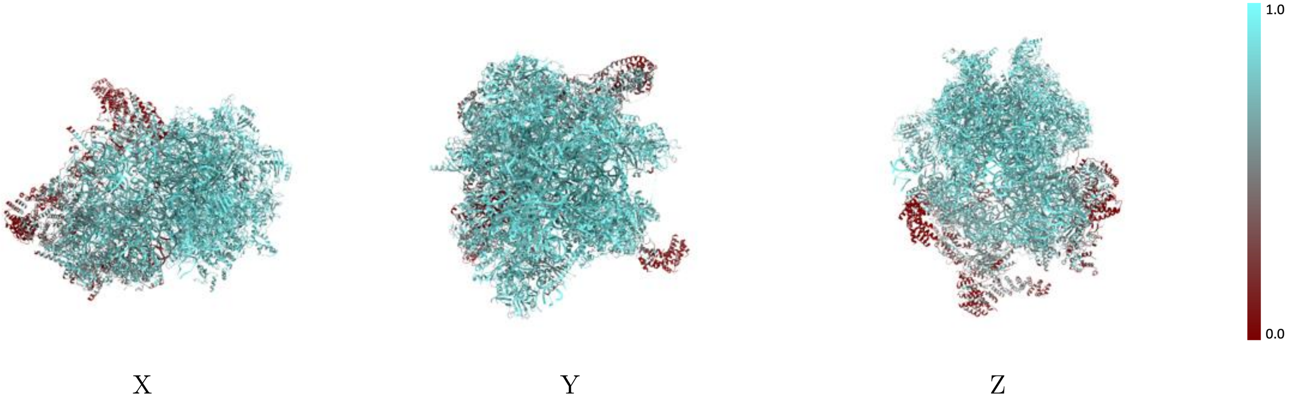
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

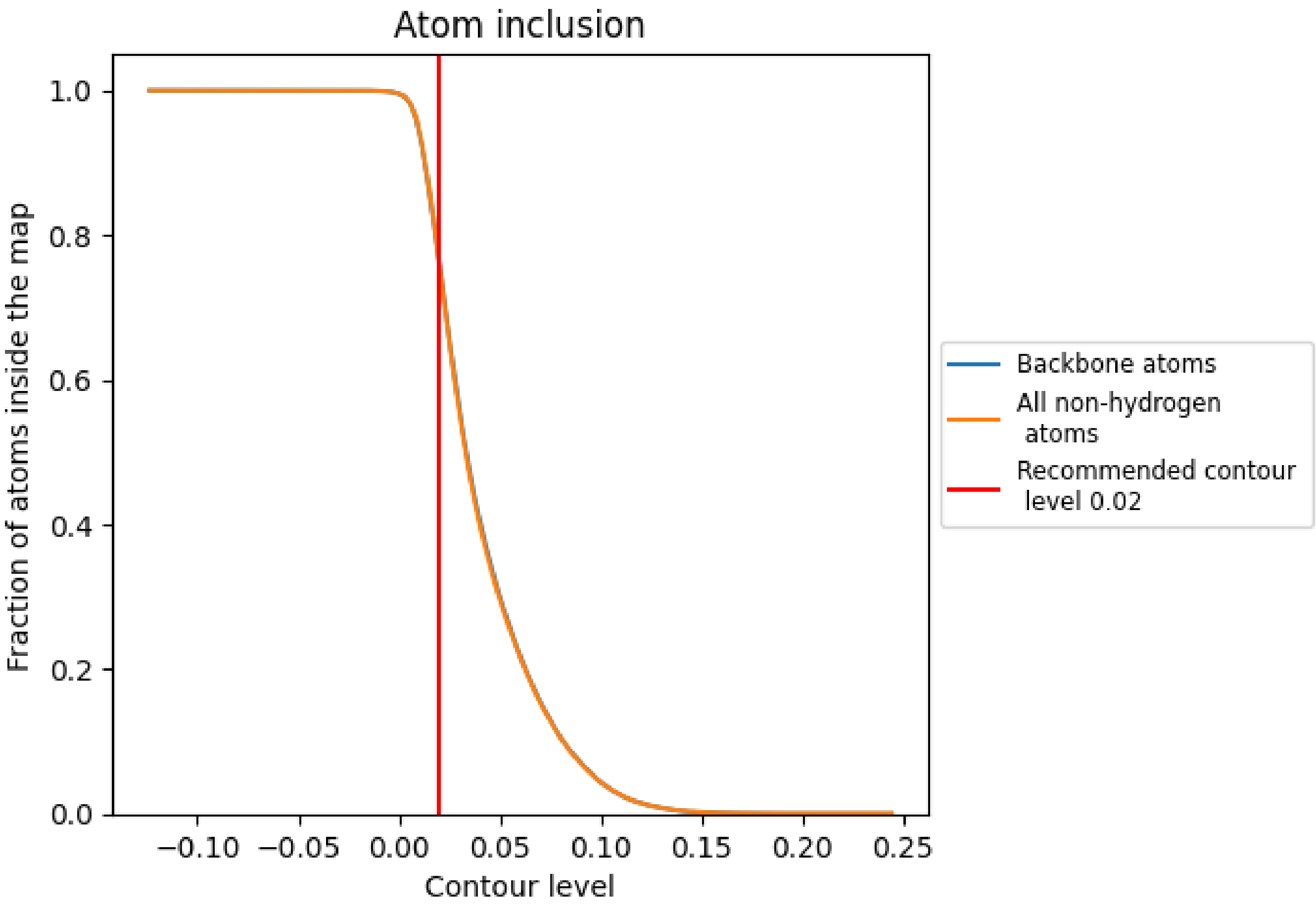
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.7566	0.3480
0	0.8312	0.4140
1	0.8521	0.4090
2	0.9111	0.5090
3	0.8997	0.5010
4	0.9233	0.4730
5	0.8511	0.4010
6	0.8105	0.3530
7	0.8159	0.3660
8	0.6130	0.2280
9	0.8212	0.3930
A0	0.4226	0.1660
A1	0.4364	0.1900
A2	0.6190	0.2530
A3	0.7612	0.3660
A4	0.2551	0.1590
AA	0.9011	0.3120
AB	0.7040	0.2630
AC	0.5442	0.2180
AD	0.5762	0.2700
AE	0.6667	0.3280
AF	0.5717	0.2160
AG	0.5561	0.2180
AH	0.4312	0.1890
AI	0.6475	0.2900
AJ	0.7067	0.2690
AK	0.4608	0.1940
AL	0.6610	0.2720
AM	0.5652	0.1930
AN	0.6070	0.2600
AO	0.5459	0.2210
AP	0.6941	0.3120
AQ	0.6963	0.3220
AR	0.4620	0.1700
AS	0.5836	0.2390

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Chain	Atom inclusion	Q-score
AT	0.6495	0.2540
AU	0.6344	0.2070
AV	0.3563	0.1550
AW	0.5896	0.2570
AX	0.3536	0.1600
AY	0.2537	0.1750
AZ	0.5458	0.1760
XA	0.9603	0.4830
XB	0.9554	0.3170
XD	0.8790	0.4480
XE	0.8621	0.4440
XF	0.8875	0.4530
XH	0.8087	0.3640
XI	0.6042	0.2720
XJ	0.6598	0.2230
XK	0.8740	0.4570
XL	0.8825	0.4540
XM	0.8593	0.4430
XN	0.8527	0.4370
XO	0.8667	0.4240
XP	0.8356	0.3850
XQ	0.7730	0.3860
XR	0.8736	0.4730
XS	0.8676	0.4600
XT	0.8892	0.4680
XU	0.8776	0.4410
XV	0.8087	0.3720
XW	0.9014	0.4750
XX	0.8209	0.3930
XY	0.8677	0.4270
XZ	0.8885	0.4660
a	0.8283	0.4140
b	0.8875	0.4540
c	0.8414	0.3890
d	0.7828	0.3510
e	0.6591	0.1920
f	0.6874	0.2630
g	0.8653	0.4310
h	0.7988	0.3490
i	0.8893	0.4810
j	0.8378	0.4150
k	0.7843	0.3040

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Chain	Atom inclusion	Q-score
l	0.7125	0.2600
m	0.6956	0.2260
o	0.9016	0.4730
p	0.8170	0.3490
q	0.6533	0.3050
r	0.8806	0.3940
r3	0.0756	0.0790
s	0.8617	0.4190
t1	0.2181	0.1990
t2	0.1807	0.1860
t3	0.0000	0.1740
t4	0.0000	0.1200
t5	0.0000	0.1370
t6	0.0000	0.1020