



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 03:26 pm GMT

PDB ID : 6ZSD
EMDB ID : EMD-11394
Title : Human mitochondrial ribosome in complex with mRNA, P-site tRNA and E-site tRNA
Authors : Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.
Deposited on : 2020-07-15
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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 : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

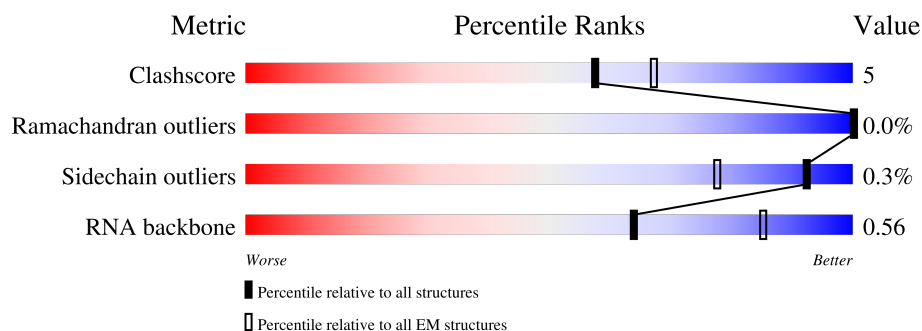
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	188	51% 7% 43%
2	1	65	68% 14% 18%
3	2	92	48% . 50%
4	3	188	39% 12% 49%
5	4	103	34% . 63%
6	5	423	80% 12% 7%
7	6	380	78% 15% 7%







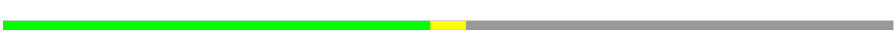





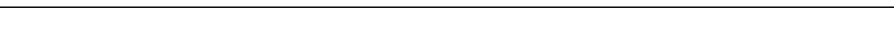

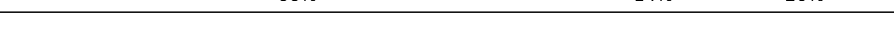

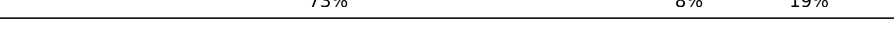








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Mol	Chain	Length	Quality of chain
8	7	338	
9	8	206	
10	9	137	
11	XA	1559	
12	A0	218	
13	A1	323	
14	A2	118	
15	A3	199	
16	A4	689	
17	AA	954	
18	AB	296	
19	AC	167	
20	AD	430	
21	AE	125	
22	AF	242	
23	AG	396	
24	AH	201	
25	AI	194	
26	AJ	138	
27	AK	128	
28	AL	257	
29	AM	137	
30	AN	130	
31	AO	258	
32	AP	142	

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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	

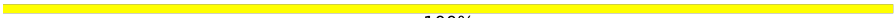








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Mol	Chain	Length	Quality of chain
58	XS	205	
59	XT	206	
60	XU	153	
61	XV	216	
62	XW	148	
63	XX	256	
64	XY	250	
65	XZ	161	
66	a	142	
67	b	215	
68	c	332	
69	d	306	
70	e	279	
71	f	212	
72	g	166	
73	h	158	
74	i	128	
75	j	123	
76	k	112	
77	l	138	
78	m	128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

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Mol	Chain	Length	Quality of chain
83	r1	12	 100%
84	r3	75	 100%
85	r4	76	 100%
86	s	439	 84% 16%
87	t1	198	 23% 77%
87	t2	198	 15% 85%
87	t3	198	 15% 85%
87	t4	198	 15% 85%
87	t5	198	 15% 85%
87	t6	198	 14% 86%

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 313735 atoms, of which 143072 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	46	Total	C	H	N	O	S	0	0
			783	233	407	83	59	1		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	38	Total	C	H	N	O	S	0	0
			703	217	362	72	48	4		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	354	Total	C	H	N	O	S	0	0
			5788	1881	2841	525	532	9		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	8	139	Total	C	H	N	O	S	0	0
			2377	747	1202	208	218	2		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	XA	1499	Total	C	H	N	O	P	0	0
			48003	14284	16171	5756	10294	1498		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XA	3107	U	UNK	conflict	GB 1025814679
XA	3200	A	U	conflict	GB 1025814679

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AA	924	Total	C	H	N	O	P	0	0
			29599	8800	9971	3540	6364	924		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AF	201	Total	C	H	N	O	S	0	0
			3383	1069	1715	305	283	11		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
31	AO	185	Total	C	H	N	O	S	0	0
			3017	970	1489	285	267	6		

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	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
41	AY	113	Total	C	H	N	O	S	0	0
			1868	621	912	157	176	2		

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

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

- Molecule 43 is a RNA chain called mitochondrial tRNA^{Val}.

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
45	XE	304	Total	C	H	N	O	S	0	0
			4799	1539	2403	416	430	11		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
71	f	143	Total	C	H	N	O	S	0	0
			2314	737	1165	187	221	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	C	H	N	O	S	0	0
			2738	858	1359	267	249	5		

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

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

- Molecule 83 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	r1	12	Total	C	N	O	P		
			216	108	24	72	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
84	r3	75	Total	C	N	O	P		
			1459	711	222	451	75	0	0

- Molecule 85 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	r4	76	Total	C	N	O	P		
			1486	723	230	457	76	0	0

- Molecule 86 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 87 is a protein called 39S ribosomal protein L12, mitochondrial.

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

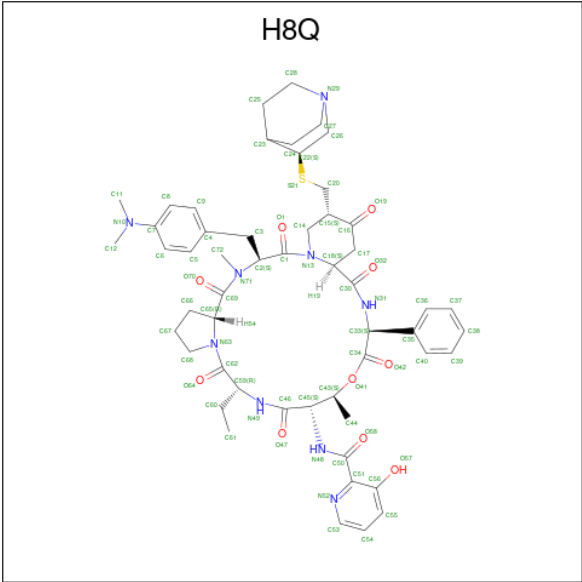
- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
88	0	1	Total 1	Zn 1	0
88	4	1	Total 1	Zn 1	0
88	AB	1	Total 1	Zn 1	0
88	AO	1	Total 1	Zn 1	0
88	AP	1	Total 1	Zn 1	0
88	AT	1	Total 1	Zn 1	0
88	XI	1	Total 1	Zn 1	0

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

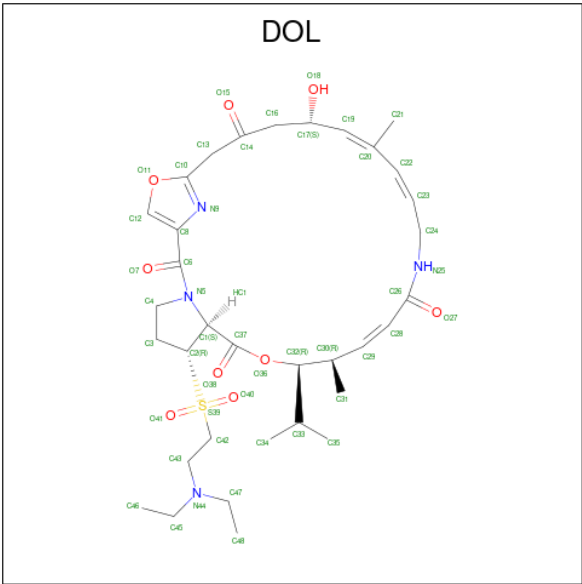
Mol	Chain	Residues	Atoms		AltConf
89	XA	143	Total 143	Mg 143	0
89	AA	46	Total 46	Mg 46	0
89	XD	1	Total 1	Mg 1	0
89	XE	1	Total 1	Mg 1	0
89	XI	1	Total 1	Mg 1	0
89	XM	1	Total 1	Mg 1	0
89	XW	1	Total 1	Mg 1	0
89	g	1	Total 1	Mg 1	0

- Molecule 90 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: C₅₃H₆₇N₉O₁₀S).



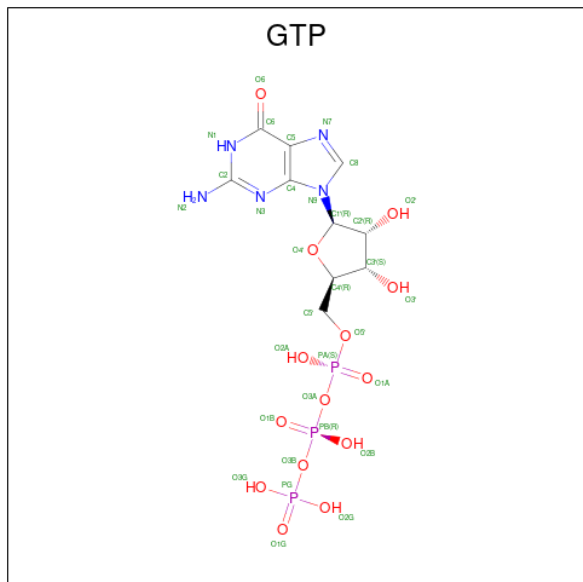
Mol	Chain	Residues	Atoms						AltConf
90	XA	1	Total	C	H	N	O	S	0
			140	53	67	9	10	1	

- Molecule 91 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: C₃₄H₅₀N₄O₉S).



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

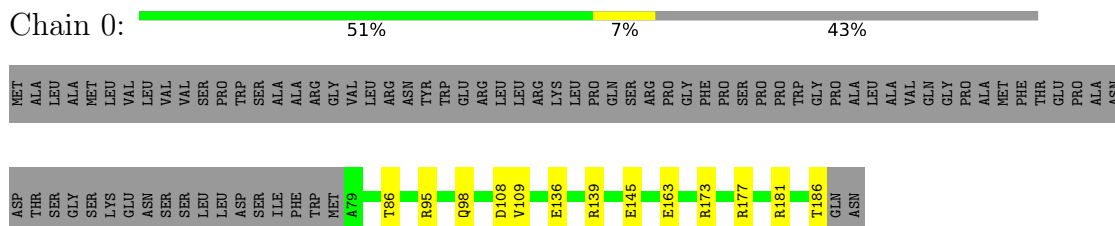
- Molecule 92 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



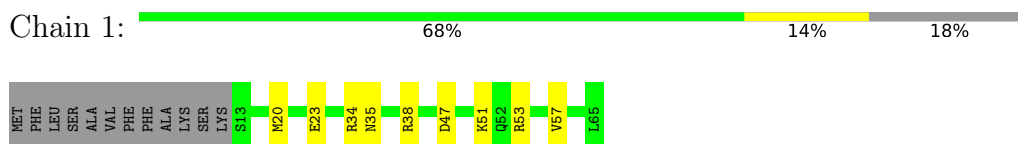
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

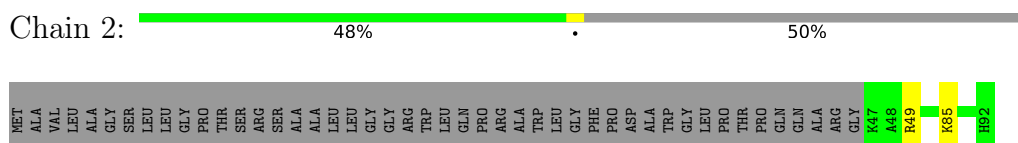
- Molecule 1: 39S ribosomal protein L32, mitochondrial



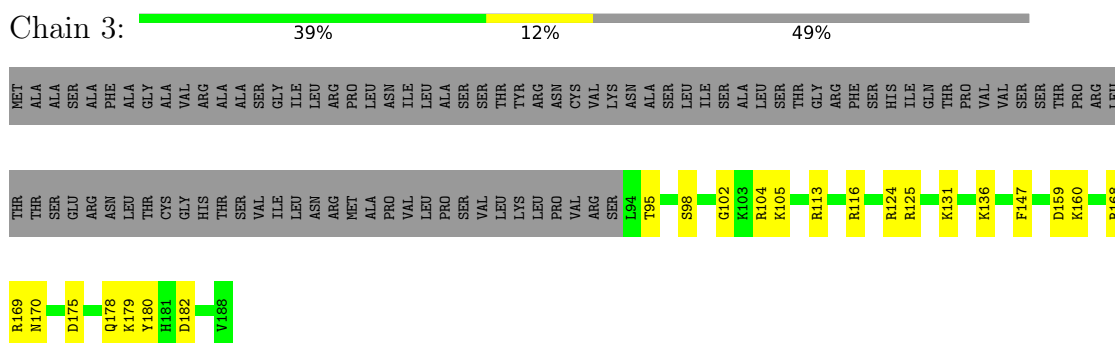
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial

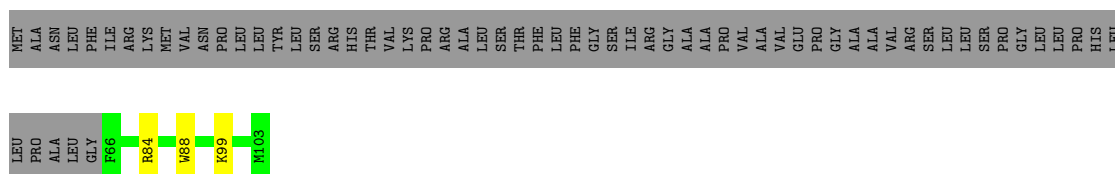


- Molecule 4: 39S ribosomal protein L35, mitochondrial

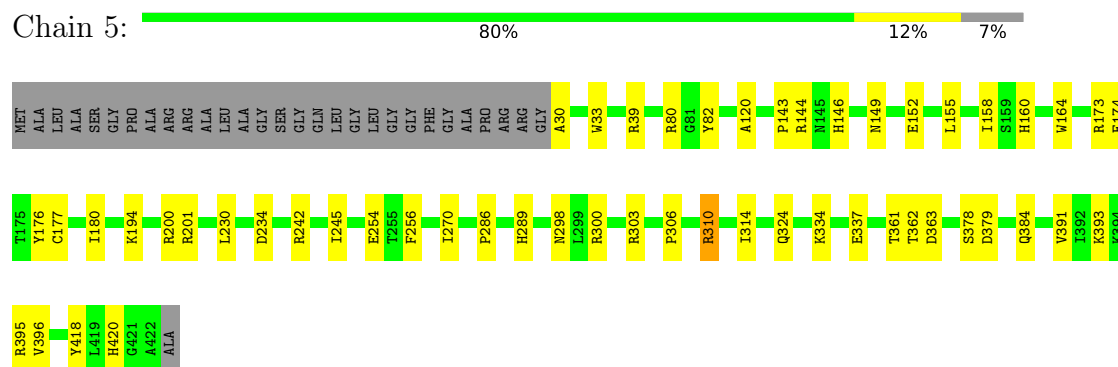


- Molecule 5: 39S ribosomal protein L36, mitochondrial

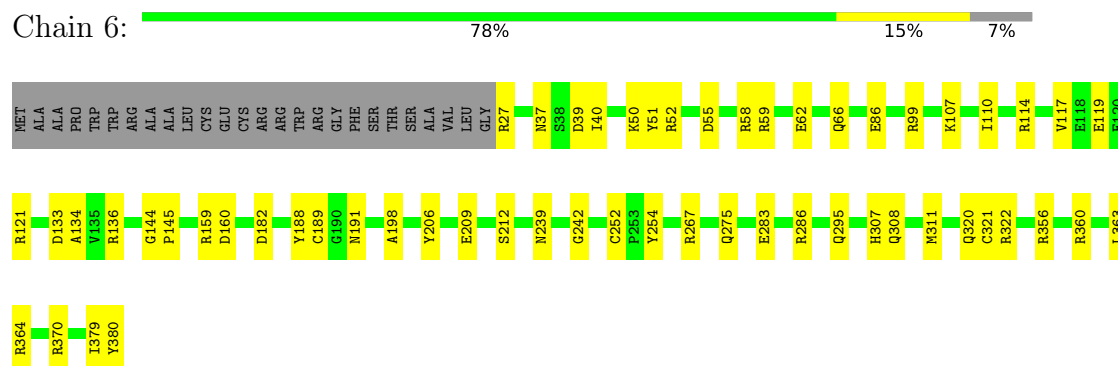




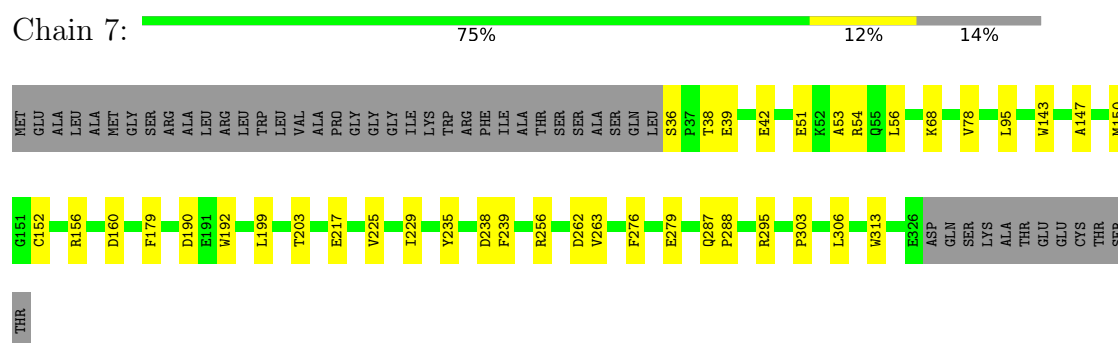
- Molecule 6: 39S ribosomal protein L37, mitochondrial



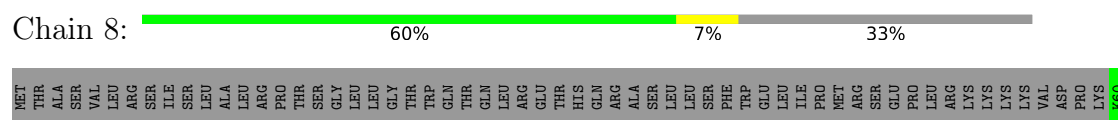
- Molecule 7: 39S ribosomal protein L38, mitochondrial



- Molecule 8: 39S ribosomal protein L39, mitochondrial

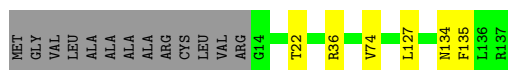


- Molecule 9: 39S ribosomal protein L40, mitochondrial



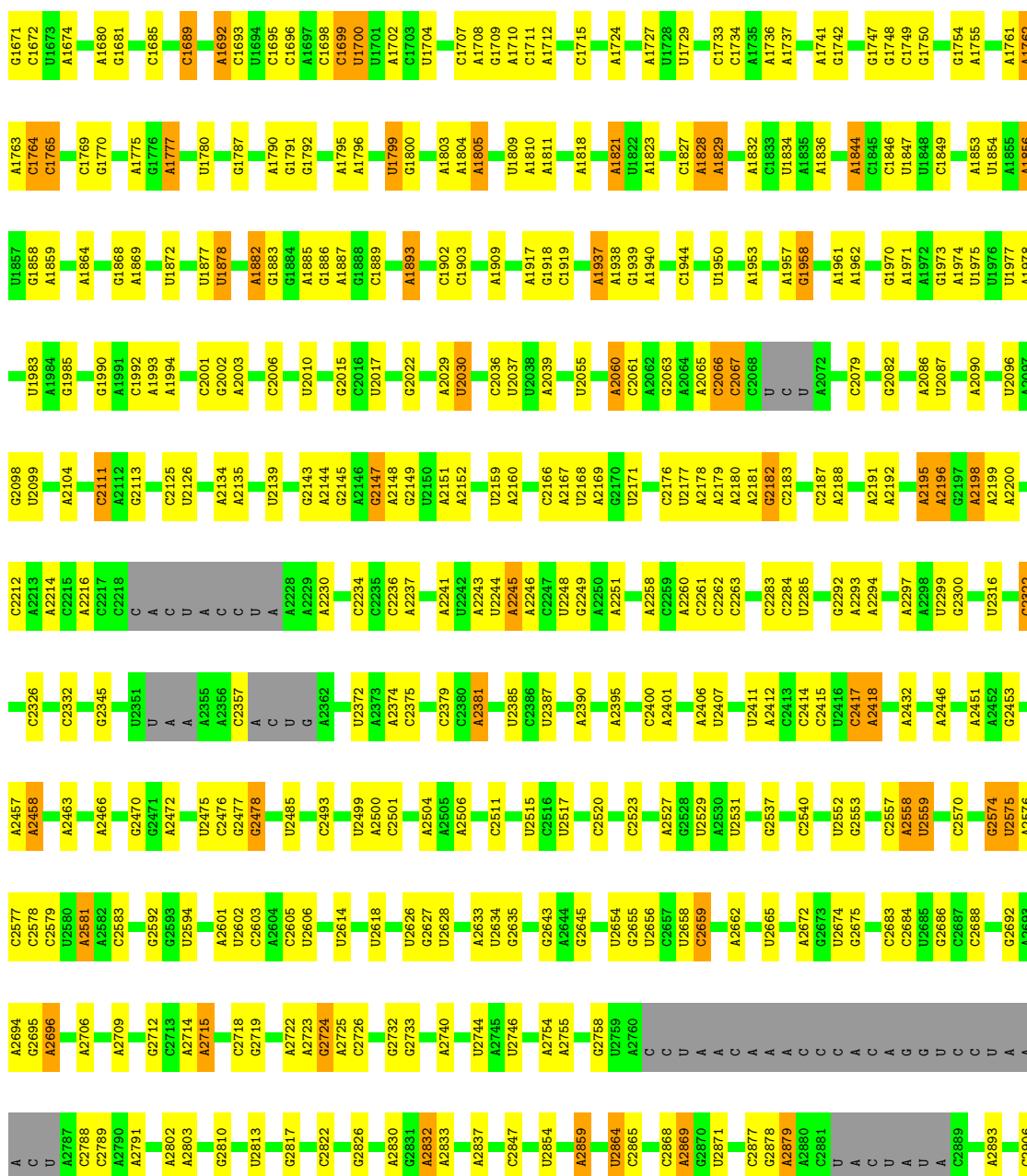
- Molecule 10: 39S ribosomal protein L41, mitochondrial

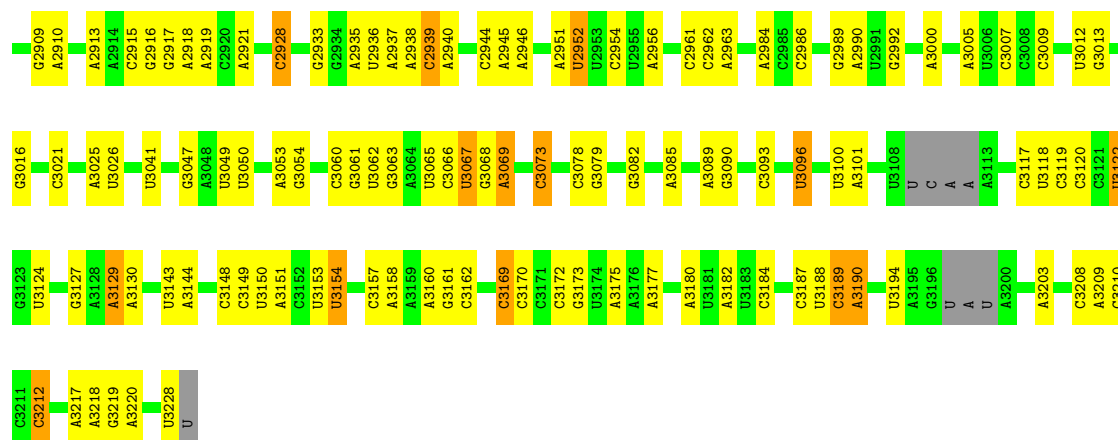
Chain 9: 86% . 9%



- Molecule 11: 16S mitochondrial rRNA

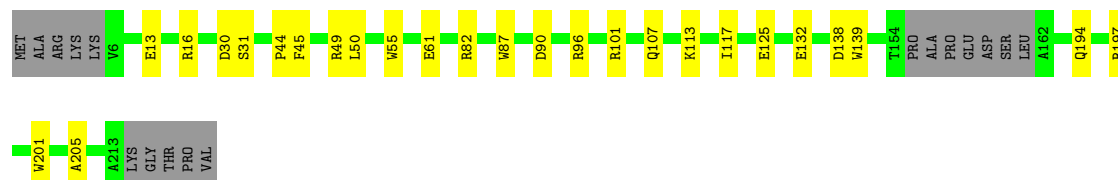
Chain XA: 65% 27% . .





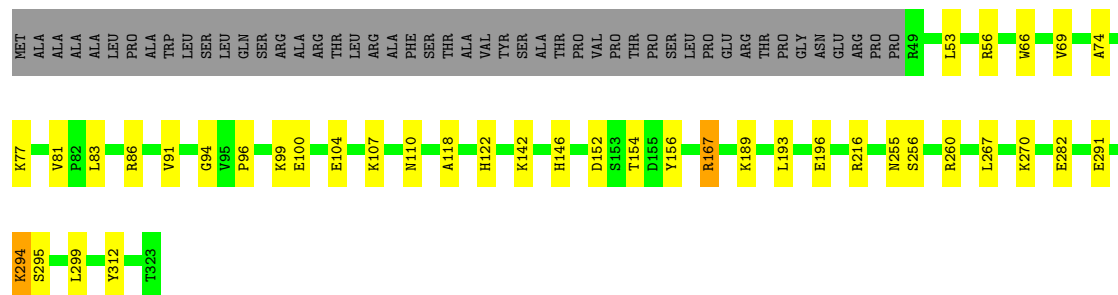
- Molecule 12: 28S ribosomal protein S34, mitochondrial

Chain A0: 80% 12% 8%



- Molecule 13: 28S ribosomal protein S35, mitochondrial

Chain A1: 73% 12% 15%



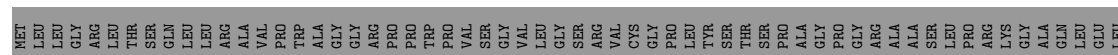
- Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

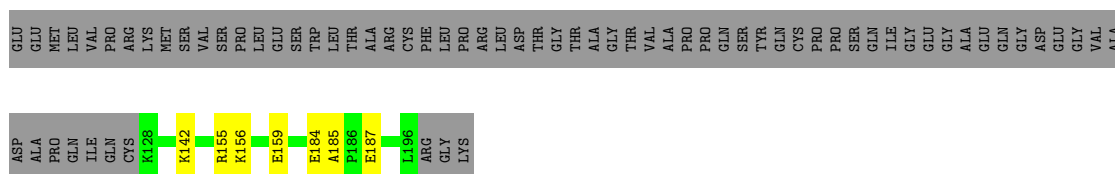
Chain A2: 76% 22% 2%



- Molecule 15: Aurora kinase A-interacting protein

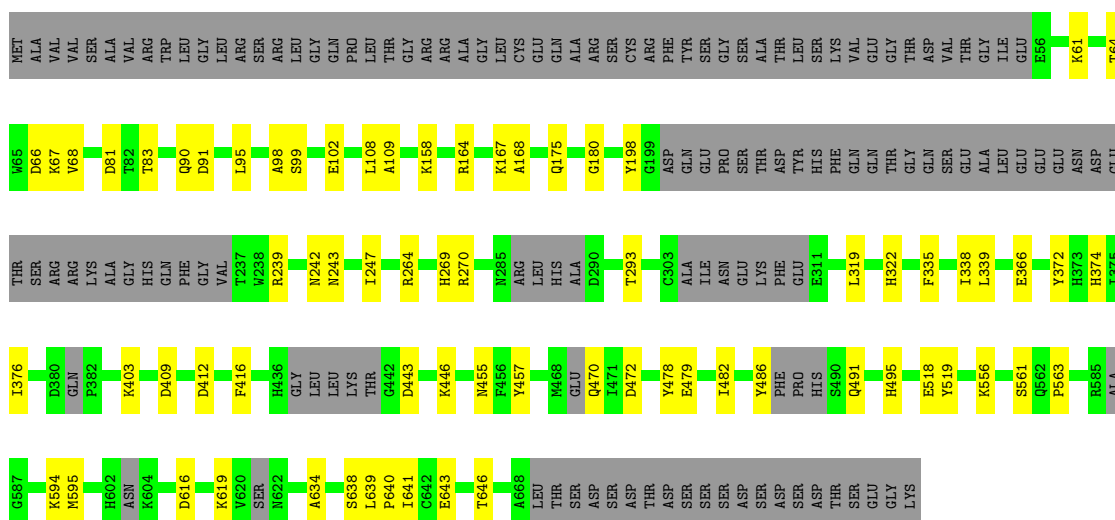
Chain A3: 31% 65% 4%





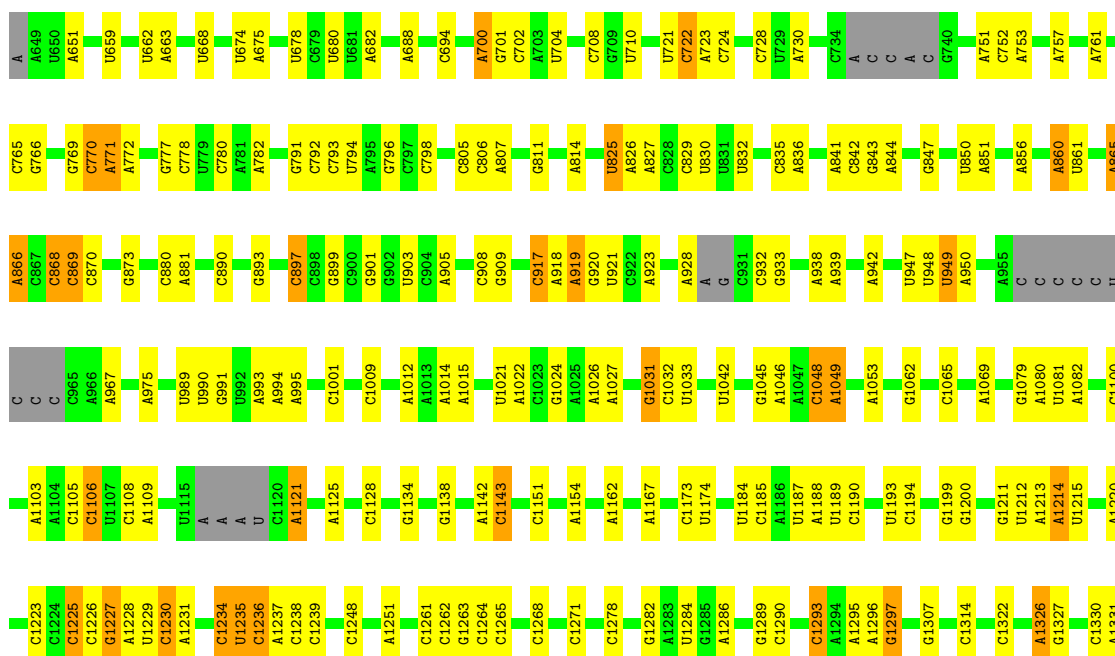
- Molecule 16: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4: 70% 10% 20%



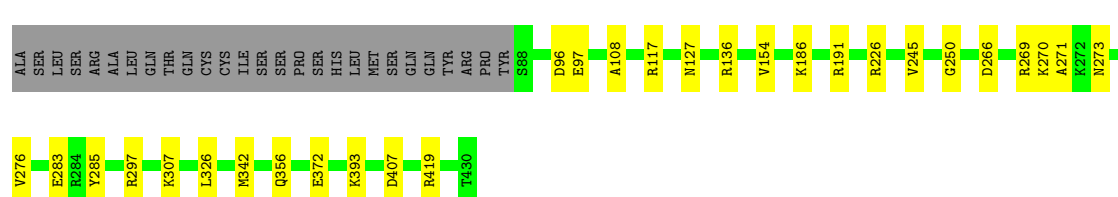
- Molecule 17: 12S mitochondrial rRNA

Chain AA: 66% 26% . .

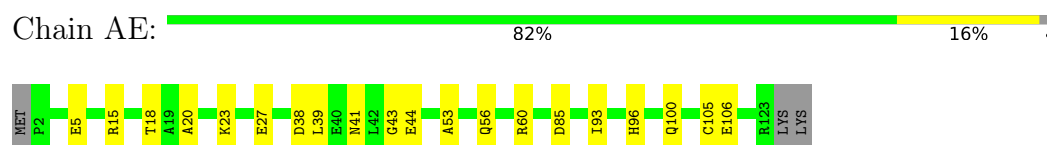


- Molecule 18: 28S ribosomal protein S2, mitochondrial

- Molecule 19: 28S ribosomal protein S24, mitochondrial



- Molecule 21: 28S ribosomal protein S6, mitochondrial

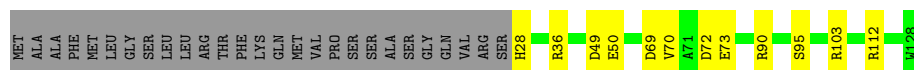


- Molecule 22: 28S ribosomal protein S7, mitochondrial



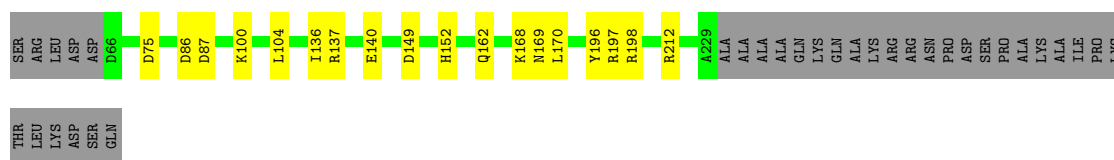
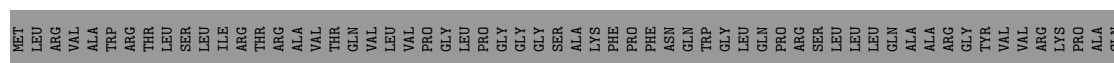
- Molecule 27: 28S ribosomal protein S14, mitochondrial

Chain AK: 70% 9% 21%



- Molecule 28: 28S ribosomal protein S15, mitochondrial

Chain AL: 57% 7% 36%



- Molecule 29: 28S ribosomal protein S16, mitochondrial

Chain AM: 76% 9% 15%



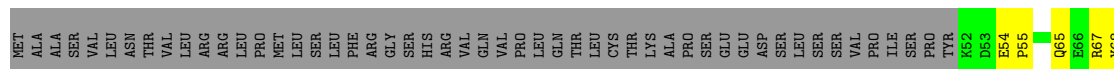
- Molecule 30: 28S ribosomal protein S17, mitochondrial

Chain AN: 72% 11% 18%



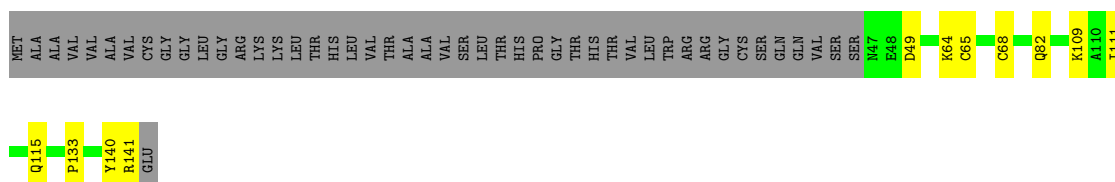
- Molecule 31: 28S ribosomal protein S18b, mitochondrial

Chain AO: 62% 10% 28%



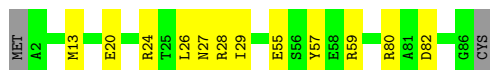
- Molecule 32: 28S ribosomal protein S18c, mitochondrial

Chain AP: 59% 8% 33%



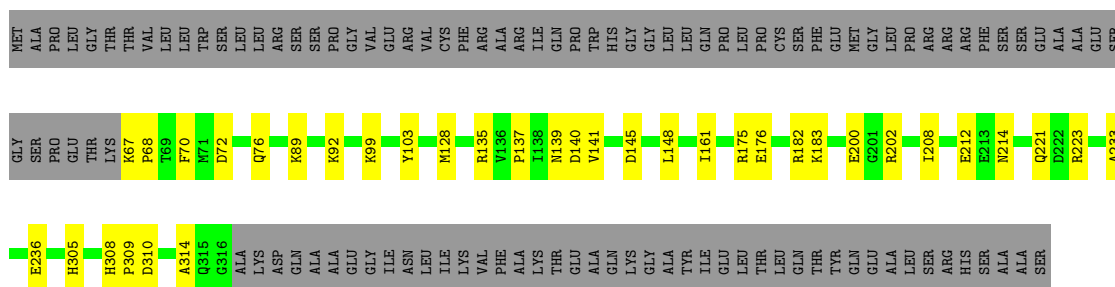
- Molecule 33: 28S ribosomal protein S21, mitochondrial

Chain AQ: 84% 14%



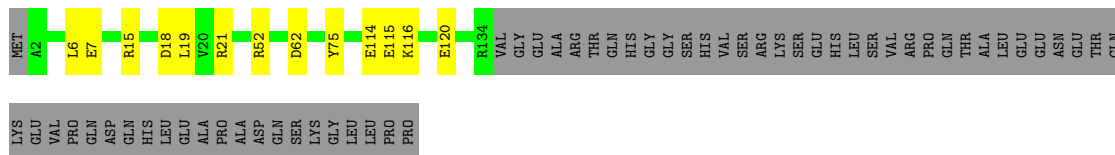
- Molecule 34: 28S ribosomal protein S22, mitochondrial

Chain AR: 59% 10% 31%



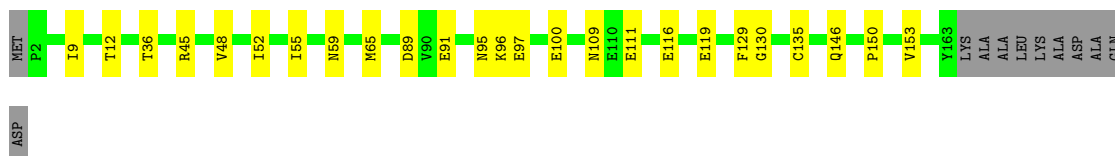
- Molecule 35: 28S ribosomal protein S23, mitochondrial

Chain AS: 63% 7% 30%



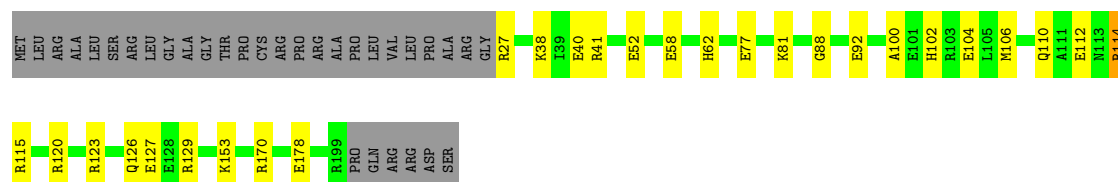
- Molecule 36: 28S ribosomal protein S25, mitochondrial

Chain AT: 79% 14% 6%

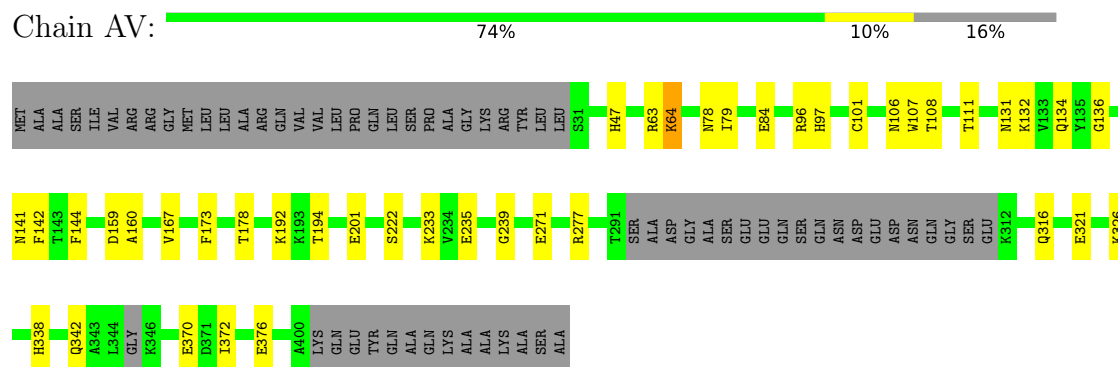


- Molecule 37: 28S ribosomal protein S26, mitochondrial

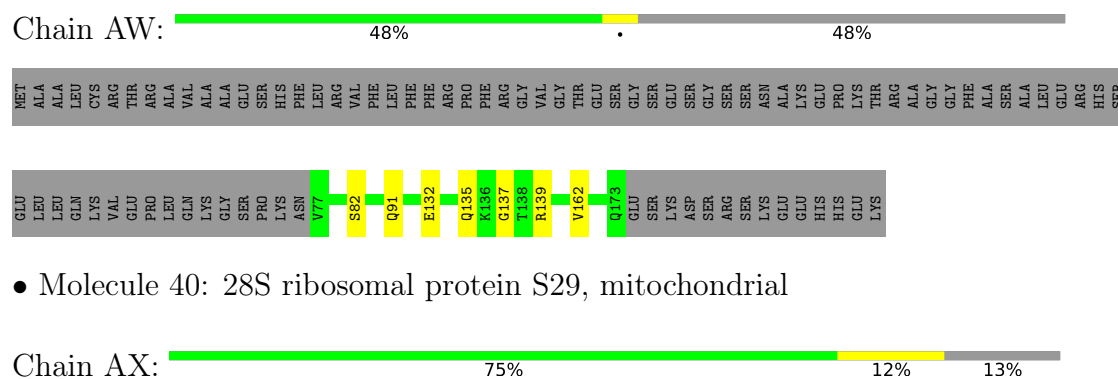
Chain AU: 71% 13% 16%



- Molecule 38: 28S ribosomal protein S27, mitochondrial



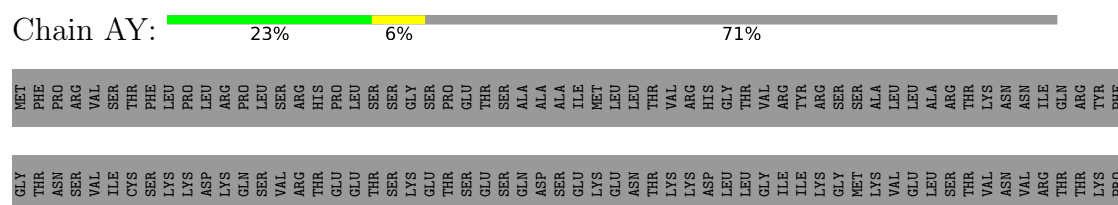
- Molecule 39: 28S ribosomal protein S28, mitochondrial

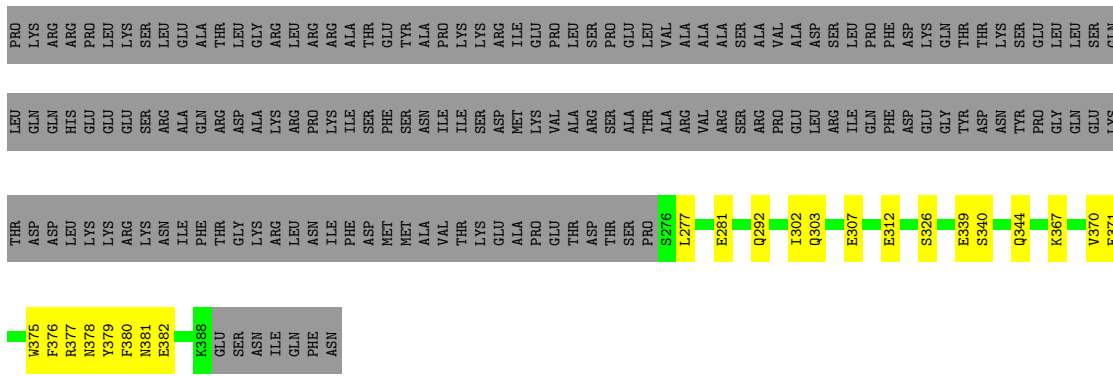


- Molecule 40: 28S ribosomal protein S29, mitochondrial



- Molecule 41: 28S ribosomal protein S31, mitochondrial





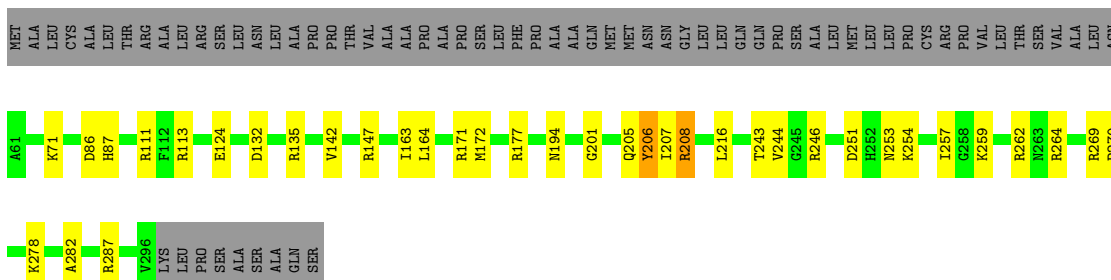
- Molecule 42: 28S ribosomal protein S33, mitochondrial



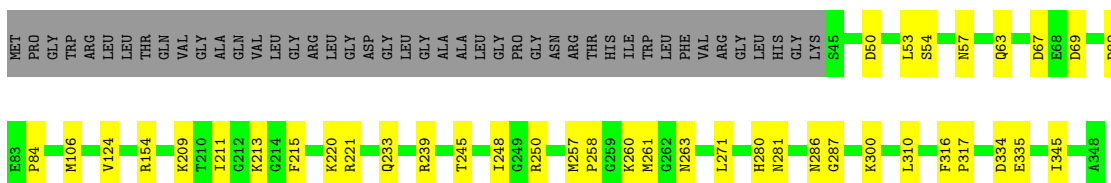
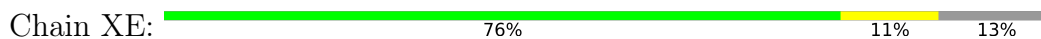
- Molecule 43: mitochondrial tRNA^{Val}



- Molecule 44: 39S ribosomal protein L2, mitochondrial

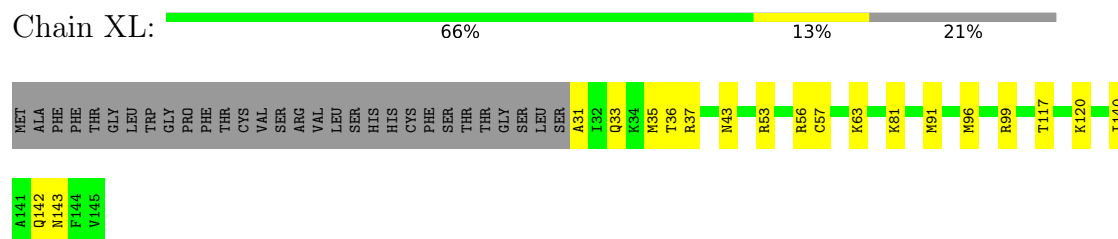


- Molecule 45: 39S ribosomal protein L3, mitochondrial

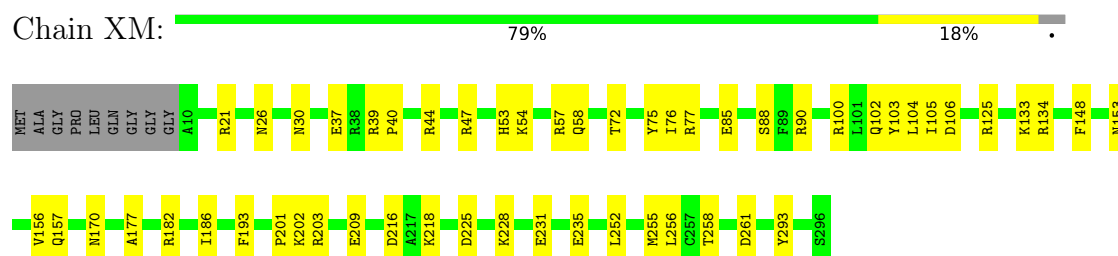


- Molecule 46: 39S ribosomal protein L4, mitochondrial

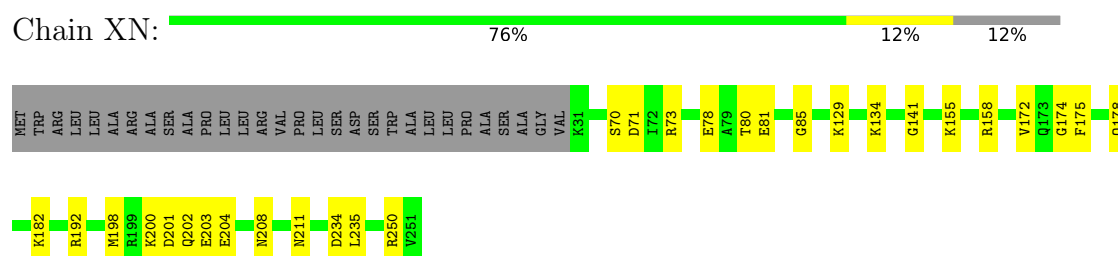
- Molecule 51: 39S ribosomal protein L14, mitochondrial



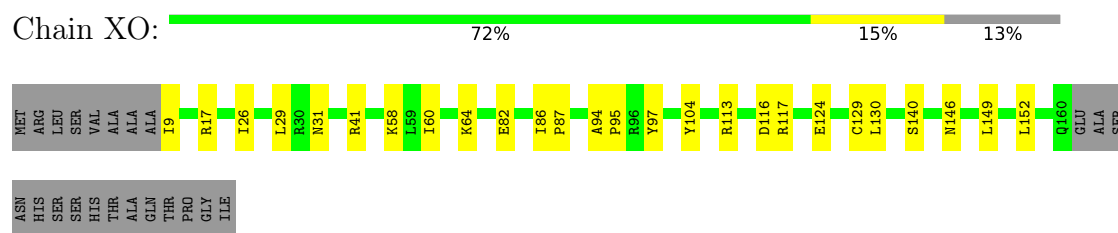
- Molecule 52: 39S ribosomal protein L15, mitochondrial



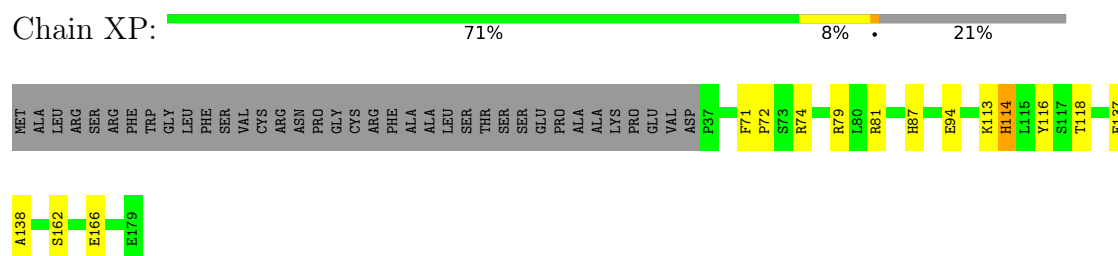
- Molecule 53: 39S ribosomal protein L16, mitochondrial




- Molecule 54: 39S ribosomal protein L17, mitochondrial

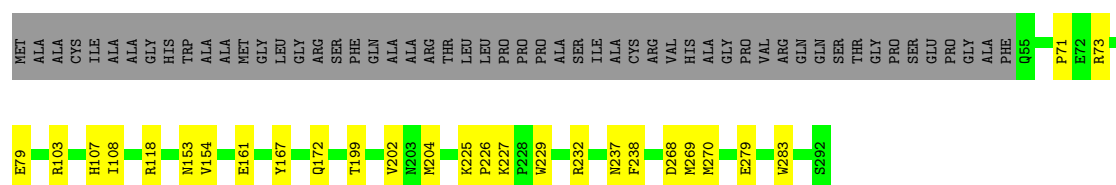


- Molecule 55: 39S ribosomal protein L18, mitochondrial




- Molecule 56: 39S ribosomal protein L19, mitochondrial

Chain XQ:  72% 9% 18%



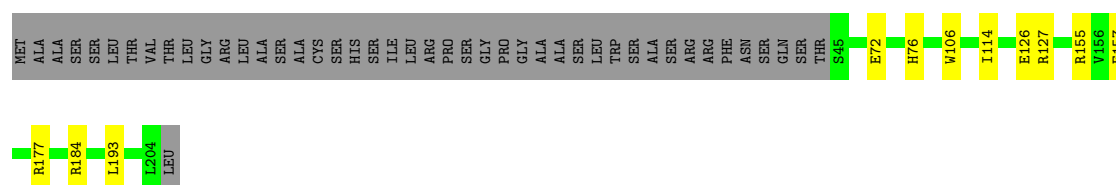
- Molecule 57: 39S ribosomal protein L20, mitochondrial

Chain XR:  83% 11% 6%



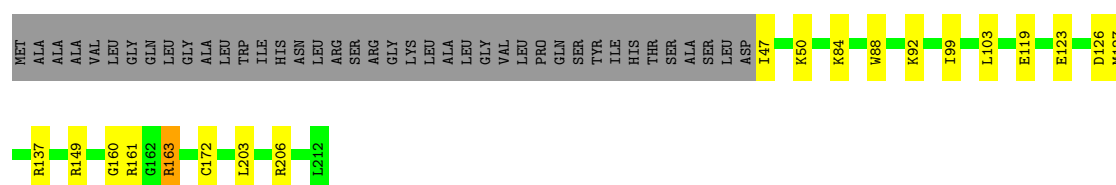
- Molecule 58: 39S ribosomal protein L21, mitochondrial

Chain XS:  73% 5% 22%




- Molecule 59: 39S ribosomal protein L22, mitochondrial

Chain XT:  71% 9% 19%




- Molecule 60: 39S ribosomal protein L23, mitochondrial

Chain XU:  81% 11% 8%



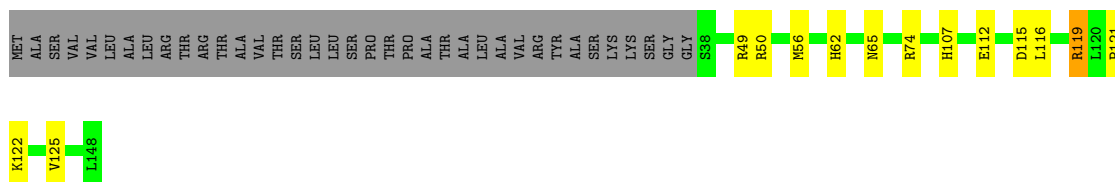
- Molecule 61: 39S ribosomal protein L24, mitochondrial

Chain XV:  86% 8% 6%



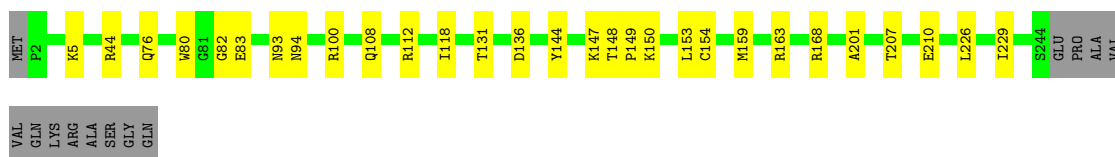
- Molecule 62: 39S ribosomal protein L27, mitochondrial

Chain XW: 66% 9% 25%



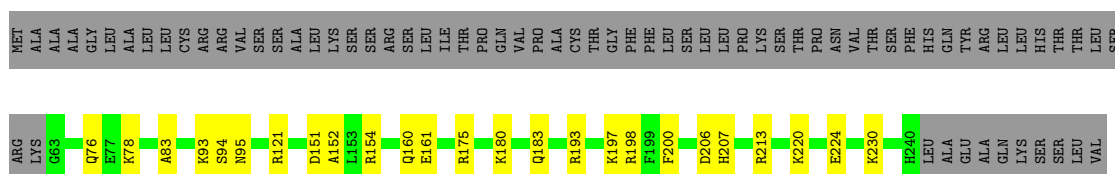
- Molecule 63: 39S ribosomal protein L28, mitochondrial

Chain XX: 84% 11% 5%



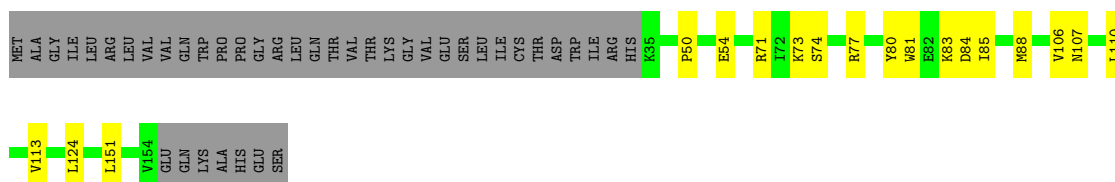
- Molecule 64: 39S ribosomal protein L47, mitochondrial

Chain XY: 61% 10% 29%



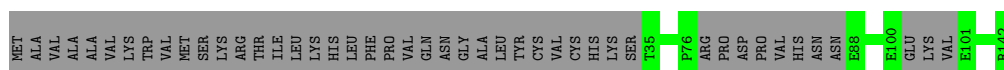
- Molecule 65: 39S ribosomal protein L30, mitochondrial

Chain XZ: 63% 11% 25%



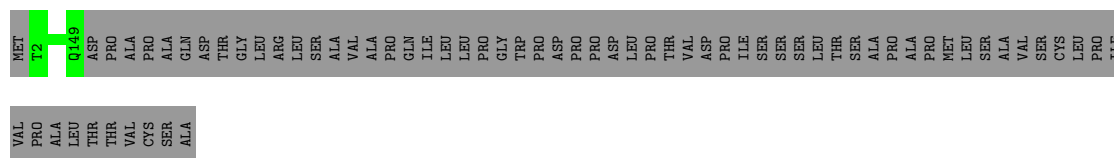
- Molecule 66: 39S ribosomal protein L42, mitochondrial

Chain a: 68% 32%




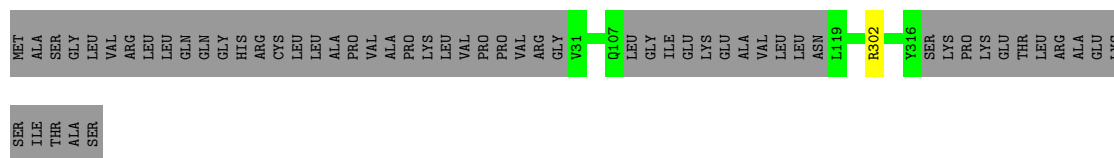
- Molecule 67: 39S ribosomal protein L43, mitochondrial

Chain b:  69% 31%



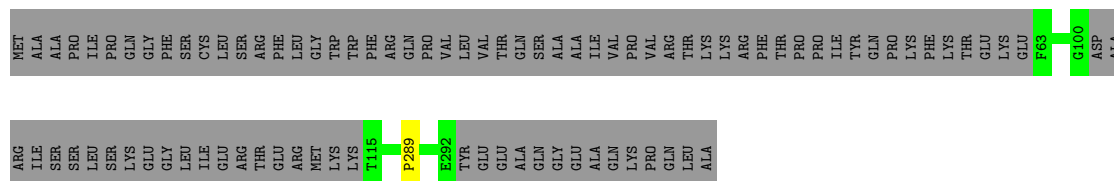
- Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c:  83% 17%




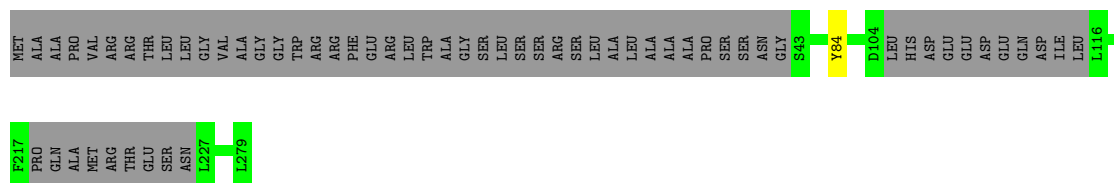
- Molecule 69: 39S ribosomal protein L45, mitochondrial

Chain d:  70% 29%



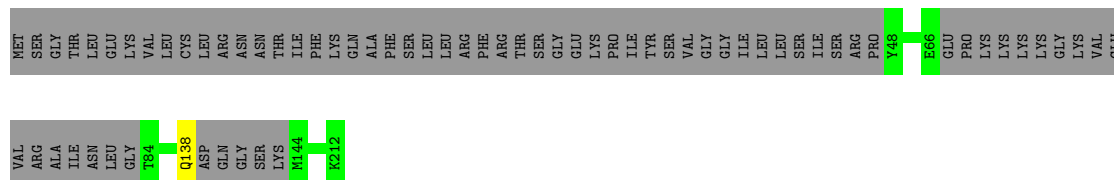
- Molecule 70: 39S ribosomal protein L46, mitochondrial

Chain e:  77% 22%




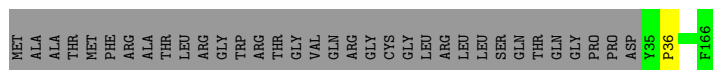
- Molecule 71: 39S ribosomal protein L48, mitochondrial

Chain f:  67% 33%



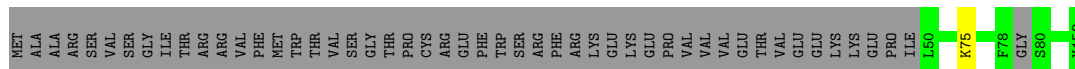
- Molecule 72: 39S ribosomal protein L49, mitochondrial

Chain g:  79% 20%



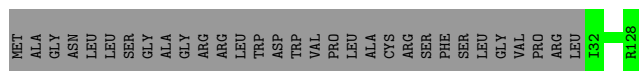
- Molecule 73: 39S ribosomal protein L50, mitochondrial

Chain h:  68% 32%



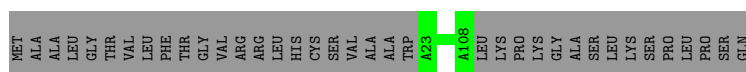
- Molecule 74: 39S ribosomal protein L51, mitochondrial

Chain i:  76% 24%




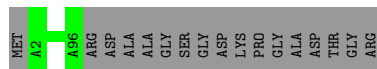
- Molecule 75: 39S ribosomal protein L52, mitochondrial

Chain j:  70% 30%



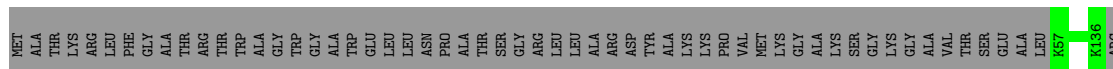
- Molecule 76: 39S ribosomal protein L53, mitochondrial

Chain k:  85% 15%



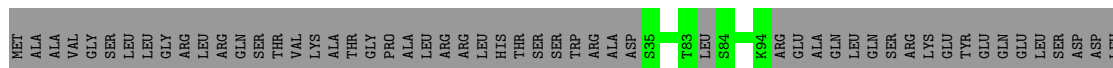
- Molecule 77: 39S ribosomal protein L54, mitochondrial

Chain l:  58% 42%



- Molecule 78: 39S ribosomal protein L55, mitochondrial

Chain m:  47% 53%



HIS
VAL
GLU
ARG
THR
TYR
ARG
GLN
PHE
TRP
THR
ARG
THR
LYS
LYS

- Molecule 79: Ribosomal protein 63, mitochondrial

Chain o:  92% 8%

MET
PHE
LEU
THR
ALA
LEU
LEU
TRP
R9
S102

- Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:  62% 38%

MET
ALA
THR
ARG
CYS
LEU
ARG
TRP
GLY
LEU
SER
ARG
ALA
GLY
VAL
TRP
LEU
LEU
PRO
PRO
ALA
PRO
CYS
ARG
CYS
PRO
ARG
ARG
ALA
LEU
HIS
LYS
GLN
LYS
ASP
GLY
THR
E38
V61
PRO
ASN
GLY
ALA
LYS
GLN
ALA
ASP
SER
D70
S83
SER
GLY
PRO
GLY
GLY
GLN
ASN
VAL

ASN
LYS
V95
THR
PRO
LYS
GLU
PRO
THR
LYS
GLY
ASP
VAL
K174
I193
HIS
SER
VAL
LYS
THR
SER
ARG
VAL
ASP
MET
ASP


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

Chain q:  73% 26%

MET
ALA
SER
VAL
GLN
ARG
ALA
ARG
SER
LEU
LEU
GLY
VAL
ALA
THR
LEU
ALA
PRO
GLY
SER
SER
GLY
Y25
R140
K188
ARG
LEU
LYS
GLU
LYS
GLN
LYS
ARG
LYS
LYS
GLU
ALA
ALA
ALA
ALA
LEU
ALA
ALA
ALA
VAL
VAL
ALA
GLN
ASP
PRO
ALA
ALA
SER
GLY
ALA

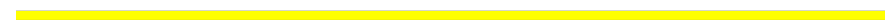
PRO
SER
SER

- Molecule 82: 39S ribosomal protein S18a, mitochondrial

Chain r:  78% 22%

MET
ALA
ALA
LEU
LYS
ALA
LEU
VAL
SER
SER
CYS
GLY
ARG
LEU
LEU
ARG
GLY
LEU
ALA
GLY
PRO
ALA
ALA
THR
SER
TRP
SER
ARG
LEU
PRO
ALA
ARG
GLY
F35
T41
GLN
E43
P136
GLU
VAL
VAL
VAL
PRO
LYS
SER
LYS
PRO
Q146
H196

- Molecule 83: mRNA

Chain r1:  100%

Y5P46
Y5P47
Y5P48
Y5P49
Y5P50
Y5P51
Y5P52
Y5P53
Y5P54
Y5P55
Y5P56
Y5P57

- Molecule 84: P-site tRNA

Chain r3:  100%

Y5P1
Y5P2
A3
A4
A5
A6
Y5P7
A8
A9
A10
A11
Y5P12
Y5P13
A14
A15
Y5P16
Y5P17
A17A
A18
A19
Y5P20
A21
A22
A23
Y5P24
Y5P25
A26
Y5P27
Y5P28
A29
A30
A31
Y5P32
Y5P33
Y5P34
A35
Y5P36
A37
Y5P38
Y5P39
Y5P40
Y5P41
A42
A43
A44
A45
A46
Y5P47
A48
Y5P49
Y5P50
A51
A52
Y5P53
Y5P54
A55
Y5P56
A57
Y5P58
Y5P59

85%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24491	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/895	0.45	0/1201
2	1	0.27	0/444	0.48	0/591
3	2	0.35	0/382	0.43	0/507
4	3	0.35	0/852	0.45	0/1136
5	4	0.29	0/349	0.45	0/461
6	5	0.28	0/3299	0.43	0/4495
7	6	0.28	0/3041	0.42	0/4137
8	7	0.26	0/2420	0.42	0/3270
9	8	1.79	1/1199 (0.1%)	0.46	2/1612 (0.1%)
10	9	0.29	0/1024	0.42	0/1379
11	XA	0.39	0/35612	0.78	1/55425 (0.0%)
12	A0	0.23	0/1727	0.42	0/2338
13	A1	0.24	0/2276	0.40	0/3079
14	A2	0.26	0/939	0.42	0/1256
15	A3	0.29	0/621	0.46	0/820
16	A4	0.25	0/4559	0.41	0/6149
17	AA	0.27	0/21952	0.76	1/34164 (0.0%)
18	AB	0.26	0/1819	0.41	0/2462
19	AC	0.27	0/1112	0.42	0/1505
20	AD	0.25	0/2768	0.44	0/3707
21	AE	0.26	0/989	0.44	0/1335
22	AF	0.25	0/1708	0.40	0/2291
23	AG	0.25	0/2559	0.41	0/3429
24	AH	0.26	0/1128	0.43	0/1529
25	AI	0.26	0/1031	0.43	0/1390
26	AJ	0.26	0/854	0.45	0/1148
27	AK	0.24	0/879	0.43	0/1182
28	AL	0.26	0/1406	0.40	0/1878
29	AM	0.25	0/941	0.41	0/1265
30	AN	0.26	0/864	0.44	0/1169
31	AO	0.25	0/1580	0.40	0/2150
32	AP	0.27	0/782	0.40	0/1050

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AQ	0.28	0/746	0.43	0/993
34	AR	0.26	0/2103	0.51	3/2842 (0.1%)
35	AS	0.26	0/1127	0.40	0/1518
36	AT	0.26	0/1361	0.42	0/1829
37	AU	0.24	0/1482	0.39	0/1987
38	AV	0.24	0/2925	0.40	0/3948
39	AW	0.25	0/778	0.45	0/1048
40	AX	0.25	0/2886	0.43	0/3909
41	AY	0.25	0/985	0.39	0/1329
42	AZ	0.25	0/748	0.39	0/1000
43	XB	0.22	0/1400	0.73	0/2168
44	XD	0.30	0/1879	0.48	0/2527
45	XE	0.30	0/2465	0.45	0/3344
46	XF	0.34	0/2071	0.45	0/2817
47	XH	0.28	0/798	0.44	0/1073
48	XI	0.26	0/1727	0.43	0/2340
49	XJ	0.24	0/1309	0.40	0/1764
50	XK	0.31	0/1495	0.41	0/2029
51	XL	0.29	0/904	0.44	0/1218
52	XM	0.32	0/2359	0.45	0/3185
53	XN	0.30	0/1825	0.46	0/2458
54	XO	0.28	0/1269	0.45	0/1708
55	XP	0.28	0/1190	0.44	0/1611
56	XQ	0.27	0/2026	0.44	0/2734
57	XR	0.33	0/1174	0.45	0/1572
58	XS	0.33	0/1311	0.47	0/1778
59	XT	0.33	0/1402	0.44	0/1886
60	XU	0.30	0/1200	0.42	0/1623
61	XV	0.27	0/1693	0.43	0/2297
62	XW	0.33	0/893	0.47	0/1204
63	XX	0.31	1/2090 (0.0%)	0.43	0/2825
64	XY	0.28	0/1571	0.40	0/2106
65	XZ	0.31	0/1003	0.46	0/1354
66	a	0.29	0/838	0.44	0/1138
67	b	0.31	0/1202	0.47	0/1626
68	c	0.27	0/2264	0.42	0/3059
69	d	0.26	0/1807	0.42	0/2450
70	e	1.45	6/1797 (0.3%)	0.43	0/2422
71	f	0.27	0/1169	0.43	0/1576
72	g	0.35	1/1134 (0.1%)	0.45	0/1547
73	h	0.25	0/905	0.44	0/1233
74	i	0.33	0/849	0.47	0/1135
75	j	0.28	0/703	0.41	0/947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	k	0.24	0/743	0.44	0/1003
77	l	0.24	0/692	0.38	0/939
78	m	0.24	0/508	0.45	0/682
79	o	0.31	0/818	0.44	0/1097
80	p	0.25	0/1071	0.43	0/1433
81	q	0.26	0/1413	0.42	0/1906
82	r	0.28	0/1282	0.42	0/1734
86	s	0.29	0/3114	0.45	0/4225
87	t1	0.25	0/366	0.38	0/497
87	t2	0.22	0/238	0.38	0/319
87	t3	0.23	0/238	0.37	0/319
87	t4	0.23	0/229	0.36	0/308
87	t5	0.23	0/229	0.37	0/308
87	t6	0.24	0/213	0.40	0/286
All	All	0.36	9/176028 (0.0%)	0.58	7/249723 (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	1
50	XK	0	1
55	XP	0	1
71	f	0	1
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	99	ARG	CG-CD	61.33	3.05	1.51
70	e	84	TYR	CD2-CE2	32.53	1.88	1.39
70	e	84	TYR	CD1-CE1	31.48	1.86	1.39
70	e	84	TYR	CE2-CZ	22.46	1.67	1.38
70	e	84	TYR	CE1-CZ	21.25	1.66	1.38
70	e	84	TYR	CG-CD1	18.96	1.63	1.39
70	e	84	TYR	CG-CD2	17.05	1.61	1.39
72	g	36	PRO	N-CD	6.05	1.56	1.47
63	XX	149	PRO	N-CD	5.45	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AR	309	PRO	O-C-N	11.63	141.32	122.70
34	AR	309	PRO	CA-C-N	-8.78	97.89	117.20
34	AR	309	PRO	C-N-CA	-5.91	106.92	121.70
9	8	99	ARG	CG-CD-NE	5.87	124.12	111.80
11	XA	2098	G	O4'-C1'-N9	5.61	112.69	108.20
9	8	99	ARG	CB-CG-CD	5.61	126.17	111.60
17	AA	765	C	C2-N1-C1'	5.54	124.89	118.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	XD	206	TYR	Peptide
48	XI	197	LEU	Peptide
50	XK	137	ILE	Peptide
55	XP	114	HIS	Peptide
71	f	138	GLN	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	7	0
3	2	376	407	406	2	0
4	3	831	883	883	16	0
5	4	341	362	362	4	0
6	5	3204	3201	3201	30	0
7	6	2947	2841	2840	41	0
8	7	2365	2373	2372	24	0
9	8	1175	1202	1202	9	0
10	9	996	987	987	4	0
11	XA	31832	16171	16171	219	0
12	A0	1684	1685	1685	16	0
13	A1	2230	2261	2261	38	0
14	A2	925	964	964	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A3	610	682	682	5	0
16	A4	4470	4485	4486	67	0
17	AA	19628	9971	9972	134	0
18	AB	1776	1769	1769	15	0
19	AC	1082	1088	1088	13	0
20	AD	2716	2785	2785	28	0
21	AE	972	1001	1001	14	0
22	AF	1668	1715	1716	23	0
23	AG	2505	2492	2490	28	0
24	AH	1105	1136	1136	18	0
25	AI	1011	1052	1052	13	0
26	AJ	838	887	887	16	0
27	AK	861	885	885	13	0
28	AL	1382	1472	1472	15	0
29	AM	920	951	951	9	0
30	AN	846	908	908	10	0
31	AO	1528	1489	1489	20	0
32	AP	765	796	796	8	0
33	AQ	734	749	749	9	0
34	AR	2060	2074	2074	30	0
35	AS	1100	1103	1103	10	0
36	AT	1330	1342	1343	16	0
37	AU	1461	1471	1471	21	0
38	AV	2867	2863	2862	25	0
39	AW	766	785	785	5	0
40	AX	2814	2805	2804	30	0
41	AY	956	912	911	20	0
42	AZ	731	734	734	7	0
43	XB	1255	640	640	5	0
44	XD	1842	1896	1896	27	0
45	XE	2396	2403	2402	29	0
46	XF	2013	2045	2044	29	0
47	XH	784	832	832	10	0
48	XI	1691	1783	1783	14	0
49	XJ	1291	1367	1364	7	0
50	XK	1451	1448	1448	9	0
51	XL	889	941	941	14	0
52	XM	2305	2378	2378	36	0
53	XN	1778	1808	1808	18	0
54	XO	1245	1283	1283	17	0
55	XP	1164	1162	1162	12	0
56	XQ	1978	2022	2022	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	XR	1153	1214	1214	15	0
58	XS	1284	1354	1354	8	0
59	XT	1368	1410	1410	15	0
60	XU	1171	1164	1164	11	0
61	XV	1648	1656	1654	12	0
62	XW	871	898	898	13	0
63	XX	2035	2054	2054	21	0
64	XY	1534	1575	1575	19	0
65	XZ	978	1030	1030	13	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	1149	1165	1165	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	r1	216	0	145	0	0
84	r3	1459	0	831	0	0
85	r4	1486	0	834	0	0
86	s	3036	3023	3022	0	0
87	t1	354	379	374	0	0
87	t2	238	268	270	0	0
87	t3	238	268	270	0	0
87	t4	229	255	257	0	0
87	t5	229	255	257	0	0
87	t6	214	236	236	0	0
88	0	1	0	0	0	0
88	4	1	0	0	0	0
88	AB	1	0	0	0	0
88	AO	1	0	0	0	0
88	AP	1	0	0	0	0
88	AT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	XI	1	0	0	0	0
89	AA	46	0	0	0	0
89	XA	143	0	0	0	0
89	XD	1	0	0	0	0
89	XE	1	0	0	0	0
89	XI	1	0	0	0	0
89	XM	1	0	0	0	0
89	XW	1	0	0	0	0
89	g	1	0	0	0	0
90	XA	73	67	0	4	0
91	XA	48	50	50	0	0
92	AX	32	10	12	0	0
All	All	170663	143072	144806	1142	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 (1142) 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)
16:A4:67:LYS:HE2	41:AY:312:GLU:OE2	1.41	1.17
13:A1:77:LYS:CD	16:A4:91:ASP:OD2	1.94	1.13
13:A1:77:LYS:CG	16:A4:91:ASP:OD2	2.08	1.01
13:A1:77:LYS:HD2	16:A4:91:ASP:OD2	1.61	0.98
34:AR:305:HIS:HD2	34:AR:314:ALA:HB2	1.27	0.97
13:A1:77:LYS:HG3	16:A4:91:ASP:OD2	1.66	0.93
34:AR:305:HIS:HD2	34:AR:314:ALA:CB	1.83	0.92
16:A4:67:LYS:CE	41:AY:312:GLU:OE2	2.19	0.91
53:XN:134:LYS:NZ	53:XN:141:GLY:O	2.04	0.90
17:AA:1032:C:OP1	32:AP:109:LYS:NZ	2.04	0.89
44:XD:132:ASP:OD2	44:XD:135:ARG:NH1	2.05	0.89
17:AA:728:C:OP1	30:AN:5:ARG:NH2	2.05	0.88
7:6:356:ARG:NH1	11:XA:2090:A:OP1	2.06	0.88
48:XI:51:THR:O	53:XN:250:ARG:NH1	2.07	0.88
11:XA:1777:A:N6	11:XA:1780:U:OP2	2.08	0.87
22:AF:79:ALA:O	23:AG:312:GLN:NE2	2.08	0.87
11:XA:1680:A:OP1	64:XY:230:LYS:NZ	2.08	0.86
37:AU:126:GLN:OE1	37:AU:129:ARG:NH2	2.09	0.86
63:XX:144:TYR:O	63:XX:148:THR:HG23	1.75	0.86
34:AR:305:HIS:CD2	34:AR:314:ALA:HB2	2.11	0.85
11:XA:2537:G:O2'	11:XA:2634:U:OP2	1.95	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:XU:11:ARG:NH2	61:XV:212:LYS:O	2.09	0.84
17:AA:1530:A:OP1	38:AV:64:LYS:NZ	2.11	0.84
11:XA:3063:G:O2'	11:XA:3066:C:OP2	1.96	0.83
12:A0:49:ARG:NH2	37:AU:41:ARG:O	2.12	0.83
11:XA:2261:C:O2'	58:XS:184:ARG:NH1	2.11	0.83
16:A4:108:LEU:CD2	20:AD:154:VAL:HG11	2.09	0.82
52:XM:202:LYS:NZ	52:XM:293:TYR:O	2.11	0.82
23:AG:310:ARG:NH1	40:AX:383:LEU:O	2.12	0.81
7:6:160:ASP:OD2	7:6:267:ARG:NH1	2.13	0.81
27:AK:72:ASP:OD1	27:AK:73:GLU:N	2.13	0.81
29:AM:93:LEU:O	34:AR:175:ARG:NH2	2.14	0.81
11:XA:3068:G:N2	11:XA:3068:G:OP2	2.13	0.81
23:AG:103:ASP:OD1	23:AG:106:ARG:NH2	2.14	0.81
7:6:117:VAL:O	7:6:121:ARG:NH2	2.13	0.81
11:XA:2187:C:O3'	49:XJ:106:LYS:NZ	2.14	0.81
11:XA:1957:A:O4'	59:XT:163:ARG:NH1	2.14	0.80
26:AJ:50:GLY:O	26:AJ:89:ARG:NH1	2.14	0.80
13:A1:154:THR:OG1	24:AH:172:VAL:O	1.99	0.80
29:AM:55:ASP:OD2	36:AT:146:GLN:NE2	2.14	0.80
17:AA:868:C:OP2	17:AA:870:C:N4	2.15	0.80
51:XL:31:ALA:N	51:XL:91:MET:SD	2.54	0.80
23:AG:198:ARG:N	23:AG:246:ARG:O	2.13	0.80
52:XM:53:HIS:O	52:XM:58:GLN:NE2	2.15	0.80
17:AA:659:U:OP1	20:AD:226:ARG:NH2	2.15	0.79
11:XA:1699:C:OP2	64:XY:197:LYS:NZ	2.14	0.79
20:AD:307:LYS:NZ	34:AR:103:TYR:OH	2.16	0.79
1:0:139:ARG:NH2	11:XA:2322:C:OP1	2.16	0.79
11:XA:2724:G:OP1	46:XF:131:LYS:NZ	2.15	0.79
25:AI:71:SER:O	25:AI:74:ARG:NH1	2.15	0.79
17:AA:780:C:N3	28:AL:197:ARG:NH2	2.31	0.79
17:AA:1589:C:OP1	25:AI:187:ARG:NH1	2.16	0.79
14:A2:38:ARG:NH2	17:AA:1184:U:OP1	2.16	0.79
16:A4:108:LEU:CD2	20:AD:154:VAL:CG1	2.61	0.78
11:XA:3203:A:O3'	45:XE:300:LYS:NZ	2.17	0.78
4:3:104:ARG:NH1	4:3:160:LYS:O	2.16	0.78
15:A3:155:ARG:NH2	17:AA:1154:A:OP2	2.16	0.78
17:AA:825:U:N3	17:AA:827:A:OP1	2.17	0.78
11:XA:2166:C:O2	11:XA:2214:A:N6	2.17	0.78
31:AO:185:SER:O	34:AR:183:LYS:NZ	2.17	0.78
14:A2:9:ARG:NH2	17:AA:1021:U:OP2	2.16	0.77
40:AX:53:GLU:N	40:AX:67:HIS:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:XH:134:PRO:O	47:XH:138:LYS:NZ	2.17	0.77
17:AA:1557:A:O2'	26:AJ:72:LYS:NZ	2.18	0.77
35:AS:6:LEU:O	35:AS:15:ARG:NH1	2.17	0.77
24:AH:122:GLN:OE1	27:AK:112:ARG:NH1	2.18	0.77
6:5:33:TRP:O	6:5:39:ARG:NH2	2.18	0.77
4:3:175:ASP:O	4:3:178:GLN:NE2	2.18	0.77
22:AF:126:TYR:O	22:AF:134:GLN:NE2	2.18	0.77
58:XS:72:GLU:O	58:XS:76:HIS:ND1	2.16	0.77
49:XJ:85:PRO:O	49:XJ:124:LYS:NZ	2.18	0.77
60:XU:16:GLN:NE2	60:XU:17:LEU:O	2.18	0.77
8:7:190:ASP:O	8:7:295:ARG:NH1	2.17	0.77
22:AF:52:ARG:NH2	23:AG:360:GLU:OE1	2.17	0.76
22:AF:122:GLN:NE2	22:AF:138:GLU:O	2.18	0.76
27:AK:90:ARG:NH2	27:AK:95:SER:O	2.18	0.76
46:XF:75:GLU:OE2	46:XF:210:ARG:NE	2.18	0.76
9:8:110:GLU:OE2	9:8:114:ARG:NE	2.18	0.76
56:XQ:71:PRO:O	56:XQ:73:ARG:NH1	2.18	0.76
17:AA:860:A:N7	17:AA:919:A:O2'	2.18	0.76
47:XH:84:GLU:OE1	63:XX:44:ARG:NH2	2.18	0.76
11:XA:2954:C:O2	53:XN:182:LYS:NZ	2.18	0.76
7:6:27:ARG:N	11:XA:2832:A:N1	2.34	0.76
11:XA:1800:G:N1	11:XA:1803:A:OP2	2.19	0.76
32:AP:140:TYR:O	32:AP:141:ARG:NE	2.18	0.76
1:0:163:GLU:N	1:0:163:GLU:OE1	2.18	0.75
11:XA:2248:U:OP1	57:XR:99:ARG:NH2	2.17	0.75
26:AJ:96:PRO:O	26:AJ:127:ARG:NH2	2.19	0.75
7:6:136:ARG:NH1	55:XP:137:GLU:OE2	2.19	0.75
34:AR:176:GLU:OE2	34:AR:182:ARG:NE	2.20	0.74
11:XA:1689:C:OP2	63:XX:5:LYS:NZ	2.20	0.74
17:AA:701:G:N2	17:AA:841:A:O2'	2.20	0.74
17:AA:826:A:OP1	26:AJ:55:ARG:NH1	2.20	0.74
56:XQ:118:ARG:NH2	56:XQ:202:VAL:O	2.19	0.74
16:A4:108:LEU:HD21	20:AD:154:VAL:HG11	1.68	0.74
18:AB:137:TYR:O	18:AB:264:ARG:NH2	2.21	0.74
11:XA:1700:U:O4	64:XY:193:ARG:NH2	2.20	0.74
23:AG:382:PRO:O	24:AH:131:ARG:NH1	2.20	0.74
16:A4:269:HIS:O	16:A4:270:ARG:NE	2.20	0.74
16:A4:108:LEU:HD21	20:AD:154:VAL:CG1	2.18	0.74
38:AV:173:PHE:O	38:AV:178:THR:OG1	2.04	0.74
54:XO:82:GLU:N	54:XO:82:GLU:OE1	2.21	0.74
14:A2:60:GLU:O	14:A2:62:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AY:340:SER:OG	41:AY:377:ARG:NH2	2.21	0.73
37:AU:77:GLU:OE1	37:AU:81:LYS:NZ	2.22	0.73
38:AV:192:LYS:NZ	38:AV:194:THR:O	2.21	0.73
13:A1:74:ALA:O	13:A1:110:ASN:ND2	2.21	0.73
14:A2:42:GLU:N	22:AF:241:TRP:O	2.22	0.73
21:AE:105:CYS:SG	32:AP:64:LYS:NZ	2.61	0.73
36:AT:89:ASP:OD2	37:AU:120:ARG:NH2	2.22	0.73
18:AB:219:THR:O	18:AB:233:THR:OG1	2.05	0.73
8:7:238:ASP:OD1	8:7:239:PHE:N	2.22	0.73
61:XV:150:SER:O	61:XV:152:ARG:NH1	2.22	0.73
29:AM:20:ARG:NH1	29:AM:42:PRO:O	2.21	0.73
42:AZ:26:THR:HG1	42:AZ:30:SER:HG	1.33	0.73
24:AH:74:LYS:N	24:AH:175:THR:O	2.22	0.73
11:XA:1729:U:OP2	63:XX:100:ARG:NH1	2.22	0.72
22:AF:129:ALA:O	22:AF:134:GLN:NE2	2.21	0.72
6:5:30:ALA:N	44:XD:201:GLY:O	2.22	0.72
5:4:84:ARG:NE	11:XA:3188:U:OP2	2.21	0.72
45:XE:345:ILE:O	56:XQ:172:GLN:NE2	2.22	0.72
11:XA:2864:U:O5'	62:XW:50:ARG:NH1	2.22	0.72
14:A2:12:ARG:NH2	17:AA:1125:A:O4'	2.23	0.72
40:AX:121:ALA:N	40:AX:299:ASN:OD1	2.22	0.72
17:AA:1314:C:N3	22:AF:36:ARG:NH2	2.38	0.72
49:XJ:154:ARG:NH1	49:XJ:155:VAL:O	2.23	0.72
2:1:23:GLU:N	2:1:23:GLU:OE1	2.23	0.72
52:XM:72:THR:OG1	52:XM:77:ARG:NH2	2.23	0.72
10:9:22:THR:OG1	10:9:36:ARG:NH1	2.22	0.72
17:AA:947:U:OP1	28:AL:162:GLN:NE2	2.22	0.71
38:AV:96:ARG:NH1	38:AV:101:CYS:SG	2.63	0.71
40:AX:206:GLU:OE1	40:AX:249:ARG:NH1	2.23	0.71
16:A4:479:GLU:HA	16:A4:482:ILE:HD12	1.71	0.71
40:AX:111:TYR:O	40:AX:115:THR:OG1	2.08	0.71
22:AF:231:GLU:O	22:AF:234:ARG:NE	2.23	0.71
52:XM:148:PHE:O	52:XM:170:ASN:ND2	2.23	0.71
11:XA:2144:A:OP1	57:XR:57:ARG:NH1	2.24	0.71
40:AX:174:ASN:OD1	40:AX:177:ARG:NH1	2.23	0.71
46:XF:167:MET:SD	46:XF:276:GLN:NE2	2.63	0.71
52:XM:203:ARG:NH2	52:XM:261:ASP:O	2.23	0.71
20:AD:97:GLU:N	20:AD:97:GLU:OE1	2.22	0.71
23:AG:272:SER:OG	23:AG:347:ALA:O	2.08	0.71
38:AV:132:LYS:O	38:AV:136:GLY:N	2.23	0.71
48:XI:224:HIS:O	48:XI:228:GLN:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AY:303:GLN:NE2	41:AY:307:GLU:OE1	2.24	0.70
53:XN:201:ASP:OD1	53:XN:202:GLN:N	2.24	0.70
11:XA:2712:G:N2	45:XE:257:MET:SD	2.64	0.70
34:AR:305:HIS:CD2	34:AR:314:ALA:HA	2.27	0.70
37:AU:40:GLU:N	37:AU:40:GLU:OE1	2.23	0.70
16:A4:470:GLN:OE1	16:A4:472:ASP:N	2.25	0.70
21:AE:27:GLU:OE1	37:AU:170:ARG:NH1	2.23	0.70
7:6:360:ARG:NH2	11:XA:2869:A:N7	2.39	0.70
40:AX:56:PRO:O	40:AX:59:HIS:NE2	2.24	0.70
13:A1:256:SER:O	13:A1:260:ARG:NH1	2.24	0.69
32:AP:65:CYS:SG	32:AP:68:CYS:N	2.65	0.69
45:XE:69:ASP:OD1	45:XE:154:ARG:NH1	2.26	0.69
52:XM:153:ASN:ND2	52:XM:256:LEU:O	2.25	0.69
59:XT:126:ASP:OD1	59:XT:127:MET:N	2.24	0.69
61:XV:181:ASP:O	64:XY:93:LYS:NZ	2.23	0.69
11:XA:1696:C:OP2	64:XY:180:LYS:NZ	2.24	0.69
6:5:144:ARG:O	6:5:194:LYS:NZ	2.26	0.69
2:1:53:ARG:NH2	11:XA:2879:A:O2'	2.26	0.69
11:XA:2293:A:N6	52:XM:37:GLU:OE2	2.26	0.69
1:0:95:ARG:NH1	11:XA:1821:A:OP2	2.25	0.69
11:XA:2167:A:N6	11:XA:2212:C:OP2	2.26	0.69
13:A1:154:THR:OG1	24:AH:171:GLU:OE2	2.10	0.69
20:AD:283:GLU:O	20:AD:356:GLN:NE2	2.27	0.68
22:AF:70:LYS:O	23:AG:365:ARG:NH1	2.26	0.68
11:XA:2457:A:O2'	54:XO:17:ARG:NH2	2.27	0.68
19:AC:89:ASP:OD1	19:AC:90:VAL:N	2.26	0.68
34:AR:305:HIS:CD2	34:AR:314:ALA:CA	2.77	0.68
11:XA:2634:U:OP1	44:XD:278:LYS:NZ	2.27	0.68
13:A1:77:LYS:CE	16:A4:91:ASP:OD2	2.41	0.68
11:XA:1878:U:O3'	46:XF:92:ARG:NH2	2.27	0.67
11:XA:2928:C:OP2	11:XA:3073:C:O2'	2.12	0.67
45:XE:54:SER:OG	45:XE:57:ASN:OD1	2.11	0.67
7:6:55:ASP:OD2	7:6:59:ARG:NH1	2.27	0.67
11:XA:2515:U:O2'	44:XD:282:ALA:O	2.11	0.67
63:XX:80:TRP:O	63:XX:131:THR:OG1	2.13	0.67
25:AI:81:GLU:O	25:AI:148:ARG:NH1	2.27	0.67
11:XA:1962:A:OP2	11:XA:2501:C:N4	2.27	0.67
18:AB:111:LEU:O	18:AB:113:HIS:ND1	2.27	0.67
40:AX:266:ASN:ND2	40:AX:311:SER:O	2.28	0.67
62:XW:62:HIS:N	62:XW:65:ASN:OD1	2.26	0.67
11:XA:3078:C:N4	11:XA:3079:G:O6	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A0:13:GLU:OE1	12:A0:16:ARG:NH1	2.28	0.67
56:XQ:226:PRO:O	56:XQ:229:TRP:NE1	2.28	0.67
29:AM:59:ASN:ND2	29:AM:63:GLU:OE2	2.28	0.67
34:AR:70:PHE:O	34:AR:76:GLN:NE2	2.28	0.67
50:XK:36:SER:O	50:XK:40:GLN:NE2	2.27	0.67
30:AN:62:ASP:OD1	30:AN:88:VAL:N	2.27	0.66
11:XA:3012:U:O4'	11:XA:3173:G:N2	2.27	0.66
46:XF:126:LYS:NZ	46:XF:130:GLN:OE1	2.28	0.66
3:2:49:ARG:NH2	11:XA:2500:A:N1	2.43	0.66
11:XA:2195:A:O2'	11:XA:2196:A:O5'	2.13	0.66
11:XA:2466:A:OP1	56:XQ:232:ARG:NH1	2.28	0.66
4:3:179:LYS:O	7:6:370:ARG:NH2	2.28	0.66
56:XQ:103:ARG:NH2	56:XQ:167:TYR:OH	2.27	0.66
64:XY:76:GLN:NE2	64:XY:78:LYS:O	2.28	0.66
6:5:149:ASN:ND2	6:5:152:GLU:OE2	2.29	0.66
28:AL:149:ASP:OD2	28:AL:152:HIS:ND1	2.29	0.66
54:XO:58:LYS:NZ	56:XQ:270:MET:SD	2.67	0.66
17:AA:1293:C:N4	33:AQ:80:ARG:O	2.28	0.66
11:XA:2755:A:O2'	63:XX:112:ARG:NH2	2.29	0.66
42:AZ:54:ASN:ND2	42:AZ:57:THR:OG1	2.29	0.66
17:AA:798:C:OP1	29:AM:10:LYS:N	2.29	0.66
16:A4:478:TYR:CE2	16:A4:482:ILE:HD11	2.31	0.66
21:AE:5:GLU:OE2	21:AE:96:HIS:ND1	2.28	0.66
7:6:212:SER:OG	7:6:275:GLN:O	2.14	0.65
7:6:283:GLU:OE2	7:6:307:HIS:NE2	2.29	0.65
11:XA:3220:A:OP1	45:XE:260:LYS:NZ	2.29	0.65
60:XU:9:LEU:N	64:XY:183:GLN:OE1	2.29	0.65
4:3:113:ARG:NH1	52:XM:75:TYR:O	2.30	0.65
7:6:114:ARG:NH1	43:XB:1643:A:OP1	2.30	0.65
11:XA:2191:A:N6	11:XA:2198:A:OP2	2.30	0.65
53:XN:234:ASP:OD1	53:XN:235:LEU:N	2.30	0.65
4:3:98:SER:OG	4:3:102:GLY:N	2.30	0.65
48:XI:101:ASN:OD1	48:XI:151:ASN:N	2.30	0.65
16:A4:198:TYR:O	16:A4:239:ARG:NH1	2.28	0.65
17:AA:769:G:N2	17:AA:772:A:OP2	2.28	0.64
27:AK:28:HIS:NE2	42:AZ:60:GLU:OE2	2.29	0.64
26:AJ:84:ARG:NH1	26:AJ:85:LEU:O	2.31	0.64
2:1:34:ARG:NH2	2:1:38:ARG:O	2.30	0.64
17:AA:1053:A:N1	17:AA:1100:C:O2'	2.31	0.64
18:AB:149:ARG:NH2	33:AQ:82:ASP:OD1	2.31	0.64
19:AC:113:ARG:NH2	24:AH:166:GLU:OE1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AP:82:GLN:NE2	32:AP:133:PRO:O	2.30	0.64
63:XX:118:ILE:O	63:XX:168:ARG:NH1	2.30	0.64
17:AA:1389:G:N2	17:AA:1416:A:N7	2.46	0.64
11:XA:3127:G:O2'	11:XA:3130:A:N6	2.30	0.64
16:A4:478:TYR:CD2	16:A4:482:ILE:HD11	2.32	0.64
1:O:181:ARG:NH1	1:O:186:THR:O	2.31	0.63
17:AA:1411:G:O3'	40:AX:279:LYS:NZ	2.31	0.63
17:AA:1433:A:N3	17:AA:1458:A:N6	2.46	0.63
47:XH:58:ARG:NH1	47:XH:77:HIS:O	2.30	0.63
22:AF:119:LYS:NZ	40:AX:398:LEU:O	2.31	0.63
50:XK:10:GLN:NE2	59:XT:203:LEU:O	2.30	0.63
6:5:334:LYS:N	6:5:362:THR:OG1	2.30	0.63
33:AQ:20:GLU:OE1	33:AQ:24:ARG:NH1	2.32	0.63
34:AR:305:HIS:HD2	34:AR:314:ALA:CA	2.10	0.63
17:AA:826:A:N7	26:AJ:55:ARG:NE	2.46	0.63
38:AV:131:ASN:ND2	38:AV:134:GLN:OE1	2.32	0.63
11:XA:1761:A:O2'	11:XA:1762:A:O5'	2.16	0.63
17:AA:678:U:N3	17:AA:920:G:O6	2.32	0.63
6:5:174:GLU:OE1	6:5:298:ASN:ND2	2.33	0.62
16:A4:455:ASN:O	16:A4:486:TYR:OH	2.17	0.62
17:AA:751:A:OP1	30:AN:47:LYS:NZ	2.31	0.62
51:XL:35:MET:N	51:XL:57:CYS:O	2.30	0.62
10:9:74:VAL:O	64:XY:83:ALA:N	2.32	0.62
25:AI:79:LYS:N	25:AI:82:GLU:OE2	2.31	0.62
16:A4:108:LEU:HD22	20:AD:154:VAL:HG11	1.82	0.62
22:AF:151:ASN:O	22:AF:223:LYS:NZ	2.33	0.62
36:AT:91:GLU:OE2	37:AU:123:ARG:NH1	2.33	0.62
11:XA:1689:C:O2	64:XY:213:ARG:NH2	2.33	0.62
38:AV:321:GLU:O	38:AV:326:LYS:NZ	2.32	0.62
11:XA:2531:U:O4	44:XD:246:ARG:NH2	2.33	0.61
11:XA:2643:G:O2'	11:XA:2645:G:OP2	2.18	0.61
16:A4:67:LYS:HE2	41:AY:312:GLU:CD	2.19	0.61
28:AL:169:ASN:OD1	28:AL:170:LEU:N	2.33	0.61
12:A0:87:TRP:O	31:AO:215:ARG:NH2	2.33	0.61
11:XA:2655:G:N2	11:XA:2659:C:O2'	2.33	0.61
4:3:113:ARG:NH2	11:XA:1750:G:OP2	2.33	0.61
4:3:168:ARG:NH2	4:3:170:ASN:OD1	2.33	0.61
38:AV:222:SER:OG	38:AV:277:ARG:NH1	2.33	0.61
17:AA:668:U:O2'	31:AO:83:GLY:O	2.18	0.61
34:AR:308:HIS:C	34:AR:310:ASP:H	1.98	0.61
56:XQ:279:GLU:OE2	56:XQ:283:TRP:NE1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AD:136:ARG:N	42:AZ:67:PHE:O	2.34	0.60
11:XA:2822:C:O2'	11:XA:2915:C:OP2	2.19	0.60
17:AA:752:C:O2'	17:AA:793:C:N4	2.34	0.60
36:AT:95:ASN:OD1	36:AT:96:LYS:N	2.34	0.60
7:6:308:GLN:NE2	7:6:311:MET:SD	2.74	0.60
18:AB:77:GLU:OE2	18:AB:259:ARG:NH1	2.34	0.60
11:XA:2581:A:O2'	11:XA:2583:C:N4	2.34	0.60
56:XQ:227:LYS:O	56:XQ:229:TRP:N	2.35	0.60
9:8:100:GLU:N	9:8:100:GLU:OE1	2.34	0.60
23:AG:219:MET:SD	23:AG:223:ARG:NH2	2.75	0.60
1:0:136:GLU:OE1	1:0:177:ARG:NH2	2.35	0.60
61:XV:54:TRP:NE1	61:XV:56:LEU:O	2.35	0.60
11:XA:2294:A:OP2	52:XM:39:ARG:NH2	2.33	0.59
36:AT:109:ASN:ND2	36:AT:111:GLU:OE2	2.35	0.59
45:XE:63:GLN:NE2	45:XE:67:ASP:OD2	2.35	0.59
11:XA:3082:G:N2	11:XA:3085:A:OP2	2.32	0.59
16:A4:67:LYS:CE	41:AY:312:GLU:CD	2.69	0.59
16:A4:99:SER:N	16:A4:102:GLU:OE2	2.33	0.59
34:AR:305:HIS:CD2	34:AR:314:ALA:CB	2.75	0.59
6:5:143:PRO:HA	6:5:146:HIS:HD1	1.66	0.59
11:XA:2499:U:OP2	11:XA:2504:A:N6	2.26	0.59
13:A1:77:LYS:HE3	16:A4:91:ASP:OD1	2.03	0.59
11:XA:1958:G:OP2	59:XT:160:GLY:N	2.36	0.59
17:AA:1162:A:OP1	26:AJ:47:ARG:NH1	2.31	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
17:AA:897:C:OP1	26:AJ:114:ARG:NH2	2.35	0.59
61:XV:66:GLU:N	61:XV:66:GLU:OE1	2.35	0.59
8:7:192:TRP:O	8:7:295:ARG:NH1	2.36	0.59
20:AD:127:ASN:O	42:AZ:72:ARG:NH1	2.35	0.58
11:XA:2063:G:N2	62:XW:56:MET:SD	2.76	0.58
38:AV:201:GLU:OE1	38:AV:233:LYS:NZ	2.35	0.58
53:XN:80:THR:OG1	53:XN:81:GLU:OE1	2.20	0.58
62:XW:115:ASP:O	62:XW:119:ARG:NE	2.33	0.58
13:A1:83:LEU:O	13:A1:99:LYS:NZ	2.35	0.58
11:XA:3066:C:O2'	45:XE:233:GLN:OE1	2.22	0.58
41:AY:292:GLN:OE1	41:AY:292:GLN:N	2.37	0.58
58:XS:126:GLU:N	58:XS:126:GLU:OE1	2.36	0.58
13:A1:77:LYS:HE3	16:A4:91:ASP:OD2	2.03	0.58
13:A1:81:VAL:O	13:A1:99:LYS:NZ	2.37	0.58
37:AU:110:GLN:O	37:AU:114:ARG:NE	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A1:100:GLU:O	19:AC:156:GLN:NE2	2.36	0.58
13:A1:312:TYR:OH	40:AX:338:ASP:O	2.22	0.58
49:XJ:27:GLY:O	49:XJ:58:LYS:NZ	2.36	0.58
17:AA:1048:C:O2'	17:AA:1049:A:OP1	2.22	0.57
26:AJ:107:ILE:N	26:AJ:131:ASP:OD2	2.31	0.57
40:AX:214:GLU:OE2	40:AX:232:ARG:NH2	2.37	0.57
55:XP:79:ARG:NH1	55:XP:94:GLU:OE2	2.35	0.57
10:9:127:LEU:O	10:9:134:ASN:ND2	2.36	0.57
46:XF:215:SER:OG	46:XF:257:GLN:N	2.35	0.57
11:XA:1856:A:OP2	11:XA:2986:C:O2'	2.21	0.57
11:XA:2472:A:O2'	11:XA:2478:G:N7	2.33	0.57
13:A1:118:ALA:O	13:A1:122:HIS:ND1	2.37	0.57
18:AB:109:SER:OG	35:AS:62:ASP:OD1	2.22	0.57
62:XW:115:ASP:OD1	62:XW:116:LEU:N	2.38	0.57
11:XA:2511:C:O2'	44:XD:257:ILE:O	2.20	0.57
14:A2:102:ASN:OD1	14:A2:103:LYS:N	2.38	0.57
39:AW:132:GLU:O	39:AW:135:GLN:NE2	2.34	0.57
11:XA:1844:A:OP2	57:XR:48:ARG:NH2	2.37	0.57
14:A2:24:ASN:OD1	14:A2:25:LYS:N	2.37	0.57
11:XA:1755:A:O2'	47:XH:64:LEU:O	2.16	0.57
11:XA:1889:C:OP1	52:XM:133:LYS:NZ	2.36	0.57
17:AA:1014:A:O2'	17:AA:1031:G:O4'	2.20	0.57
31:AO:228:SER:OG	37:AU:52:GLU:OE2	2.21	0.57
33:AQ:55:GLU:OE2	33:AQ:59:ARG:NE	2.38	0.57
34:AR:202:ARG:NE	34:AR:233:ALA:O	2.37	0.57
6:5:201:ARG:NH2	6:5:418:TYR:O	2.37	0.56
11:XA:1805:A:OP2	61:XV:94:HIS:NE2	2.38	0.56
50:XK:110:GLY:O	50:XK:114:LYS:NZ	2.37	0.56
11:XA:2744:U:O2'	11:XA:2746:U:O4	2.21	0.56
17:AA:869:C:OP2	31:AO:97:ARG:NH2	2.37	0.56
20:AD:283:GLU:OE2	35:AS:21:ARG:NH1	2.37	0.56
34:AR:308:HIS:C	34:AR:310:ASP:N	2.57	0.56
44:XD:111:ARG:NH1	44:XD:243:THR:OG1	2.38	0.56
10:9:134:ASN:OD1	10:9:135:PHE:N	2.38	0.56
11:XA:2192:A:OP1	49:XJ:142:ARG:NE	2.37	0.56
45:XE:124:VAL:O	45:XE:281:ASN:ND2	2.38	0.56
56:XQ:268:ASP:OD1	56:XQ:269:MET:N	2.38	0.56
52:XM:88:SER:O	52:XM:134:ARG:NE	2.39	0.56
30:AN:31:THR:OG1	36:AT:65:MET:SD	2.64	0.56
32:AP:49:ASP:OD2	39:AW:82:SER:N	2.38	0.56
7:6:119:GLU:N	7:6:119:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:283:GLU:OE1	7:6:283:GLU:N	2.37	0.56
11:XA:1864:A:OP1	57:XR:17:ARG:NH1	2.36	0.56
20:AD:342:MET:SD	20:AD:342:MET:N	2.75	0.56
51:XL:43:ASN:ND2	51:XL:117:THR:OG1	2.39	0.56
15:A3:142:LYS:NZ	17:AA:1490:U:OP1	2.38	0.56
17:AA:1429:C:OP1	23:AG:388:ARG:NH2	2.38	0.56
40:AX:170:GLN:OE1	40:AX:175:LYS:NZ	2.36	0.56
20:AD:285:TYR:OH	20:AD:372:GLU:OE1	2.24	0.56
11:XA:2813:U:N3	11:XA:2817:G:OP2	2.38	0.55
17:AA:769:G:OP1	30:AN:24:LYS:NZ	2.39	0.55
57:XR:149:HIS:O	65:XZ:151:LEU:N	2.39	0.55
19:AC:74:GLY:O	27:AK:103:ARG:NH2	2.38	0.55
23:AG:276:ARG:NH1	23:AG:373:ASP:OD2	2.39	0.55
51:XL:120:LYS:O	51:XL:143:ASN:ND2	2.40	0.55
11:XA:2171:U:N3	11:XA:2198:A:N7	2.52	0.55
65:XZ:84:ASP:OD1	65:XZ:85:ILE:N	2.39	0.55
13:A1:282:GLU:N	13:A1:282:GLU:OE1	2.39	0.55
45:XE:286:ASN:OD1	45:XE:287:GLY:N	2.40	0.55
59:XT:84:LYS:N	59:XT:172:CYS:SG	2.80	0.55
60:XU:30:ARG:O	64:XY:121:ARG:NH1	2.39	0.55
17:AA:1278:C:OP2	20:AD:269:ARG:NH1	2.39	0.55
16:A4:175:GLN:O	16:A4:180:GLY:N	2.40	0.55
17:AA:1108:C:N4	17:AA:1125:A:N7	2.53	0.55
32:AP:111:ILE:HG22	32:AP:115:GLN:HE22	1.70	0.55
39:AW:137:GLY:O	39:AW:139:ARG:NH1	2.40	0.55
11:XA:2658:U:O2	51:XL:33:GLN:NE2	2.38	0.55
13:A1:156:TYR:O	13:A1:167:ARG:NH1	2.40	0.55
16:A4:264:ARG:HE	16:A4:293:THR:HG22	1.72	0.55
33:AQ:27:ASN:OD1	33:AQ:28:ARG:N	2.40	0.55
54:XO:129:CYS:SG	54:XO:130:LEU:N	2.80	0.55
25:AI:94:ASN:OD1	25:AI:95:THR:N	2.39	0.55
37:AU:58:GLU:OE2	37:AU:62:HIS:NE2	2.39	0.55
23:AG:295:VAL:N	23:AG:298:ILE:O	2.40	0.55
21:AE:44:GLU:OE1	21:AE:60:ARG:NH2	2.40	0.55
2:1:47:ASP:O	2:1:51:LYS:N	2.38	0.54
11:XA:2614:U:O3'	51:XL:53:ARG:NH1	2.39	0.54
17:AA:948:U:OP2	17:AA:1045:G:N2	2.39	0.54
36:AT:130:GLY:N	36:AT:135:CYS:SG	2.80	0.54
38:AV:370:GLU:OE2	38:AV:370:GLU:N	2.40	0.54
12:A0:30:ASP:OD1	12:A0:31:SER:N	2.40	0.54
18:AB:103:GLU:OE2	35:AS:52:ARG:NH2	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AS:7:GLU:N	35:AS:7:GLU:OE1	2.39	0.54
60:XU:71:ARG:NH2	60:XU:73:GLN:OE1	2.40	0.54
4:3:124:ARG:NH2	11:XA:2868:C:OP1	2.40	0.54
17:AA:1322:C:OP1	19:AC:43:ARG:NH1	2.38	0.54
63:XX:83:GLU:N	63:XX:83:GLU:OE1	2.40	0.54
12:A0:96:ARG:N	12:A0:117:ILE:O	2.38	0.54
12:A0:132:GLU:OE1	12:A0:205:ALA:N	2.41	0.54
17:AA:722:C:N3	17:AA:798:C:O2'	2.41	0.54
17:AA:1033:U:O2'	21:AE:93:ILE:O	2.26	0.54
36:AT:97:GLU:OE1	36:AT:97:GLU:N	2.39	0.54
11:XA:2065:A:OP2	62:XW:74:ARG:NH1	2.38	0.54
22:AF:207:HIS:NE2	22:AF:211:GLU:OE2	2.41	0.54
46:XF:220:ASP:O	46:XF:245:ALA:N	2.41	0.54
1:0:108:ASP:OD1	1:0:109:VAL:N	2.41	0.54
7:6:86:GLU:OE2	7:6:86:GLU:N	2.39	0.54
17:AA:700:A:OP2	37:AU:27:ARG:NH1	2.40	0.54
19:AC:76:LEU:O	27:AK:103:ARG:NH2	2.38	0.54
11:XA:2506:A:N6	11:XA:3093:C:O4'	2.39	0.54
11:XA:2754:A:N3	63:XX:108:GLN:NE2	2.56	0.54
17:AA:1265:C:OP1	27:AK:112:ARG:NH1	2.34	0.54
18:AB:211:ASP:OD1	18:AB:212:ALA:N	2.41	0.54
11:XA:2472:A:OP1	51:XL:37:ARG:NH2	2.37	0.54
53:XN:71:ASP:OD2	53:XN:129:LYS:NZ	2.37	0.53
17:AA:949:U:OP1	28:AL:168:LYS:NZ	2.41	0.53
36:AT:9:ILE:O	36:AT:12:THR:OG1	2.25	0.53
11:XA:2111:C:OP1	48:XI:35:ARG:NH1	2.42	0.53
30:AN:53:ASP:OD2	30:AN:57:GLN:N	2.41	0.53
17:AA:1347:G:OP1	27:AK:36:ARG:NH1	2.36	0.53
12:A0:90:ASP:OD1	31:AO:215:ARG:NH1	2.42	0.53
13:A1:77:LYS:HE3	16:A4:91:ASP:CG	2.29	0.53
52:XM:216:ASP:OD1	52:XM:218:LYS:N	2.42	0.53
11:XA:1883:G:N7	46:XF:281:ARG:NH1	2.56	0.53
11:XA:3096:U:C5	90:XA:5144:H8Q:O42	2.61	0.53
17:AA:1430:A:OP1	23:AG:388:ARG:NH2	2.38	0.53
23:AG:244:PHE:O	23:AG:246:ARG:NH1	2.42	0.53
8:7:36:SER:N	8:7:39:GLU:OE2	2.42	0.53
55:XP:71:PHE:HB3	55:XP:72:PRO:HD3	1.91	0.53
7:6:252:CYS:SG	7:6:286:ARG:NH2	2.81	0.53
7:6:364:ARG:NE	11:XA:2859:A:OP2	2.35	0.53
31:AO:65:GLN:O	31:AO:69:GLY:N	2.40	0.53
8:7:152:CYS:SG	8:7:156:ARG:NH1	2.80	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2029:A:O2'	11:XA:2030:U:OP1	2.25	0.53
17:AA:1143:C:N4	17:AA:1576:G:OP1	2.41	0.53
40:AX:157:ASP:OD1	40:AX:158:ALA:N	2.42	0.53
13:A1:56:ARG:NH2	16:A4:83:THR:O	2.41	0.53
44:XD:86:ASP:OD2	44:XD:87:HIS:ND1	2.41	0.53
54:XO:41:ARG:NE	54:XO:124:GLU:OE1	2.36	0.53
11:XA:1747:G:OP2	11:XA:1749:C:N4	2.41	0.52
11:XA:3119:C:C2	11:XA:3120:C:C5	2.97	0.52
31:AO:81:HIS:ND1	31:AO:82:LYS:O	2.42	0.52
38:AV:159:ASP:OD1	38:AV:160:ALA:N	2.41	0.52
17:AA:1049:A:OP2	28:AL:198:ARG:NH2	2.42	0.52
17:AA:1234:C:O2'	17:AA:1235:U:OP1	2.23	0.52
17:AA:1431:G:N2	17:AA:1458:A:OP2	2.39	0.52
64:XY:154:ARG:NH1	64:XY:160:GLN:O	2.42	0.52
64:XY:206:ASP:OD1	64:XY:207:HIS:N	2.43	0.52
16:A4:108:LEU:CD2	20:AD:154:VAL:HG12	2.39	0.52
17:AA:1526:U:O2'	17:AA:1527:A:O4'	2.20	0.52
35:AS:18:ASP:OD1	35:AS:19:LEU:N	2.42	0.52
45:XE:334:ASP:OD1	45:XE:335:GLU:N	2.39	0.52
18:AB:94:LYS:NZ	18:AB:112:ASP:OD1	2.41	0.52
11:XA:1742:G:O2'	11:XA:1754:G:O6	2.25	0.52
14:A2:113:ASN:OD1	14:A2:114:LYS:N	2.42	0.52
25:AI:158:ARG:NH2	25:AI:177:ASP:OD2	2.43	0.52
6:5:300:ARG:HA	6:5:303:ARG:HE	1.75	0.52
12:A0:50:LEU:O	12:A0:55:TRP:NE1	2.42	0.52
37:AU:178:GLU:N	37:AU:178:GLU:OE1	2.41	0.52
63:XX:150:LYS:HG3	63:XX:159:MET:CE	2.39	0.52
18:AB:153:TYR:O	18:AB:157:ASN:ND2	2.43	0.52
38:AV:47:HIS:N	38:AV:78:ASN:OD1	2.43	0.52
47:XH:108:ARG:NH1	47:XH:143:GLU:OE2	2.38	0.52
8:7:262:ASP:OD1	8:7:263:VAL:N	2.42	0.52
20:AD:266:ASP:OD1	20:AD:269:ARG:NH2	2.43	0.52
54:XO:64:LYS:NZ	54:XO:97:TYR:O	2.39	0.52
44:XD:113:ARG:O	44:XD:147:ARG:NH2	2.43	0.52
44:XD:264:ARG:HE	44:XD:270:PRO:HD3	1.75	0.52
35:AS:75:TYR:OH	39:AW:91:GLN:O	2.27	0.51
7:6:239:ASN:OD1	7:6:275:GLN:NE2	2.42	0.51
11:XA:1769:C:N4	46:XF:105:ASN:OD1	2.43	0.51
11:XA:3050:U:O3'	51:XL:63:LYS:NZ	2.42	0.51
13:A1:53:LEU:HB2	16:A4:518:GLU:OE2	2.10	0.51
38:AV:271:GLU:N	38:AV:271:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A1:152:ASP:N	13:A1:152:ASP:OD1	2.42	0.51
65:XZ:71:ARG:NH1	65:XZ:73:LYS:O	2.43	0.51
11:XA:1847:U:OP1	52:XM:47:ARG:NE	2.43	0.51
16:A4:478:TYR:O	16:A4:482:ILE:HG13	2.11	0.51
11:XA:2139:U:OP2	65:XZ:74:SER:N	2.36	0.51
11:XA:2148:A:OP2	57:XR:65:ARG:NH1	2.43	0.51
16:A4:98:ALA:N	16:A4:102:GLU:OE2	2.44	0.51
27:AK:49:ASP:OD1	27:AK:50:GLU:N	2.43	0.51
7:6:133:ASP:OD1	7:6:134:ALA:N	2.42	0.51
12:A0:61:GLU:OE2	12:A0:139:TRP:N	2.43	0.51
17:AA:901:G:OP1	20:AD:117:ARG:NH1	2.44	0.51
47:XH:95:GLU:OE2	47:XH:112:VAL:N	2.44	0.51
48:XI:181:ILE:O	48:XI:184:THR:N	2.42	0.51
58:XS:127:ARG:NH2	58:XS:157:GLU:OE1	2.39	0.51
11:XA:1877:U:O3'	52:XM:30:ASN:ND2	2.44	0.51
11:XA:2182:G:O2'	11:XA:2183:C:O4'	2.23	0.51
13:A1:196:GLU:N	13:A1:196:GLU:OE1	2.44	0.51
29:AM:71:ASP:OD1	29:AM:72:ARG:N	2.44	0.51
11:XA:2145:G:O2'	11:XA:2147:G:OP1	2.28	0.51
17:AA:873:G:O2'	17:AA:921:U:O2	2.28	0.51
11:XA:1672:C:OP1	59:XT:50:LYS:N	2.44	0.50
17:AA:710:U:OP2	29:AM:13:ARG:NH1	2.45	0.50
16:A4:95:LEU:HD11	19:AC:132:TYR:HB2	1.93	0.50
38:AV:235:GLU:O	38:AV:239:GLY:N	2.45	0.50
41:AY:344:GLN:N	41:AY:344:GLN:OE1	2.45	0.50
7:6:114:ARG:NH2	55:XP:116:TYR:O	2.45	0.50
11:XA:2082:G:N2	65:XZ:88:MET:SD	2.74	0.50
22:AF:108:ARG:O	22:AF:112:ILE:HG12	2.10	0.50
4:3:116:ARG:NH2	4:3:159:ASP:OD1	2.45	0.50
11:XA:2104:A:OP1	53:XN:73:ARG:NH1	2.37	0.50
46:XF:191:ASP:OD1	46:XF:192:SER:N	2.45	0.50
55:XP:81:ARG:NH1	55:XP:94:GLU:OE1	2.43	0.50
1:0:98:GLN:NE2	11:XA:2709:A:N3	2.60	0.50
6:5:384:GLN:NE2	11:XA:2395:A:O2'	2.44	0.50
7:6:198:ALA:O	7:6:254:TYR:OH	2.26	0.50
11:XA:2665:U:OP2	54:XO:17:ARG:HD2	2.12	0.50
17:AA:1517:A:O2'	17:AA:1518:C:O4'	2.28	0.50
23:AG:312:GLN:OE1	23:AG:345:ARG:NH2	2.45	0.50
38:AV:108:THR:O	38:AV:111:THR:OG1	2.27	0.50
46:XF:199:ASP:N	46:XF:199:ASP:OD1	2.43	0.50
63:XX:76:GLN:NE2	63:XX:154:CYS:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:51:GLU:OE2	8:7:54:ARG:NH2	2.42	0.50
11:XA:2182:G:N2	11:XA:2199:A:N3	2.59	0.50
40:AX:161:TRP:NE1	40:AX:183:GLU:OE2	2.45	0.50
6:5:160:HIS:HA	6:5:164:TRP:HB2	1.93	0.50
6:5:337:GLU:N	6:5:337:GLU:OE1	2.45	0.50
22:AF:35:SER:OG	22:AF:36:ARG:N	2.43	0.50
28:AL:75:ASP:OD2	37:AU:153:LYS:NZ	2.38	0.50
45:XE:316:PHE:HB3	45:XE:317:PRO:HD3	1.94	0.50
17:AA:1199:G:N1	17:AA:1424:U:N3	2.60	0.50
46:XF:103:GLN:OE1	46:XF:249:ASN:ND2	2.44	0.50
52:XM:255:MET:O	52:XM:258:THR:OG1	2.28	0.50
23:AG:379:ARG:NH2	24:AH:133:GLN:OE1	2.44	0.49
47:XH:120:ARG:NH2	63:XX:136:ASP:OD2	2.43	0.49
3:2:85:LYS:NZ	11:XA:1792:G:OP2	2.42	0.49
11:XA:2387:U:O2'	11:XA:2406:A:N6	2.45	0.49
21:AE:85:ASP:OD1	44:XD:171:ARG:NH1	2.42	0.49
24:AH:161:GLN:HA	24:AH:164:LEU:CD1	2.42	0.49
34:AR:135:ARG:NH1	34:AR:236:GLU:OE2	2.45	0.49
34:AR:200:GLU:N	34:AR:200:GLU:OE2	2.40	0.49
2:1:20:MET:SD	2:1:20:MET:N	2.85	0.49
6:5:361:THR:OG1	6:5:363:ASP:OD1	2.27	0.49
24:AH:75:ARG:N	24:AH:175:THR:OG1	2.45	0.49
17:AA:1225:C:O2'	17:AA:1449:G:O2'	2.28	0.49
40:AX:171:SER:OG	40:AX:178:PHE:O	2.31	0.49
11:XA:2149:G:OP2	57:XR:65:ARG:NH2	2.46	0.49
11:XA:2715:A:O2'	45:XE:245:THR:O	2.29	0.49
11:XA:2939:C:H2'	11:XA:2940:A:O4'	2.11	0.49
17:AA:1048:C:O2'	28:AL:196:TYR:O	2.18	0.49
17:AA:1079:G:O6	17:AA:1080:A:N6	2.40	0.49
11:XA:1674:A:N7	59:XT:47:ILE:N	2.61	0.49
11:XA:2662:A:OP1	45:XE:220:LYS:NZ	2.37	0.49
17:AA:1289:G:O2'	17:AA:1297:G:OP2	2.27	0.49
46:XF:49:ARG:NH1	46:XF:270:GLU:OE1	2.42	0.49
11:XA:2830:A:N6	11:XA:2837:A:OP2	2.36	0.49
11:XA:1787:G:N2	11:XA:1790:A:OP2	2.39	0.49
11:XA:1990:G:OP1	44:XD:269:ARG:NH2	2.42	0.49
37:AU:52:GLU:N	37:AU:52:GLU:OE1	2.43	0.49
17:AA:1024:G:N2	17:AA:1027:A:OP2	2.43	0.49
17:AA:1227:G:OP1	24:AH:128:LYS:NZ	2.42	0.49
65:XZ:106:VAL:O	65:XZ:110:LEU:HD23	2.13	0.49
12:A0:82:ARG:NH2	12:A0:138:ASP:O	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A1:216:ARG:NH1	41:AY:326:SER:O	2.45	0.48
17:AA:1264:C:O3'	27:AK:112:ARG:NH2	2.46	0.48
21:AE:53:ALA:N	21:AE:56:GLN:O	2.39	0.48
23:AG:276:ARG:HG3	23:AG:277:LYS:H	1.78	0.48
13:A1:142:LYS:O	13:A1:146:HIS:ND1	2.43	0.48
53:XN:85:GLY:O	53:XN:192:ARG:NH2	2.43	0.48
11:XA:2017:U:OP1	52:XM:54:LYS:NZ	2.41	0.48
14:A2:50:SER:O	14:A2:53:MET:HG2	2.13	0.48
17:AA:850:U:O2'	37:AU:27:ARG:NH2	2.46	0.48
54:XO:140:SER:O	54:XO:146:ASN:ND2	2.46	0.48
17:AA:662:U:H2'	17:AA:663:A:O4'	2.14	0.48
17:AA:843:G:N1	17:AA:847:G:O6	2.46	0.48
17:AA:989:U:OP1	25:AI:94:ASN:ND2	2.45	0.48
23:AG:362:GLU:OE2	23:AG:365:ARG:NH1	2.44	0.48
9:8:186:GLN:N	9:8:186:GLN:OE1	2.46	0.48
16:A4:61:LYS:HA	24:AH:69:PRO:HA	1.94	0.48
17:AA:1212:U:O2'	17:AA:1214:A:N6	2.45	0.48
13:A1:255:ASN:OD1	13:A1:256:SER:N	2.47	0.48
22:AF:114:THR:HG22	22:AF:202:PRO:HA	1.94	0.48
40:AX:51:THR:O	40:AX:67:HIS:N	2.45	0.48
51:XL:140:ILE:O	51:XL:142:GLN:NE2	2.47	0.48
32:AP:111:ILE:O	32:AP:115:GLN:NE2	2.47	0.48
56:XQ:108:ILE:O	56:XQ:108:ILE:HG13	2.14	0.48
8:7:287:GLN:N	8:7:288:PRO:CD	2.77	0.48
46:XF:91:PRO:O	46:XF:176:VAL:HG21	2.14	0.48
63:XX:148:THR:HG21	63:XX:153:LEU:HD13	1.96	0.48
4:3:131:LYS:NZ	11:XA:2909:G:O6	2.41	0.48
6:5:177:CYS:O	6:5:180:ILE:HG22	2.14	0.48
17:AA:1516:G:O6	17:AA:1517:A:N6	2.47	0.48
45:XE:280:HIS:O	45:XE:281:ASN:OD1	2.32	0.48
1:0:86:THR:OG1	11:XA:2684:C:OP1	2.26	0.48
11:XA:2529:U:O2'	44:XD:206:TYR:O	2.32	0.48
11:XA:2529:U:N3	44:XD:205:GLN:OE1	2.44	0.48
11:XA:2939:C:O2'	11:XA:2940:A:H5'	2.14	0.48
13:A1:86:ARG:NH1	13:A1:96:PRO:O	2.45	0.48
22:AF:201:MET:N	22:AF:202:PRO:HD2	2.29	0.48
46:XF:280:TYR:CE2	52:XM:125:ARG:HD3	2.49	0.48
50:XK:130:ASP:OD1	50:XK:131:GLU:N	2.46	0.48
4:3:169:ARG:NH2	4:3:182:ASP:OD1	2.47	0.47
8:7:203:THR:HG21	8:7:279:GLU:HB2	1.96	0.47
43:XB:1644:G:O6	55:XP:87:HIS:NE2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:XH:84:GLU:OE2	47:XH:89:ARG:NH2	2.47	0.47
7:6:62:GLU:O	7:6:66:GLN:OE1	2.31	0.47
17:AA:1121:A:OP2	20:AD:297:ARG:NH2	2.47	0.47
17:AA:1462:G:C2	17:AA:1463:G:C5	3.02	0.47
11:XA:2381:A:N6	11:XA:2412:A:N1	2.62	0.47
14:A2:32:ARG:NH1	17:AA:1599:A:OP2	2.47	0.47
34:AR:137:PRO:O	34:AR:139:ASN:ND2	2.48	0.47
52:XM:225:ASP:OD2	52:XM:228:LYS:NZ	2.47	0.47
61:XV:103:ASP:OD1	61:XV:104:TYR:N	2.47	0.47
7:6:320:GLN:N	7:6:320:GLN:OE1	2.48	0.47
22:AF:201:MET:N	22:AF:201:MET:SD	2.87	0.47
31:AO:161:GLY:O	34:AR:223:ARG:NH2	2.48	0.47
48:XI:163:GLU:O	48:XI:166:ARG:HG3	2.14	0.47
11:XA:1672:C:O2'	59:XT:149:ARG:O	2.32	0.47
42:AZ:77:ASP:O	42:AZ:80:ASP:OD1	2.33	0.47
11:XA:2096:U:O4	52:XM:57:ARG:NH1	2.46	0.47
11:XA:2293:A:C6	52:XM:39:ARG:HD2	2.49	0.47
11:XA:2529:U:OP2	44:XD:208:ARG:NH1	2.48	0.47
11:XA:3047:G:O3'	51:XL:81:LYS:NZ	2.48	0.47
16:A4:366:GLU:OE1	16:A4:366:GLU:N	2.42	0.47
17:AA:1234:C:H2'	17:AA:1234:C:O2	2.14	0.47
17:AA:1526:U:O2'	17:AA:1526:U:O2	2.32	0.47
17:AA:1598:G:OP1	33:AQ:57:TYR:OH	2.27	0.47
21:AE:56:GLN:OE1	21:AE:56:GLN:N	2.47	0.47
22:AF:38:SER:OG	22:AF:40:GLU:OE1	2.10	0.47
36:AT:36:THR:O	36:AT:45:ARG:NE	2.48	0.47
13:A1:69:VAL:HA	16:A4:81:ASP:OD2	2.15	0.47
17:AA:1225:C:HO2'	17:AA:1449:G:HO2'	1.63	0.47
17:AA:1239:C:O2	17:AA:1351:G:N2	2.47	0.47
21:AE:96:HIS:O	21:AE:100:GLN:NE2	2.41	0.47
7:6:50:LYS:HA	62:XW:121:PRO:HA	1.96	0.47
7:6:286:ARG:NE	7:6:295:GLN:O	2.44	0.47
11:XA:1834:U:C4	59:XT:206:ARG:HA	2.50	0.47
11:XA:1878:U:O2'	46:XF:92:ARG:NH2	2.48	0.47
11:XA:2951:A:H2'	11:XA:2952:U:H6	1.80	0.47
41:AY:367:LYS:O	41:AY:370:VAL:HG12	2.14	0.47
41:AY:378:ASN:O	41:AY:382:GLU:OE1	2.32	0.47
11:XA:2552:U:C2	11:XA:2553:G:C8	3.03	0.47
11:XA:2826:G:OP1	62:XW:49:ARG:NH1	2.44	0.47
17:AA:782:A:O2'	30:AN:46:ARG:NH1	2.47	0.47
22:AF:111:MET:O	22:AF:114:THR:OG1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:XD:124:GLU:HG3	44:XD:142:VAL:HG22	1.97	0.47
11:XA:2385:U:OP1	44:XD:71:LYS:NZ	2.45	0.46
52:XM:193:PHE:CZ	52:XM:201:PRO:HD3	2.50	0.46
65:XZ:80:TYR:HA	65:XZ:83:LYS:HG2	1.97	0.46
2:1:34:ARG:NH2	2:1:35:ASN:O	2.48	0.46
7:6:188:TYR:N	7:6:191:ASN:OD1	2.46	0.46
7:6:206:TYR:OH	7:6:242:GLY:O	2.14	0.46
52:XM:100:ARG:O	52:XM:104:LEU:HG	2.15	0.46
53:XN:78:GLU:OE2	53:XN:158:ARG:NE	2.48	0.46
57:XR:36:ASN:OD1	57:XR:37:ARG:N	2.49	0.46
65:XZ:81:TRP:O	65:XZ:84:ASP:OD1	2.34	0.46
8:7:143:TRP:HE3	8:7:179:PHE:HB3	1.81	0.46
17:AA:1200:G:N2	17:AA:1418:G:O2'	2.49	0.46
26:AJ:47:ARG:HE	26:AJ:48:LYS:H	1.62	0.46
63:XX:147:LYS:O	63:XX:147:LYS:HG2	2.15	0.46
64:XY:151:ASP:OD1	64:XY:152:ALA:N	2.48	0.46
11:XA:3148:C:O2'	45:XE:106:MET:SD	2.73	0.46
40:AX:130:LYS:O	40:AX:130:LYS:HG3	2.15	0.46
44:XD:216:LEU:HD23	44:XD:216:LEU:H	1.81	0.46
61:XV:148:THR:HG22	61:XV:149:ARG:H	1.80	0.46
8:7:306:LEU:O	8:7:306:LEU:HG	2.15	0.46
11:XA:3175:A:OP2	11:XA:3187:C:N4	2.48	0.46
12:A0:101:ARG:NH1	17:AA:1528:A:OP1	2.48	0.46
14:A2:17:ARG:NE	17:AA:1022:A:OP2	2.48	0.46
16:A4:95:LEU:HD11	19:AC:132:TYR:CB	2.45	0.46
17:AA:1400:U:OP2	42:AZ:32:LYS:NZ	2.48	0.46
18:AB:156:GLU:OE1	23:AG:163:HIS:ND1	2.48	0.46
17:AA:701:G:OP1	37:AU:38:LYS:NZ	2.47	0.46
17:AA:928:A:O3'	20:AD:419:ARG:NH1	2.48	0.46
37:AU:88:GLY:O	37:AU:92:GLU:OE1	2.32	0.46
54:XO:86:ILE:HB	54:XO:87:PRO:HD3	1.98	0.46
11:XA:2182:G:H2'	11:XA:2183:C:C6	2.51	0.46
11:XA:3066:C:C2'	11:XA:3067:U:H5'	2.46	0.46
16:A4:90:GLN:CG	19:AC:133:TYR:HE1	2.29	0.46
52:XM:85:GLU:O	52:XM:90:ARG:NH2	2.49	0.46
65:XZ:107:ASN:HA	65:XZ:110:LEU:CD2	2.46	0.46
6:5:242:ARG:HA	6:5:245:ILE:HG12	1.97	0.46
9:8:165:ASP:OD1	9:8:165:ASP:N	2.48	0.46
11:XA:1671:G:C6	11:XA:1818:A:N1	2.83	0.46
11:XA:2086:A:H2'	11:XA:2087:U:C6	2.51	0.46
14:A2:9:ARG:O	14:A2:20:VAL:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:AV:144:PHE:CZ	38:AV:167:VAL:HG21	2.51	0.46
41:AY:377:ARG:O	41:AY:381:ASN:ND2	2.47	0.46
21:AE:38:ASP:OD1	21:AE:39:LEU:N	2.45	0.46
34:AR:221:GLN:OE1	34:AR:223:ARG:NH2	2.48	0.46
40:AX:69:ASN:OD1	40:AX:70:ILE:N	2.48	0.46
57:XR:65:ARG:O	57:XR:69:ILE:HG12	2.16	0.46
7:6:37:ASN:ND2	62:XW:125:VAL:O	2.42	0.46
11:XA:2151:A:OP2	11:XA:2249:G:N1	2.40	0.46
25:AI:140:LYS:NZ	25:AI:168:GLY:O	2.46	0.46
30:AN:59:THR:OG1	30:AN:62:ASP:OD2	2.24	0.46
44:XD:253:ASN:OD1	44:XD:254:LYS:N	2.49	0.46
6:5:201:ARG:NH2	6:5:420:HIS:O	2.50	0.45
6:5:391:VAL:O	6:5:391:VAL:HG13	2.16	0.45
7:6:39:ASP:OD1	7:6:40:ILE:N	2.49	0.45
11:XA:3096:U:H2'	90:XA:5144:H8Q:C40	2.46	0.45
16:A4:67:LYS:CD	41:AY:312:GLU:OE2	2.64	0.45
17:AA:1012:A:O2'	17:AA:1065:C:N4	2.47	0.45
41:AY:367:LYS:O	41:AY:371:GLU:OE1	2.33	0.45
43:XB:1620:A:N3	43:XB:1620:A:H2'	2.31	0.45
11:XA:1868:G:H2'	52:XM:40:PRO:HG3	1.97	0.45
11:XA:3061:G:H2'	11:XA:3062:U:O4'	2.16	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
34:AR:176:GLU:N	34:AR:176:GLU:OE1	2.49	0.45
50:XK:24:LYS:O	50:XK:26:GLN:NE2	2.49	0.45
53:XN:204:GLU:OE1	53:XN:208:ASN:ND2	2.48	0.45
54:XO:113:ARG:NH1	54:XO:116:ASP:OD2	2.49	0.45
57:XR:96:GLU:OE1	57:XR:96:GLU:N	2.49	0.45
16:A4:164:ARG:H	16:A4:167:LYS:HE3	1.82	0.45
45:XE:257:MET:HB2	45:XE:258:PRO:CD	2.47	0.45
46:XF:70:ARG:NE	46:XF:194:GLU:OE1	2.49	0.45
14:A2:44:THR:HG22	14:A2:45:CYS:N	2.31	0.45
4:3:131:LYS:O	4:3:136:LYS:NZ	2.48	0.45
11:XA:2574:G:O2'	11:XA:2575:U:P	2.75	0.45
59:XT:99:ILE:O	59:XT:103:LEU:HD23	2.17	0.45
11:XA:1939:G:O2'	11:XA:1973:G:H4'	2.16	0.45
11:XA:2139:U:O4	65:XZ:77:ARG:NH1	2.49	0.45
20:AD:191:ARG:NH1	31:AO:79:ARG:O	2.49	0.45
52:XM:231:GLU:O	52:XM:235:GLU:OE1	2.34	0.45
5:4:99:LYS:NZ	11:XA:3013:G:O3'	2.48	0.45
11:XA:2060:A:O2'	11:XA:2061:C:OP2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:XA:5144:H8Q:O57	90:XA:5144:H8Q:O58	2.33	0.45
27:AK:70:VAL:HA	27:AK:73:GLU:OE2	2.17	0.45
36:AT:48:VAL:HA	36:AT:52:ILE:HD13	1.98	0.45
45:XE:209:LYS:NZ	45:XE:263:ASN:OD1	2.43	0.45
46:XF:177:ALA:HB1	46:XF:253:MET:SD	2.57	0.45
56:XQ:199:THR:O	56:XQ:199:THR:HG23	2.17	0.45
63:XX:207:THR:N	63:XX:210:GLU:OE2	2.38	0.45
8:7:199:LEU:O	8:7:203:THR:HG23	2.17	0.45
8:7:279:GLU:OE2	8:7:313:TRP:NE1	2.50	0.45
21:AE:106:GLU:OE1	21:AE:106:GLU:N	2.49	0.45
28:AL:86:ASP:OD1	28:AL:87:ASP:N	2.50	0.45
29:AM:50:GLN:NE2	36:AT:129:PHE:O	2.47	0.45
7:6:182:ASP:OD1	7:6:182:ASP:N	2.50	0.45
11:XA:2458:A:O2'	45:XE:215:PHE:O	2.27	0.45
45:XE:310:LEU:HG	45:XE:310:LEU:O	2.17	0.45
55:XP:162:SER:O	55:XP:166:GLU:OE1	2.35	0.45
60:XU:31:PRO:O	64:XY:121:ARG:NH2	2.50	0.45
11:XA:3118:U:C2	11:XA:3119:C:C5	3.05	0.45
14:A2:53:MET:SD	22:AF:234:ARG:HD2	2.57	0.45
17:AA:1199:G:N1	17:AA:1424:U:C4	2.85	0.45
17:AA:1428:G:OP1	23:AG:390:LYS:NZ	2.45	0.45
17:AA:1433:A:C4	17:AA:1458:A:N6	2.84	0.45
18:AB:82:ARG:NH2	18:AB:86:ASP:OD1	2.48	0.45
56:XQ:225:LYS:HG2	56:XQ:226:PRO:HD2	1.99	0.45
6:5:80:ARG:NH2	6:5:82:TYR:OH	2.50	0.44
7:6:379:ILE:HD13	11:XA:1882:A:C5	2.52	0.44
11:XA:2234:C:O2'	11:XA:2688:C:O2'	2.29	0.44
24:AH:126:ILE:O	24:AH:127:TYR:CG	2.70	0.44
47:XH:134:PRO:HA	47:XH:137:LYS:HG2	1.99	0.44
6:5:270:ILE:HG22	6:5:270:ILE:O	2.17	0.44
6:5:286:PRO:O	6:5:324:GLN:NE2	2.50	0.44
16:A4:482:ILE:CG2	16:A4:519:TYR:HE2	2.30	0.44
18:AB:239:ASN:ND2	18:AB:242:SER:OG	2.51	0.44
44:XD:172:MET:SD	44:XD:172:MET:N	2.88	0.44
46:XF:142:ARG:HA	46:XF:149:GLY:HA2	1.99	0.44
47:XH:133:SER:OG	47:XH:135:GLU:HG3	2.17	0.44
60:XU:58:GLU:OE2	60:XU:65:VAL:N	2.46	0.44
6:5:230:LEU:O	6:5:289:HIS:N	2.47	0.44
11:XA:2195:A:HO2'	11:XA:2196:A:P	2.39	0.44
31:AO:148:LYS:O	31:AO:151:THR:OG1	2.27	0.44
38:AV:96:ARG:NH1	38:AV:101:CYS:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:XF:228:GLN:HA	46:XF:231:VAL:HG12	1.99	0.44
48:XI:50:VAL:O	53:XN:211:ASN:ND2	2.50	0.44
5:4:88:TRP:NE1	11:XA:2160:A:OP2	2.39	0.44
7:6:209:GLU:N	7:6:209:GLU:OE1	2.51	0.44
11:XA:1791:G:HO2'	11:XA:2006:C:HO2'	1.63	0.44
17:AA:1262:C:C4	17:AA:1263:G:C5	3.06	0.44
28:AL:136:ILE:O	28:AL:140:GLU:OE1	2.36	0.44
37:AU:112:GLU:OE2	37:AU:115:ARG:NH1	2.50	0.44
41:AY:277:LEU:O	41:AY:281:GLU:OE1	2.36	0.44
48:XI:137:ASP:N	48:XI:137:ASP:OD1	2.50	0.44
62:XW:112:GLU:O	62:XW:115:ASP:OD1	2.35	0.44
11:XA:3153:U:C2'	11:XA:3154:U:H5'	2.48	0.44
17:AA:682:A:N6	17:AA:865:A:H61	2.16	0.44
17:AA:723:A:OP1	17:AA:724:C:N4	2.45	0.44
17:AA:1214:A:O2'	17:AA:1238:C:O2	2.31	0.44
55:XP:72:PRO:O	55:XP:74:ARG:NH2	2.50	0.44
9:8:104:VAL:HG23	9:8:104:VAL:O	2.18	0.44
11:XA:1849:C:OP2	52:XM:53:HIS:NE2	2.51	0.44
11:XA:2111:C:H1'	11:XA:2944:C:O2'	2.18	0.44
11:XA:3143:U:O4	11:XA:3144:A:N6	2.51	0.44
17:AA:1459:A:O2'	17:AA:1460:C:O4'	2.33	0.44
21:AE:41:ASN:OD1	21:AE:43:GLY:N	2.51	0.44
61:XV:163:ASP:N	61:XV:163:ASP:OD1	2.51	0.44
11:XA:1692:A:O2'	64:XY:175:ARG:NH1	2.51	0.44
17:AA:702:C:O2'	17:AA:842:C:O2	2.27	0.44
40:AX:337:LEU:HG	40:AX:337:LEU:O	2.17	0.44
62:XW:115:ASP:C	62:XW:119:ARG:HE	2.16	0.44
7:6:159:ARG:NH2	7:6:160:ASP:OD1	2.51	0.44
11:XA:2453:G:O6	11:XA:2672:A:N6	2.50	0.44
17:AA:1106:C:O2'	17:AA:1108:C:OP2	2.28	0.44
17:AA:1278:C:OP2	20:AD:270:LYS:NZ	2.49	0.44
29:AM:68:LEU:O	34:AR:161:ILE:N	2.51	0.44
31:AO:125:GLN:OE1	31:AO:125:GLN:N	2.49	0.44
40:AX:297:MET:O	40:AX:297:MET:HG2	2.18	0.44
52:XM:103:TYR:O	52:XM:106:ASP:OD1	2.36	0.44
55:XP:71:PHE:HB2	62:XW:107:HIS:HA	2.00	0.44
4:3:113:ARG:HH12	52:XM:76:ILE:HA	1.82	0.44
11:XA:3169:C:O2'	11:XA:3170:C:O4'	2.31	0.44
12:A0:107:GLN:O	38:AV:97:HIS:NE2	2.48	0.44
46:XF:102:TRP:CZ2	46:XF:164:MET:HE1	2.53	0.44
54:XO:149:LEU:HA	54:XO:152:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:XZ:50:PRO:O	65:XZ:54:GLU:OE1	2.35	0.44
11:XA:1828:A:H4'	11:XA:1829:A:C8	2.53	0.43
11:XA:1953:A:O2'	11:XA:2463:A:OP1	2.35	0.43
11:XA:1961:A:O4'	59:XT:161:ARG:HA	2.18	0.43
17:AA:708:C:O2'	17:AA:842:C:OP1	2.36	0.43
17:AA:826:A:N7	26:AJ:55:ARG:CZ	2.81	0.43
26:AJ:49:LEU:HD23	26:AJ:50:GLY:H	1.83	0.43
52:XM:156:VAL:O	52:XM:177:ALA:N	2.51	0.43
56:XQ:107:HIS:O	56:XQ:108:ILE:HG13	2.17	0.43
59:XT:123:GLU:O	59:XT:126:ASP:OD1	2.36	0.43
60:XU:80:ARG:NH2	60:XU:84:ASN:OD1	2.51	0.43
61:XV:147:SER:OG	61:XV:152:ARG:N	2.49	0.43
36:AT:96:LYS:O	36:AT:100:GLU:OE1	2.37	0.43
52:XM:156:VAL:HG22	52:XM:157:GLN:H	1.83	0.43
53:XN:70:SER:O	53:XN:155:LYS:NZ	2.51	0.43
8:7:38:THR:O	8:7:42:GLU:OE1	2.37	0.43
11:XA:1775:A:OP1	46:XF:148:GLY:N	2.42	0.43
11:XA:1846:C:OP2	58:XS:177:ARG:N	2.39	0.43
17:AA:918:A:O2'	17:AA:919:A:O4'	2.35	0.43
17:AA:1449:G:C2	17:AA:1450:C:C6	3.06	0.43
38:AV:79:ILE:HG12	38:AV:84:GLU:HB3	2.01	0.43
41:AY:375:TRP:CZ2	41:AY:379:TYR:CE2	3.06	0.43
48:XI:34:THR:OG1	48:XI:36:HIS:O	2.31	0.43
48:XI:181:ILE:O	48:XI:184:THR:OG1	2.29	0.43
52:XM:21:ARG:O	52:XM:26:ASN:ND2	2.51	0.43
20:AD:407:ASP:OD1	20:AD:407:ASP:N	2.45	0.43
31:AO:67:ARG:NH2	31:AO:68:TYR:OH	2.51	0.43
34:AR:89:LYS:O	34:AR:92:LYS:NZ	2.48	0.43
38:AV:106:ASN:OD1	38:AV:107:TRP:N	2.52	0.43
9:8:138:ALA:O	9:8:141:GLU:HG3	2.18	0.43
38:AV:316:GLN:NE2	38:AV:321:GLU:O	2.52	0.43
40:AX:63:HIS:O	40:AX:63:HIS:ND1	2.51	0.43
40:AX:164:ASN:OD1	40:AX:166:ARG:NH1	2.51	0.43
53:XN:174:GLY:O	53:XN:178:GLN:OE1	2.36	0.43
53:XN:200:LYS:O	53:XN:203:GLU:HG3	2.18	0.43
11:XA:2714:A:P	45:XE:239:ARG:HH11	2.42	0.43
17:AA:777:G:C2	17:AA:778:C:C6	3.07	0.43
23:AG:321:ASP:C	23:AG:321:ASP:OD1	2.57	0.43
30:AN:85:VAL:HG13	30:AN:86:PHE:N	2.34	0.43
46:XF:77:VAL:O	46:XF:77:VAL:HG13	2.18	0.43
56:XQ:237:ASN:OD1	56:XQ:238:PHE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:XY:161:GLU:OE1	64:XY:161:GLU:N	2.51	0.43
6:5:254:GLU:OE2	6:5:256:PHE:N	2.49	0.43
7:6:144:GLY:N	7:6:145:PRO:CD	2.82	0.43
11:XA:1799:U:H2'	11:XA:1800:G:O4'	2.19	0.43
11:XA:2066:C:O2'	11:XA:2067:C:OP1	2.33	0.43
14:A2:64:ASP:OD1	14:A2:65:ALA:N	2.52	0.43
16:A4:634:ALA:HB3	16:A4:641:ILE:HG21	2.01	0.43
17:AA:990:U:H2'	17:AA:991:G:O4'	2.18	0.43
17:AA:1282:G:N2	17:AA:1286:A:OP2	2.38	0.43
26:AJ:49:LEU:HD23	26:AJ:50:GLY:N	2.34	0.43
30:AN:66:LEU:HD13	30:AN:79:HIS:HB3	2.00	0.43
35:AS:116:LYS:O	35:AS:120:GLU:OE1	2.36	0.43
40:AX:169:LEU:O	40:AX:179:ASP:N	2.51	0.43
44:XD:177:ARG:O	44:XD:244:VAL:HG11	2.19	0.43
58:XS:106:TRP:CD2	58:XS:114:ILE:HD11	2.54	0.43
63:XX:93:ASN:O	63:XX:94:ASN:OD1	2.36	0.43
1:0:145:GLU:OE2	1:0:173:ARG:NH2	2.51	0.43
11:XA:2692:G:N1	11:XA:2696:A:OP2	2.38	0.43
11:XA:2802:A:H2'	11:XA:2803:A:O4'	2.18	0.43
13:A1:53:LEU:CB	16:A4:518:GLU:HG2	2.49	0.43
16:A4:64:THR:HG22	24:AH:64:THR:HG23	2.01	0.43
17:AA:806:C:OP2	17:AA:807:A:N6	2.37	0.43
23:AG:107:ALA:O	23:AG:111:LEU:HD23	2.19	0.43
34:AR:212:GLU:OE2	34:AR:212:GLU:N	2.51	0.43
8:7:160:ASP:OD1	8:7:160:ASP:N	2.51	0.43
11:XA:1795:A:H2'	11:XA:1796:A:O4'	2.18	0.43
11:XA:2216:A:N3	48:XI:150:HIS:NE2	2.63	0.43
11:XA:2674:U:H2'	11:XA:2675:G:O4'	2.19	0.43
43:XB:1630:A:N1	43:XB:1637:C:N4	2.66	0.43
48:XI:66:PRO:O	48:XI:67:SER:OG	2.33	0.43
48:XI:181:ILE:O	48:XI:182:ASP:OD1	2.37	0.43
60:XU:44:ILE:HB	60:XU:45:PRO:CD	2.49	0.43
63:XX:148:THR:O	63:XX:148:THR:OG1	2.36	0.43
7:6:58:ARG:O	7:6:62:GLU:OE1	2.37	0.43
11:XA:1698:C:O2'	11:XA:1702:A:N3	2.45	0.43
11:XA:2938:A:OP1	11:XA:2984:A:N6	2.52	0.43
12:A0:194:GLN:O	12:A0:197:ARG:NH1	2.52	0.43
13:A1:53:LEU:HB3	16:A4:518:GLU:HG2	2.01	0.43
17:AA:995:A:P	25:AI:120:ALA:HB2	2.59	0.43
17:AA:1211:G:N1	17:AA:1354:A:C6	2.87	0.43
25:AI:151:VAL:HG21	25:AI:158:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AO:107:ILE:HD11	31:AO:146:GLN:HB3	2.01	0.43
6:5:143:PRO:HA	6:5:146:HIS:ND1	2.31	0.42
11:XA:1885:A:OP2	46:XF:168:LYS:NZ	2.52	0.42
11:XA:2143:G:C6	11:XA:2258:A:C2	3.07	0.42
11:XA:2933:G:N2	11:XA:2936:U:O2	2.41	0.42
11:XA:3096:U:H3'	90:XA:5144:H8Q:C39	2.49	0.42
17:AA:805:C:O4'	17:AA:805:C:O2	2.36	0.42
40:AX:159:HIS:NE2	40:AX:266:ASN:OD1	2.52	0.42
41:AY:376:PHE:O	41:AY:380:PHE:CD2	2.71	0.42
44:XD:251:ASP:OD1	44:XD:251:ASP:C	2.57	0.42
54:XO:113:ARG:O	54:XO:117:ARG:NH1	2.52	0.42
6:5:200:ARG:NH1	6:5:234:ASP:OD2	2.52	0.42
8:7:95:LEU:O	59:XT:137:ARG:NH2	2.45	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:770:C:O2'	17:AA:771:A:OP1	2.32	0.42
34:AR:128:MET:SD	34:AR:128:MET:N	2.88	0.42
44:XD:163:ILE:HG22	44:XD:164:LEU:N	2.33	0.42
45:XE:271:LEU:HD12	45:XE:286:ASN:O	2.19	0.42
46:XF:90:ALA:O	46:XF:176:VAL:HG23	2.18	0.42
49:XJ:75:ASP:O	49:XJ:76:ARG:HB3	2.20	0.42
54:XO:60:ILE:HD11	54:XO:104:TYR:CG	2.53	0.42
57:XR:85:ALA:O	57:XR:89:ASN:OD1	2.37	0.42
6:5:173:ARG:HA	6:5:176:TYR:CE2	2.53	0.42
17:AA:908:C:N4	17:AA:909:G:O6	2.52	0.42
18:AB:186:THR:HG23	18:AB:186:THR:O	2.20	0.42
38:AV:372:ILE:O	38:AV:376:GLU:OE1	2.36	0.42
8:7:238:ASP:OD1	8:7:238:ASP:C	2.58	0.42
11:XA:3148:C:OP1	45:XE:211:ILE:HG12	2.19	0.42
17:AA:1134:G:N7	26:AJ:35:GLN:NE2	2.67	0.42
20:AD:250:GLY:N	20:AD:326:LEU:O	2.52	0.42
27:AK:69:ASP:O	27:AK:73:GLU:OE1	2.37	0.42
28:AL:137:ARG:HA	28:AL:140:GLU:OE2	2.19	0.42
43:XB:1607:U:O2'	43:XB:1608:G:H5'	2.20	0.42
58:XS:114:ILE:CG2	58:XS:193:LEU:HB2	2.48	0.42
4:3:125:ARG:HE	4:3:147:PHE:HE1	1.66	0.42
11:XA:2326:C:O2'	54:XO:31:ASN:OD1	2.30	0.42
46:XF:237:LEU:HD11	46:XF:240:PHE:HB2	2.01	0.42
56:XQ:118:ARG:NH2	56:XQ:204:MET:O	2.53	0.42
58:XS:155:ARG:NE	58:XS:157:GLU:OE2	2.52	0.42
60:XU:40:VAL:HG12	60:XU:41:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2726:C:O2	11:XA:2937:A:N1	2.53	0.42
11:XA:3212:C:O2	11:XA:3212:C:O4'	2.36	0.42
16:A4:638:SER:OG	16:A4:640:PRO:HD2	2.20	0.42
23:AG:140:TRP:HA	23:AG:146:PRO:HA	2.02	0.42
31:AO:163:LEU:HD23	31:AO:163:LEU:H	1.83	0.42
56:XQ:225:LYS:CG	56:XQ:226:PRO:HD2	2.49	0.42
4:3:95:THR:HG21	4:3:105:LYS:HD3	2.01	0.42
7:6:51:TYR:CZ	62:XW:122:LYS:HA	2.54	0.42
8:7:53:ALA:HA	8:7:56:LEU:CD2	2.50	0.42
11:XA:1917:A:C8	11:XA:1983:U:C4	3.08	0.42
11:XA:1970:G:H2'	11:XA:1971:A:O4'	2.19	0.42
11:XA:2605:C:OP2	11:XA:2606:U:O2'	2.29	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
17:AA:1235:U:H5''	17:AA:1236:C:OP2	2.20	0.42
17:AA:1265:C:H4'	24:AH:122:GLN:HG3	2.01	0.42
26:AJ:49:LEU:HD23	26:AJ:51:PRO:HD2	2.02	0.42
35:AS:15:ARG:O	35:AS:18:ASP:OD1	2.38	0.42
36:AT:55:ILE:O	36:AT:59:ASN:OD1	2.38	0.42
37:AU:102:HIS:O	37:AU:106:MET:SD	2.78	0.42
60:XU:13:GLY:O	61:XV:211:LYS:NZ	2.45	0.42
63:XX:82:GLY:N	63:XX:83:GLU:OE1	2.53	0.42
11:XA:1939:G:O5'	44:XD:259:LYS:NZ	2.49	0.42
11:XA:2470:G:O2'	51:XL:36:THR:HG22	2.20	0.42
11:XA:2517:U:OP1	44:XD:287:ARG:NH2	2.53	0.42
11:XA:2714:A:OP2	45:XE:239:ARG:NH1	2.53	0.42
11:XA:3180:A:C4	11:XA:3190:A:C6	3.08	0.42
12:A0:44:PRO:O	12:A0:45:PHE:HB3	2.19	0.42
13:A1:267:LEU:O	13:A1:270:LYS:NZ	2.43	0.42
16:A4:68:VAL:HG13	41:AY:302:ILE:HG23	2.01	0.42
16:A4:109:ALA:O	19:AC:134:PHE:HD1	2.02	0.42
36:AT:116:GLU:O	36:AT:119:GLU:HG3	2.20	0.42
40:AX:393:ARG:O	40:AX:397:TYR:CD2	2.72	0.42
41:AY:377:ARG:HA	41:AY:380:PHE:CE2	2.55	0.42
50:XK:7:ALA:HB3	50:XK:8:PRO:HD3	2.01	0.42
61:XV:77:VAL:HG23	61:XV:89:GLY:N	2.35	0.42
16:A4:335:PHE:HA	16:A4:338:ILE:HG22	2.01	0.42
27:AK:72:ASP:OD1	27:AK:72:ASP:C	2.56	0.42
34:AR:140:ASP:OD1	34:AR:141:VAL:N	2.53	0.42
52:XM:102:GLN:HA	52:XM:105:ILE:HG12	2.00	0.42
55:XP:87:HIS:O	55:XP:118:THR:OG1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:XX:207:THR:OG1	63:XX:210:GLU:OE1	2.37	0.42
2:1:23:GLU:OE2	2:1:57:VAL:N	2.51	0.42
8:7:68:LYS:HG2	8:7:78:VAL:HG12	2.01	0.42
11:XA:3122:U:O2	11:XA:3122:U:O4'	2.37	0.42
16:A4:640:PRO:O	16:A4:643:GLU:HG2	2.20	0.42
23:AG:115:GLY:N	24:AH:84:ASP:OD2	2.53	0.42
25:AI:181:ILE:HG13	25:AI:181:ILE:O	2.20	0.42
33:AQ:26:LEU:O	33:AQ:29:ILE:HG22	2.19	0.42
45:XE:221:ARG:HA	45:XE:261:MET:SD	2.60	0.42
51:XL:96:MET:SD	51:XL:96:MET:N	2.93	0.42
53:XN:172:VAL:HG13	53:XN:175:PHE:CZ	2.55	0.42
53:XN:198:MET:O	53:XN:201:ASP:OD1	2.38	0.42
64:XY:94:SER:OG	64:XY:95:ASN:N	2.53	0.42
11:XA:2944:C:H2'	11:XA:2945:A:O4'	2.20	0.41
22:AF:116:GLU:O	22:AF:120:ARG:HG2	2.19	0.41
34:AR:67:LYS:N	34:AR:68:PRO:CD	2.83	0.41
6:5:306:PRO:O	6:5:310:ARG:NE	2.47	0.41
11:XA:2400:C:O2'	11:XA:2401:A:O5'	2.36	0.41
17:AA:1231:A:O2'	17:AA:1236:C:N4	2.48	0.41
17:AA:1464:G:H2'	17:AA:1465:C:C6	2.56	0.41
25:AI:174:SER:OG	33:AQ:13:MET:SD	2.78	0.41
31:AO:151:THR:O	31:AO:154:ILE:HG22	2.20	0.41
46:XF:284:TYR:HB2	46:XF:285:PRO:HD2	2.02	0.41
50:XK:42:LEU:O	57:XR:74:ALA:HB2	2.20	0.41
59:XT:88:TRP:CZ3	59:XT:92:LYS:HD2	2.55	0.41
65:XZ:124:LEU:HD12	65:XZ:124:LEU:O	2.21	0.41
7:6:379:ILE:O	7:6:380:TYR:CG	2.73	0.41
8:7:235:TYR:O	8:7:238:ASP:OD1	2.38	0.41
11:XA:2411:U:O4	11:XA:2412:A:N6	2.54	0.41
16:A4:455:ASN:HA	16:A4:486:TYR:CE1	2.55	0.41
17:AA:1440:G:H2'	17:AA:1441:A:C8	2.55	0.41
23:AG:200:LEU:O	23:AG:218:TYR:OH	2.35	0.41
24:AH:123:SER:OG	24:AH:124:VAL:N	2.50	0.41
39:AW:162:VAL:HG12	39:AW:162:VAL:O	2.20	0.41
45:XE:50:ASP:HA	45:XE:53:LEU:HD21	2.02	0.41
57:XR:17:ARG:HA	57:XR:20:ARG:HG2	2.02	0.41
59:XT:119:GLU:O	59:XT:123:GLU:OE1	2.37	0.41
63:XX:163:ARG:HG3	63:XX:201:ALA:O	2.20	0.41
11:XA:2714:A:N6	11:XA:3101:A:O2'	2.50	0.41
20:AD:273:ASN:HA	20:AD:276:VAL:HG12	2.03	0.41
31:AO:105:CYS:HB2	31:AO:106:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:XN:201:ASP:OD1	53:XN:201:ASP:C	2.59	0.41
57:XR:73:THR:HG22	57:XR:77:GLN:OE1	2.21	0.41
17:AA:1024:G:C4	17:AA:1026:A:OP2	2.74	0.41
17:AA:1399:A:H2'	17:AA:1400:U:C6	2.55	0.41
6:5:393:LYS:O	6:5:396:VAL:HG12	2.21	0.41
7:6:321:CYS:SG	7:6:322:ARG:N	2.93	0.41
9:8:169:PHE:HB2	9:8:170:PRO:HD3	2.03	0.41
13:A1:53:LEU:HB2	16:A4:518:GLU:CG	2.51	0.41
13:A1:66:TRP:CG	23:AG:91:MET:HG2	2.55	0.41
13:A1:91:VAL:O	13:A1:94:GLY:N	2.54	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:865:A:H2'	17:AA:866:A:N9	2.36	0.41
17:AA:1578:A:H2'	17:AA:1579:C:C6	2.56	0.41
20:AD:245:VAL:HG22	20:AD:271:ALA:HB1	2.02	0.41
22:AF:112:ILE:HD12	40:AX:397:TYR:CD1	2.56	0.41
22:AF:192:ARG:HG3	22:AF:192:ARG:O	2.21	0.41
23:AG:171:ASN:O	23:AG:175:HIS:ND1	2.50	0.41
26:AJ:61:VAL:O	26:AJ:84:ARG:N	2.51	0.41
40:AX:371:ALA:O	40:AX:373:THR:N	2.53	0.41
44:XD:194:ASN:OD1	44:XD:243:THR:HG23	2.21	0.41
45:XE:82:ASP:O	45:XE:84:PRO:HD3	2.20	0.41
52:XM:133:LYS:C	52:XM:134:ARG:HG2	2.40	0.41
64:XY:220:LYS:O	64:XY:224:GLU:OE1	2.38	0.41
4:3:180:TYR:CD2	7:6:363:LEU:HD21	2.56	0.41
11:XA:2475:U:C2	11:XA:2477:G:OP2	2.74	0.41
11:XA:3127:G:C2	11:XA:3129:A:OP2	2.74	0.41
12:A0:125:GLU:OE1	12:A0:125:GLU:N	2.53	0.41
28:AL:100:LYS:O	28:AL:104:LEU:HG	2.20	0.41
31:AO:54:GLU:N	31:AO:55:PRO:CD	2.84	0.41
34:AR:145:ASP:OD2	34:AR:148:LEU:N	2.50	0.41
38:AV:63:ARG:O	38:AV:64:LYS:HG3	2.21	0.41
50:XK:135:GLU:HA	50:XK:138:LEU:CD2	2.51	0.41
54:XO:26:ILE:HA	54:XO:29:LEU:CD2	2.50	0.41
11:XA:3117:C:C2	11:XA:3118:U:C5	3.09	0.41
13:A1:291:GLU:O	13:A1:294:LYS:HG3	2.20	0.41
17:AA:842:C:H2'	17:AA:843:G:O4'	2.21	0.41
17:AA:1173:C:H2'	17:AA:1174:U:C6	2.55	0.41
17:AA:1485:G:H2'	17:AA:1486:C:O4'	2.20	0.41
31:AO:148:LYS:O	31:AO:152:GLN:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:AQ:24:ARG:O	33:AQ:27:ASN:OD1	2.39	0.41
48:XI:112:MET:O	48:XI:116:LEU:HD23	2.21	0.41
51:XL:99:ARG:NH1	56:XQ:161:GLU:OE2	2.54	0.41
56:XQ:79:GLU:OE2	56:XQ:167:TYR:OH	2.30	0.41
6:5:120:ALA:HB3	6:5:314:ILE:HD11	2.03	0.41
7:6:189:CYS:O	55:XP:138:ALA:HA	2.21	0.41
8:7:147:ALA:O	8:7:150:MET:HG2	2.21	0.41
8:7:217:GLU:HG2	8:7:256:ARG:HB3	2.02	0.41
8:7:225:VAL:O	8:7:229:ILE:HG12	2.21	0.41
11:XA:1882:A:N6	11:XA:1893:A:O4'	2.54	0.41
11:XA:2151:A:H2'	11:XA:2152:A:C8	2.56	0.41
11:XA:2417:C:H5''	11:XA:2418:A:OP1	2.21	0.41
11:XA:2476:C:N3	11:XA:3069:A:H5'	2.35	0.41
12:A0:201:TRP:CD2	17:AA:844:A:C2	3.09	0.41
13:A1:295:SER:O	13:A1:299:LEU:HD23	2.21	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
18:AB:60:ASP:OD2	18:AB:64:ASN:ND2	2.54	0.41
37:AU:123:ARG:O	37:AU:127:GLU:OE1	2.38	0.41
38:AV:141:ASN:OD1	38:AV:142:PHE:N	2.54	0.41
40:AX:350:PRO:O	40:AX:354:GLU:OE1	2.39	0.41
52:XM:182:ARG:O	52:XM:186:ILE:HD12	2.21	0.41
52:XM:209:GLU:N	52:XM:209:GLU:OE1	2.53	0.41
55:XP:113:LYS:HG3	55:XP:114:HIS:N	2.36	0.41
56:XQ:153:ASN:OD1	56:XQ:154:VAL:N	2.54	0.41
63:XX:226:LEU:HA	63:XX:229:ILE:HG12	2.02	0.41
5:4:99:LYS:NZ	11:XA:3013:G:O2'	2.49	0.41
6:5:155:LEU:HA	6:5:158:ILE:HG22	2.02	0.41
7:6:107:LYS:HA	7:6:110:ILE:HG22	2.03	0.41
9:8:128:GLU:O	9:8:131:MET:HG3	2.21	0.41
11:XA:2401:A:OP1	44:XD:262:ARG:NH1	2.54	0.41
11:XA:3013:G:O6	11:XA:3025:A:C6	2.74	0.41
11:XA:3025:A:C2	11:XA:3026:U:C5	3.09	0.41
19:AC:58:ALA:HB1	19:AC:59:PRO:HD2	2.02	0.41
35:AS:114:GLU:HG2	35:AS:115:GLU:N	2.36	0.41
40:AX:374:GLU:HG2	40:AX:375:GLU:N	2.35	0.41
45:XE:248:ILE:HG13	45:XE:250:ARG:HG2	2.03	0.41
11:XA:3169:C:H2'	11:XA:3170:C:C6	2.56	0.40
17:AA:917:C:OP2	31:AO:91:ARG:NH2	2.55	0.40
19:AC:86:THR:O	19:AC:89:ASP:OD1	2.39	0.40
19:AC:89:ASP:OD1	19:AC:89:ASP:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AD:96:ASP:OD1	20:AD:96:ASP:N	2.54	0.40
25:AI:69:GLU:HA	25:AI:70:GLU:HA	1.91	0.40
9:8:116:LEU:O	9:8:119:LYS:HG3	2.22	0.40
11:XA:1858:G:H2'	11:XA:1859:A:O4'	2.21	0.40
11:XA:1977:U:H2'	11:XA:1978:A:H8	1.86	0.40
11:XA:2558:A:C4'	11:XA:2559:U:OP2	2.68	0.40
11:XA:3149:C:N4	11:XA:3161:G:N7	2.69	0.40
11:XA:3189:C:C2'	11:XA:3190:A:OP2	2.70	0.40
13:A1:104:GLU:HA	13:A1:107:LYS:HG2	2.02	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:N	2.54	0.40
17:AA:1326:A:N3	20:AD:108:ALA:HB3	2.36	0.40
23:AG:376:VAL:HG12	23:AG:377:ARG:N	2.36	0.40
24:AH:178:GLU:OE1	24:AH:178:GLU:N	2.54	0.40
37:AU:100:ALA:O	37:AU:104:GLU:OE1	2.38	0.40
65:XZ:110:LEU:HA	65:XZ:113:VAL:HG22	2.04	0.40
13:A1:189:LYS:O	13:A1:193:LEU:HD23	2.21	0.40
14:A2:48:GLU:O	14:A2:51:VAL:HG12	2.22	0.40
15:A3:156:LYS:O	15:A3:159:GLU:HG3	2.21	0.40
15:A3:184:GLU:HG3	15:A3:185:ALA:H	1.87	0.40
21:AE:20:ALA:O	21:AE:23:LYS:HG2	2.21	0.40
49:XJ:107:GLU:OE1	49:XJ:109:ALA:N	2.51	0.40
50:XK:73:GLU:OE1	50:XK:73:GLU:N	2.54	0.40
11:XA:1764:C:H3'	11:XA:1765:C:C5'	2.52	0.40
11:XA:2292:G:N1	57:XR:10:LEU:N	2.69	0.40
11:XA:2372:U:O2	11:XA:2372:U:O4'	2.39	0.40
14:A2:95:GLU:HA	14:A2:95:GLU:OE2	2.22	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:674:U:O4'	17:AA:826:A:H2	2.04	0.40
21:AE:15:ARG:HA	21:AE:18:THR:OG1	2.22	0.40
24:AH:170:MET:SD	24:AH:172:VAL:HG13	2.62	0.40
36:AT:150:PRO:HA	36:AT:153:VAL:O	2.21	0.40
51:XL:36:THR:O	51:XL:56:ARG:HA	2.21	0.40
64:XY:198:ARG:HG3	64:XY:200:PHE:CE1	2.56	0.40
6:5:378:SER:OG	6:5:379:ASP:N	2.55	0.40
8:7:276:PHE:H	8:7:303:PRO:HA	1.85	0.40
11:XA:1937:A:H2'	11:XA:1938:A:O4'	2.22	0.40
11:XA:2245:A:H1'	11:XA:2246:A:C8	2.56	0.40
11:XA:2877:C:H2'	11:XA:2878:G:O4'	2.22	0.40
11:XA:3009:C:O2	11:XA:3009:C:O5'	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A3:187:GLU:O	28:AL:212:ARG:NH2	2.42	0.40
17:AA:1230:C:N4	17:AA:1447:G:C4	2.90	0.40
17:AA:1262:C:C2	17:AA:1334:G:N2	2.90	0.40
17:AA:1592:U:O2'	17:AA:1593:U:H5'	2.21	0.40
28:AL:137:ARG:HA	28:AL:140:GLU:CD	2.42	0.40
34:AR:72:ASP:N	34:AR:72:ASP:OD1	2.55	0.40
34:AR:208:ILE:O	34:AR:214:ASN:ND2	2.53	0.40
38:AV:338:HIS:ND1	38:AV:342:GLN:OE1	2.54	0.40
41:AY:339:GLU:N	41:AY:339:GLU:OE1	2.54	0.40
45:XE:213:LYS:O	54:XO:9:ILE:HG21	2.22	0.40
46:XF:52:GLU:N	46:XF:52:GLU:OE1	2.55	0.40
46:XF:141:ILE:O	46:XF:142:ARG:HB2	2.21	0.40
52:XM:252:LEU:H	52:XM:252:LEU:HD23	1.87	0.40
54:XO:94:ALA:HB3	54:XO:95:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	102 (96%)	4 (4%)	0	100	100
2	1	51/65 (78%)	50 (98%)	1 (2%)	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
6	5	391/423 (92%)	366 (94%)	25 (6%)	0	100	100
7	6	350/380 (92%)	327 (93%)	23 (7%)	0	100	100
8	7	285/338 (84%)	266 (93%)	19 (7%)	0	100	100
9	8	137/206 (66%)	133 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	9	122/137 (89%)	117 (96%)	5 (4%)	0	100	100
12	A0	197/218 (90%)	186 (94%)	11 (6%)	0	100	100
13	A1	273/323 (84%)	258 (94%)	15 (6%)	0	100	100
14	A2	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
15	A3	67/199 (34%)	66 (98%)	1 (2%)	0	100	100
16	A4	526/689 (76%)	493 (94%)	33 (6%)	0	100	100
18	AB	216/296 (73%)	209 (97%)	7 (3%)	0	100	100
19	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
20	AD	341/430 (79%)	325 (95%)	16 (5%)	0	100	100
21	AE	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
22	AF	197/242 (81%)	194 (98%)	3 (2%)	0	100	100
23	AG	300/396 (76%)	289 (96%)	11 (4%)	0	100	100
24	AH	133/201 (66%)	123 (92%)	10 (8%)	0	100	100
25	AI	134/194 (69%)	128 (96%)	6 (4%)	0	100	100
26	AJ	106/138 (77%)	99 (93%)	7 (7%)	0	100	100
27	AK	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
28	AL	162/257 (63%)	159 (98%)	3 (2%)	0	100	100
29	AM	114/137 (83%)	111 (97%)	3 (3%)	0	100	100
30	AN	105/130 (81%)	101 (96%)	4 (4%)	0	100	100
31	AO	183/258 (71%)	178 (97%)	5 (3%)	0	100	100
32	AP	93/142 (66%)	87 (94%)	6 (6%)	0	100	100
33	AQ	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
34	AR	248/360 (69%)	237 (96%)	11 (4%)	0	100	100
35	AS	131/190 (69%)	124 (95%)	7 (5%)	0	100	100
36	AT	160/173 (92%)	149 (93%)	11 (7%)	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%)	92 (97%)	3 (3%)	0	100	100
40	AX	346/398 (87%)	327 (94%)	19 (6%)	0	100	100
41	AY	111/395 (28%)	103 (93%)	8 (7%)	0	100	100
42	AZ	84/106 (79%)	82 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	XD	234/305 (77%)	222 (95%)	10 (4%)	2 (1%)	17	54
45	XE	302/348 (87%)	286 (95%)	16 (5%)	0	100	100
46	XF	248/311 (80%)	241 (97%)	7 (3%)	0	100	100
47	XH	93/267 (35%)	90 (97%)	3 (3%)	0	100	100
48	XI	209/261 (80%)	193 (92%)	16 (8%)	0	100	100
49	XJ	168/192 (88%)	157 (94%)	11 (6%)	0	100	100
50	XK	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
51	XL	113/145 (78%)	107 (95%)	6 (5%)	0	100	100
52	XM	285/296 (96%)	276 (97%)	9 (3%)	0	100	100
53	XN	219/251 (87%)	210 (96%)	9 (4%)	0	100	100
54	XO	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
55	XP	141/180 (78%)	133 (94%)	8 (6%)	0	100	100
56	XQ	236/292 (81%)	225 (95%)	11 (5%)	0	100	100
57	XR	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
58	XS	158/205 (77%)	152 (96%)	6 (4%)	0	100	100
59	XT	164/206 (80%)	159 (97%)	5 (3%)	0	100	100
60	XU	137/153 (90%)	132 (96%)	5 (4%)	0	100	100
61	XV	200/216 (93%)	192 (96%)	8 (4%)	0	100	100
62	XW	109/148 (74%)	103 (94%)	6 (6%)	0	100	100
63	XX	241/256 (94%)	234 (97%)	7 (3%)	0	100	100
64	XY	176/250 (70%)	171 (97%)	5 (3%)	0	100	100
65	XZ	118/161 (73%)	115 (98%)	3 (2%)	0	100	100
66	a	93/142 (66%)	84 (90%)	9 (10%)	0	100	100
67	b	146/215 (68%)	134 (92%)	12 (8%)	0	100	100
68	c	271/332 (82%)	260 (96%)	11 (4%)	0	100	100
69	d	212/306 (69%)	200 (94%)	11 (5%)	1 (0%)	29	66
70	e	211/279 (76%)	204 (97%)	7 (3%)	0	100	100
71	f	139/212 (66%)	133 (96%)	6 (4%)	0	100	100
72	g	130/166 (78%)	123 (95%)	7 (5%)	0	100	100
73	h	106/158 (67%)	100 (94%)	6 (6%)	0	100	100
74	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	j	84/123 (68%)	83 (99%)	1 (1%)	0	100	100
76	k	93/112 (83%)	86 (92%)	7 (8%)	0	100	100
77	l	78/138 (56%)	70 (90%)	8 (10%)	0	100	100
78	m	58/128 (45%)	54 (93%)	4 (7%)	0	100	100
79	o	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
80	p	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
81	q	162/222 (73%)	160 (99%)	2 (1%)	0	100	100
82	r	144/196 (74%)	140 (97%)	4 (3%)	0	100	100
86	s	366/439 (83%)	348 (95%)	18 (5%)	0	100	100
87	t1	45/198 (23%)	42 (93%)	3 (7%)	0	100	100
87	t2	28/198 (14%)	28 (100%)	0	0	100	100
87	t3	28/198 (14%)	28 (100%)	0	0	100	100
87	t4	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
87	t5	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
87	t6	25/198 (13%)	25 (100%)	0	0	100	100
All	All	13788/19160 (72%)	13164 (96%)	621 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	XD	207	ILE
44	XD	208	ARG
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	351 (99%)	2 (1%)	86	93
7	6	313/332 (94%)	311 (99%)	2 (1%)	86	93
8	7	267/303 (88%)	267 (100%)	0	100	100
9	8	128/190 (67%)	127 (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	93
13	A1	253/291 (87%)	251 (99%)	2 (1%)	81	89
14	A2	99/101 (98%)	97 (98%)	2 (2%)	55	74
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%)	152 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	304 (99%)	3 (1%)	76	86
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%)	190 (100%)	0	100	100
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%)	154 (99%)	1 (1%)	86	93
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%)	125 (100%)	0	100	100
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%)	145 (99%)	1 (1%)	84	91
60	XU	126/135 (93%)	126 (100%)	0	100	100
61	XV	179/191 (94%)	179 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	188 (100%)	0	100	100
71	f	128/188 (68%)	128 (100%)	0	100	100
72	g	122/148 (82%)	122 (100%)	0	100	100
73	h	103/148 (70%)	102 (99%)	1 (1%)	76	86
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%)	140 (99%)	1 (1%)	84	91
82	r	138/169 (82%)	138 (100%)	0	100	100
86	s	326/381 (86%)	326 (100%)	0	100	100
87	t1	41/158 (26%)	40 (98%)	1 (2%)	49	71
87	t2	29/158 (18%)	29 (100%)	0	100	100
87	t3	29/158 (18%)	29 (100%)	0	100	100
87	t4	28/158 (18%)	28 (100%)	0	100	100
87	t5	28/158 (18%)	28 (100%)	0	100	100
87	t6	26/158 (16%)	26 (100%)	0	100	100
All	All	12397/16507 (75%)	12366 (100%)	31 (0%)	92	96

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	5	310	ARG
6	5	395	ARG
7	6	52	ARG
7	6	99	ARG
9	8	119	LYS
12	A0	113	LYS
13	A1	167	ARG

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Mol	Chain	Res	Type
13	A1	294	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	393	LYS
34	AR	99	LYS
37	AU	114	ARG
38	AV	64	LYS
40	AX	163	LYS
40	AX	232	ARG
40	AX	275	LYS
49	XJ	154	ARG
50	XK	150	LYS
52	XM	44	ARG
59	XT	163	ARG
62	XW	119	ARG
68	c	302	ARG
73	h	75	LYS
81	q	140	ARG
87	t1	21[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
14	A2	59	ASN
14	A2	90	GLN
16	A4	72	GLN
16	A4	242	ASN
16	A4	566	GLN
16	A4	590	GLN
16	A4	656	ASN
18	AB	239	ASN
27	AK	60	ASN
31	AO	160	HIS
33	AQ	79	ASN
34	AR	139	ASN
35	AS	91	ASN
38	AV	342	GLN

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Mol	Chain	Res	Type
40	AX	110	HIS
40	AX	347	ASN
40	AX	394	HIS
46	XF	241	ASN
48	XI	235	GLN
49	XJ	47	ASN
55	XP	96	GLN
67	b	90	HIS
72	g	93	ASN
75	j	107	ASN
76	k	15	GLN
77	l	135	ASN
86	s	343	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	XA	1490/1559 (95%)	268 (17%)	7 (0%)
17	AA	916/954 (96%)	160 (17%)	3 (0%)
43	XB	54/72 (75%)	10 (18%)	0
83	r1	0/12	-	-
84	r3	0/75	-	-
85	r4	0/76	-	-
All	All	2460/2748 (89%)	438 (17%)	10 (0%)

All (438) 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

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Mol	Chain	Res	Type
11	XA	1711	C
11	XA	1712	A
11	XA	1715	C
11	XA	1724	A
11	XA	1727	A
11	XA	1733	C
11	XA	1734	C
11	XA	1736	A
11	XA	1737	A
11	XA	1741	A
11	XA	1748	G
11	XA	1762	A
11	XA	1763	A
11	XA	1764	C
11	XA	1765	C
11	XA	1770	G
11	XA	1777	A
11	XA	1799	U
11	XA	1804	A
11	XA	1805	A
11	XA	1809	U
11	XA	1810	A
11	XA	1811	A
11	XA	1821	A
11	XA	1823	A
11	XA	1827	C
11	XA	1828	A
11	XA	1829	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

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Mol	Chain	Res	Type
11	XA	1903	C
11	XA	1909	A
11	XA	1918	G
11	XA	1919	C
11	XA	1937	A
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	1992	C
11	XA	1993	A
11	XA	1994	A
11	XA	2001	C
11	XA	2002	G
11	XA	2003	A
11	XA	2010	U
11	XA	2015	G
11	XA	2022	G
11	XA	2030	U
11	XA	2036	C
11	XA	2037	U
11	XA	2039	A
11	XA	2055	U
11	XA	2060	A
11	XA	2067	C
11	XA	2079	C
11	XA	2099	U
11	XA	2111	C
11	XA	2113	G
11	XA	2125	C
11	XA	2126	U
11	XA	2134	A
11	XA	2135	A
11	XA	2147	G
11	XA	2159	U
11	XA	2168	U
11	XA	2169	A
11	XA	2176	C
11	XA	2177	U

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Mol	Chain	Res	Type
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	2236	C
11	XA	2237	A
11	XA	2241	A
11	XA	2243	A
11	XA	2244	U
11	XA	2245	A
11	XA	2251	A
11	XA	2260	A
11	XA	2262	C
11	XA	2263	C
11	XA	2283	C
11	XA	2284	C
11	XA	2285	U
11	XA	2297	A
11	XA	2299	U
11	XA	2300	G
11	XA	2316	U
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	2379	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

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Mol	Chain	Res	Type
11	XA	2446	A
11	XA	2451	A
11	XA	2458	A
11	XA	2478	G
11	XA	2485	U
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	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	2601	A
11	XA	2602	U
11	XA	2603	C
11	XA	2618	U
11	XA	2626	U
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

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Mol	Chain	Res	Type
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	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
11	XA	2913	A
11	XA	2916	G
11	XA	2917	G
11	XA	2918	A
11	XA	2919	A
11	XA	2921	A
11	XA	2928	C
11	XA	2935	A
11	XA	2939	C
11	XA	2946	A
11	XA	2952	U
11	XA	2956	A
11	XA	2962	C
11	XA	2963	A
11	XA	2989	G
11	XA	2990	A

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Mol	Chain	Res	Type
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	3060	C
11	XA	3065	U
11	XA	3067	U
11	XA	3069	A
11	XA	3073	C
11	XA	3089	A
11	XA	3090	G
11	XA	3096	U
11	XA	3100	U
11	XA	3122	U
11	XA	3124	U
11	XA	3129	A
11	XA	3150	U
11	XA	3151	A
11	XA	3154	U
11	XA	3157	C
11	XA	3158	A
11	XA	3160	A
11	XA	3162	C
11	XA	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	3208	C
11	XA	3209	A
11	XA	3210	C
11	XA	3212	C
11	XA	3217	A

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Mol	Chain	Res	Type
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	829	C
17	AA	830	U
17	AA	832	U
17	AA	835	C
17	AA	836	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

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Mol	Chain	Res	Type
17	AA	899	G
17	AA	903	U
17	AA	905	A
17	AA	917	C
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	949	U
17	AA	950	A
17	AA	967	A
17	AA	975	A
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	1046	A
17	AA	1049	A
17	AA	1062	G
17	AA	1069	A
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	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	1187	U
17	AA	1188	A

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Mol	Chain	Res	Type
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	1251	A
17	AA	1261	C
17	AA	1268	C
17	AA	1271	C
17	AA	1284	U
17	AA	1290	C
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

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Mol	Chain	Res	Type
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	1422	G
17	AA	1424	U
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	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
17	AA	1540	A
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	1591	C
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

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Mol	Chain	Res	Type
43	XB	1620	A
43	XB	1621	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 ⓘ

163 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	$\# Z > 2$
84	Y5P	r3	32	84	14,19,20	3.12	3 (21%)	18,26,29	0.56	0
85	P5P	r4	35	85	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r3	51	84	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r4	40	85	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
84	Y5P	r3	69	84	14,19,20	3.13	3 (21%)	18,26,29	0.61	0
85	P5P	r4	28	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r4	60	85	14,19,20	3.13	3 (21%)	18,26,29	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	Y5P	r3	20	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
85	Y5P	r4	4	85	14,19,20	3.12	3 (21%)	18,26,29	0.63	0
85	Y5P	r4	59	85	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
85	P5P	r4	14	85	16,23,24	0.95	1 (6%)	14,33,36	1.96	3 (21%)
85	Y5P	r4	16	85	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
84	P5P	r3	30	84	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
85	P5P	r4	10	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
85	P5P	r4	65	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r3	70	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
85	P5P	r4	24	85	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r4	72	85	14,19,20	3.12	3 (21%)	18,26,29	0.58	0
84	P5P	r3	42	84	16,23,24	0.96	1 (6%)	14,33,36	2.01	3 (21%)
83	Y5P	r1	54	83	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
84	P5P	r3	4	84	16,23,24	0.97	1 (6%)	14,33,36	2.01	3 (21%)
85	P5P	r4	7	85	16,23,24	0.97	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r1	51	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
85	P5P	r4	69	85	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r1	50	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
84	P5P	r3	22	84	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
85	Y5P	r4	17	85	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
85	Y5P	r4	2	85	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
84	P5P	r3	35	84	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
84	Y5P	r3	54	84	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
84	P5P	r3	52	84	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r3	29	84	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
85	P5P	r4	53	85	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r4	46	85	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r4	32	85	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
85	P5P	r4	19	85	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r4	42	85	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
84	Y5P	r3	7	84	14,19,20	3.12	3 (21%)	18,26,29	0.61	0
83	Y5P	r1	49	83	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
85	Y5P	r4	47	85	14,19,20	3.16	3 (21%)	18,26,29	0.64	0
85	Y5P	r4	39	85	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
84	P5P	r3	8	84	16,23,24	0.96	1 (6%)	14,33,36	2.02	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	Y5P	r3	13	84	14,19,20	3.13	3 (21%)	18,26,29	0.62	0
85	P5P	r4	36	85	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
85	P5P	r4	22	85	16,23,24	0.94	1 (6%)	14,33,36	2.02	3 (21%)
83	Y5P	r1	56	83	14,19,20	3.14	3 (21%)	18,26,29	0.62	0
83	Y5P	r1	57	83	14,19,20	3.15	3 (21%)	18,26,29	0.59	0
84	P5P	r3	46	84	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
84	Y5P	r3	72	84	14,19,20	3.09	3 (21%)	18,26,29	0.61	0
85	P5P	r4	29	85	16,23,24	0.95	1 (6%)	14,33,36	2.02	3 (21%)
85	Y5P	r4	11	85	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
85	Y5P	r4	43	85	14,19,20	3.14	3 (21%)	18,26,29	0.60	0
84	Y5P	r3	2	84	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	Y5P	r4	13	85	14,19,20	3.15	3 (21%)	18,26,29	0.54	0
85	Y5P	r4	50	85	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
84	P5P	r3	68	84	16,23,24	0.94	1 (6%)	14,33,36	2.02	3 (21%)
84	Y5P	r3	39	84	14,19,20	3.12	3 (21%)	18,26,29	0.56	0
84	P5P	r3	18	84	16,23,24	0.97	1 (6%)	14,33,36	1.98	3 (21%)
84	Y5P	r3	27	84	14,19,20	3.12	3 (21%)	18,26,29	0.55	0
85	P5P	r4	27	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r3	26	84	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r4	12	85	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
84	P5P	r3	44	84	16,23,24	0.96	1 (6%)	14,33,36	1.96	3 (21%)
84	P5P	r3	19	84	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
85	Y5P	r4	74	85	14,19,20	3.15	3 (21%)	18,26,29	0.58	0
84	P5P	r3	43	84	16,23,24	0.94	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r4	56	85	14,19,20	3.14	3 (21%)	18,26,29	0.60	0
84	Y5P	r3	61	84	14,19,20	3.12	3 (21%)	18,26,29	0.58	0
85	P5P	r4	31	85	16,23,24	0.93	1 (6%)	14,33,36	2.03	3 (21%)
85	Y5P	r4	49	85	14,19,20	3.15	3 (21%)	18,26,29	0.58	0
85	Y5P	r4	48	85	14,19,20	3.14	3 (21%)	18,26,29	0.60	0
85	P5P	r4	64	85	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r3	23	84	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
85	P5P	r4	70	85	16,23,24	0.94	1 (6%)	14,33,36	1.97	3 (21%)
84	Y5P	r3	25	84	14,19,20	3.10	3 (21%)	18,26,29	0.60	0
84	Y5P	r3	41	84	14,19,20	3.12	3 (21%)	18,26,29	0.64	0
84	Y5P	r3	63	84	14,19,20	3.13	3 (21%)	18,26,29	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	P5P	r4	9	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	P5P	r4	63	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r3	47	84	14,19,20	3.12	3 (21%)	18,26,29	0.59	0
84	P5P	r3	11	84	16,23,24	0.95	1 (6%)	14,33,36	1.96	3 (21%)
84	Y5P	r3	73	84	14,19,20	3.08	3 (21%)	18,26,29	0.54	0
85	Y5P	r4	66	85	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
83	Y5P	r1	53	83	14,19,20	3.10	3 (21%)	18,26,29	0.66	0
84	P5P	r3	48	84	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r4	3	85	14,19,20	3.12	3 (21%)	18,26,29	0.54	0
84	P5P	r3	17(A)	84	16,23,24	0.95	1 (6%)	14,33,36	2.05	3 (21%)
84	Y5P	r3	36	84	14,19,20	3.11	3 (21%)	18,26,29	0.65	0
85	P5P	r4	37	85	20,24,24	0.88	1 (5%)	21,36,36	4.64	9 (42%)
84	Y5P	r3	53	84	14,19,20	3.13	3 (21%)	18,26,29	0.61	0
85	P5P	r4	26	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
83	Y5P	r1	47	83	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
85	P5P	r4	44	85	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r4	5	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r3	16	84	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
85	P5P	r4	34	85,17	16,23,24	0.97	1 (6%)	14,33,36	1.98	3 (21%)
84	P5P	r3	57	84	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
84	P5P	r3	6	84	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r4	54	85	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
85	Y5P	r4	68	85	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
85	P5P	r4	15	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r4	75	85	14,19,20	3.13	3 (21%)	18,26,29	0.71	0
84	Y5P	r3	58	84	14,19,20	3.12	3 (21%)	18,26,29	0.63	0
85	P5P	r4	30	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r4	8	85	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
84	P5P	r3	45	84	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
84	Y5P	r3	62	84	14,19,20	3.12	3 (21%)	18,26,29	0.62	0
85	P5P	r4	6	85	16,23,24	0.95	1 (6%)	14,33,36	2.02	3 (21%)
85	P5P	r4	52	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r3	33	84	14,19,20	3.12	3 (21%)	18,26,29	0.60	0
85	P5P	r4	21	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
84	P5P	r3	5	84	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	Y5P	r4	67	85	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
84	Y5P	r3	1	84	18,20,20	2.76	3 (16%)	25,29,29	0.69	0
84	P5P	r3	37	84	16,23,24	0.94	1 (6%)	14,33,36	1.97	3 (21%)
84	Y5P	r3	49	84	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
85	P5P	r4	71	85	16,23,24	0.94	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r1	46	83	14,19,20	3.13	3 (21%)	18,26,29	0.61	0
84	P5P	r3	10	84	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r4	61	85	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
84	P5P	r3	31	84	16,23,24	0.95	1 (6%)	14,33,36	2.03	3 (21%)
84	P5P	r3	9	84	16,23,24	0.96	1 (6%)	14,33,36	2.01	3 (21%)
84	P5P	r3	3	84	16,23,24	0.96	1 (6%)	14,33,36	2.03	3 (21%)
85	P5P	r4	73	85	16,23,24	0.98	1 (6%)	14,33,36	2.01	3 (21%)
85	Y5P	r4	25	85	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
85	P5P	r4	58	85	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
85	P5P	r4	18	85	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r4	41	85	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
84	P5P	r3	55	84	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r4	62	85	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
84	Y5P	r3	60	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
84	Y5P	r3	50	84	14,19,20	3.12	3 (21%)	18,26,29	0.61	0
84	Y5P	r3	59	84	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
84	Y5P	r3	40	84	14,19,20	3.10	3 (21%)	18,26,29	0.61	0
84	Y5P	r3	64	84	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
84	P5P	r3	14	84	16,23,24	0.93	1 (6%)	14,33,36	2.02	3 (21%)
85	Y5P	r4	55	85	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
85	P5P	r4	76	85,11	16,23,24	0.97	1 (6%)	14,33,36	2.09	3 (21%)
83	Y5P	r1	52	83	14,19,20	3.12	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	55	83	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
84	Y5P	r3	17	-	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
85	P5P	r4	1	85	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r3	21	84	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r4	20	85	14,19,20	3.15	3 (21%)	18,26,29	0.59	0
85	Y5P	r4	51	85	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	P5P	r4	57	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r4	33	85	14,19,20	3.13	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
84	P5P	r3	15	84	16,23,24	0.98	1 (6%)	14,33,36	1.93	3 (21%)
84	P5P	r3	66	84	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r4	23	85	16,23,24	0.96	1 (6%)	14,33,36	2.02	3 (21%)
84	Y5P	r3	34	84	14,19,20	3.12	3 (21%)	18,26,29	0.58	0
84	Y5P	r3	38	84	14,19,20	3.12	3 (21%)	18,26,29	0.56	0
85	P5P	r4	38	85	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
84	Y5P	r3	12	84	14,19,20	3.12	3 (21%)	18,26,29	0.59	0
84	Y5P	r3	28	84	14,19,20	3.12	3 (21%)	18,26,29	0.59	0
84	Y5P	r3	56	84	14,19,20	3.13	3 (21%)	18,26,29	0.63	0
84	P5P	r3	74	84	16,23,24	0.94	1 (6%)	14,33,36	1.94	3 (21%)
84	P5P	r3	71	84	16,23,24	0.94	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r4	45	85	14,19,20	3.13	3 (21%)	18,26,29	0.55	0
83	Y5P	r1	48	83	14,19,20	3.12	3 (21%)	18,26,29	0.57	0
84	Y5P	r3	67	84	14,19,20	3.11	3 (21%)	18,26,29	0.59	0
84	Y5P	r3	65	84	14,19,20	3.12	3 (21%)	18,26,29	0.61	0
84	Y5P	r3	24	84	14,19,20	3.11	3 (21%)	18,26,29	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	Y5P	r3	32	84	-	1/7/33/34	0/2/2/2
85	P5P	r4	35	85	-	0/3/25/26	0/3/3/3
84	P5P	r3	51	84	-	2/3/25/26	0/3/3/3
85	Y5P	r4	40	85	-	1/7/33/34	0/2/2/2
84	Y5P	r3	69	84	-	3/7/33/34	0/2/2/2
85	P5P	r4	28	85	-	2/3/25/26	0/3/3/3
85	Y5P	r4	60	85	-	1/7/33/34	0/2/2/2
84	Y5P	r3	20	84	-	1/7/33/34	0/2/2/2
85	Y5P	r4	4	85	-	1/7/33/34	0/2/2/2
85	Y5P	r4	59	85	-	2/7/33/34	0/2/2/2
85	P5P	r4	14	85	-	0/3/25/26	0/3/3/3
85	Y5P	r4	16	85	-	1/7/33/34	0/2/2/2
84	P5P	r3	30	84	-	0/3/25/26	0/3/3/3
85	P5P	r4	10	85	-	1/3/25/26	0/3/3/3
85	P5P	r4	65	85	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	Y5P	r3	70	84	-	1/7/33/34	0/2/2/2
85	P5P	r4	24	85	-	0/3/25/26	0/3/3/3
85	Y5P	r4	72	85	-	3/7/33/34	0/2/2/2
84	P5P	r3	42	84	-	0/3/25/26	0/3/3/3
83	Y5P	r1	54	83	-	1/7/33/34	0/2/2/2
84	P5P	r3	4	84	-	3/3/25/26	0/3/3/3
85	P5P	r4	7	85	-	2/3/25/26	0/3/3/3
83	Y5P	r1	51	83	-	1/7/33/34	0/2/2/2
85	P5P	r4	69	85	-	0/3/25/26	0/3/3/3
83	Y5P	r1	50	83	-	1/7/33/34	0/2/2/2
84	P5P	r3	22	84	-	0/3/25/26	0/3/3/3
85	Y5P	r4	17	85	-	3/7/33/34	0/2/2/2
85	Y5P	r4	2	85	-	1/7/33/34	0/2/2/2
84	P5P	r3	35	84	-	0/3/25/26	0/3/3/3
84	Y5P	r3	54	84	-	1/7/33/34	0/2/2/2
84	P5P	r3	52	84	-	0/3/25/26	0/3/3/3
84	P5P	r3	29	84	-	0/3/25/26	0/3/3/3
85	P5P	r4	53	85	-	0/3/25/26	0/3/3/3
85	P5P	r4	46	85	-	0/3/25/26	0/3/3/3
85	Y5P	r4	32	85	-	3/7/33/34	0/2/2/2
85	P5P	r4	19	85	-	0/3/25/26	0/3/3/3
85	Y5P	r4	42	85	-	1/7/33/34	0/2/2/2
84	Y5P	r3	7	84	-	3/7/33/34	0/2/2/2
83	Y5P	r1	49	83	-	2/7/33/34	0/2/2/2
85	Y5P	r4	47	85	-	4/7/33/34	0/2/2/2
85	Y5P	r4	39	85	-	1/7/33/34	0/2/2/2
84	P5P	r3	8	84	-	0/3/25/26	0/3/3/3
84	Y5P	r3	13	84	-	5/7/33/34	0/2/2/2
85	P5P	r4	36	85	-	0/3/25/26	0/3/3/3
85	P5P	r4	22	85	-	3/3/25/26	0/3/3/3
83	Y5P	r1	56	83	-	4/7/33/34	0/2/2/2
83	Y5P	r1	57	83	-	2/7/33/34	0/2/2/2
84	P5P	r3	46	84	-	2/3/25/26	0/3/3/3
84	Y5P	r3	72	84	-	2/7/33/34	0/2/2/2
85	P5P	r4	29	85	-	2/3/25/26	0/3/3/3
85	Y5P	r4	11	85	-	1/7/33/34	0/2/2/2
85	Y5P	r4	43	85	-	1/7/33/34	0/2/2/2
84	Y5P	r3	2	84	-	2/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	Y5P	r4	13	85	-	3/7/33/34	0/2/2/2
85	Y5P	r4	50	85	-	2/7/33/34	0/2/2/2
84	P5P	r3	68	84	-	0/3/25/26	0/3/3/3
84	Y5P	r3	39	84	-	1/7/33/34	0/2/2/2
84	P5P	r3	18	84	-	3/3/25/26	0/3/3/3
84	Y5P	r3	27	84	-	1/7/33/34	0/2/2/2
85	P5P	r4	27	85	-	2/3/25/26	0/3/3/3
84	P5P	r3	26	84	-	0/3/25/26	0/3/3/3
85	Y5P	r4	12	85	-	1/7/33/34	0/2/2/2
84	P5P	r3	44	84	-	0/3/25/26	0/3/3/3
84	P5P	r3	19	84	-	2/3/25/26	0/3/3/3
85	Y5P	r4	74	85	-	6/7/33/34	0/2/2/2
84	P5P	r3	43	84	-	1/3/25/26	0/3/3/3
85	Y5P	r4	56	85	-	3/7/33/34	0/2/2/2
84	Y5P	r3	61	84	-	3/7/33/34	0/2/2/2
85	P5P	r4	31	85	-	1/3/25/26	0/3/3/3
85	Y5P	r4	49	85	-	3/7/33/34	0/2/2/2
85	Y5P	r4	48	85	-	3/7/33/34	0/2/2/2
85	P5P	r4	64	85	-	2/3/25/26	0/3/3/3
84	P5P	r3	23	84	-	0/3/25/26	0/3/3/3
85	P5P	r4	70	85	-	0/3/25/26	0/3/3/3
84	Y5P	r3	25	84	-	1/7/33/34	0/2/2/2
84	Y5P	r3	41	84	-	1/7/33/34	0/2/2/2
84	Y5P	r3	63	84	-	3/7/33/34	0/2/2/2
85	P5P	r4	9	85	-	2/3/25/26	0/3/3/3
85	P5P	r4	63	85	-	0/3/25/26	0/3/3/3
84	Y5P	r3	47	84	-	2/7/33/34	0/2/2/2
84	P5P	r3	11	84	-	0/3/25/26	0/3/3/3
84	Y5P	r3	73	84	-	1/7/33/34	0/2/2/2
85	Y5P	r4	66	85	-	3/7/33/34	0/2/2/2
83	Y5P	r1	53	83	-	6/7/33/34	0/2/2/2
84	P5P	r3	48	84	-	0/3/25/26	0/3/3/3
85	Y5P	r4	3	85	-	1/7/33/34	0/2/2/2
84	P5P	r3	17(A)	84	-	3/3/25/26	0/3/3/3
84	Y5P	r3	36	84	-	1/7/33/34	0/2/2/2
85	P5P	r4	37	85	-	2/6/26/26	0/3/3/3
84	Y5P	r3	53	84	-	3/7/33/34	0/2/2/2
85	P5P	r4	26	85	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	Y5P	r1	47	83	-	3/7/33/34	0/2/2/2
85	P5P	r4	44	85	-	0/3/25/26	0/3/3/3
85	P5P	r4	5	85	-	0/3/25/26	0/3/3/3
84	Y5P	r3	16	84	-	2/7/33/34	0/2/2/2
85	P5P	r4	34	85,17	-	2/3/25/26	0/3/3/3
84	P5P	r3	57	84	-	1/3/25/26	0/3/3/3
84	P5P	r3	6	84	-	0/3/25/26	0/3/3/3
85	Y5P	r4	54	85	-	1/7/33/34	0/2/2/2
85	Y5P	r4	68	85	-	1/7/33/34	0/2/2/2
85	P5P	r4	15	85	-	0/3/25/26	0/3/3/3
85	Y5P	r4	75	85	-	5/7/33/34	0/2/2/2
84	Y5P	r3	58	84	-	2/7/33/34	0/2/2/2
85	P5P	r4	30	85	-	1/3/25/26	0/3/3/3
85	Y5P	r4	8	85	-	1/7/33/34	0/2/2/2
84	P5P	r3	45	84	-	0/3/25/26	0/3/3/3
84	Y5P	r3	62	84	-	2/7/33/34	0/2/2/2
85	P5P	r4	6	85	-	2/3/25/26	0/3/3/3
85	P5P	r4	52	85	-	2/3/25/26	0/3/3/3
84	Y5P	r3	33	84	-	1/7/33/34	0/2/2/2
85	P5P	r4	21	85	-	1/3/25/26	0/3/3/3
84	P5P	r3	5	84	-	2/3/25/26	0/3/3/3
85	Y5P	r4	67	85	-	2/7/33/34	0/2/2/2
84	Y5P	r3	1	84	-	6/10/34/34	0/2/2/2
84	P5P	r3	37	84	-	0/3/25/26	0/3/3/3
84	Y5P	r3	49	84	-	2/7/33/34	0/2/2/2
85	P5P	r4	71	85	-	0/3/25/26	0/3/3/3
83	Y5P	r1	46	83	-	4/7/33/34	0/2/2/2
84	P5P	r3	10	84	-	0/3/25/26	0/3/3/3
85	Y5P	r4	61	85	-	2/7/33/34	0/2/2/2
84	P5P	r3	31	84	-	0/3/25/26	0/3/3/3
84	P5P	r3	9	84	-	0/3/25/26	0/3/3/3
84	P5P	r3	3	84	-	3/3/25/26	0/3/3/3
85	P5P	r4	73	85	-	3/3/25/26	0/3/3/3
85	Y5P	r4	25	85	-	3/7/33/34	0/2/2/2
85	P5P	r4	58	85	-	0/3/25/26	0/3/3/3
85	P5P	r4	18	85	-	2/3/25/26	0/3/3/3
85	Y5P	r4	41	85	-	4/7/33/34	0/2/2/2
84	P5P	r3	55	84	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	Y5P	r4	62	85	-	1/7/33/34	0/2/2/2
84	Y5P	r3	60	84	-	1/7/33/34	0/2/2/2
84	Y5P	r3	50	84	-	4/7/33/34	0/2/2/2
84	Y5P	r3	59	84	-	4/7/33/34	0/2/2/2
84	Y5P	r3	40	84	-	3/7/33/34	0/2/2/2
84	Y5P	r3	64	84	-	1/7/33/34	0/2/2/2
84	P5P	r3	14	84	-	1/3/25/26	0/3/3/3
85	Y5P	r4	55	85	-	1/7/33/34	0/2/2/2
85	P5P	r4	76	85,11	-	3/3/25/26	0/3/3/3
83	Y5P	r1	52	83	-	2/7/33/34	0/2/2/2
83	Y5P	r1	55	83	-	3/7/33/34	0/2/2/2
84	Y5P	r3	17	-	-	2/7/33/34	0/2/2/2
85	P5P	r4	1	85	-	2/3/25/26	0/3/3/3
84	P5P	r3	21	84	-	3/3/25/26	0/3/3/3
85	Y5P	r4	20	85	-	3/7/33/34	0/2/2/2
85	Y5P	r4	51	85	-	1/7/33/34	0/2/2/2
85	P5P	r4	57	85	-	0/3/25/26	0/3/3/3
85	Y5P	r4	33	85	-	2/7/33/34	0/2/2/2
84	P5P	r3	15	84	-	0/3/25/26	0/3/3/3
84	P5P	r3	66	84	-	0/3/25/26	0/3/3/3
85	P5P	r4	23	85	-	3/3/25/26	0/3/3/3
84	Y5P	r3	34	84	-	3/7/33/34	0/2/2/2
84	Y5P	r3	38	84	-	1/7/33/34	0/2/2/2
85	P5P	r4	38	85	-	2/3/25/26	0/3/3/3
84	Y5P	r3	12	84	-	1/7/33/34	0/2/2/2
84	Y5P	r3	28	84	-	1/7/33/34	0/2/2/2
84	Y5P	r3	56	84	-	4/7/33/34	0/2/2/2
84	P5P	r3	74	84	-	0/3/25/26	0/3/3/3
84	P5P	r3	71	84	-	0/3/25/26	0/3/3/3
85	Y5P	r4	45	85	-	4/7/33/34	0/2/2/2
83	Y5P	r1	48	83	-	1/7/33/34	0/2/2/2
84	Y5P	r3	67	84	-	1/7/33/34	0/2/2/2
84	Y5P	r3	65	84	-	3/7/33/34	0/2/2/2
84	Y5P	r3	24	84	-	1/7/33/34	0/2/2/2

All (339) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r4	47	Y5P	C6-C5	10.61	1.52	1.33
85	r4	61	Y5P	C6-C5	10.60	1.52	1.33
85	r4	49	Y5P	C6-C5	10.59	1.52	1.33
83	r1	57	Y5P	C6-C5	10.58	1.52	1.33
84	r3	16	Y5P	C6-C5	10.57	1.52	1.33
83	r1	47	Y5P	C6-C5	10.57	1.52	1.33
85	r4	68	Y5P	C6-C5	10.56	1.52	1.33
85	r4	75	Y5P	C6-C5	10.56	1.52	1.33
85	r4	42	Y5P	C6-C5	10.55	1.52	1.33
85	r4	13	Y5P	C6-C5	10.55	1.52	1.33
84	r3	59	Y5P	C6-C5	10.55	1.52	1.33
83	r1	49	Y5P	C6-C5	10.55	1.52	1.33
83	r1	54	Y5P	C6-C5	10.54	1.52	1.33
85	r4	17	Y5P	C6-C5	10.54	1.52	1.33
85	r4	67	Y5P	C6-C5	10.54	1.52	1.33
83	r1	51	Y5P	C6-C5	10.54	1.52	1.33
83	r1	55	Y5P	C6-C5	10.54	1.52	1.33
85	r4	55	Y5P	C6-C5	10.54	1.52	1.33
84	r3	17	Y5P	C6-C5	10.54	1.52	1.33
84	r3	33	Y5P	C6-C5	10.54	1.52	1.33
85	r4	54	Y5P	C6-C5	10.54	1.52	1.33
85	r4	41	Y5P	C6-C5	10.53	1.52	1.33
85	r4	66	Y5P	C6-C5	10.53	1.52	1.33
83	r1	48	Y5P	C6-C5	10.53	1.52	1.33
84	r3	38	Y5P	C6-C5	10.53	1.52	1.33
85	r4	74	Y5P	C6-C5	10.53	1.52	1.33
84	r3	2	Y5P	C6-C5	10.52	1.52	1.33
85	r4	43	Y5P	C6-C5	10.52	1.52	1.33
84	r3	70	Y5P	C6-C5	10.52	1.52	1.33
85	r4	20	Y5P	C6-C5	10.52	1.52	1.33
83	r1	50	Y5P	C6-C5	10.52	1.52	1.33
85	r4	11	Y5P	C6-C5	10.52	1.52	1.33
85	r4	48	Y5P	C6-C5	10.52	1.52	1.33
83	r1	56	Y5P	C6-C5	10.52	1.52	1.33
84	r3	27	Y5P	C6-C5	10.52	1.52	1.33
85	r4	33	Y5P	C6-C5	10.52	1.52	1.33
84	r3	39	Y5P	C6-C5	10.52	1.52	1.33
84	r3	69	Y5P	C6-C5	10.51	1.52	1.33
85	r4	62	Y5P	C6-C5	10.51	1.52	1.33
85	r4	2	Y5P	C6-C5	10.51	1.52	1.33
85	r4	8	Y5P	C6-C5	10.51	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r4	12	Y5P	C6-C5	10.51	1.52	1.33
84	r3	64	Y5P	C6-C5	10.51	1.52	1.33
85	r4	45	Y5P	C6-C5	10.51	1.52	1.33
84	r3	20	Y5P	C6-C5	10.51	1.52	1.33
85	r4	40	Y5P	C6-C5	10.51	1.52	1.33
84	r3	13	Y5P	C6-C5	10.51	1.52	1.33
84	r3	41	Y5P	C6-C5	10.51	1.52	1.33
85	r4	39	Y5P	C6-C5	10.51	1.52	1.33
85	r4	32	Y5P	C6-C5	10.51	1.52	1.33
85	r4	25	Y5P	C6-C5	10.50	1.52	1.33
85	r4	3	Y5P	C6-C5	10.50	1.52	1.33
83	r1	46	Y5P	C6-C5	10.50	1.52	1.33
84	r3	32	Y5P	C6-C5	10.50	1.52	1.33
84	r3	47	Y5P	C6-C5	10.50	1.52	1.33
84	r3	56	Y5P	C6-C5	10.50	1.52	1.33
85	r4	72	Y5P	C6-C5	10.50	1.52	1.33
84	r3	7	Y5P	C6-C5	10.49	1.52	1.33
85	r4	16	Y5P	C6-C5	10.49	1.52	1.33
84	r3	49	Y5P	C6-C5	10.49	1.52	1.33
84	r3	28	Y5P	C6-C5	10.49	1.52	1.33
84	r3	67	Y5P	C6-C5	10.49	1.52	1.33
85	r4	51	Y5P	C6-C5	10.49	1.52	1.33
84	r3	54	Y5P	C6-C5	10.49	1.52	1.33
84	r3	50	Y5P	C6-C5	10.48	1.52	1.33
85	r4	56	Y5P	C6-C5	10.48	1.52	1.33
85	r4	59	Y5P	C6-C5	10.48	1.52	1.33
85	r4	60	Y5P	C6-C5	10.48	1.52	1.33
84	r3	53	Y5P	C6-C5	10.48	1.52	1.33
84	r3	63	Y5P	C6-C5	10.48	1.52	1.33
84	r3	60	Y5P	C6-C5	10.47	1.52	1.33
84	r3	12	Y5P	C6-C5	10.47	1.52	1.33
84	r3	34	Y5P	C6-C5	10.47	1.52	1.33
83	r1	52	Y5P	C6-C5	10.46	1.52	1.33
84	r3	36	Y5P	C6-C5	10.46	1.52	1.33
84	r3	24	Y5P	C6-C5	10.46	1.52	1.33
84	r3	1	Y5P	C6-C5	10.46	1.52	1.33
84	r3	65	Y5P	C6-C5	10.46	1.52	1.33
85	r4	50	Y5P	C6-C5	10.46	1.52	1.33
84	r3	58	Y5P	C6-C5	10.46	1.52	1.33
84	r3	61	Y5P	C6-C5	10.45	1.52	1.33
85	r4	4	Y5P	C6-C5	10.44	1.52	1.33
84	r3	62	Y5P	C6-C5	10.44	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r3	40	Y5P	C6-C5	10.44	1.52	1.33
84	r3	73	Y5P	C6-C5	10.44	1.52	1.33
84	r3	72	Y5P	C6-C5	10.43	1.52	1.33
83	r1	53	Y5P	C6-C5	10.42	1.51	1.33
84	r3	25	Y5P	C6-C5	10.41	1.51	1.33
85	r4	56	Y5P	C2-N1	3.93	1.45	1.36
84	r3	53	Y5P	C2-N1	3.90	1.45	1.36
84	r3	65	Y5P	C2-N1	3.90	1.45	1.36
85	r4	20	Y5P	C2-N1	3.89	1.45	1.36
85	r4	12	Y5P	C2-N1	3.88	1.45	1.36
85	r4	16	Y5P	C2-N1	3.88	1.45	1.36
84	r3	49	Y5P	C2-N1	3.87	1.45	1.36
83	r1	56	Y5P	C2-N1	3.87	1.45	1.36
83	r1	53	Y5P	C2-N1	3.87	1.45	1.36
84	r3	17	Y5P	C2-N1	3.87	1.45	1.36
84	r3	13	Y5P	C2-N1	3.87	1.45	1.36
85	r4	40	Y5P	C2-N1	3.86	1.45	1.36
85	r4	50	Y5P	C2-N1	3.86	1.45	1.36
85	r4	62	Y5P	C2-N1	3.86	1.45	1.36
84	r3	54	Y5P	C2-N1	3.86	1.45	1.36
85	r4	60	Y5P	C2-N1	3.86	1.45	1.36
85	r4	67	Y5P	C2-N1	3.86	1.45	1.36
84	r3	63	Y5P	C2-N1	3.85	1.45	1.36
84	r3	62	Y5P	C2-N1	3.85	1.45	1.36
85	r4	43	Y5P	C2-N1	3.85	1.45	1.36
84	r3	1	Y5P	C2-N1	3.84	1.45	1.36
83	r1	57	Y5P	C2-N1	3.84	1.45	1.36
84	r3	56	Y5P	C2-N1	3.84	1.45	1.36
83	r1	46	Y5P	C2-N1	3.84	1.45	1.36
83	r1	54	Y5P	C2-N1	3.84	1.45	1.36
84	r3	50	Y5P	C2-N1	3.84	1.45	1.36
85	r4	8	Y5P	C2-N1	3.84	1.45	1.36
85	r4	54	Y5P	C2-N1	3.84	1.45	1.36
85	r4	47	Y5P	C2-N1	3.83	1.45	1.36
85	r4	11	Y5P	C2-N1	3.83	1.45	1.36
85	r4	66	Y5P	C2-N1	3.83	1.45	1.36
85	r4	48	Y5P	C2-N1	3.83	1.45	1.36
83	r1	50	Y5P	C2-N1	3.82	1.45	1.36
85	r4	45	Y5P	C2-N1	3.82	1.45	1.36
85	r4	59	Y5P	C2-N1	3.82	1.45	1.36
84	r3	70	Y5P	C2-N1	3.82	1.45	1.36
83	r1	55	Y5P	C2-N1	3.82	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r3	20	Y5P	C2-N1	3.82	1.45	1.36
85	r4	33	Y5P	C2-N1	3.82	1.45	1.36
85	r4	17	Y5P	C2-N1	3.82	1.45	1.36
84	r3	58	Y5P	C2-N1	3.82	1.45	1.36
83	r1	52	Y5P	C2-N1	3.82	1.45	1.36
84	r3	60	Y5P	C2-N1	3.81	1.45	1.36
84	r3	7	Y5P	C2-N1	3.81	1.45	1.36
85	r4	2	Y5P	C2-N1	3.81	1.45	1.36
83	r1	49	Y5P	C2-N1	3.81	1.45	1.36
84	r3	12	Y5P	C2-N1	3.81	1.45	1.36
84	r3	25	Y5P	C2-N1	3.81	1.45	1.36
84	r3	28	Y5P	C2-N1	3.81	1.45	1.36
85	r4	41	Y5P	C2-N1	3.81	1.45	1.36
85	r4	68	Y5P	C2-N1	3.80	1.45	1.36
85	r4	74	Y5P	C2-N1	3.80	1.45	1.36
84	r3	16	Y5P	C2-N1	3.80	1.45	1.36
84	r3	34	Y5P	C2-N1	3.80	1.45	1.36
85	r4	4	Y5P	C2-N1	3.80	1.45	1.36
85	r4	32	Y5P	C2-N1	3.80	1.45	1.36
85	r4	13	Y5P	C2-N1	3.80	1.45	1.36
85	r4	51	Y5P	C2-N1	3.79	1.45	1.36
85	r4	55	Y5P	C2-N1	3.79	1.45	1.36
83	r1	51	Y5P	C2-N1	3.79	1.45	1.36
84	r3	64	Y5P	C2-N1	3.79	1.45	1.36
84	r3	59	Y5P	C2-N1	3.78	1.45	1.36
84	r3	61	Y5P	C2-N1	3.78	1.45	1.36
85	r4	42	Y5P	C2-N1	3.77	1.45	1.36
85	r4	49	Y5P	C2-N1	3.77	1.45	1.36
85	r4	61	Y5P	C2-N1	3.77	1.45	1.36
85	r4	39	Y5P	C2-N1	3.77	1.45	1.36
84	r3	2	Y5P	C2-N1	3.77	1.45	1.36
85	r4	25	Y5P	C2-N1	3.77	1.45	1.36
85	r4	3	Y5P	C2-N1	3.76	1.45	1.36
84	r3	67	Y5P	C2-N1	3.76	1.45	1.36
84	r3	47	Y5P	C2-N1	3.76	1.45	1.36
84	r3	24	Y5P	C2-N1	3.76	1.45	1.36
84	r3	36	Y5P	C2-N1	3.76	1.45	1.36
84	r3	32	Y5P	C2-N1	3.75	1.45	1.36
84	r3	27	Y5P	C2-N1	3.75	1.45	1.36
83	r1	48	Y5P	C2-N1	3.75	1.45	1.36
84	r3	69	Y5P	C2-N1	3.75	1.45	1.36
84	r3	40	Y5P	C2-N1	3.74	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r3	38	Y5P	C2-N1	3.74	1.45	1.36
83	r1	47	Y5P	C2-N1	3.74	1.45	1.36
84	r3	72	Y5P	C2-N1	3.73	1.45	1.36
84	r3	33	Y5P	C2-N1	3.73	1.45	1.36
85	r4	72	Y5P	C2-N1	3.72	1.45	1.36
84	r3	41	Y5P	C2-N1	3.71	1.45	1.36
85	r4	75	Y5P	C2-N1	3.71	1.45	1.36
84	r3	39	Y5P	C2-N1	3.70	1.44	1.36
84	r3	73	Y5P	C2-N1	3.63	1.44	1.36
85	r4	32	Y5P	C6-N1	2.70	1.44	1.37
85	r4	50	Y5P	C6-N1	2.69	1.44	1.37
84	r3	60	Y5P	C6-N1	2.68	1.44	1.37
83	r1	52	Y5P	C6-N1	2.68	1.44	1.37
84	r3	17	Y5P	C6-N1	2.68	1.44	1.37
85	r4	66	Y5P	C6-N1	2.67	1.44	1.37
85	r4	55	Y5P	C6-N1	2.67	1.44	1.37
85	r4	41	Y5P	C6-N1	2.67	1.44	1.37
85	r4	61	Y5P	C6-N1	2.67	1.44	1.37
83	r1	51	Y5P	C6-N1	2.67	1.44	1.37
85	r4	16	Y5P	C6-N1	2.67	1.43	1.37
85	r4	62	Y5P	C6-N1	2.67	1.43	1.37
85	r4	40	Y5P	C6-N1	2.67	1.43	1.37
84	r3	62	Y5P	C6-N1	2.67	1.43	1.37
85	r4	47	Y5P	C6-N1	2.67	1.43	1.37
85	r4	17	Y5P	C6-N1	2.66	1.43	1.37
85	r4	2	Y5P	C6-N1	2.66	1.43	1.37
85	r4	51	Y5P	C6-N1	2.66	1.43	1.37
85	r4	60	Y5P	C6-N1	2.66	1.43	1.37
83	r1	56	Y5P	C6-N1	2.66	1.43	1.37
85	r4	4	Y5P	C6-N1	2.66	1.43	1.37
84	r3	13	Y5P	C6-N1	2.66	1.43	1.37
84	r3	63	Y5P	C6-N1	2.66	1.43	1.37
85	r4	74	Y5P	C6-N1	2.66	1.43	1.37
84	r3	47	Y5P	C6-N1	2.66	1.43	1.37
84	r3	16	Y5P	C6-N1	2.65	1.43	1.37
85	r4	11	Y5P	C6-N1	2.65	1.43	1.37
83	r1	57	Y5P	C6-N1	2.65	1.43	1.37
84	r3	54	Y5P	C6-N1	2.65	1.43	1.37
83	r1	46	Y5P	C6-N1	2.65	1.43	1.37
85	r4	13	Y5P	C6-N1	2.65	1.43	1.37
84	r3	7	Y5P	C6-N1	2.65	1.43	1.37
83	r1	50	Y5P	C6-N1	2.65	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r3	53	Y5P	C6-N1	2.65	1.43	1.37
85	r4	42	Y5P	C6-N1	2.65	1.43	1.37
84	r3	1	Y5P	C6-N1	2.65	1.43	1.37
85	r4	3	Y5P	C6-N1	2.65	1.43	1.37
83	r1	47	Y5P	C6-N1	2.64	1.43	1.37
84	r3	56	Y5P	C6-N1	2.64	1.43	1.37
83	r1	49	Y5P	C6-N1	2.64	1.43	1.37
84	r3	59	Y5P	C6-N1	2.64	1.43	1.37
85	r4	20	Y5P	C6-N1	2.64	1.43	1.37
85	r4	25	Y5P	C6-N1	2.64	1.43	1.37
85	r4	49	Y5P	C6-N1	2.64	1.43	1.37
83	r1	55	Y5P	C6-N1	2.64	1.43	1.37
85	r4	43	Y5P	C6-N1	2.64	1.43	1.37
84	r3	2	Y5P	C6-N1	2.64	1.43	1.37
85	r4	39	Y5P	C6-N1	2.64	1.43	1.37
84	r3	34	Y5P	C6-N1	2.64	1.43	1.37
85	r4	56	Y5P	C6-N1	2.63	1.43	1.37
85	r4	59	Y5P	C6-N1	2.63	1.43	1.37
84	r3	20	Y5P	C6-N1	2.63	1.43	1.37
84	r3	49	Y5P	C6-N1	2.63	1.43	1.37
84	r3	38	Y5P	C6-N1	2.63	1.43	1.37
84	r3	58	Y5P	C6-N1	2.63	1.43	1.37
83	r1	48	Y5P	C6-N1	2.63	1.43	1.37
84	r3	33	Y5P	C6-N1	2.63	1.43	1.37
85	r4	54	Y5P	C6-N1	2.63	1.43	1.37
84	r3	24	Y5P	C6-N1	2.62	1.43	1.37
84	r3	61	Y5P	C6-N1	2.62	1.43	1.37
84	r3	28	Y5P	C6-N1	2.62	1.43	1.37
85	r4	68	Y5P	C6-N1	2.62	1.43	1.37
84	r3	69	Y5P	C6-N1	2.62	1.43	1.37
85	r4	48	Y5P	C6-N1	2.62	1.43	1.37
83	r1	54	Y5P	C6-N1	2.62	1.43	1.37
84	r3	36	Y5P	C6-N1	2.62	1.43	1.37
84	r3	12	Y5P	C6-N1	2.62	1.43	1.37
84	r3	65	Y5P	C6-N1	2.62	1.43	1.37
85	r4	75	Y5P	C6-N1	2.62	1.43	1.37
84	r3	27	Y5P	C6-N1	2.62	1.43	1.37
84	r3	67	Y5P	C6-N1	2.61	1.43	1.37
85	r4	8	Y5P	C6-N1	2.61	1.43	1.37
85	r4	33	Y5P	C6-N1	2.61	1.43	1.37
85	r4	45	Y5P	C6-N1	2.61	1.43	1.37
85	r4	67	Y5P	C6-N1	2.61	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r3	25	Y5P	C6-N1	2.61	1.43	1.37
84	r3	50	Y5P	C6-N1	2.61	1.43	1.37
84	r3	64	Y5P	C6-N1	2.60	1.43	1.37
85	r4	12	Y5P	C6-N1	2.60	1.43	1.37
84	r3	32	Y5P	C6-N1	2.60	1.43	1.37
84	r3	70	Y5P	C6-N1	2.59	1.43	1.37
85	r4	72	Y5P	C6-N1	2.59	1.43	1.37
84	r3	41	Y5P	C6-N1	2.59	1.43	1.37
84	r3	40	Y5P	C6-N1	2.59	1.43	1.37
84	r3	72	Y5P	C6-N1	2.57	1.43	1.37
84	r3	39	Y5P	C6-N1	2.57	1.43	1.37
83	r1	53	Y5P	C6-N1	2.57	1.43	1.37
84	r3	73	Y5P	C6-N1	2.54	1.43	1.37
84	r3	31	P5P	C5-C4	-2.27	1.34	1.40
84	r3	29	P5P	C5-C4	-2.26	1.35	1.40
84	r3	26	P5P	C5-C4	-2.25	1.35	1.40
84	r3	44	P5P	C5-C4	-2.24	1.35	1.40
84	r3	35	P5P	C5-C4	-2.24	1.35	1.40
84	r3	66	P5P	C5-C4	-2.24	1.35	1.40
84	r3	43	P5P	C5-C4	-2.24	1.35	1.40
85	r4	69	P5P	C5-C4	-2.23	1.35	1.40
84	r3	42	P5P	C5-C4	-2.23	1.35	1.40
84	r3	30	P5P	C5-C4	-2.23	1.35	1.40
85	r4	64	P5P	C5-C4	-2.23	1.35	1.40
84	r3	6	P5P	C5-C4	-2.23	1.35	1.40
84	r3	23	P5P	C5-C4	-2.23	1.35	1.40
84	r3	52	P5P	C5-C4	-2.23	1.35	1.40
85	r4	1	P5P	C5-C4	-2.23	1.35	1.40
84	r3	51	P5P	C5-C4	-2.22	1.35	1.40
84	r3	71	P5P	C5-C4	-2.22	1.35	1.40
84	r3	3	P5P	C5-C4	-2.22	1.35	1.40
84	r3	11	P5P	C5-C4	-2.22	1.35	1.40
84	r3	10	P5P	C5-C4	-2.22	1.35	1.40
84	r3	4	P5P	C5-C4	-2.21	1.35	1.40
84	r3	18	P5P	C5-C4	-2.21	1.35	1.40
85	r4	24	P5P	C5-C4	-2.21	1.35	1.40
85	r4	73	P5P	C5-C4	-2.21	1.35	1.40
85	r4	70	P5P	C5-C4	-2.21	1.35	1.40
85	r4	28	P5P	C5-C4	-2.21	1.35	1.40
85	r4	65	P5P	C5-C4	-2.21	1.35	1.40
85	r4	44	P5P	C5-C4	-2.21	1.35	1.40
85	r4	15	P5P	C5-C4	-2.21	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r4	52	P5P	C5-C4	-2.21	1.35	1.40
85	r4	53	P5P	C5-C4	-2.21	1.35	1.40
84	r3	68	P5P	C5-C4	-2.20	1.35	1.40
85	r4	36	P5P	C5-C4	-2.20	1.35	1.40
85	r4	34	P5P	C5-C4	-2.20	1.35	1.40
85	r4	21	P5P	C5-C4	-2.20	1.35	1.40
84	r3	21	P5P	C5-C4	-2.20	1.35	1.40
85	r4	37	P5P	C5-C4	-2.20	1.35	1.40
84	r3	48	P5P	C5-C4	-2.20	1.35	1.40
84	r3	22	P5P	C5-C4	-2.20	1.35	1.40
84	r3	17(A)	P5P	C5-C4	-2.20	1.35	1.40
85	r4	58	P5P	C5-C4	-2.20	1.35	1.40
85	r4	5	P5P	C5-C4	-2.20	1.35	1.40
84	r3	37	P5P	C5-C4	-2.20	1.35	1.40
85	r4	46	P5P	C5-C4	-2.20	1.35	1.40
85	r4	71	P5P	C5-C4	-2.19	1.35	1.40
85	r4	35	P5P	C5-C4	-2.19	1.35	1.40
85	r4	57	P5P	C5-C4	-2.19	1.35	1.40
85	r4	30	P5P	C5-C4	-2.19	1.35	1.40
85	r4	38	P5P	C5-C4	-2.19	1.35	1.40
84	r3	46	P5P	C5-C4	-2.19	1.35	1.40
85	r4	76	P5P	C5-C4	-2.19	1.35	1.40
84	r3	15	P5P	C5-C4	-2.19	1.35	1.40
85	r4	6	P5P	C5-C4	-2.18	1.35	1.40
85	r4	9	P5P	C5-C4	-2.18	1.35	1.40
84	r3	19	P5P	C5-C4	-2.18	1.35	1.40
84	r3	74	P5P	C5-C4	-2.18	1.35	1.40
85	r4	26	P5P	C5-C4	-2.18	1.35	1.40
85	r4	29	P5P	C5-C4	-2.18	1.35	1.40
85	r4	63	P5P	C5-C4	-2.18	1.35	1.40
85	r4	31	P5P	C5-C4	-2.18	1.35	1.40
84	r3	45	P5P	C5-C4	-2.18	1.35	1.40
84	r3	5	P5P	C5-C4	-2.18	1.35	1.40
85	r4	7	P5P	C5-C4	-2.18	1.35	1.40
85	r4	10	P5P	C5-C4	-2.17	1.35	1.40
85	r4	23	P5P	C5-C4	-2.17	1.35	1.40
84	r3	9	P5P	C5-C4	-2.17	1.35	1.40
85	r4	19	P5P	C5-C4	-2.17	1.35	1.40
85	r4	14	P5P	C5-C4	-2.17	1.35	1.40
84	r3	14	P5P	C5-C4	-2.17	1.35	1.40
85	r4	27	P5P	C5-C4	-2.17	1.35	1.40
84	r3	8	P5P	C5-C4	-2.17	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r4	18	P5P	C5-C4	-2.16	1.35	1.40
84	r3	57	P5P	C5-C4	-2.16	1.35	1.40
84	r3	55	P5P	C5-C4	-2.14	1.35	1.40
85	r4	22	P5P	C5-C4	-2.11	1.35	1.40

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r4	37	P5P	OP2-P-O5'	-10.22	79.54	106.73
85	r4	37	P5P	O5'-P-OP1	-9.64	79.44	106.47
85	r4	37	P5P	OP2-P-OP1	8.11	142.43	110.68
85	r4	37	P5P	OP3-P-O5'	7.02	125.41	106.73
85	r4	37	P5P	OP3-P-OP1	-6.87	83.80	110.68
85	r4	37	P5P	OP3-P-OP2	-6.32	83.50	107.64
84	r3	31	P5P	N1-C2-N3	-6.03	119.94	127.65
85	r4	52	P5P	N1-C2-N3	-6.02	119.94	127.65
85	r4	73	P5P	N1-C2-N3	-6.01	119.95	127.65
84	r3	29	P5P	N1-C2-N3	-6.00	119.97	127.65
84	r3	52	P5P	N1-C2-N3	-6.00	119.97	127.65
85	r4	63	P5P	N1-C2-N3	-5.99	119.98	127.65
84	r3	51	P5P	N1-C2-N3	-5.99	119.98	127.65
85	r4	24	P5P	N1-C2-N3	-5.99	119.99	127.65
84	r3	42	P5P	N1-C2-N3	-5.99	119.99	127.65
85	r4	29	P5P	N1-C2-N3	-5.98	119.99	127.65
85	r4	65	P5P	N1-C2-N3	-5.97	120.00	127.65
84	r3	3	P5P	N1-C2-N3	-5.97	120.01	127.65
84	r3	30	P5P	N1-C2-N3	-5.97	120.01	127.65
84	r3	22	P5P	N1-C2-N3	-5.97	120.01	127.65
85	r4	6	P5P	N1-C2-N3	-5.96	120.02	127.65
85	r4	1	P5P	N1-C2-N3	-5.96	120.03	127.65
85	r4	35	P5P	N1-C2-N3	-5.96	120.03	127.65
85	r4	53	P5P	N1-C2-N3	-5.96	120.03	127.65
85	r4	69	P5P	N1-C2-N3	-5.96	120.03	127.65
84	r3	19	P5P	N1-C2-N3	-5.95	120.04	127.65
85	r4	71	P5P	N1-C2-N3	-5.95	120.04	127.65
84	r3	68	P5P	N1-C2-N3	-5.95	120.04	127.65
84	r3	9	P5P	N1-C2-N3	-5.94	120.04	127.65
84	r3	23	P5P	N1-C2-N3	-5.94	120.05	127.65
85	r4	15	P5P	N1-C2-N3	-5.94	120.06	127.65
85	r4	44	P5P	N1-C2-N3	-5.94	120.06	127.65
85	r4	64	P5P	N1-C2-N3	-5.93	120.06	127.65
84	r3	66	P5P	N1-C2-N3	-5.93	120.06	127.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r4	28	P5P	N1-C2-N3	-5.93	120.06	127.65
84	r3	17(A)	P5P	N1-C2-N3	-5.93	120.06	127.65
85	r4	46	P5P	N1-C2-N3	-5.93	120.07	127.65
85	r4	57	P5P	N1-C2-N3	-5.93	120.07	127.65
84	r3	26	P5P	N1-C2-N3	-5.92	120.07	127.65
85	r4	30	P5P	N1-C2-N3	-5.92	120.07	127.65
85	r4	9	P5P	N1-C2-N3	-5.92	120.07	127.65
85	r4	38	P5P	N1-C2-N3	-5.92	120.08	127.65
84	r3	43	P5P	N1-C2-N3	-5.92	120.08	127.65
84	r3	35	P5P	N1-C2-N3	-5.92	120.08	127.65
84	r3	18	P5P	N1-C2-N3	-5.91	120.08	127.65
84	r3	21	P5P	N1-C2-N3	-5.91	120.08	127.65
85	r4	5	P5P	N1-C2-N3	-5.91	120.08	127.65
84	r3	8	P5P	N1-C2-N3	-5.91	120.09	127.65
85	r4	19	P5P	N1-C2-N3	-5.91	120.09	127.65
85	r4	23	P5P	N1-C2-N3	-5.91	120.09	127.65
85	r4	21	P5P	N1-C2-N3	-5.90	120.10	127.65
85	r4	70	P5P	N1-C2-N3	-5.90	120.10	127.65
85	r4	58	P5P	N1-C2-N3	-5.90	120.11	127.65
85	r4	76	P5P	N1-C2-N3	-5.90	120.11	127.65
85	r4	18	P5P	N1-C2-N3	-5.89	120.11	127.65
85	r4	10	P5P	N1-C2-N3	-5.89	120.12	127.65
85	r4	26	P5P	N1-C2-N3	-5.89	120.12	127.65
84	r3	4	P5P	N1-C2-N3	-5.89	120.12	127.65
84	r3	37	P5P	N1-C2-N3	-5.89	120.12	127.65
84	r3	48	P5P	N1-C2-N3	-5.89	120.12	127.65
84	r3	44	P5P	N1-C2-N3	-5.88	120.12	127.65
84	r3	71	P5P	N1-C2-N3	-5.88	120.13	127.65
85	r4	7	P5P	N1-C2-N3	-5.88	120.13	127.65
84	r3	11	P5P	N1-C2-N3	-5.88	120.13	127.65
85	r4	14	P5P	N1-C2-N3	-5.87	120.13	127.65
84	r3	10	P5P	N1-C2-N3	-5.87	120.13	127.65
85	r4	34	P5P	N1-C2-N3	-5.87	120.13	127.65
84	r3	6	P5P	N1-C2-N3	-5.87	120.13	127.65
85	r4	36	P5P	N1-C2-N3	-5.87	120.14	127.65
85	r4	27	P5P	N1-C2-N3	-5.87	120.14	127.65
85	r4	37	P5P	N1-C2-N3	-5.86	120.14	127.65
85	r4	31	P5P	N1-C2-N3	-5.86	120.16	127.65
84	r3	5	P5P	N1-C2-N3	-5.86	120.16	127.65
85	r4	22	P5P	N1-C2-N3	-5.85	120.17	127.65
84	r3	15	P5P	N1-C2-N3	-5.82	120.20	127.65
84	r3	45	P5P	N1-C2-N3	-5.80	120.23	127.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r3	55	P5P	N1-C2-N3	-5.79	120.24	127.65
84	r3	57	P5P	N1-C2-N3	-5.76	120.27	127.65
84	r3	14	P5P	N1-C2-N3	-5.74	120.30	127.65
84	r3	74	P5P	N1-C2-N3	-5.71	120.34	127.65
84	r3	46	P5P	N1-C2-N3	-5.71	120.34	127.65
85	r4	76	P5P	C1'-N9-C4	3.50	132.80	126.64
84	r3	14	P5P	C1'-N9-C4	3.43	132.67	126.64
85	r4	22	P5P	C1'-N9-C4	3.26	132.37	126.64
85	r4	31	P5P	C1'-N9-C4	3.26	132.37	126.64
84	r3	8	P5P	C1'-N9-C4	3.25	132.35	126.64
85	r4	23	P5P	C1'-N9-C4	3.23	132.32	126.64
84	r3	55	P5P	C1'-N9-C4	3.21	132.29	126.64
84	r3	57	P5P	C1'-N9-C4	3.20	132.27	126.64
85	r4	1	P5P	C6-N1-C2	3.19	120.41	115.84
85	r4	52	P5P	C6-N1-C2	3.18	120.39	115.84
84	r3	31	P5P	C6-N1-C2	3.16	120.36	115.84
84	r3	22	P5P	C6-N1-C2	3.16	120.36	115.84
85	r4	24	P5P	C6-N1-C2	3.14	120.34	115.84
85	r4	10	P5P	C1'-N9-C4	3.14	132.15	126.64
84	r3	68	P5P	C6-N1-C2	3.13	120.33	115.84
84	r3	29	P5P	C6-N1-C2	3.13	120.33	115.84
84	r3	52	P5P	C6-N1-C2	3.13	120.32	115.84
84	r3	19	P5P	C6-N1-C2	3.12	120.31	115.84
84	r3	46	P5P	C1'-N9-C4	3.12	132.12	126.64
85	r4	71	P5P	C6-N1-C2	3.11	120.30	115.84
85	r4	31	P5P	C6-N1-C2	3.11	120.29	115.84
84	r3	35	P5P	C6-N1-C2	3.11	120.29	115.84
85	r4	29	P5P	C6-N1-C2	3.10	120.28	115.84
84	r3	51	P5P	C6-N1-C2	3.10	120.28	115.84
85	r4	53	P5P	C6-N1-C2	3.10	120.28	115.84
84	r3	23	P5P	C6-N1-C2	3.10	120.28	115.84
85	r4	44	P5P	C6-N1-C2	3.10	120.28	115.84
85	r4	65	P5P	C6-N1-C2	3.10	120.28	115.84
85	r4	29	P5P	C1'-N9-C4	3.10	132.08	126.64
85	r4	46	P5P	C6-N1-C2	3.09	120.27	115.84
84	r3	30	P5P	C6-N1-C2	3.09	120.27	115.84
85	r4	69	P5P	C6-N1-C2	3.09	120.26	115.84
85	r4	6	P5P	C6-N1-C2	3.09	120.26	115.84
84	r3	10	P5P	C6-N1-C2	3.08	120.26	115.84
85	r4	23	P5P	C6-N1-C2	3.08	120.25	115.84
85	r4	9	P5P	C6-N1-C2	3.08	120.25	115.84
85	r4	18	P5P	C6-N1-C2	3.08	120.25	115.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r3	42	P5P	C6-N1-C2	3.08	120.25	115.84
85	r4	35	P5P	C6-N1-C2	3.08	120.25	115.84
85	r4	64	P5P	C6-N1-C2	3.07	120.24	115.84
85	r4	63	P5P	C6-N1-C2	3.07	120.24	115.84
84	r3	3	P5P	C6-N1-C2	3.07	120.24	115.84
84	r3	9	P5P	C6-N1-C2	3.07	120.24	115.84
85	r4	36	P5P	C6-N1-C2	3.07	120.23	115.84
85	r4	19	P5P	C6-N1-C2	3.07	120.23	115.84
85	r4	10	P5P	C6-N1-C2	3.07	120.23	115.84
84	r3	8	P5P	C6-N1-C2	3.06	120.23	115.84
85	r4	5	P5P	C6-N1-C2	3.06	120.23	115.84
84	r3	26	P5P	C6-N1-C2	3.05	120.21	115.84
85	r4	21	P5P	C6-N1-C2	3.05	120.21	115.84
85	r4	38	P5P	C6-N1-C2	3.05	120.21	115.84
84	r3	43	P5P	C6-N1-C2	3.05	120.21	115.84
85	r4	30	P5P	C6-N1-C2	3.05	120.21	115.84
85	r4	15	P5P	C6-N1-C2	3.05	120.20	115.84
84	r3	15	P5P	C6-N1-C2	3.04	120.20	115.84
85	r4	73	P5P	C6-N1-C2	3.04	120.20	115.84
84	r3	3	P5P	C1'-N9-C4	3.04	131.98	126.64
85	r4	57	P5P	C6-N1-C2	3.04	120.19	115.84
84	r3	48	P5P	C6-N1-C2	3.03	120.19	115.84
85	r4	27	P5P	C6-N1-C2	3.03	120.19	115.84
84	r3	37	P5P	C6-N1-C2	3.03	120.18	115.84
85	r4	26	P5P	C6-N1-C2	3.03	120.18	115.84
84	r3	21	P5P	C6-N1-C2	3.03	120.18	115.84
85	r4	28	P5P	C6-N1-C2	3.03	120.18	115.84
84	r3	74	P5P	C6-N1-C2	3.03	120.17	115.84
84	r3	66	P5P	C6-N1-C2	3.02	120.17	115.84
85	r4	70	P5P	C6-N1-C2	3.02	120.17	115.84
84	r3	4	P5P	C6-N1-C2	3.02	120.16	115.84
84	r3	6	P5P	C6-N1-C2	3.02	120.16	115.84
85	r4	34	P5P	C6-N1-C2	3.02	120.16	115.84
84	r3	68	P5P	C1'-N9-C4	3.02	131.94	126.64
85	r4	58	P5P	C6-N1-C2	3.02	120.16	115.84
85	r4	14	P5P	C6-N1-C2	3.02	120.16	115.84
84	r3	5	P5P	C6-N1-C2	3.01	120.16	115.84
84	r3	17(A)	P5P	C6-N1-C2	3.01	120.16	115.84
84	r3	45	P5P	C1'-N9-C4	3.01	131.93	126.64
84	r3	44	P5P	C6-N1-C2	3.01	120.15	115.84
84	r3	45	P5P	C6-N1-C2	3.01	120.15	115.84
85	r4	37	P5P	C6-N1-C2	3.01	120.14	115.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r4	76	P5P	C6-N1-C2	3.00	120.14	115.84
84	r3	18	P5P	C6-N1-C2	3.00	120.14	115.84
84	r3	71	P5P	C6-N1-C2	3.00	120.14	115.84
85	r4	22	P5P	C6-N1-C2	2.99	120.13	115.84
84	r3	11	P5P	C6-N1-C2	2.99	120.12	115.84
85	r4	26	P5P	C1'-N9-C4	2.98	131.88	126.64
84	r3	55	P5P	C6-N1-C2	2.98	120.11	115.84
85	r4	6	P5P	C1'-N9-C4	2.98	131.88	126.64
84	r3	17(A)	P5P	C1'-N9-C4	2.97	131.87	126.64
85	r4	7	P5P	C6-N1-C2	2.97	120.10	115.84
85	r4	5	P5P	C1'-N9-C4	2.97	131.86	126.64
84	r3	46	P5P	C6-N1-C2	2.95	120.06	115.84
84	r3	14	P5P	C6-N1-C2	2.95	120.06	115.84
84	r3	21	P5P	C1'-N9-C4	2.94	131.81	126.64
85	r4	73	P5P	C1'-N9-C4	2.94	131.81	126.64
84	r3	9	P5P	C1'-N9-C4	2.94	131.80	126.64
84	r3	10	P5P	C1'-N9-C4	2.92	131.78	126.64
84	r3	35	P5P	C1'-N9-C4	2.92	131.77	126.64
85	r4	36	P5P	C1'-N9-C4	2.90	131.74	126.64
84	r3	5	P5P	C1'-N9-C4	2.89	131.72	126.64
85	r4	27	P5P	C1'-N9-C4	2.89	131.72	126.64
85	r4	18	P5P	C1'-N9-C4	2.89	131.71	126.64
84	r3	57	P5P	C6-N1-C2	2.88	119.96	115.84
84	r3	23	P5P	C1'-N9-C4	2.87	131.69	126.64
85	r4	7	P5P	C1'-N9-C4	2.87	131.69	126.64
85	r4	44	P5P	C1'-N9-C4	2.87	131.68	126.64
85	r4	64	P5P	C1'-N9-C4	2.85	131.65	126.64
85	r4	28	P5P	C1'-N9-C4	2.85	131.65	126.64
85	r4	34	P5P	C1'-N9-C4	2.84	131.63	126.64
84	r3	66	P5P	C1'-N9-C4	2.82	131.60	126.64
85	r4	30	P5P	C1'-N9-C4	2.82	131.60	126.64
84	r3	4	P5P	C1'-N9-C4	2.82	131.59	126.64
84	r3	11	P5P	C1'-N9-C4	2.82	131.59	126.64
84	r3	37	P5P	C1'-N9-C4	2.82	131.59	126.64
84	r3	31	P5P	C1'-N9-C4	2.81	131.59	126.64
84	r3	22	P5P	C1'-N9-C4	2.80	131.56	126.64
85	r4	21	P5P	C1'-N9-C4	2.78	131.53	126.64
85	r4	70	P5P	C1'-N9-C4	2.78	131.53	126.64
85	r4	53	P5P	C1'-N9-C4	2.77	131.51	126.64
85	r4	1	P5P	C1'-N9-C4	2.77	131.51	126.64
85	r4	19	P5P	C1'-N9-C4	2.76	131.50	126.64
84	r3	71	P5P	C1'-N9-C4	2.76	131.49	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r4	14	P5P	C1'-N9-C4	2.75	131.48	126.64
85	r4	52	P5P	C1'-N9-C4	2.75	131.48	126.64
85	r4	9	P5P	C1'-N9-C4	2.75	131.47	126.64
84	r3	48	P5P	C1'-N9-C4	2.74	131.46	126.64
85	r4	58	P5P	C1'-N9-C4	2.73	131.44	126.64
84	r3	74	P5P	C1'-N9-C4	2.73	131.44	126.64
85	r4	65	P5P	C1'-N9-C4	2.73	131.44	126.64
84	r3	18	P5P	C1'-N9-C4	2.72	131.41	126.64
84	r3	29	P5P	C1'-N9-C4	2.71	131.41	126.64
85	r4	63	P5P	C1'-N9-C4	2.71	131.41	126.64
85	r4	69	P5P	C1'-N9-C4	2.71	131.40	126.64
84	r3	51	P5P	C1'-N9-C4	2.70	131.38	126.64
85	r4	35	P5P	C1'-N9-C4	2.70	131.38	126.64
84	r3	6	P5P	C1'-N9-C4	2.69	131.37	126.64
85	r4	71	P5P	C1'-N9-C4	2.67	131.33	126.64
85	r4	15	P5P	C1'-N9-C4	2.67	131.32	126.64
85	r4	46	P5P	C1'-N9-C4	2.66	131.32	126.64
84	r3	26	P5P	C1'-N9-C4	2.66	131.31	126.64
84	r3	19	P5P	C1'-N9-C4	2.65	131.30	126.64
85	r4	24	P5P	C1'-N9-C4	2.65	131.29	126.64
84	r3	42	P5P	C1'-N9-C4	2.65	131.29	126.64
84	r3	30	P5P	C1'-N9-C4	2.64	131.28	126.64
85	r4	57	P5P	C1'-N9-C4	2.64	131.27	126.64
85	r4	38	P5P	C1'-N9-C4	2.63	131.26	126.64
84	r3	15	P5P	C1'-N9-C4	2.63	131.25	126.64
85	r4	37	P5P	C1'-N9-C4	2.61	131.22	126.64
84	r3	44	P5P	C1'-N9-C4	2.56	131.15	126.64
84	r3	43	P5P	C1'-N9-C4	2.56	131.14	126.64
84	r3	52	P5P	C1'-N9-C4	2.41	130.87	126.64

There are no chirality outliers.

All (263) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	r1	46	Y5P	C4'-C5'-O5'-P
83	r1	46	Y5P	C3'-C4'-C5'-O5'
83	r1	46	Y5P	O4'-C1'-N1-C6
83	r1	52	Y5P	O4'-C1'-N1-C2
83	r1	53	Y5P	O4'-C4'-C5'-O5'
83	r1	54	Y5P	O4'-C1'-N1-C2
83	r1	55	Y5P	O4'-C4'-C5'-O5'
83	r1	56	Y5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
84	r3	1	Y5P	C2'-C1'-N1-C6
84	r3	4	P5P	O4'-C4'-C5'-O5'
84	r3	5	P5P	C3'-C4'-C5'-O5'
84	r3	16	Y5P	O4'-C1'-N1-C2
84	r3	19	P5P	C3'-C4'-C5'-O5'
84	r3	21	P5P	C3'-C4'-C5'-O5'
84	r3	21	P5P	O4'-C4'-C5'-O5'
84	r3	21	P5P	C4'-C5'-O5'-P
84	r3	27	Y5P	O4'-C1'-N1-C2
84	r3	28	Y5P	O4'-C1'-N1-C2
84	r3	32	Y5P	O4'-C1'-N1-C2
84	r3	33	Y5P	O4'-C1'-N1-C2
84	r3	34	Y5P	O4'-C4'-C5'-O5'
84	r3	34	Y5P	C3'-C4'-C5'-O5'
84	r3	36	Y5P	O4'-C1'-N1-C2
84	r3	38	Y5P	O4'-C1'-N1-C2
84	r3	41	Y5P	O4'-C1'-N1-C2
84	r3	50	Y5P	O4'-C1'-N1-C2
84	r3	55	P5P	O4'-C4'-C5'-O5'
84	r3	63	Y5P	O4'-C4'-C5'-O5'
84	r3	63	Y5P	C3'-C4'-C5'-O5'
84	r3	65	Y5P	O4'-C1'-N1-C2
84	r3	69	Y5P	O4'-C1'-N1-C2
84	r3	70	Y5P	O4'-C1'-N1-C2
84	r3	72	Y5P	O4'-C1'-N1-C2
85	r4	2	Y5P	O4'-C1'-N1-C2
85	r4	8	Y5P	O4'-C1'-N1-C2
85	r4	9	P5P	O4'-C4'-C5'-O5'
85	r4	13	Y5P	O4'-C4'-C5'-O5'
85	r4	13	Y5P	C3'-C4'-C5'-O5'
85	r4	13	Y5P	O4'-C1'-N1-C2
85	r4	16	Y5P	O4'-C1'-N1-C2
85	r4	21	P5P	C4'-C5'-O5'-P
85	r4	22	P5P	C3'-C4'-C5'-O5'
85	r4	22	P5P	O4'-C4'-C5'-O5'
85	r4	26	P5P	C3'-C4'-C5'-O5'
85	r4	26	P5P	O4'-C4'-C5'-O5'
85	r4	29	P5P	O4'-C4'-C5'-O5'
85	r4	32	Y5P	O4'-C4'-C5'-O5'
85	r4	37	P5P	C5'-O5'-P-OP3
85	r4	39	Y5P	O4'-C1'-N1-C2
85	r4	40	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
85	r4	41	Y5P	O4'-C4'-C5'-O5'
85	r4	41	Y5P	C3'-C4'-C5'-O5'
85	r4	47	Y5P	O4'-C4'-C5'-O5'
85	r4	48	Y5P	C3'-C4'-C5'-O5'
85	r4	52	P5P	C3'-C4'-C5'-O5'
85	r4	54	Y5P	O4'-C1'-N1-C2
85	r4	55	Y5P	O4'-C1'-N1-C2
85	r4	56	Y5P	O4'-C4'-C5'-O5'
85	r4	59	Y5P	O4'-C1'-N1-C2
85	r4	64	P5P	C3'-C4'-C5'-O5'
85	r4	64	P5P	O4'-C4'-C5'-O5'
85	r4	66	Y5P	C3'-C4'-C5'-O5'
85	r4	72	Y5P	C3'-C4'-C5'-O5'
85	r4	73	P5P	C3'-C4'-C5'-O5'
85	r4	75	Y5P	O4'-C4'-C5'-O5'
83	r1	47	Y5P	O4'-C1'-N1-C2
83	r1	48	Y5P	O4'-C1'-N1-C2
83	r1	49	Y5P	O4'-C1'-N1-C2
83	r1	50	Y5P	O4'-C1'-N1-C2
83	r1	51	Y5P	O4'-C1'-N1-C2
84	r3	7	Y5P	O4'-C1'-N1-C2
84	r3	12	Y5P	O4'-C1'-N1-C2
84	r3	17	Y5P	O4'-C1'-N1-C2
84	r3	20	Y5P	O4'-C1'-N1-C2
84	r3	24	Y5P	O4'-C1'-N1-C2
84	r3	25	Y5P	O4'-C1'-N1-C2
84	r3	34	Y5P	O4'-C1'-N1-C2
84	r3	49	Y5P	O4'-C1'-N1-C2
84	r3	53	Y5P	O4'-C1'-N1-C2
84	r3	54	Y5P	O4'-C1'-N1-C2
84	r3	59	Y5P	O4'-C1'-N1-C2
84	r3	60	Y5P	O4'-C1'-N1-C2
84	r3	61	Y5P	O4'-C1'-N1-C2
84	r3	62	Y5P	O4'-C1'-N1-C2
84	r3	63	Y5P	O4'-C1'-N1-C2
84	r3	64	Y5P	O4'-C1'-N1-C2
84	r3	67	Y5P	O4'-C1'-N1-C2
85	r4	3	Y5P	O4'-C1'-N1-C2
85	r4	12	Y5P	O4'-C1'-N1-C2
85	r4	17	Y5P	O4'-C1'-N1-C2
85	r4	20	Y5P	O4'-C1'-N1-C2
85	r4	25	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
85	r4	32	Y5P	O4'-C1'-N1-C2
85	r4	41	Y5P	O4'-C1'-N1-C2
85	r4	42	Y5P	O4'-C1'-N1-C2
85	r4	43	Y5P	O4'-C1'-N1-C2
85	r4	45	Y5P	O4'-C1'-N1-C2
85	r4	48	Y5P	O4'-C1'-N1-C2
85	r4	49	Y5P	O4'-C1'-N1-C2
85	r4	50	Y5P	O4'-C1'-N1-C2
85	r4	51	Y5P	O4'-C1'-N1-C2
85	r4	56	Y5P	O4'-C1'-N1-C2
85	r4	60	Y5P	O4'-C1'-N1-C2
85	r4	61	Y5P	O4'-C1'-N1-C2
85	r4	62	Y5P	O4'-C1'-N1-C2
85	r4	66	Y5P	O4'-C1'-N1-C2
85	r4	67	Y5P	O4'-C1'-N1-C2
85	r4	68	Y5P	O4'-C1'-N1-C2
85	r4	72	Y5P	O4'-C1'-N1-C2
84	r3	40	Y5P	O4'-C1'-N1-C6
85	r4	75	Y5P	C2'-C1'-N1-C2
84	r3	47	Y5P	C4'-C5'-O5'-P
85	r4	23	P5P	C4'-C5'-O5'-P
83	r1	47	Y5P	C3'-C4'-C5'-O5'
83	r1	53	Y5P	C3'-C4'-C5'-O5'
84	r3	3	P5P	O4'-C4'-C5'-O5'
84	r3	4	P5P	C3'-C4'-C5'-O5'
84	r3	17(A)	P5P	C3'-C4'-C5'-O5'
84	r3	17(A)	P5P	O4'-C4'-C5'-O5'
84	r3	18	P5P	O4'-C4'-C5'-O5'
84	r3	50	Y5P	O4'-C4'-C5'-O5'
84	r3	55	P5P	C3'-C4'-C5'-O5'
84	r3	59	Y5P	O4'-C4'-C5'-O5'
84	r3	61	Y5P	O4'-C4'-C5'-O5'
84	r3	61	Y5P	C3'-C4'-C5'-O5'
85	r4	6	P5P	O4'-C4'-C5'-O5'
85	r4	9	P5P	C3'-C4'-C5'-O5'
85	r4	17	Y5P	O4'-C4'-C5'-O5'
85	r4	28	P5P	O4'-C4'-C5'-O5'
85	r4	29	P5P	C3'-C4'-C5'-O5'
85	r4	32	Y5P	C3'-C4'-C5'-O5'
85	r4	45	Y5P	O4'-C4'-C5'-O5'
85	r4	45	Y5P	C3'-C4'-C5'-O5'
85	r4	52	P5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
85	r4	56	Y5P	C3'-C4'-C5'-O5'
85	r4	66	Y5P	O4'-C4'-C5'-O5'
85	r4	73	P5P	O4'-C4'-C5'-O5'
85	r4	74	Y5P	O4'-C4'-C5'-O5'
85	r4	75	Y5P	C3'-C4'-C5'-O5'
85	r4	76	P5P	O4'-C4'-C5'-O5'
85	r4	74	Y5P	O4'-C1'-N1-C6
84	r3	1	Y5P	C2'-C1'-N1-C2
85	r4	75	Y5P	C2'-C1'-N1-C6
83	r1	46	Y5P	O4'-C4'-C5'-O5'
83	r1	47	Y5P	O4'-C4'-C5'-O5'
83	r1	55	Y5P	C3'-C4'-C5'-O5'
83	r1	56	Y5P	C3'-C4'-C5'-O5'
84	r3	1	Y5P	C3'-C4'-C5'-O5'
84	r3	3	P5P	C3'-C4'-C5'-O5'
84	r3	7	Y5P	O4'-C4'-C5'-O5'
84	r3	7	Y5P	C3'-C4'-C5'-O5'
84	r3	18	P5P	C3'-C4'-C5'-O5'
84	r3	50	Y5P	C3'-C4'-C5'-O5'
84	r3	59	Y5P	C3'-C4'-C5'-O5'
85	r4	6	P5P	C3'-C4'-C5'-O5'
85	r4	38	P5P	O4'-C4'-C5'-O5'
85	r4	47	Y5P	C3'-C4'-C5'-O5'
85	r4	74	Y5P	C3'-C4'-C5'-O5'
83	r1	57	Y5P	O4'-C1'-N1-C2
84	r3	40	Y5P	C2'-C1'-N1-C2
85	r4	74	Y5P	C2'-C1'-N1-C2
84	r3	40	Y5P	C2'-C1'-N1-C6
85	r4	74	Y5P	C2'-C1'-N1-C6
84	r3	39	Y5P	O4'-C1'-N1-C2
84	r3	73	Y5P	O4'-C1'-N1-C2
85	r4	4	Y5P	O4'-C1'-N1-C2
85	r4	47	Y5P	O4'-C1'-N1-C2
85	r4	75	Y5P	O4'-C1'-N1-C2
84	r3	46	P5P	C4'-C5'-O5'-P
85	r4	20	Y5P	C4'-C5'-O5'-P
84	r3	53	Y5P	C3'-C4'-C5'-O5'
85	r4	25	Y5P	C3'-C4'-C5'-O5'
84	r3	13	Y5P	C4'-C5'-O5'-P
84	r3	1	Y5P	O4'-C4'-C5'-O5'
84	r3	51	P5P	C3'-C4'-C5'-O5'
85	r4	48	Y5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
83	r1	55	Y5P	O4'-C1'-N1-C2
85	r4	11	Y5P	O4'-C1'-N1-C2
85	r4	22	P5P	C4'-C5'-O5'-P
84	r3	5	P5P	O4'-C4'-C5'-O5'
84	r3	19	P5P	O4'-C4'-C5'-O5'
84	r3	53	Y5P	O4'-C4'-C5'-O5'
84	r3	65	Y5P	O4'-C4'-C5'-O5'
85	r4	49	Y5P	O4'-C4'-C5'-O5'
85	r4	72	Y5P	O4'-C4'-C5'-O5'
83	r1	53	Y5P	C2'-C1'-N1-C2
83	r1	53	Y5P	C2'-C1'-N1-C6
85	r4	49	Y5P	C3'-C4'-C5'-O5'
85	r4	76	P5P	C3'-C4'-C5'-O5'
84	r3	13	Y5P	C2'-C1'-N1-C2
84	r3	69	Y5P	C3'-C4'-C5'-O5'
85	r4	23	P5P	C3'-C4'-C5'-O5'
84	r3	43	P5P	C4'-C5'-O5'-P
84	r3	51	P5P	O4'-C4'-C5'-O5'
85	r4	38	P5P	C3'-C4'-C5'-O5'
85	r4	73	P5P	C4'-C5'-O5'-P
85	r4	25	Y5P	O4'-C4'-C5'-O5'
83	r1	53	Y5P	O4'-C1'-N1-C2
84	r3	47	Y5P	O4'-C1'-N1-C2
84	r3	59	Y5P	C4'-C5'-O5'-P
85	r4	34	P5P	C4'-C5'-O5'-P
85	r4	47	Y5P	C4'-C5'-O5'-P
84	r3	17	Y5P	O4'-C4'-C5'-O5'
85	r4	28	P5P	C3'-C4'-C5'-O5'
84	r3	13	Y5P	O4'-C1'-N1-C2
85	r4	1	P5P	C4'-C5'-O5'-P
85	r4	30	P5P	C4'-C5'-O5'-P
85	r4	45	Y5P	C4'-C5'-O5'-P
85	r4	17	Y5P	C3'-C4'-C5'-O5'
84	r3	13	Y5P	C2'-C1'-N1-C6
83	r1	53	Y5P	O4'-C1'-N1-C6
84	r3	1	Y5P	O4'-C1'-N1-C6
84	r3	3	P5P	C4'-C5'-O5'-P
84	r3	14	P5P	C4'-C5'-O5'-P
84	r3	69	Y5P	O4'-C4'-C5'-O5'
85	r4	27	P5P	C3'-C4'-C5'-O5'
85	r4	31	P5P	O4'-C4'-C5'-O5'
84	r3	56	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
84	r3	18	P5P	C4'-C5'-O5'-P
85	r4	18	P5P	C4'-C5'-O5'-P
84	r3	2	Y5P	O4'-C1'-N1-C2
85	r4	7	P5P	O4'-C4'-C5'-O5'
83	r1	56	Y5P	O4'-C1'-N1-C6
84	r3	56	Y5P	C2'-C1'-N1-C2
84	r3	58	Y5P	O4'-C1'-N1-C2
85	r4	33	Y5P	O4'-C1'-N1-C2
84	r3	16	Y5P	C4'-C5'-O5'-P
84	r3	17(A)	P5P	C4'-C5'-O5'-P
84	r3	50	Y5P	C4'-C5'-O5'-P
85	r4	10	P5P	C4'-C5'-O5'-P
85	r4	33	Y5P	C4'-C5'-O5'-P
83	r1	56	Y5P	C2'-C1'-N1-C6
84	r3	49	Y5P	C3'-C4'-C5'-O5'
85	r4	41	Y5P	C2'-C1'-N1-C6
84	r3	1	Y5P	O4'-C1'-N1-C2
84	r3	65	Y5P	C3'-C4'-C5'-O5'
85	r4	23	P5P	O4'-C4'-C5'-O5'
84	r3	13	Y5P	O4'-C1'-N1-C6
83	r1	49	Y5P	C2'-C1'-N1-C6
85	r4	67	Y5P	C2'-C1'-N1-C6
85	r4	76	P5P	C4'-C5'-O5'-P
85	r4	1	P5P	O4'-C4'-C5'-O5'
85	r4	27	P5P	O4'-C4'-C5'-O5'
84	r3	57	P5P	O4'-C4'-C5'-O5'
85	r4	37	P5P	C5'-O5'-P-OP2
84	r3	62	Y5P	C2'-C1'-N1-C6
84	r3	2	Y5P	C2'-C1'-N1-C2
84	r3	56	Y5P	C2'-C1'-N1-C6
84	r3	4	P5P	C4'-C5'-O5'-P
85	r4	61	Y5P	C4'-C5'-O5'-P
85	r4	74	Y5P	C4'-C5'-O5'-P
83	r1	52	Y5P	O4'-C4'-C5'-O5'
83	r1	57	Y5P	C3'-C4'-C5'-O5'
84	r3	46	P5P	C3'-C4'-C5'-O5'
85	r4	7	P5P	C3'-C4'-C5'-O5'
85	r4	18	P5P	O4'-C4'-C5'-O5'
85	r4	34	P5P	O4'-C4'-C5'-O5'
85	r4	59	Y5P	O4'-C4'-C5'-O5'
84	r3	58	Y5P	C2'-C1'-N1-C2
85	r4	20	Y5P	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
84	r3	56	Y5P	O4'-C1'-N1-C6
84	r3	72	Y5P	C4'-C5'-O5'-P
85	r4	50	Y5P	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
91	DOL	XA	5145	-	43,50,50	3.51	17 (39%)	51,70,70	2.70	9 (17%)
90	H8Q	XA	5144	-	77,80,80	1.08	5 (6%)	103,115,115	1.34	15 (14%)
92	GTP	AX	500	-	26,34,34	1.14	2 (7%)	32,54,54	1.54	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	DOL	XA	5145	-	-	21/58/77/77	0/2/3/3
90	H8Q	XA	5144	-	-	31/83/127/127	0/8/8/8
92	GTP	AX	500	-	-	8/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	XA	5145	DOL	C28-C29	9.95	1.55	1.32
91	XA	5145	DOL	C22-C23	9.59	1.57	1.32
91	XA	5145	DOL	C19-C20	7.44	1.57	1.34
91	XA	5145	DOL	C6-N5	6.54	1.49	1.34
91	XA	5145	DOL	C26-N25	6.50	1.48	1.34
91	XA	5145	DOL	C22-C20	5.59	1.58	1.45
90	XA	5144	H8Q	C20-S21	-5.24	1.76	1.82
91	XA	5145	DOL	O36-C37	5.22	1.46	1.34
91	XA	5145	DOL	C42-S39	5.19	1.86	1.78
90	XA	5144	H8Q	O41-C34	4.98	1.45	1.34
91	XA	5145	DOL	C13-C10	4.55	1.57	1.50
91	XA	5145	DOL	C16-C14	4.10	1.57	1.51
92	AX	500	GTP	C5-C6	-4.03	1.39	1.47
91	XA	5145	DOL	C28-C26	3.65	1.55	1.48
90	XA	5144	H8Q	C22-S21	-3.48	1.76	1.82
91	XA	5145	DOL	C8-C6	2.97	1.56	1.50
91	XA	5145	DOL	O27-C26	-2.75	1.19	1.24
91	XA	5145	DOL	O18-C17	-2.67	1.38	1.43
91	XA	5145	DOL	C13-C14	2.47	1.56	1.52
90	XA	5144	H8Q	O41-C43	-2.33	1.42	1.46
92	AX	500	GTP	C2-N3	2.26	1.38	1.33
91	XA	5145	DOL	C24-C23	2.11	1.58	1.50
90	XA	5144	H8Q	C35-C33	-2.07	1.49	1.52
91	XA	5145	DOL	O36-C32	-2.01	1.41	1.44

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	XA	5145	DOL	O40-S39-O41	-15.18	100.88	118.19
91	XA	5145	DOL	C24-N25-C26	-5.85	112.56	122.03
92	AX	500	GTP	PA-O3A-PB	-4.04	118.95	132.83
90	XA	5144	H8Q	O41-C34-C33	3.84	122.03	110.83
91	XA	5145	DOL	C32-O36-C37	-3.76	111.33	117.78
91	XA	5145	DOL	C23-C22-C20	-3.48	120.63	125.89
91	XA	5145	DOL	C4-N5-C1	-3.39	108.28	112.45
90	XA	5144	H8Q	C43-O41-C34	-3.29	112.74	117.51
92	AX	500	GTP	C5-C6-N1	3.27	119.72	113.95
90	XA	5144	H8Q	C3-C2-N71	-3.26	107.38	112.69
90	XA	5144	H8Q	C40-C35-C33	-3.24	115.48	120.80
92	AX	500	GTP	PB-O3B-PG	-3.21	121.80	132.83
90	XA	5144	H8Q	C50-C51-N52	3.14	121.92	115.78
92	AX	500	GTP	C8-N7-C5	3.07	108.84	102.99
92	AX	500	GTP	C2-N1-C6	-3.04	119.51	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	XA	5144	H8Q	C17-C16-C15	2.99	119.86	115.43
90	XA	5144	H8Q	O41-C34-O42	-2.97	118.38	123.94
90	XA	5144	H8Q	C36-C35-C33	2.93	125.62	120.80
91	XA	5145	DOL	C30-C29-C28	-2.87	118.60	126.44
90	XA	5144	H8Q	C35-C33-N31	-2.85	105.49	112.89
90	XA	5144	H8Q	O58-C50-C51	-2.67	116.60	120.59
91	XA	5145	DOL	O36-C32-C30	2.61	111.44	107.09
90	XA	5144	H8Q	C14-C15-C16	2.57	111.23	107.65
91	XA	5145	DOL	C3-C4-N5	2.55	105.96	103.33
91	XA	5145	DOL	C37-C1-N5	-2.51	107.90	112.26
90	XA	5144	H8Q	C17-C18-N13	-2.47	107.50	109.92
90	XA	5144	H8Q	C34-C33-N31	2.36	114.46	109.54
90	XA	5144	H8Q	C53-N52-C51	2.34	121.26	116.83
92	AX	500	GTP	O6-C6-C5	-2.13	120.21	124.37
90	XA	5144	H8Q	C2-C1-N13	2.05	122.76	117.72

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	XA	5144	H8Q	C2-C1-N13-C14
90	XA	5144	H8Q	C2-C1-N13-C18
90	XA	5144	H8Q	O1-C1-N13-C14
90	XA	5144	H8Q	O1-C1-N13-C18
90	XA	5144	H8Q	C33-C34-O41-C43
90	XA	5144	H8Q	O42-C34-O41-C43
90	XA	5144	H8Q	C59-C62-N63-C65
90	XA	5144	H8Q	C59-C62-N63-C68
90	XA	5144	H8Q	O64-C62-N63-C65
90	XA	5144	H8Q	O64-C62-N63-C68
90	XA	5144	H8Q	C66-C65-C69-N71
90	XA	5144	H8Q	C66-C65-C69-O70
90	XA	5144	H8Q	C65-C69-N71-C2
90	XA	5144	H8Q	C65-C69-N71-C72
90	XA	5144	H8Q	O70-C69-N71-C2
90	XA	5144	H8Q	O70-C69-N71-C72
91	XA	5145	DOL	C3-C2-S39-C42
91	XA	5145	DOL	C1-C2-S39-O41
91	XA	5145	DOL	C1-C2-S39-O40
91	XA	5145	DOL	C1-C2-S39-C42
91	XA	5145	DOL	C43-C42-S39-C2
91	XA	5145	DOL	C43-C42-S39-O41

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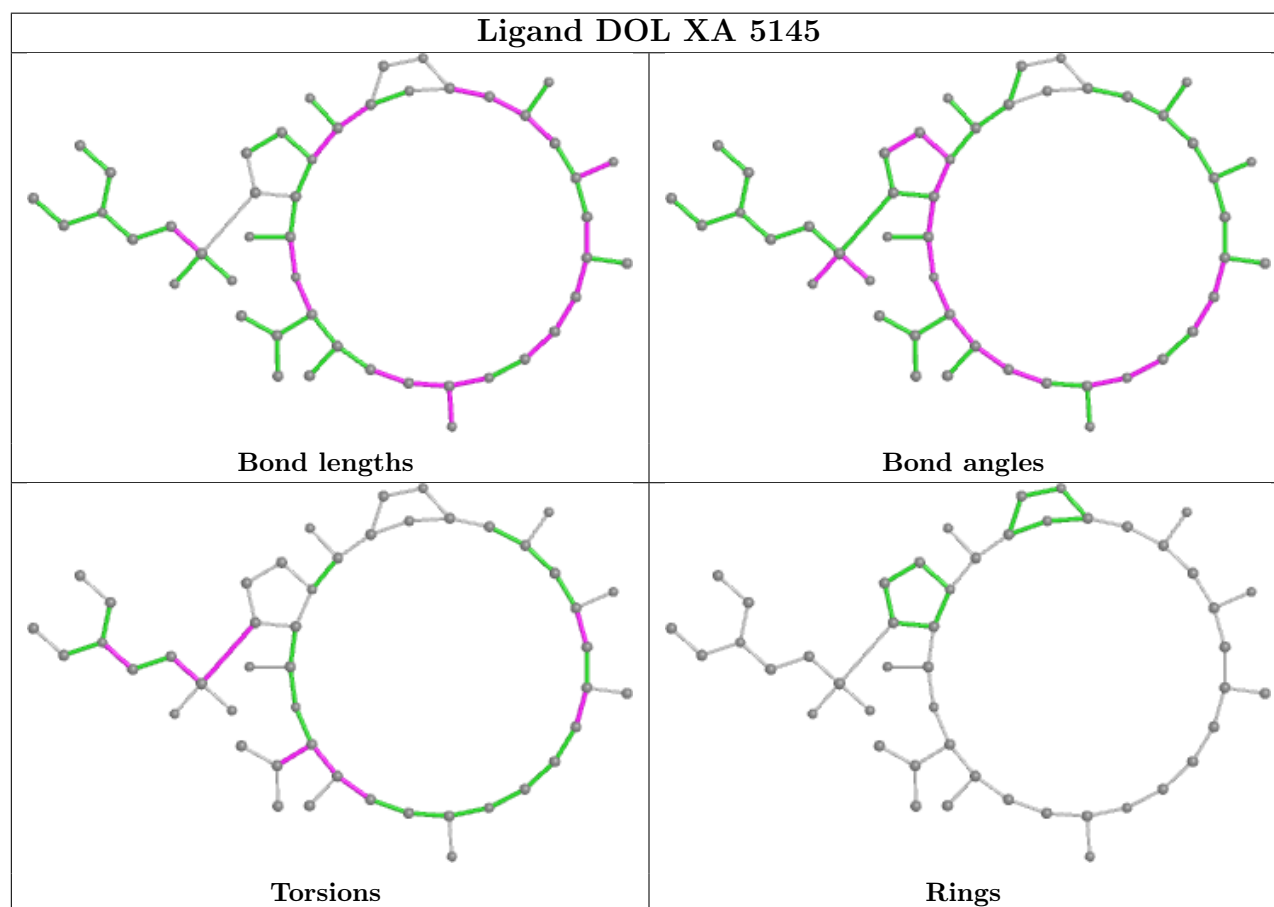
Mol	Chain	Res	Type	Atoms
91	XA	5145	DOL	C29-C30-C32-C33
91	XA	5145	DOL	C31-C30-C32-C33
92	AX	500	GTP	PB-O3B-PG-O3G
92	AX	500	GTP	C5'-O5'-PA-O3A
90	XA	5144	H8Q	C6-C7-N10-C12
90	XA	5144	H8Q	C8-C7-N10-C11
90	XA	5144	H8Q	C6-C7-N10-C11
90	XA	5144	H8Q	C8-C7-N10-C12
90	XA	5144	H8Q	C43-C45-C46-O47
91	XA	5145	DOL	C3-C2-S39-O41
90	XA	5144	H8Q	C43-C45-C46-N49
91	XA	5145	DOL	O36-C32-C33-C35
90	XA	5144	H8Q	N48-C45-C46-O47
92	AX	500	GTP	O4'-C4'-C5'-O5'
90	XA	5144	H8Q	N48-C45-C46-N49
91	XA	5145	DOL	C30-C32-C33-C34
91	XA	5145	DOL	C28-C29-C30-C31
91	XA	5145	DOL	C3-C2-S39-O40
91	XA	5145	DOL	O36-C32-C33-C34
91	XA	5145	DOL	C31-C30-C32-O36
92	AX	500	GTP	C5'-O5'-PA-O2A
91	XA	5145	DOL	C29-C30-C32-O36
92	AX	500	GTP	C3'-C4'-C5'-O5'
91	XA	5145	DOL	O18-C17-C19-C20
90	XA	5144	H8Q	N13-C1-C2-C3
90	XA	5144	H8Q	N13-C18-C30-N31
90	XA	5144	H8Q	N13-C18-C30-O32
90	XA	5144	H8Q	N31-C33-C34-O42
90	XA	5144	H8Q	C34-C33-C35-C40
90	XA	5144	H8Q	N31-C33-C34-O41
90	XA	5144	H8Q	C34-C33-C35-C36
92	AX	500	GTP	PB-O3B-PG-O1G
92	AX	500	GTP	PB-O3B-PG-O2G
91	XA	5145	DOL	C42-C43-N44-C45
92	AX	500	GTP	C5'-O5'-PA-O1A
91	XA	5145	DOL	C30-C32-C33-C35
91	XA	5145	DOL	C42-C43-N44-C47
91	XA	5145	DOL	C19-C20-C22-C23

There are no ring outliers.

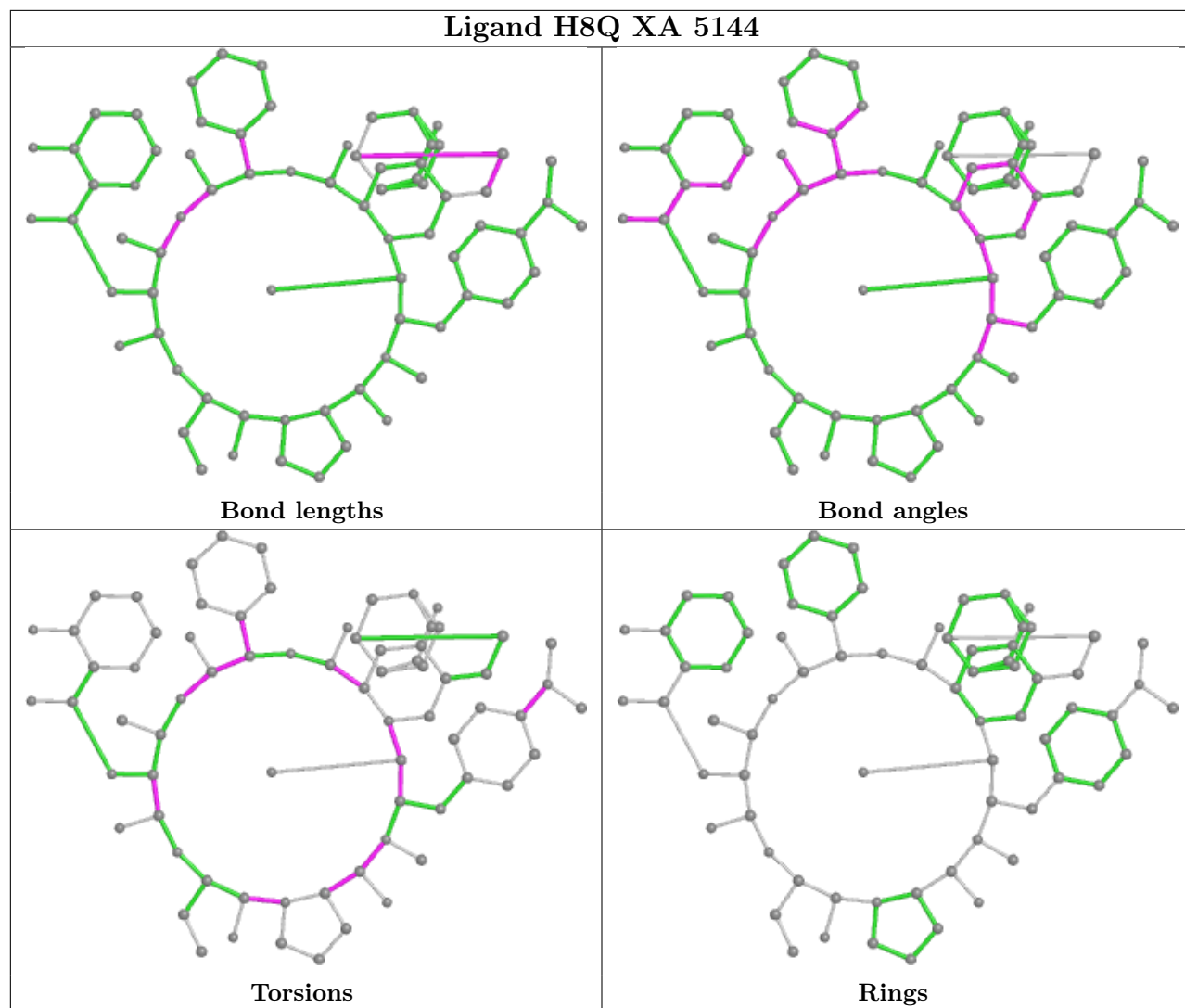
1 monomer is involved in 4 short contacts:

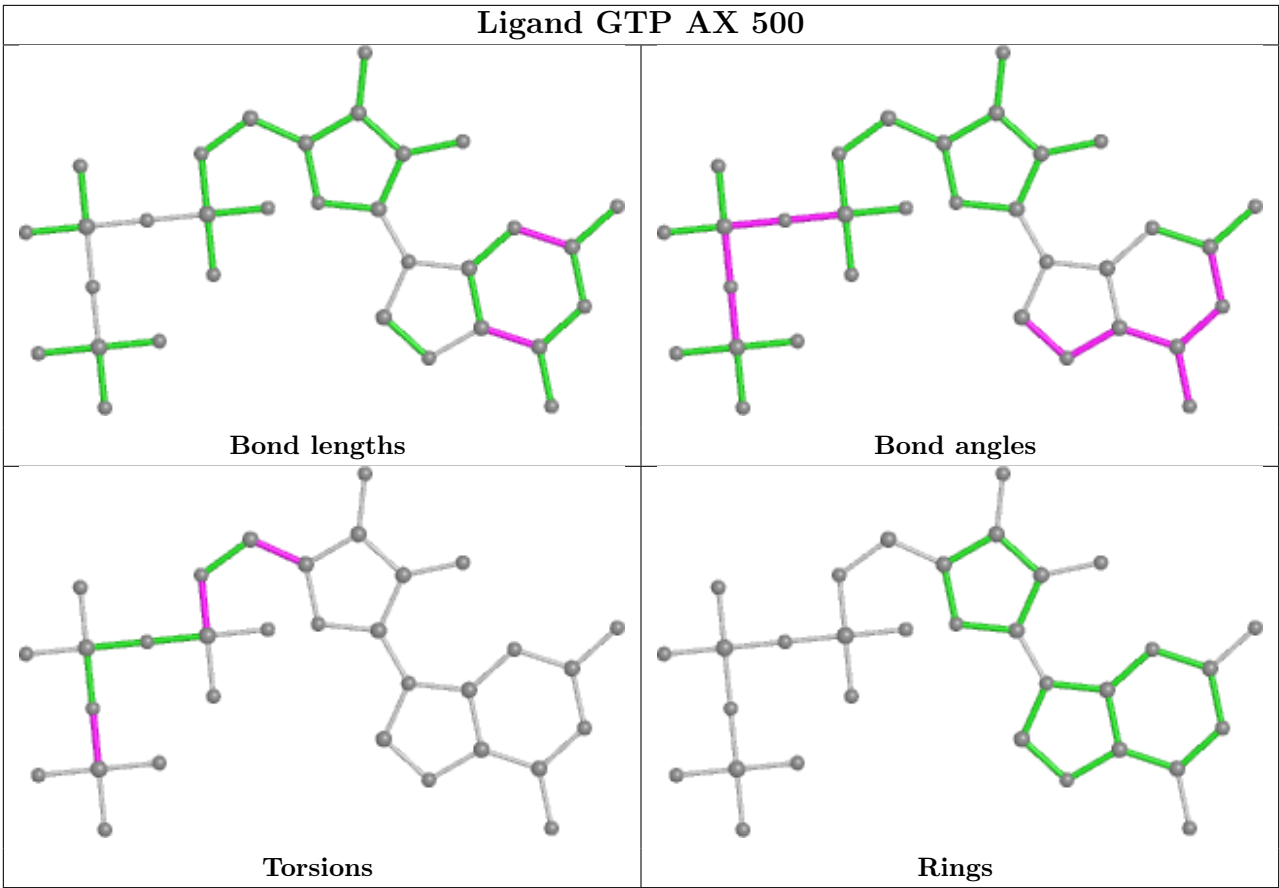
Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	XA	5144	H8Q	4	0

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



Ligand H8Q XA 5144





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
84	r3	2
16	A4	2
8	7	2
82	r	1
38	AV	1
7	6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r3	17:Y5P	O3'	17(A):P5P	P	10.13

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r3	16:Y5P	O3'	17:Y5P	P	8.44
1	A4	537:ARG	C	538:ASP	N	6.17
1	7	285:ASN	C	286:LEU	N	5.97
1	r	134:ARG	C	135:LEU	N	5.37
1	AV	269:SER	C	270:PRO	N	4.55
1	6	79:GLY	C	80:GLU	N	3.39
1	A4	143:GLU	C	144:TYR	N	3.07
1	7	185:LEU	C	186:ASP	N	3.05

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11394. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

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 ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.