



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:57 PM UTC

PDB ID : 6ZSA / pdb_00006zsa
EMDB ID : EMD-11391
Title : Human mitochondrial ribosome bound to mRNA, A-site tRNA and P-site tRNA
Authors : Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.
Deposited on : 2020-07-15
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

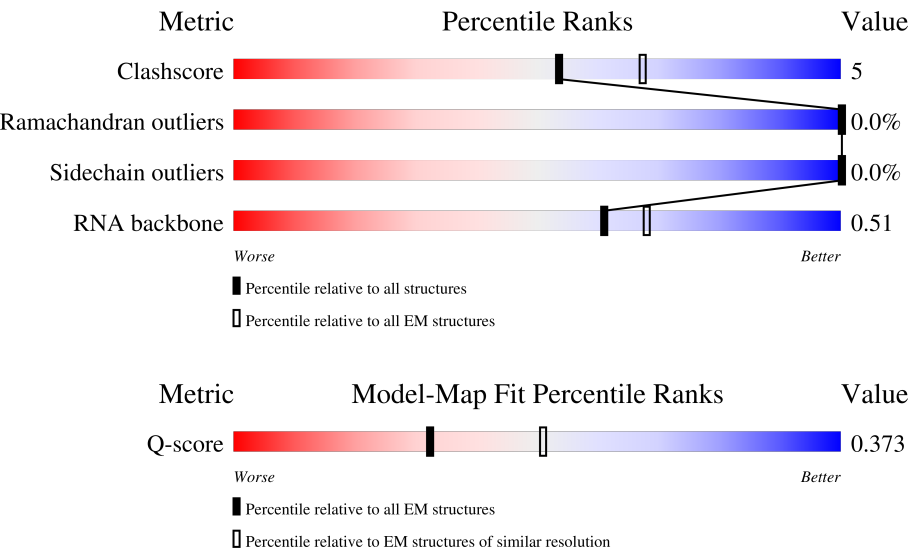
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 Å.

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



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

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

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

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Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	XA	1559	
12	A0	218	
13	A1	323	
14	A2	118	
15	A3	199	
16	A4	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	

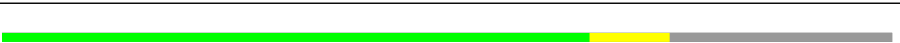
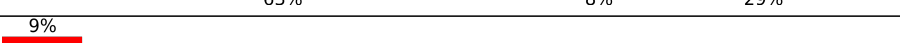
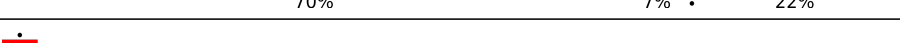
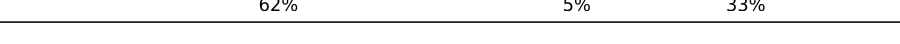
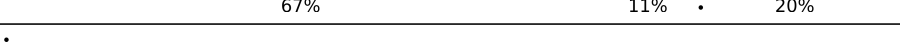
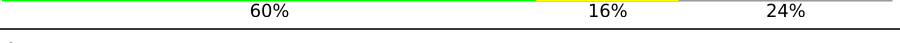
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Mol	Chain	Length	Quality of chain
29	AM	137	
30	AN	130	
31	AO	258	
32	AP	142	
33	AQ	87	
34	AR	360	
35	AS	190	
36	AT	173	
37	AU	205	
38	AV	414	
39	AW	187	
40	AX	398	
41	AY	395	
42	AZ	106	
43	XB	72	
44	XD	305	
45	XE	348	
46	XF	311	
47	XH	267	
48	XI	261	
49	XJ	192	
50	XK	178	
51	XL	145	
52	XM	296	
53	XN	251	

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Mol	Chain	Length	Quality of chain
54	XO	175	
55	XP	180	
56	XQ	292	
57	XR	149	
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	

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Mol	Chain	Length	Quality of chain
79	o	102	
80	p	206	
81	q	222	
82	r	196	
83	r1	14	
84	r2	76	
85	r3	75	
86	s	439	
87	t1	198	
87	t2	198	
87	t3	198	
87	t4	198	
87	t5	198	
87	t6	198	

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 313757 atoms, of which 143060 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
			782	233	406	83	59	1		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	291	Total	C	H	N	O	S	0	0
			4737	1514	2372	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
			48000	14284	16169	5756	10293	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
			29598	8800	9970	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
			5502	1706	2786	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
			3384	1069	1716	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
			4995	1593	2490	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
			2673	850	1343	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
			5729	1841	2862	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 tRNAVal.

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
			3739	1145	1897	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
			4798	1539	2402	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
			2639	829	1355	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	14	Total	C	N	O	P		
			252	126	28	84	14		
								0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
84	r2	76	Total	C	N	O	P		
			1486	723	230	457	76		
								0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
85	r3	75	Total	C	N	O	P		
			1459	711	222	451	75		
								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		
			732	228	378	56	70		
								2	0
87	t2	30	Total	C	H	N	O		
			502	154	265	37	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

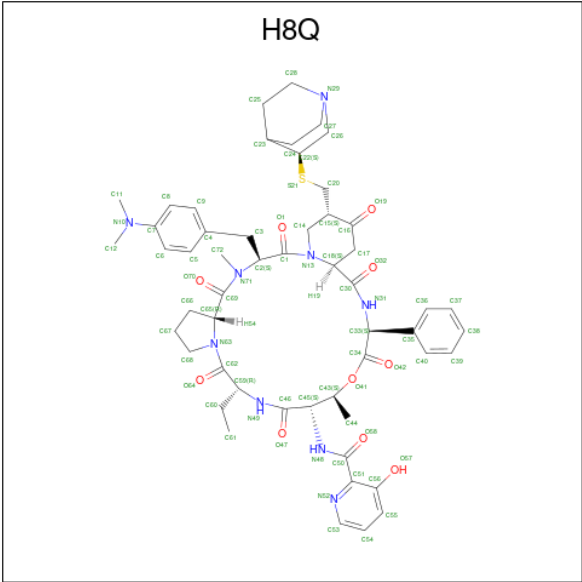
- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	r	1	Total 1	Zn 1	0

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

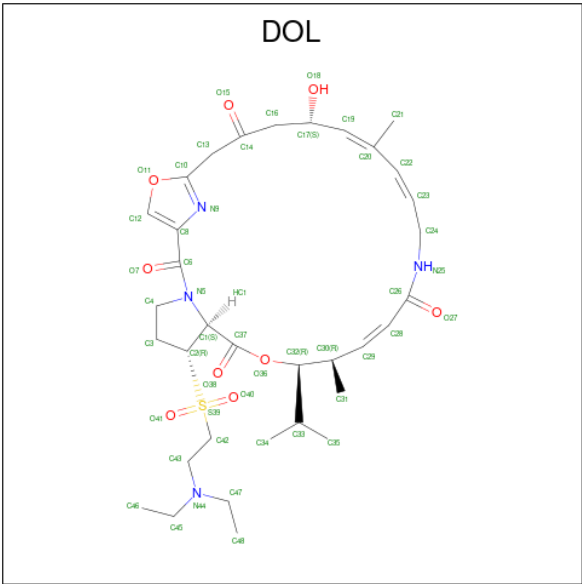
Mol	Chain	Residues	Atoms		AltConf
89	9	1	Total 1	Mg 1	0
89	XA	143	Total 143	Mg 143	0
89	AA	46	Total 46	Mg 46	0
89	XD	1	Total 1	Mg 1	0
89	XI	1	Total 1	Mg 1	0
89	XM	2	Total 2	Mg 2	0
89	g	1	Total 1	Mg 1	0

- 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 (CCD ID: H8Q) (formula: C₅₃H₆₇N₉O₁₀S).



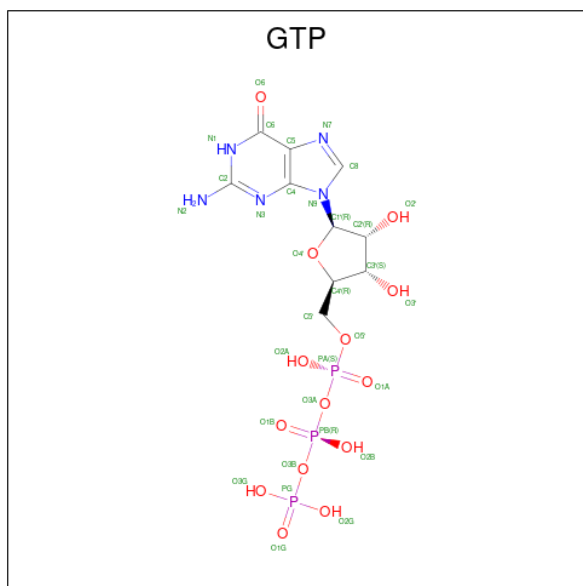
Mol	Chain	Residues	Atoms						AltConf
90	XA	1	Total	C	H	N	O	S	0
			140	53	67	9	10	1	

- 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 (CCD ID: DOL) (formula: $C_{34}H_{50}N_4O_9S$).



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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

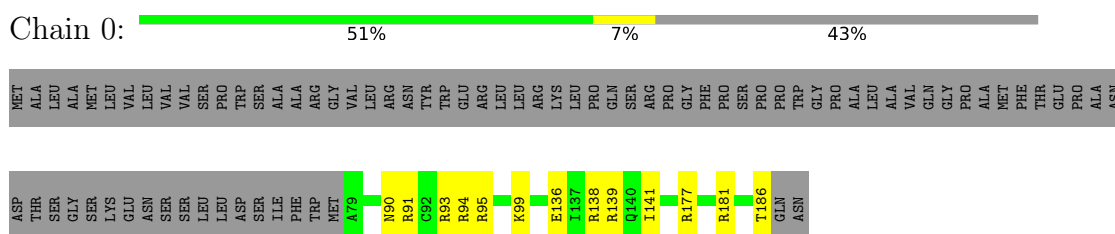


Mol	Chain	Residues	Atoms					AltConf	
92	AX	1	Total	C	H	N	O	P	0
			42	10	10	5	14	3	

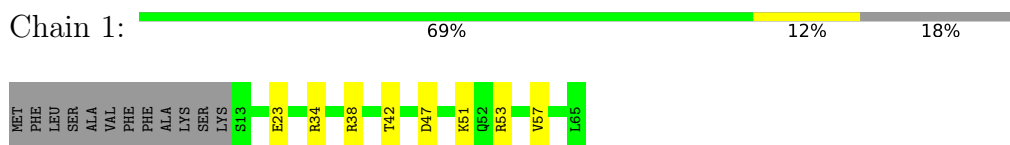
3 Residue-property plots

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

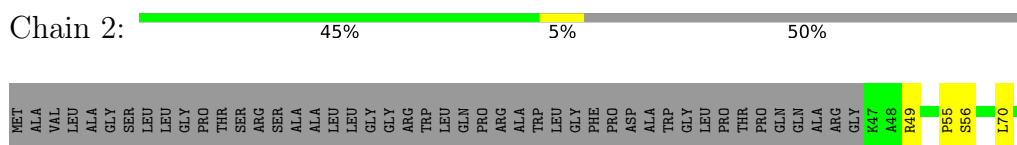
- Molecule 1: 39S ribosomal protein L32, mitochondrial



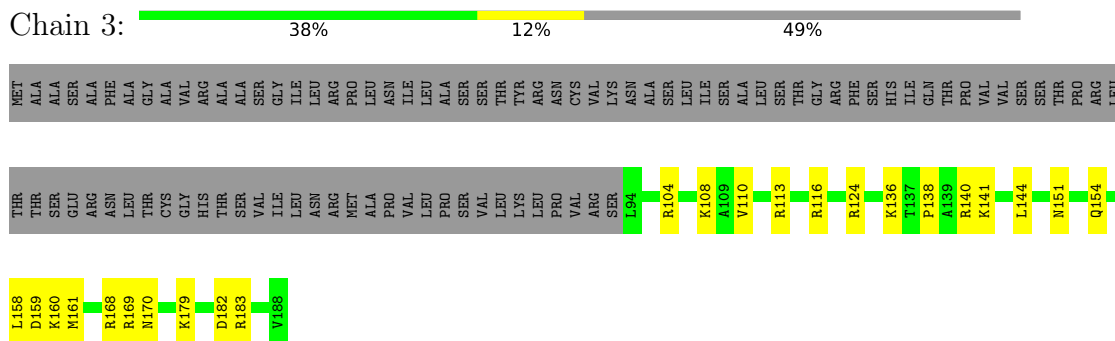
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial

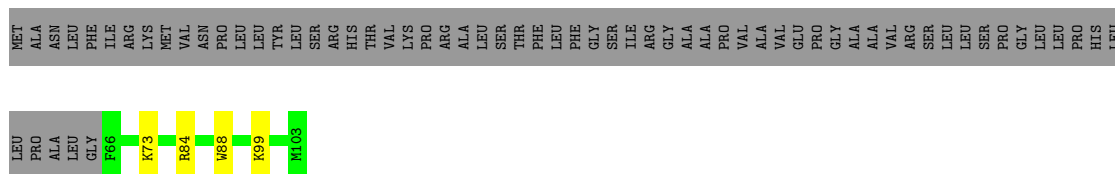


- Molecule 4: 39S ribosomal protein L35, mitochondrial



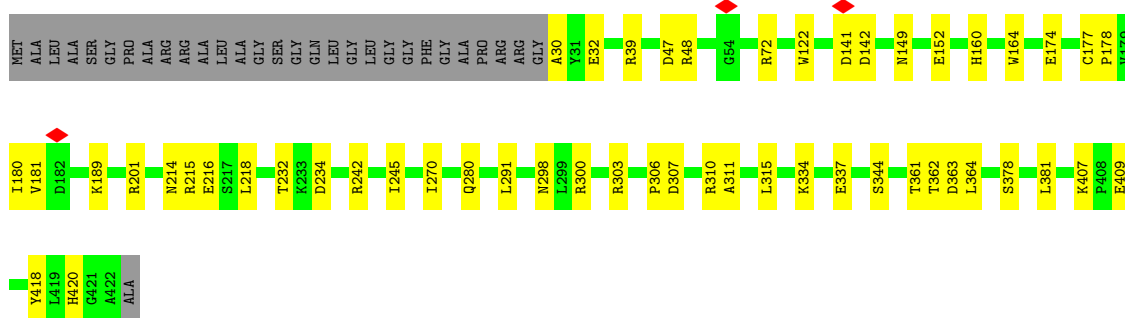
- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:  33% 63%



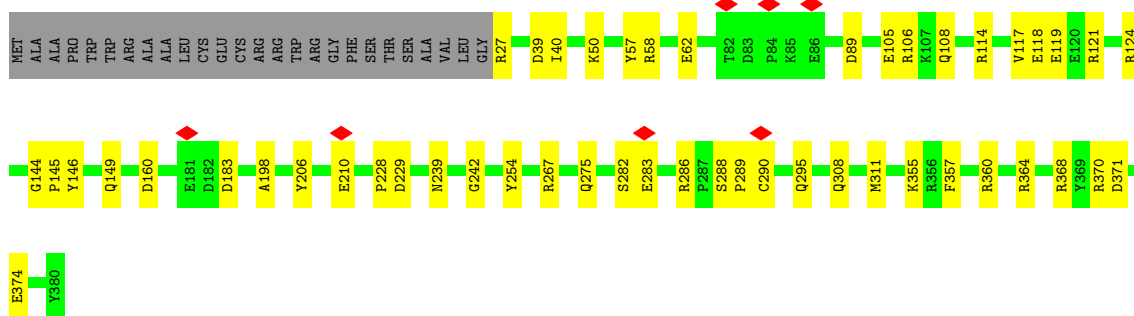
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:  81% 12% 7%



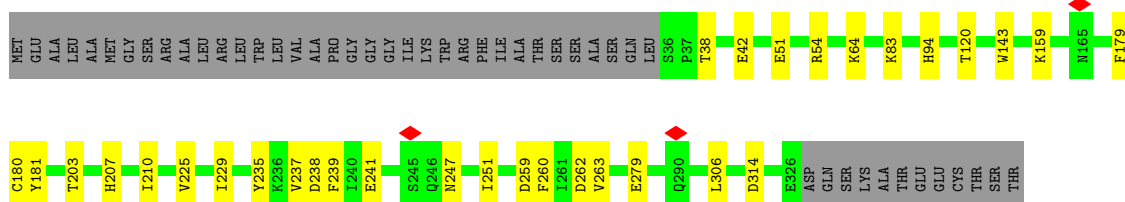
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:  80% 13% 7%

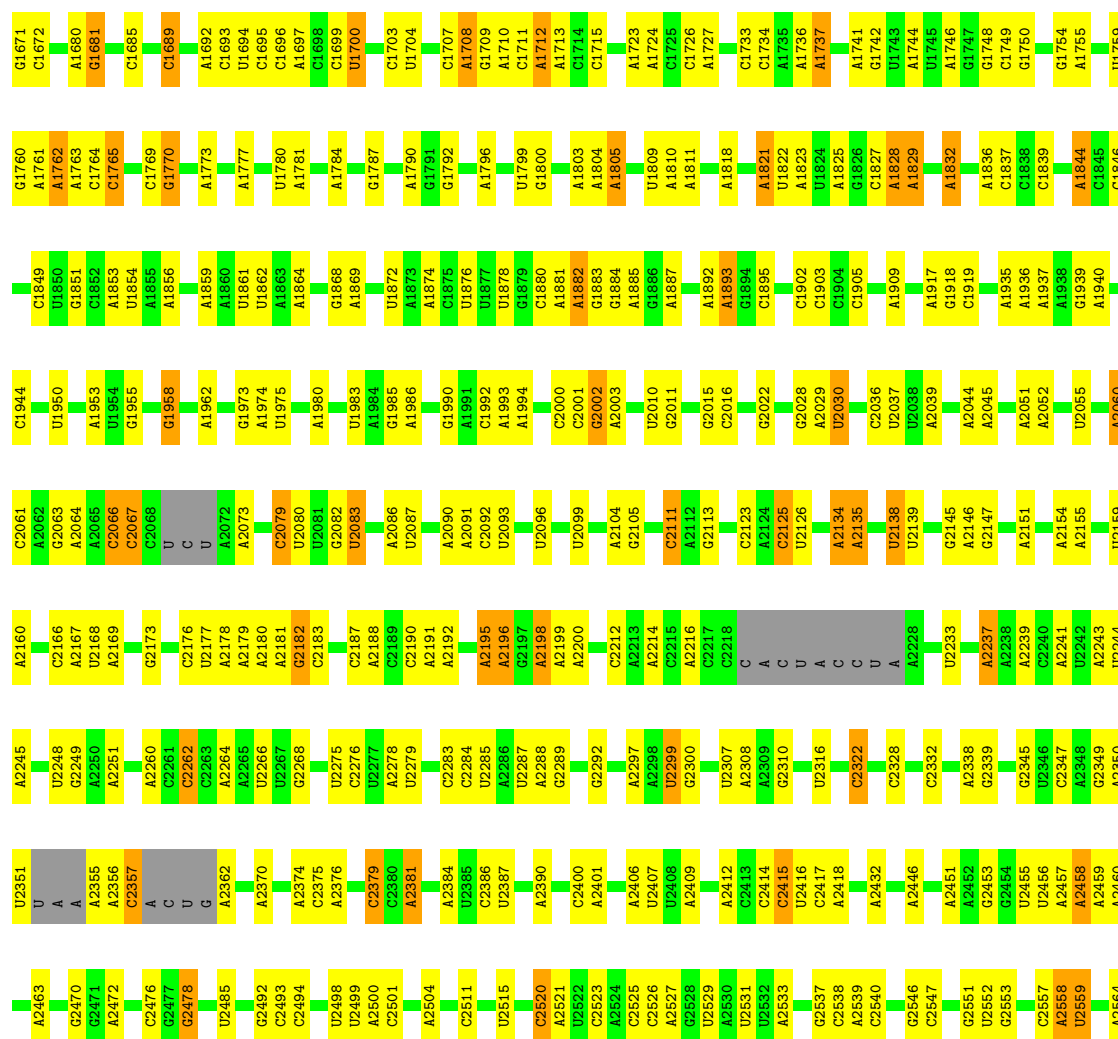
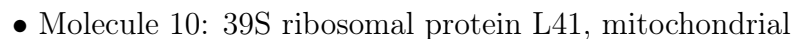


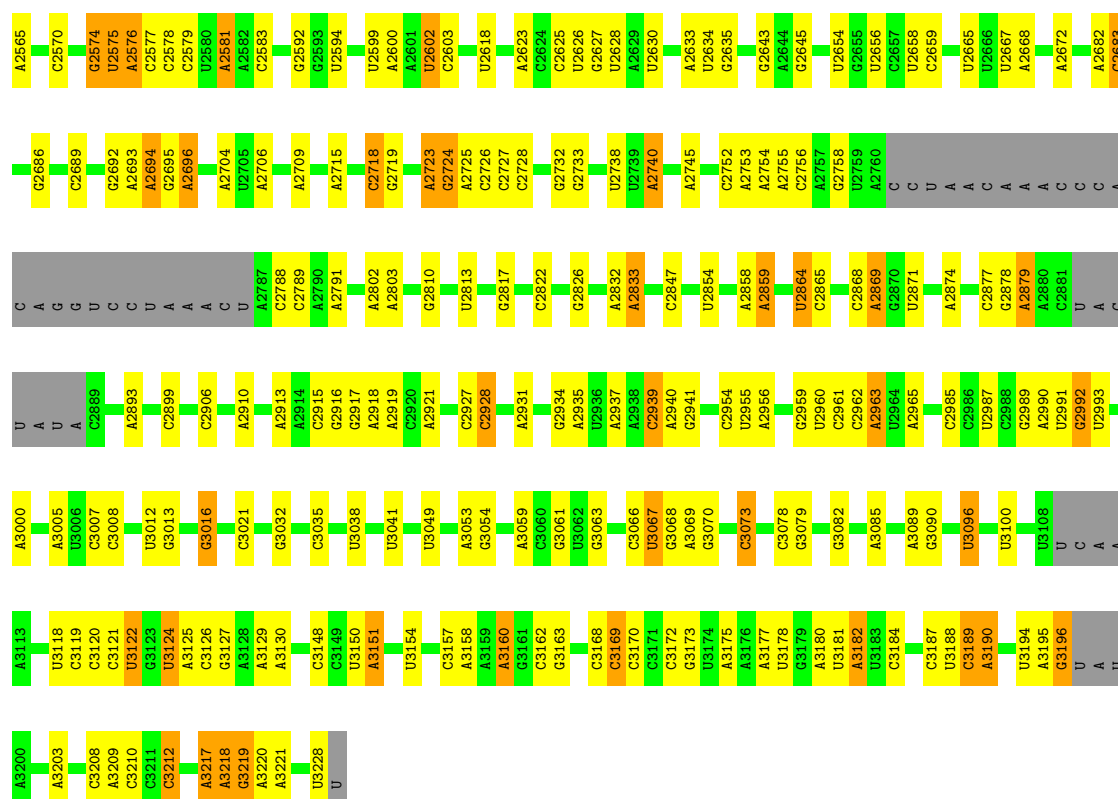
- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:  77% 9% 14%

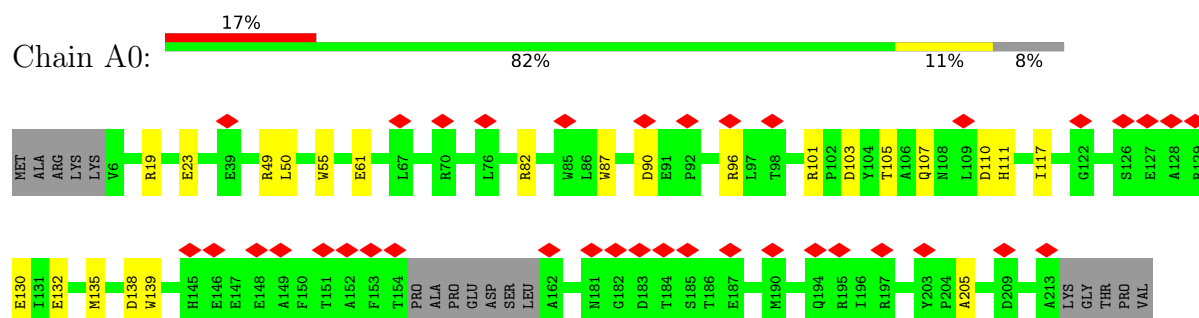


- Molecule 9: 39S ribosomal protein L40, mitochondrial

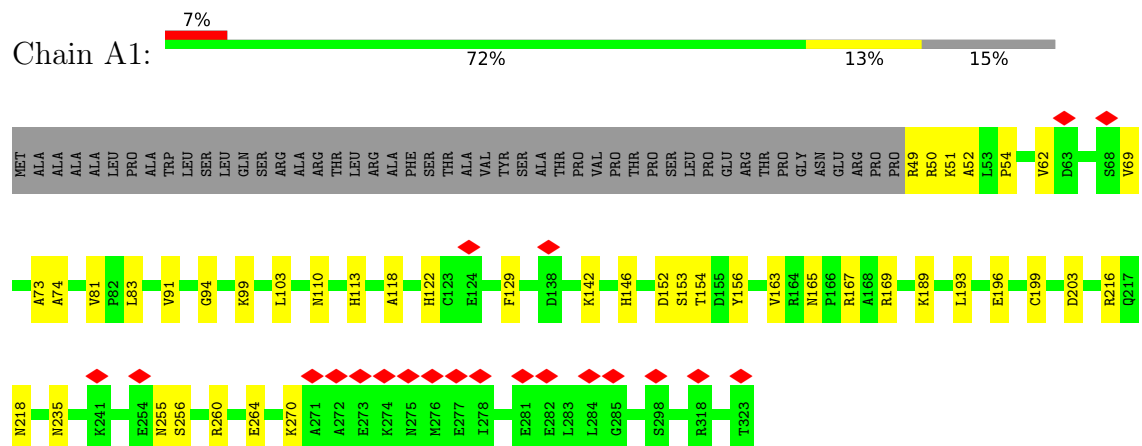




- Molecule 12: 28S ribosomal protein S34, mitochondrial

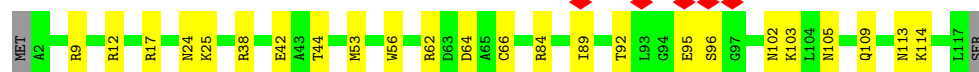


- Molecule 13: 28S ribosomal protein S35, mitochondrial



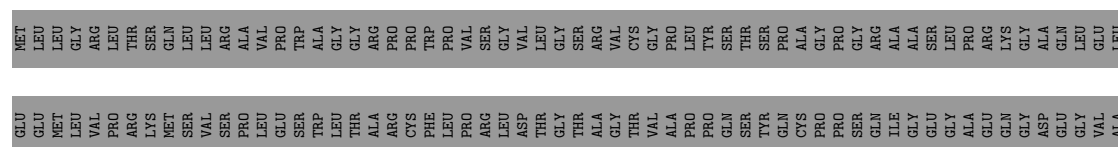
- Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2: 



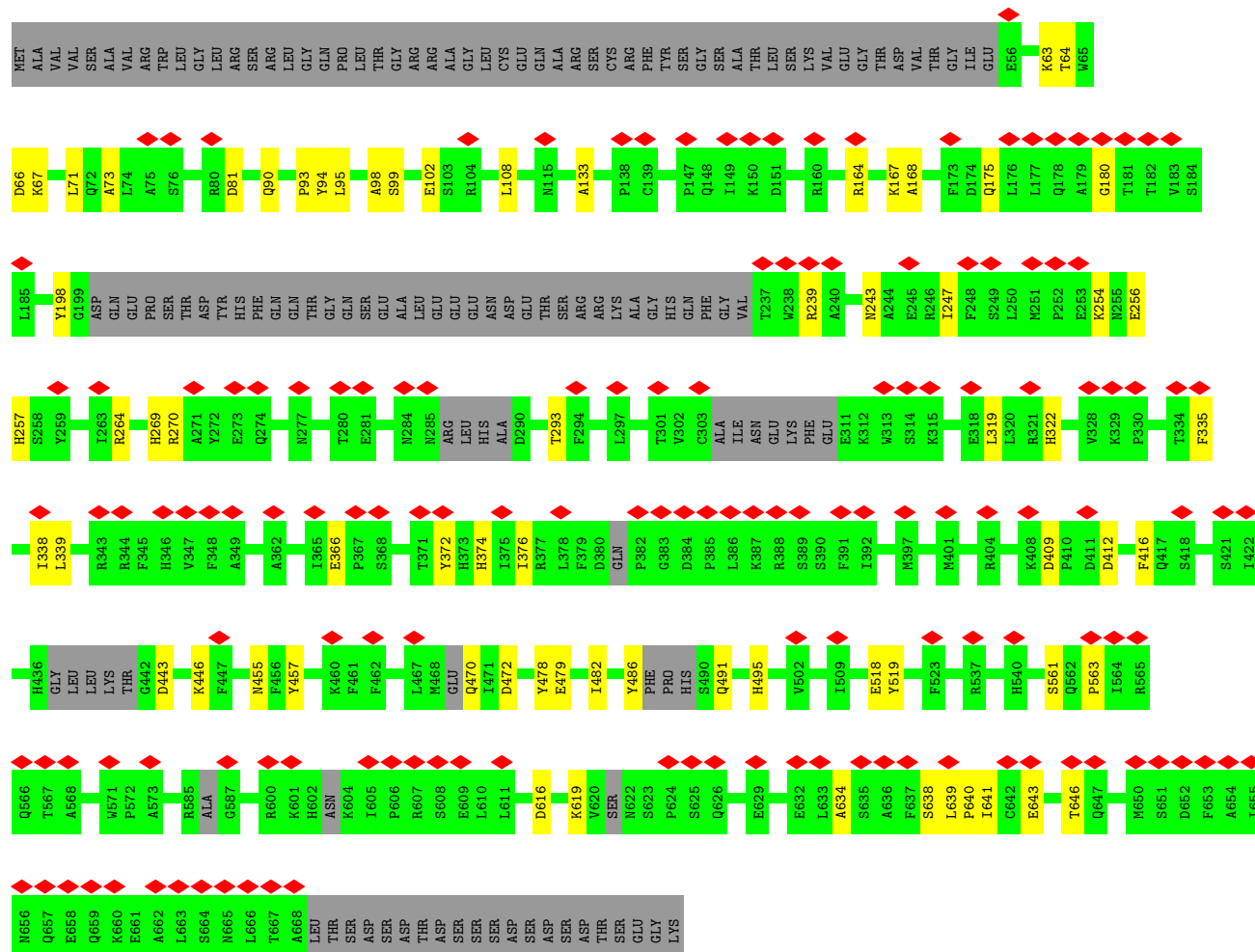
• Molecule 15: Aurora kinase A-interacting protein

Chain A3: 

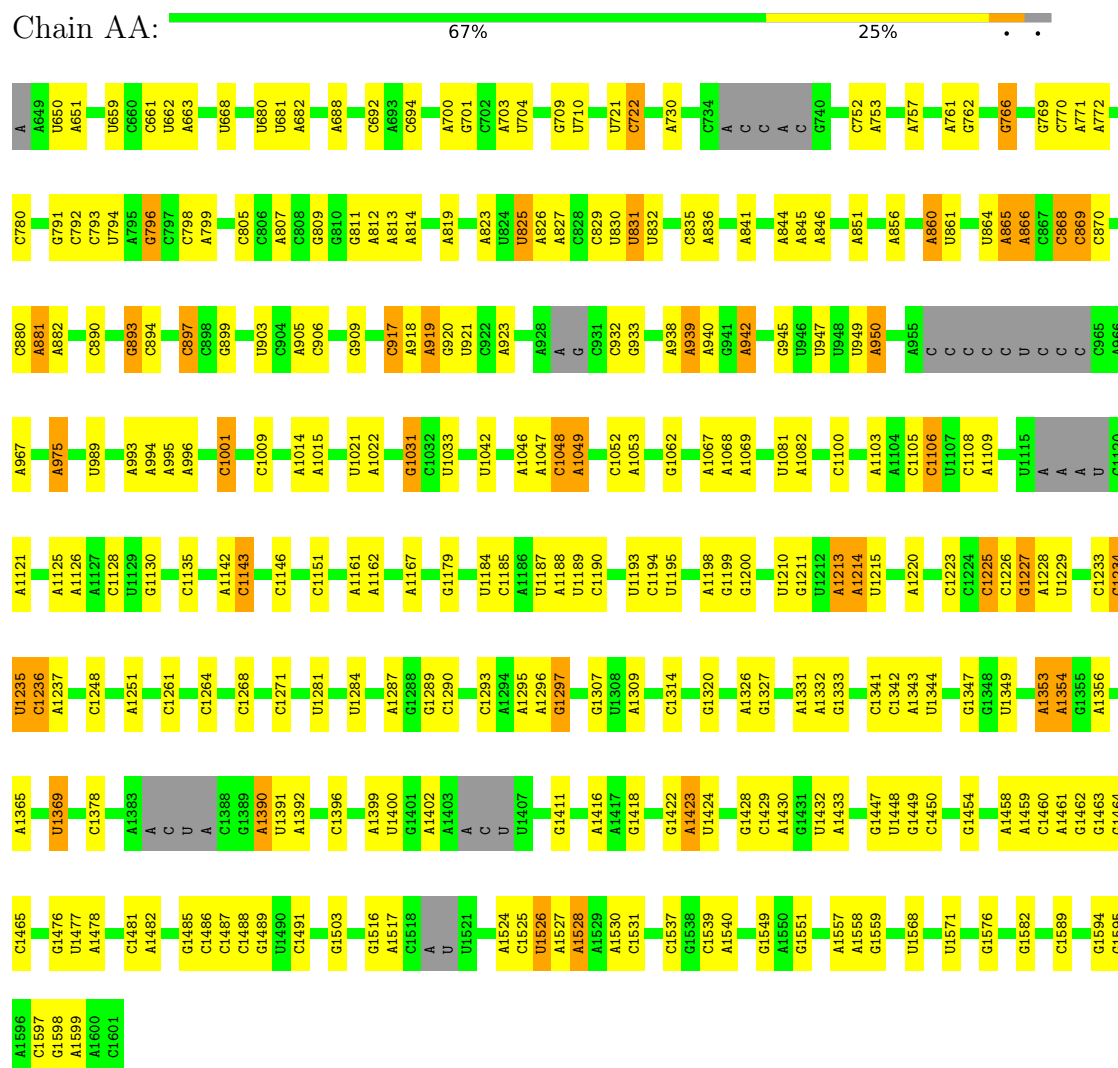


• Molecule 16: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

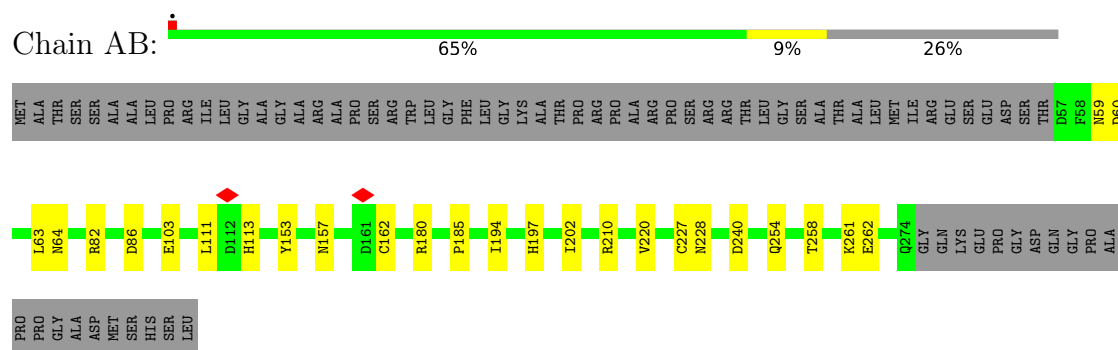
Chain A4: 



- Molecule 17: 12S mitochondrial rRNA



- Molecule 18: 28S ribosomal protein S2, mitochondrial

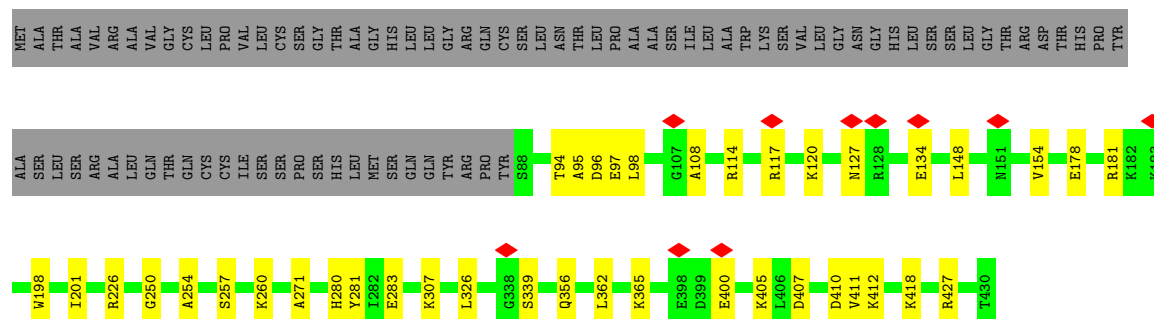
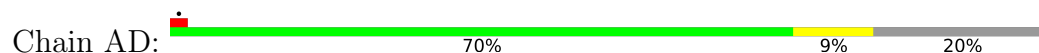


- Molecule 19: 28S ribosomal protein S24, mitochondrial

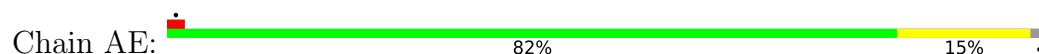




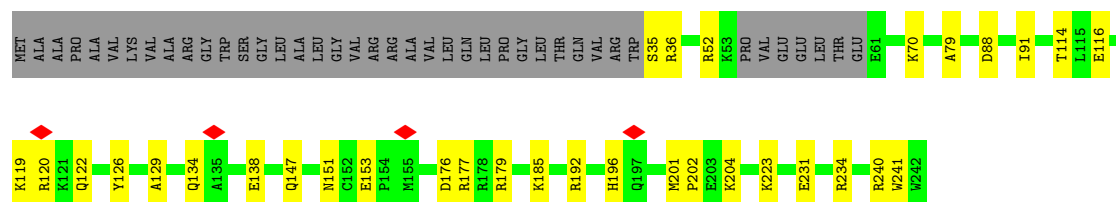
- Molecule 20: 28S ribosomal protein S5, mitochondrial



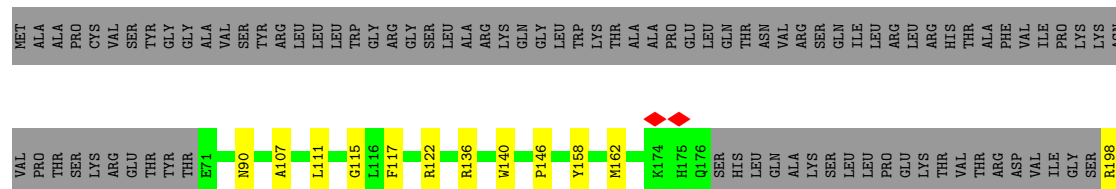
- Molecule 21: 28S ribosomal protein S6, mitochondrial

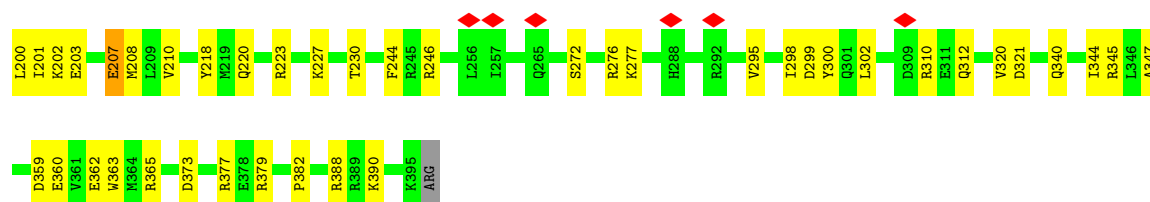


- Molecule 22: 28S ribosomal protein S7, mitochondrial



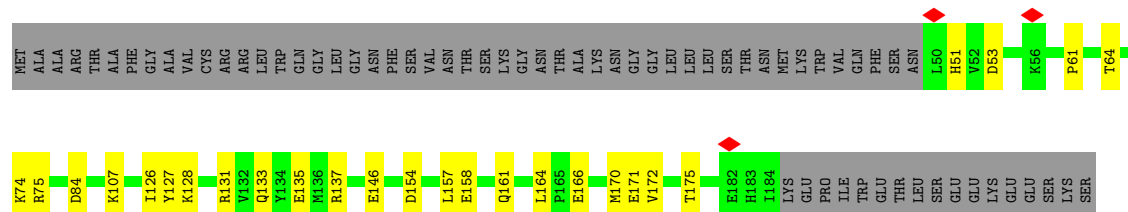
- Molecule 23: 28S ribosomal protein S9, mitochondrial





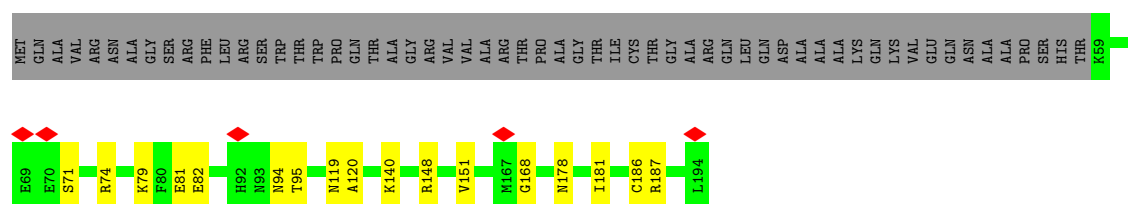
- Molecule 24: 28S ribosomal protein S10, mitochondrial

Chain AH: 54% 13% 33%



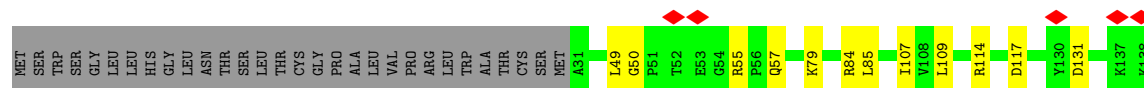
- Molecule 25: 28S ribosomal protein S11, mitochondrial

Chain AI: 61% 9% 30%



- Molecule 26: 28S ribosomal protein S12, mitochondrial

Chain AJ: 70% 9% 22%



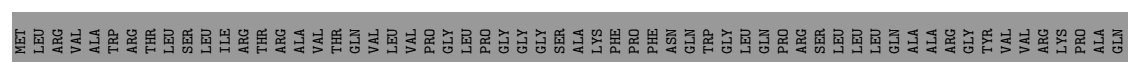
- Molecule 27: 28S ribosomal protein S14, mitochondrial

Chain AK: 67% 12% 21%

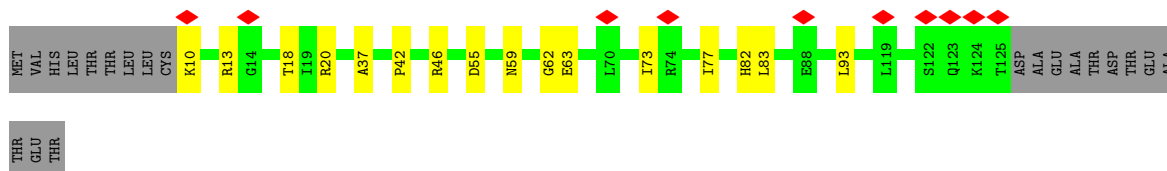
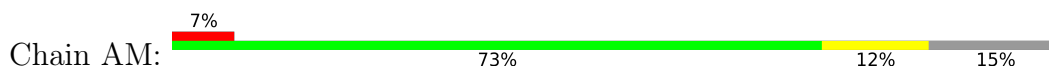


- Molecule 28: 28S ribosomal protein S15, mitochondrial

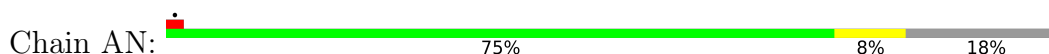
Chain AL: 55% 9% 36%



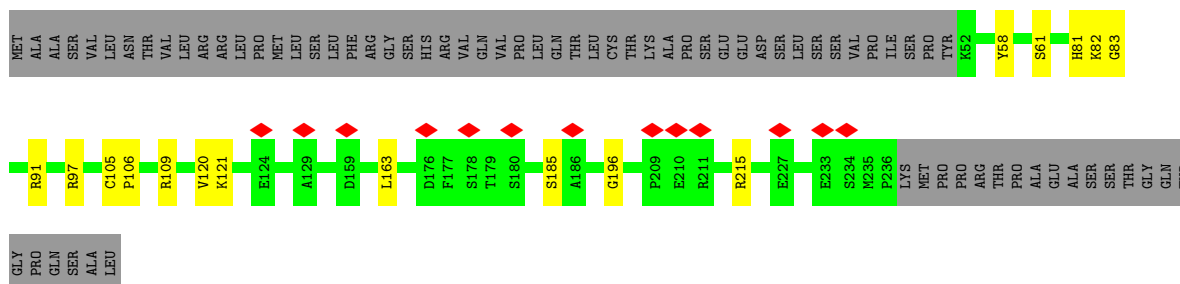
- Molecule 29: 28S ribosomal protein S16, mitochondrial



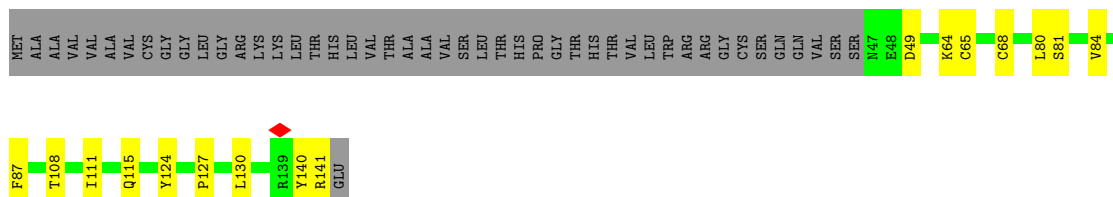
- Molecule 30: 28S ribosomal protein S17, mitochondrial



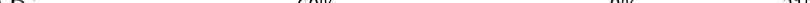
- Molecule 31: 28S ribosomal protein S18b, mitochondrial

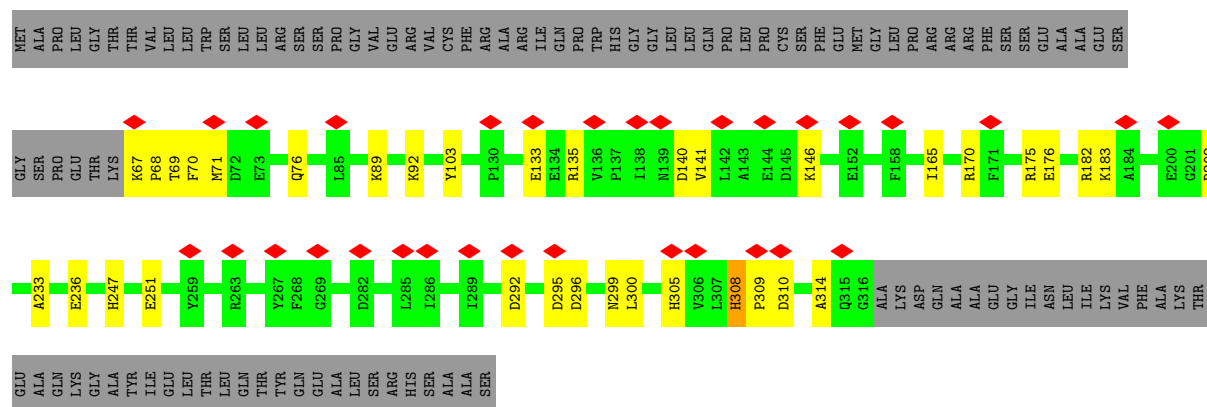


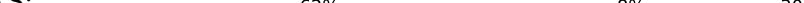
- Molecule 32: 28S ribosomal protein S18c, mitochondrial

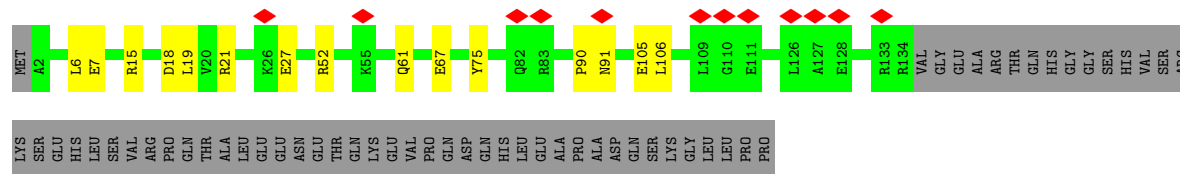


- Molecule 33: 28S ribosomal protein S21, mitochondrial

- Chain AR: 

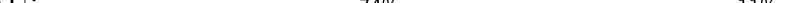


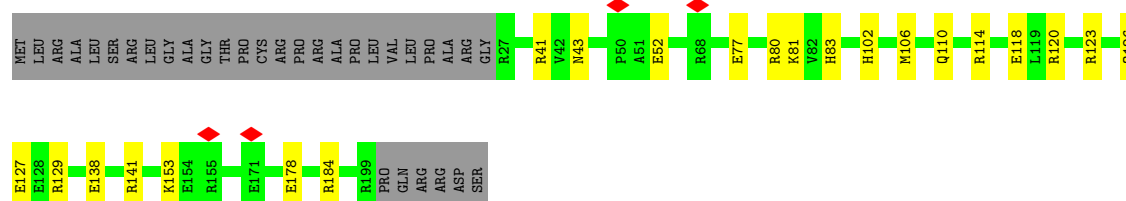
- Chain AS: 



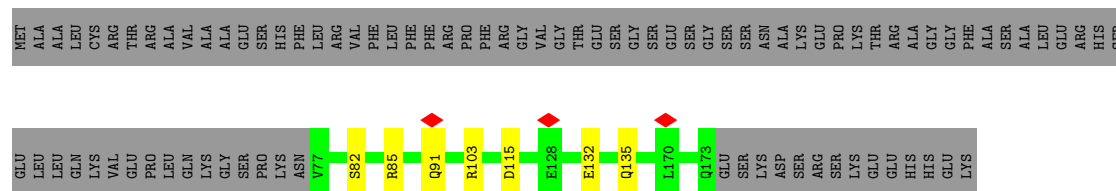
- Chain AT:



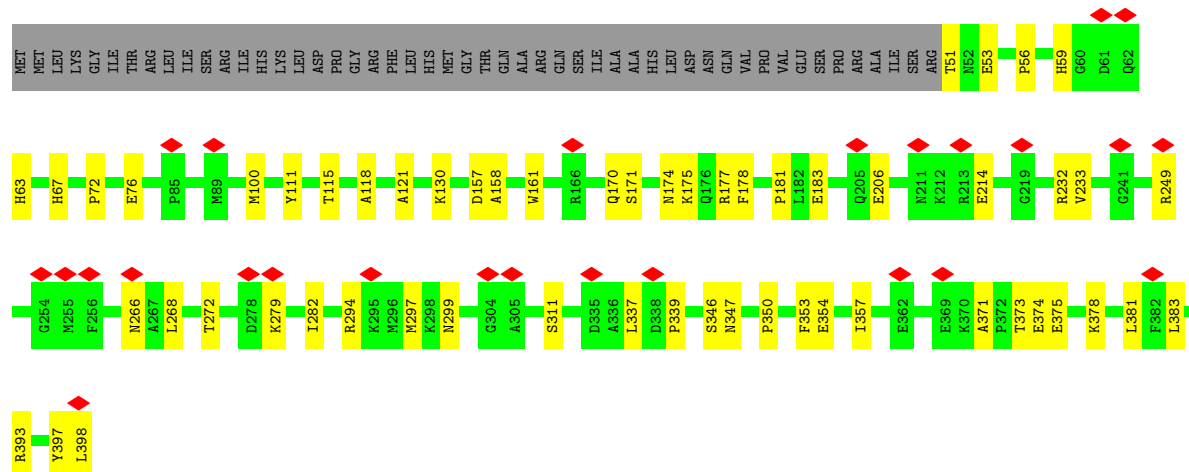
- Chain AU: 



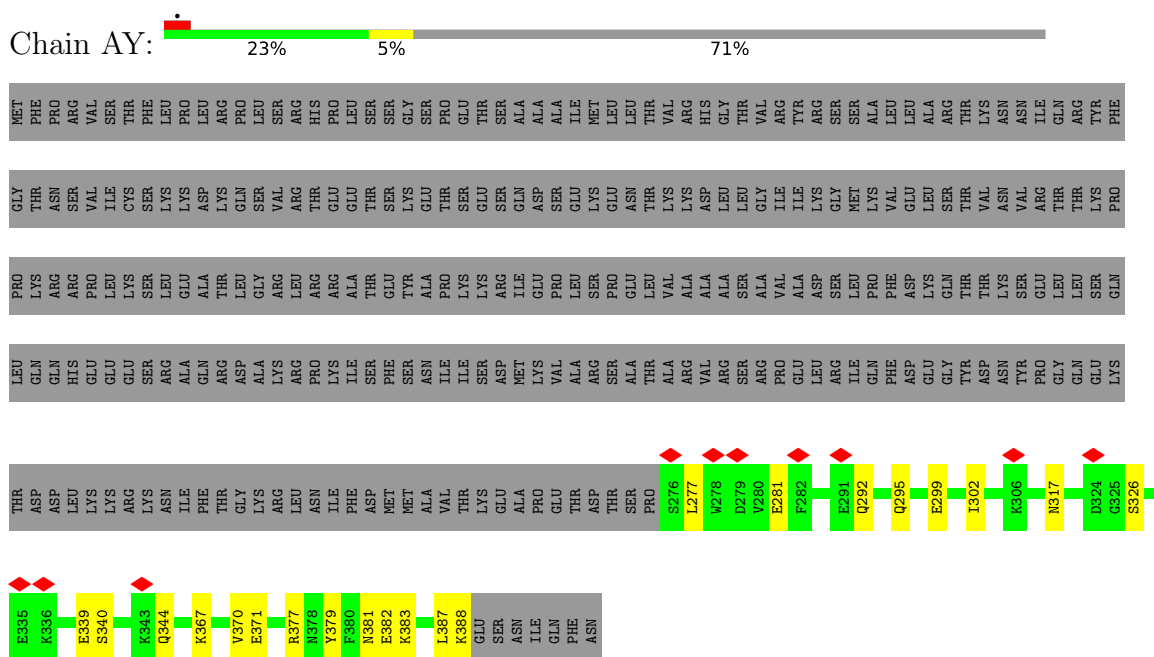
Chain AV:



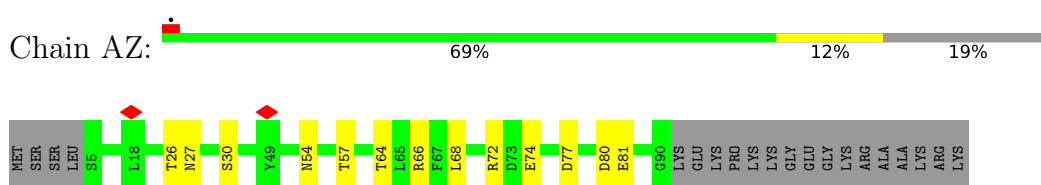
Chain AX:



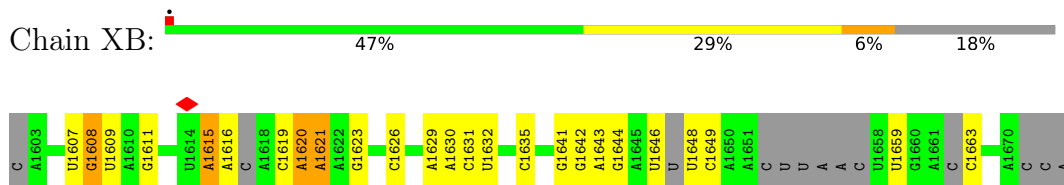
- Molecule 41: 28S ribosomal protein S31, mitochondrial



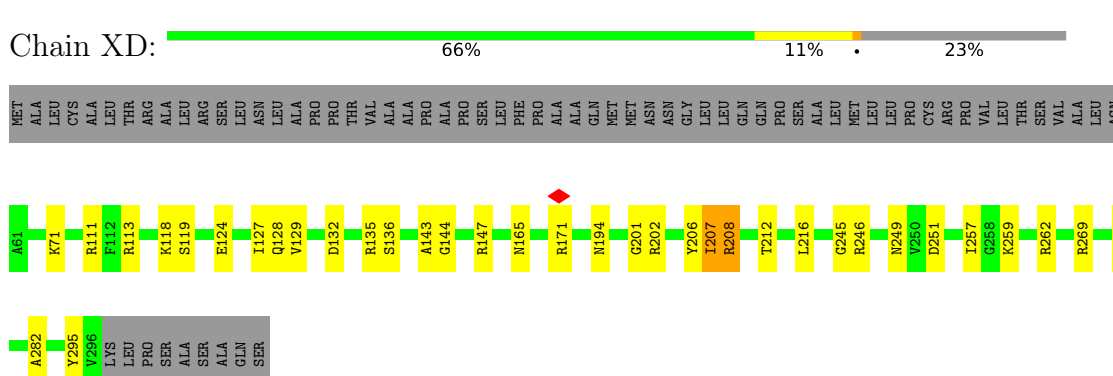
- Molecule 42: 28S ribosomal protein S33, mitochondrial



- Molecule 43: mitochondrial tRNA^{Val}



- Molecule 44: 39S ribosomal protein L2, mitochondrial



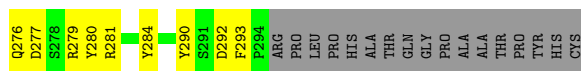
- Molecule 45: 39S ribosomal protein L3, mitochondrial

Response	Percentage
Yes	81%
No	6%
Don't know	13%



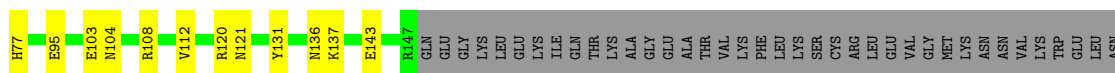
- Molecule 46: 39S ribosomal protein L4, mitochondrial

App Type	Percentage
Shopping app	64%
Social media app	17%
Productivity app	20%



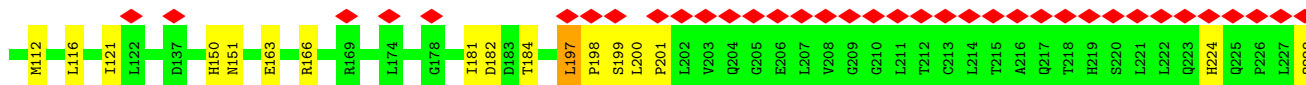
- Molecule 47: 39S ribosomal protein L9, mitochondrial

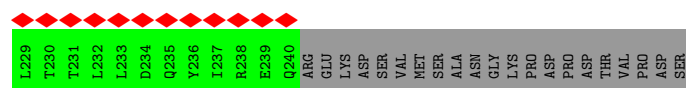
Usage Category	Percentage
Used	30%
Used but not in the last 12 months	6%
Never used	64%



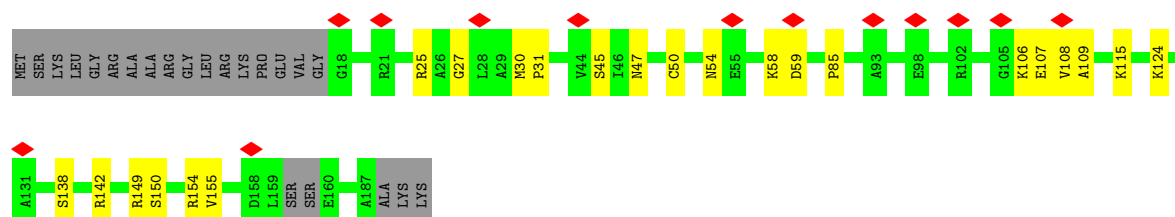
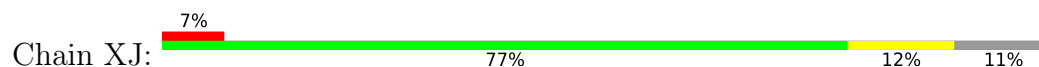
- Molecule 48: 39S ribosomal protein L10, mitochondrial

Opinion	Percentage
Doing a good job	71%
Doing a bad job	22%

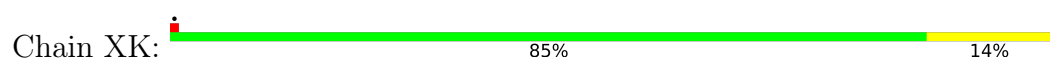




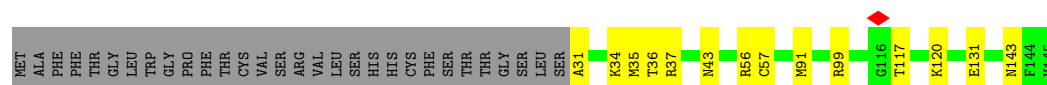
- Molecule 49: 39S ribosomal protein L11, mitochondrial



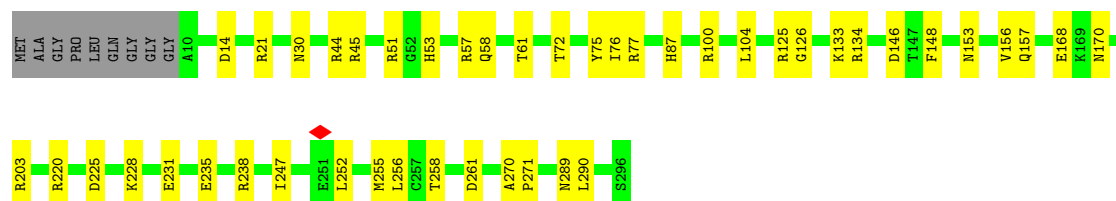
- Molecule 50: 39S ribosomal protein L13, mitochondrial



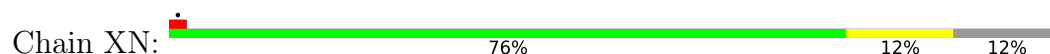
- Molecule 51: 39S ribosomal protein L14, mitochondrial

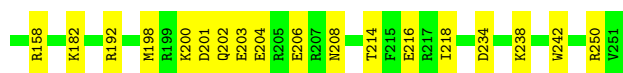


- Molecule 52: 39S ribosomal protein L15, mitochondrial



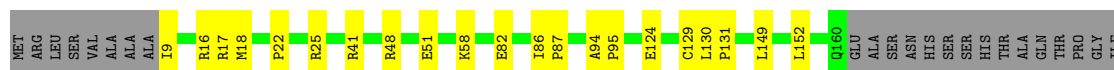
- Molecule 53: 39S ribosomal protein L16, mitochondrial





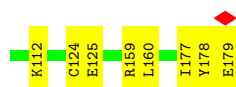
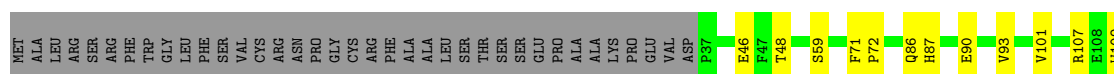
- Molecule 54: 39S ribosomal protein L17, mitochondrial

Chain XO: 75% 12% 13%



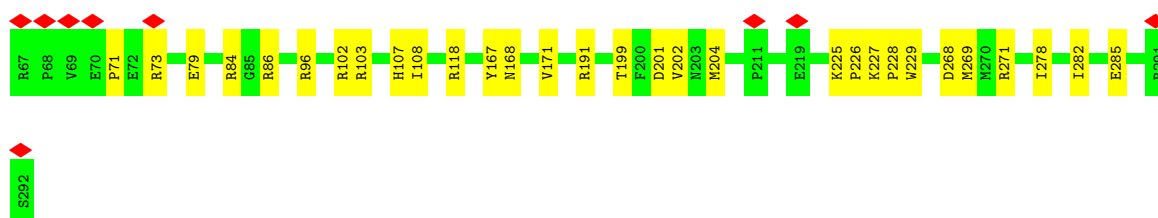
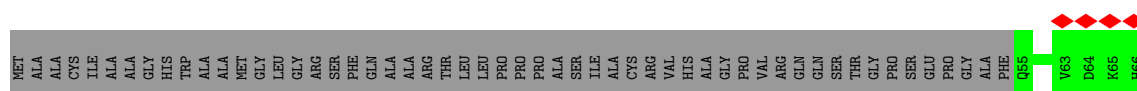
- Molecule 55: 39S ribosomal protein L18, mitochondrial

Chain XP: 68% 11% 21%



- Molecule 56: 39S ribosomal protein L19, mitochondrial

Chain XQ: 71% 10% 18%



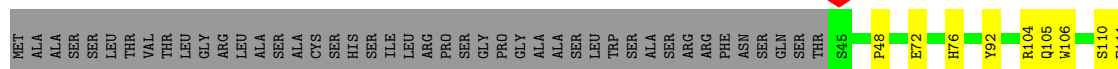
- Molecule 57: 39S ribosomal protein L20, mitochondrial

Chain XR: 77% 17% 6%



- Molecule 58: 39S ribosomal protein L21, mitochondrial

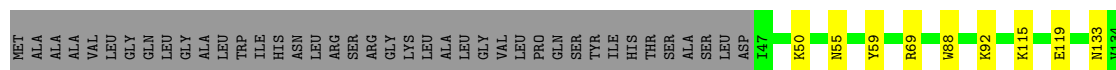
Chain XS: 69% 9% 22%





- Molecule 59: 39S ribosomal protein L22, mitochondrial

Chain XT: 73% 7% 19%



- Molecule 60: 39S ribosomal protein L23, mitochondrial

Chain XU: 82% 10% 8%



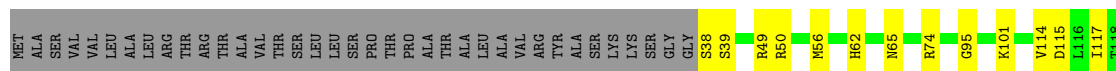
- Molecule 61: 39S ribosomal protein L24, mitochondrial

Chain XV: 81% 12% 6%



- Molecule 62: 39S ribosomal protein L27, mitochondrial

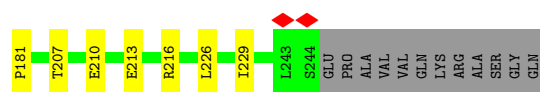
Chain XW: 63% 12% 25%



- Molecule 63: 39S ribosomal protein L28, mitochondrial

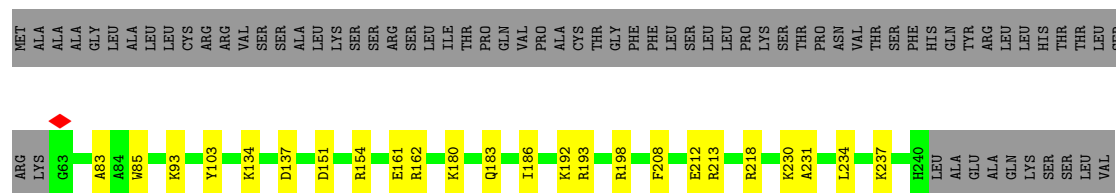
Chain XX: 79% 16% 5%





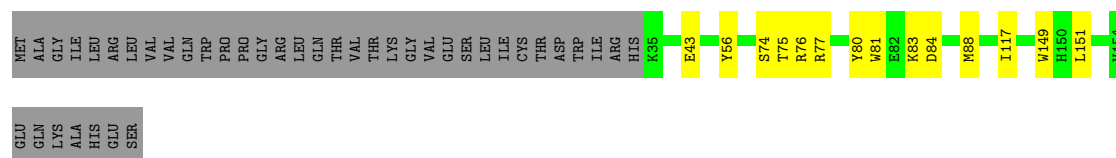
- Molecule 64: 39S ribosomal protein L47, mitochondrial

Chain XY: 62% 10% 29%



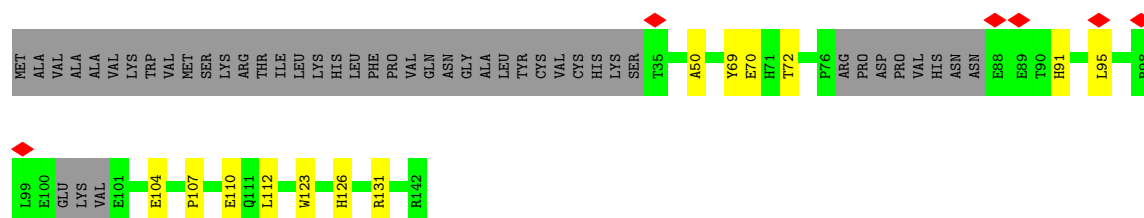
- Molecule 65: 39S ribosomal protein L30, mitochondrial

Chain XZ: 66% 9% 25%



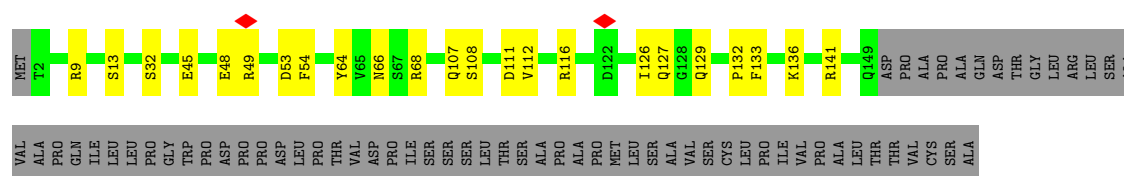
- Molecule 66: 39S ribosomal protein L42, mitochondrial

Chain a: 59% 9% 32%



- Molecule 67: 39S ribosomal protein L43, mitochondrial

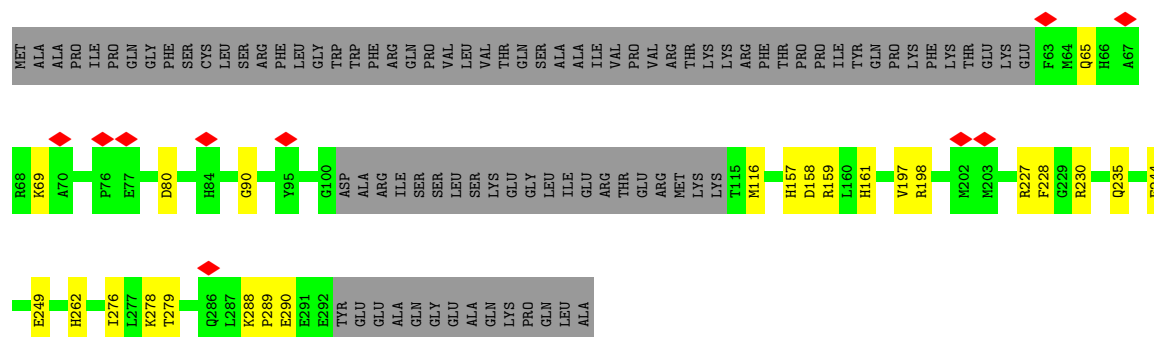
Chain b: 58% 11% 31%



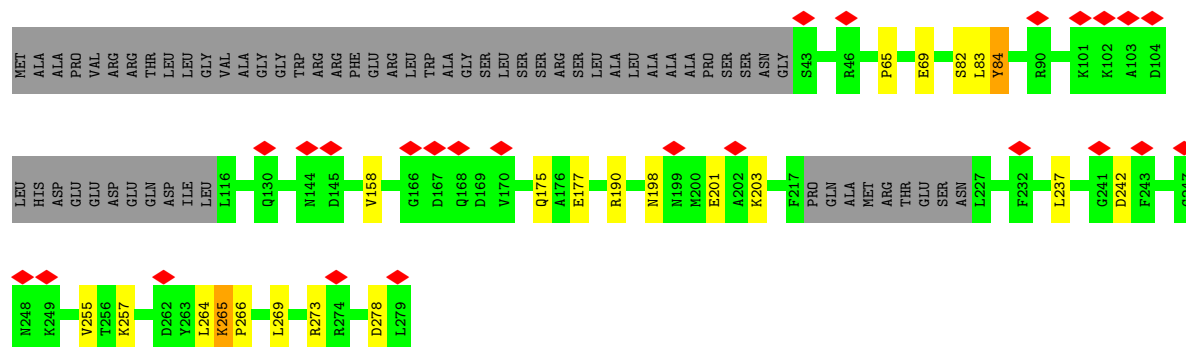
- Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c: 68% 15% 17%

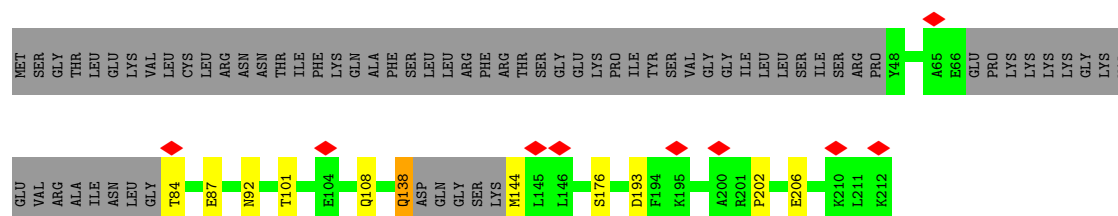
- Molecule 69: 39S ribosomal protein L45, mitochondrial



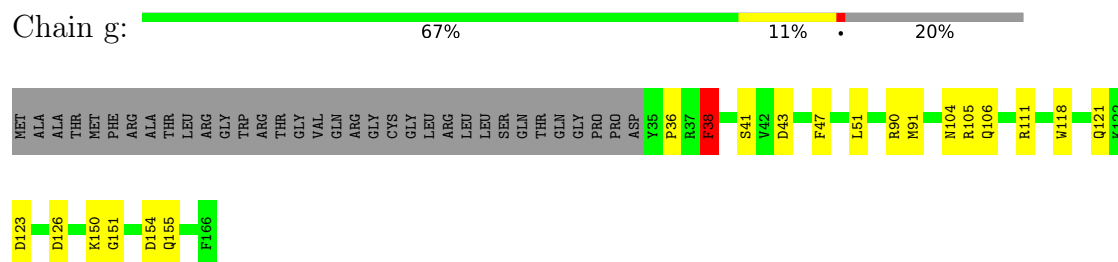
- Molecule 70: 39S ribosomal protein L46, mitochondrial



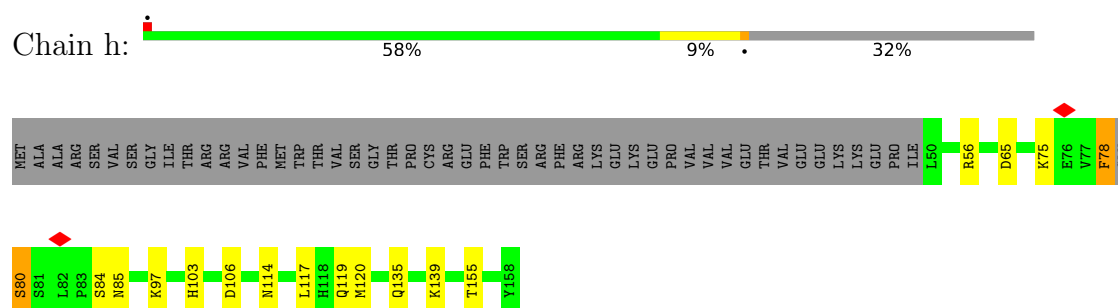
- Molecule 71: 39S ribosomal protein L48, mitochondrial



- Molecule 72: 39S ribosomal protein L49, mitochondrial



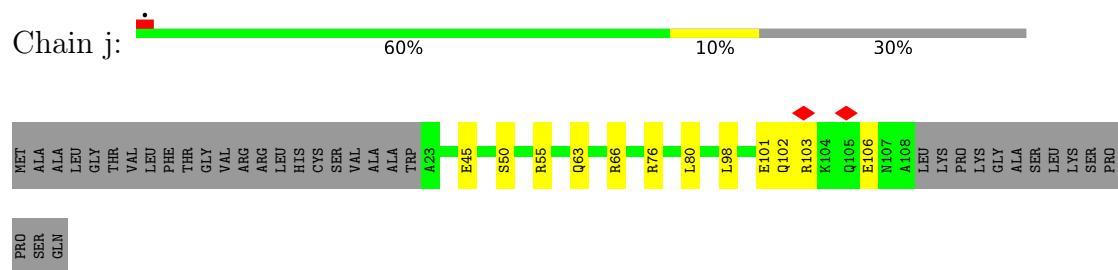
- Molecule 73: 39S ribosomal protein L50, mitochondrial



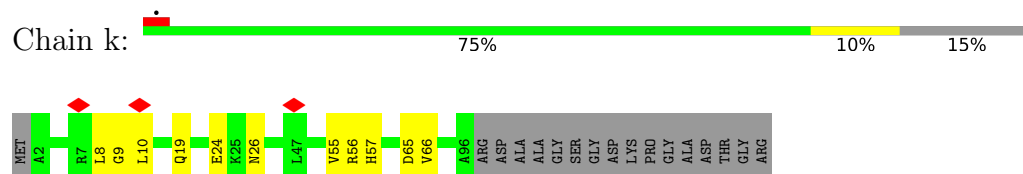
- Molecule 74: 39S ribosomal protein L51, mitochondrial



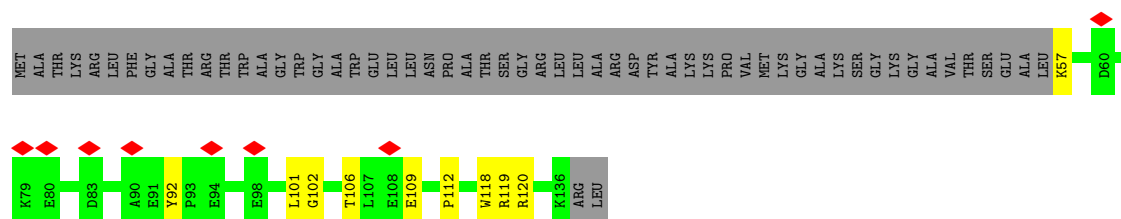
- Molecule 75: 39S ribosomal protein L52, mitochondrial



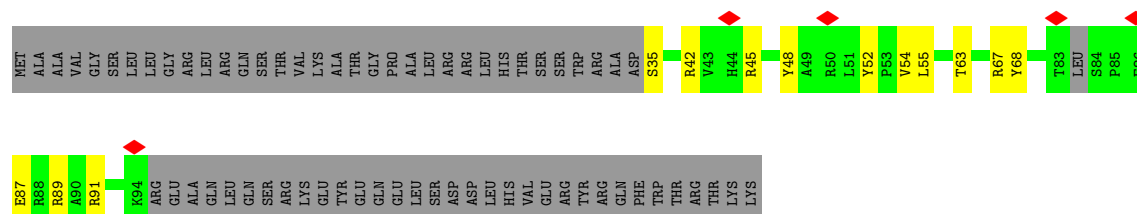
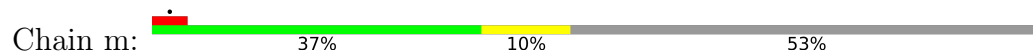
- Molecule 76: 39S ribosomal protein L53, mitochondrial



- Molecule 77: 39S ribosomal protein L54, mitochondrial



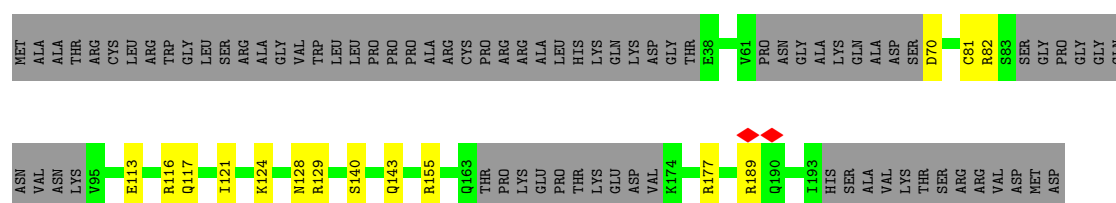
- Molecule 78: 39S ribosomal protein L55, mitochondrial



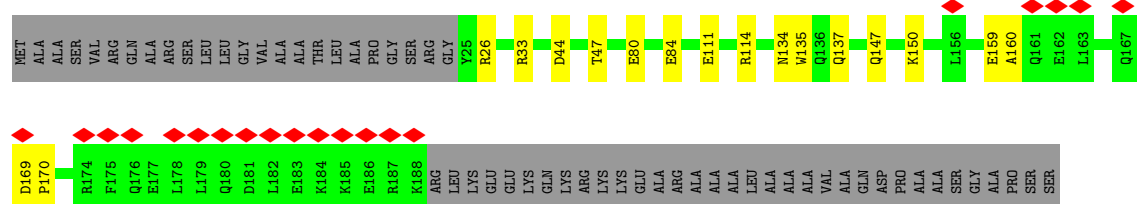
- Molecule 79: Ribosomal protein 63, mitochondrial



- Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial

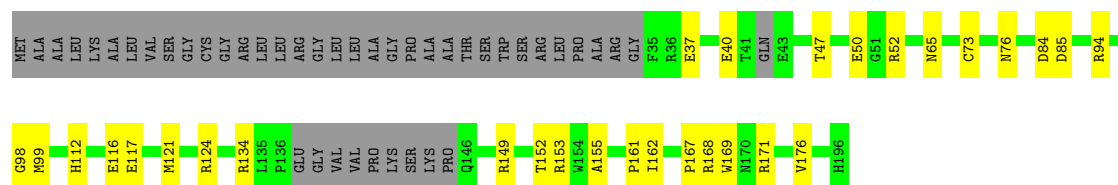


- Molecule 81: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 82: 39S ribosomal protein S18a, mitochondrial

Chain r: 

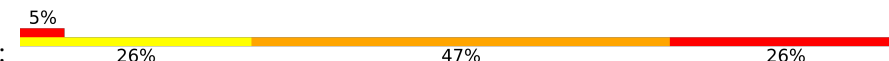


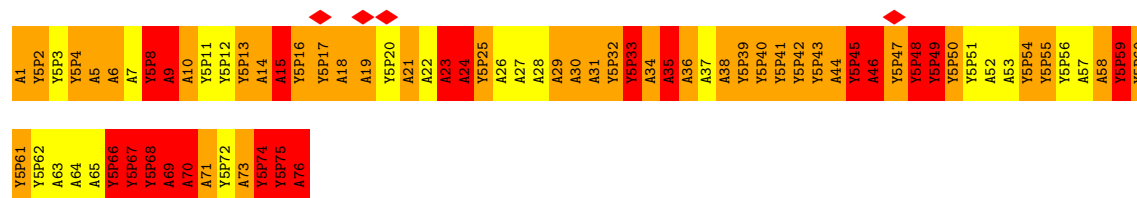
- Molecule 83: mRNA

Chain r1: 



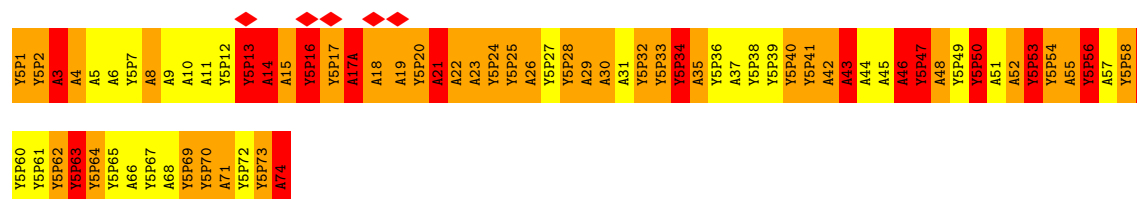
- Molecule 84: A-site tRNA

Chain r2: 



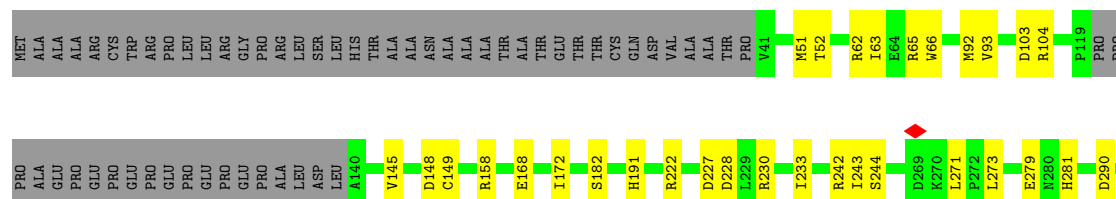
- Molecule 85: P-site tRNA

Chain r3: 



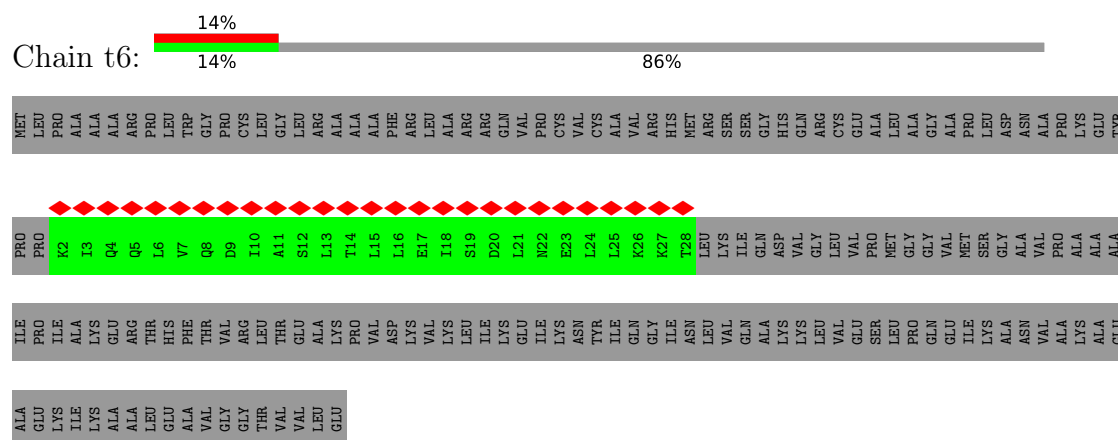
- Molecule 86: 39S ribosomal protein S30, mitochondrial

Chain s: 



- Molecule 87: 39S ribosomal protein L12, mitochondrial

- Molecule 87: 39S ribosomal protein L12, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14475	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
Maximum map value	0.255	Depositor
Minimum map value	-0.136	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.19	0/895	0.30	0/1201
2	1	0.15	0/444	0.34	0/591
3	2	0.26	0/382	0.39	0/507
4	3	0.24	0/852	0.34	0/1136
5	4	0.16	0/349	0.32	0/461
6	5	0.15	0/3298	0.32	0/4492
7	6	0.14	0/3040	0.32	0/4134
8	7	0.14	0/2419	0.30	0/3267
9	8	1.48	1/1199 (0.1%)	0.38	2/1612 (0.1%)
10	9	0.15	0/1024	0.29	0/1379
11	XA	0.17	0/35612	0.27	0/55425
12	A0	0.11	0/1727	0.32	0/2338
13	A1	0.12	0/2276	0.28	0/3079
14	A2	0.15	0/939	0.34	0/1256
15	A3	0.20	0/621	0.41	0/820
16	A4	0.12	0/4559	0.32	0/6149
17	AA	0.12	0/21952	0.23	0/34164
18	AB	0.14	0/1819	0.28	0/2462
19	AC	0.15	0/1112	0.30	0/1505
20	AD	0.15	0/2768	0.30	0/3707
21	AE	0.14	0/989	0.31	0/1335
22	AF	0.12	0/1708	0.29	0/2291
23	AG	0.13	0/2559	0.29	0/3429
24	AH	0.15	0/1128	0.33	0/1529
25	AI	0.13	0/1031	0.28	0/1390
26	AJ	0.15	0/854	0.33	0/1148
27	AK	0.15	0/879	0.35	0/1182
28	AL	0.14	0/1406	0.32	0/1878
29	AM	0.11	0/941	0.30	0/1265
30	AN	0.13	0/864	0.29	0/1169
31	AO	0.11	0/1580	0.27	0/2150
32	AP	0.14	0/782	0.29	0/1050

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AQ	0.17	0/746	0.31	0/993
34	AR	0.33	1/2103 (0.0%)	0.55	3/2842 (0.1%)
35	AS	0.13	0/1127	0.28	0/1518
36	AT	0.13	0/1361	0.32	0/1829
37	AU	0.14	0/1482	0.31	0/1987
38	AV	0.10	0/2925	0.28	0/3948
39	AW	0.12	0/778	0.25	0/1048
40	AX	0.11	0/2886	0.30	0/3909
41	AY	0.12	0/985	0.31	0/1329
42	AZ	0.14	0/748	0.31	0/1000
43	XB	0.10	0/1400	0.20	0/2168
44	XD	0.19	0/1879	0.34	0/2527
45	XE	0.18	0/2465	0.29	0/3344
46	XF	0.23	0/2071	0.35	0/2817
47	XH	0.15	0/798	0.31	0/1073
48	XI	0.14	0/1727	0.32	0/2340
49	XJ	0.10	0/1309	0.27	0/1764
50	XK	0.20	0/1495	0.33	0/2029
51	XL	0.17	0/904	0.28	0/1218
52	XM	0.20	0/2359	0.34	0/3185
53	XN	0.19	0/1825	0.34	0/2458
54	XO	0.19	0/1269	0.35	0/1708
55	XP	0.16	0/1190	0.34	0/1611
56	XQ	0.15	0/2026	0.32	0/2734
57	XR	0.24	0/1174	0.33	0/1572
58	XS	0.21	0/1311	0.33	0/1778
59	XT	0.22	0/1402	0.34	0/1886
60	XU	0.18	0/1200	0.32	0/1623
61	XV	0.15	0/1693	0.35	0/2297
62	XW	0.22	0/893	0.32	0/1204
63	XX	0.22	0/2090	0.37	0/2825
64	XY	0.18	0/1571	0.34	0/2106
65	XZ	0.23	0/1003	0.34	0/1354
66	a	0.17	0/838	0.35	0/1138
67	b	0.20	0/1202	0.36	0/1626
68	c	0.16	0/2264	0.30	0/3059
69	d	0.12	0/1807	0.28	0/2450
70	e	0.77	6/1797 (0.3%)	0.30	0/2422
71	f	0.16	0/1169	0.32	0/1576
72	g	0.32	1/1134 (0.1%)	0.48	0/1547
73	h	0.14	0/905	0.32	0/1233
74	i	0.25	0/849	0.42	0/1135
75	j	0.17	0/703	0.35	0/947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	k	0.12	0/743	0.29	0/1003
77	l	0.11	0/692	0.27	0/939
78	m	0.13	0/508	0.34	0/682
79	o	0.22	0/818	0.39	0/1097
80	p	0.13	0/1071	0.27	0/1433
81	q	0.14	0/1413	0.31	0/1906
82	r	0.16	0/1282	0.30	0/1734
86	s	0.16	0/3114	0.32	0/4225
87	t1	0.13	0/358	0.31	0/486
87	t2	0.08	0/236	0.20	0/315
87	t3	0.08	0/238	0.21	0/319
87	t4	0.07	0/229	0.21	0/308
87	t5	0.09	0/229	0.20	0/308
87	t6	0.13	0/213	0.30	0/286
All	All	0.22	9/176015 (0.0%)	0.30	5/249699 (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
70	e	0	1
71	f	0	1
73	h	0	2
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	99	ARG	CG-CD	50.89	3.05	1.52
70	e	84	TYR	CD2-CE2	16.25	1.87	1.38
70	e	84	TYR	CD1-CE1	16.03	1.86	1.38
70	e	84	TYR	CE2-CZ	12.37	1.68	1.38
34	AR	308	HIS	C-N	12.29	1.62	1.33
70	e	84	TYR	CE1-CZ	11.53	1.66	1.38
70	e	84	TYR	CG-CD1	11.49	1.63	1.39
70	e	84	TYR	CG-CD2	10.46	1.61	1.39
72	g	36	PRO	N-CD	6.25	1.56	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AR	309	PRO	O-C-N	13.83	141.32	122.64
34	AR	309	PRO	CA-C-N	-10.22	106.92	122.05
34	AR	309	PRO	C-N-CA	-10.22	106.92	122.05
9	8	99	ARG	CB-CG-CD	6.35	125.91	111.30
9	8	99	ARG	CG-CD-NE	5.46	124.02	112.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	XD	206	TYR	Peptide
48	XI	197	LEU	Peptide
70	e	265	LYS	Peptide
71	f	138	GLN	Peptide
73	h	78	PHE	Peptide
73	h	80	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	880	903	903	9	0
2	1	439	480	480	6	0
3	2	376	406	406	5	0
4	3	831	883	883	17	0
5	4	341	361	361	4	0
6	5	3204	3200	3200	38	0
7	6	2947	2839	2839	38	0
8	7	2365	2372	2371	21	0
9	8	1175	1202	1202	41	0
10	9	996	987	987	11	0
11	XA	31831	16169	16170	295	0
12	A0	1684	1685	1685	15	0
13	A1	2230	2261	2261	38	0
14	A2	925	964	964	17	0
15	A3	610	682	682	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A4	4470	4485	4486	59	0
17	AA	19628	9970	9971	130	0
18	AB	1776	1769	1769	15	0
19	AC	1082	1088	1088	16	0
20	AD	2716	2786	2785	30	0
21	AE	972	1001	1001	14	0
22	AF	1668	1716	1716	27	0
23	AG	2505	2490	2490	36	0
24	AH	1105	1136	1136	22	0
25	AI	1011	1052	1052	12	0
26	AJ	838	887	887	12	0
27	AK	861	885	885	10	0
28	AL	1382	1472	1472	19	0
29	AM	920	951	951	11	0
30	AN	846	908	908	8	0
31	AO	1528	1489	1489	13	0
32	AP	765	796	796	11	0
33	AQ	734	749	749	7	0
34	AR	2060	2074	2074	26	0
35	AS	1100	1103	1103	14	0
36	AT	1330	1343	1343	16	0
37	AU	1461	1471	1471	16	0
38	AV	2867	2862	2862	37	0
39	AW	766	785	785	5	0
40	AX	2814	2805	2804	34	0
41	AY	956	912	911	19	0
42	AZ	731	734	734	9	0
43	XB	1255	640	640	14	0
44	XD	1842	1897	1896	28	0
45	XE	2396	2402	2402	18	0
46	XF	2013	2045	2044	39	0
47	XH	784	832	832	10	0
48	XI	1691	1783	1783	18	0
49	XJ	1291	1367	1364	18	0
50	XK	1451	1448	1448	18	0
51	XL	889	941	941	10	0
52	XM	2305	2378	2377	33	0
53	XN	1778	1808	1808	22	0
54	XO	1245	1283	1283	15	0
55	XP	1164	1162	1162	14	0
56	XQ	1978	2022	2022	22	0
57	XR	1153	1214	1214	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	XS	1284	1355	1354	16	0
59	XT	1368	1410	1410	13	0
60	XU	1171	1164	1164	13	0
61	XV	1648	1656	1654	20	0
62	XW	871	898	898	15	0
63	XX	2035	2054	2054	30	0
64	XY	1534	1575	1575	22	0
65	XZ	978	1030	1030	16	0
66	a	813	777	777	10	0
67	b	1178	1180	1180	18	0
68	c	2217	2220	2220	29	0
69	d	1758	1743	1742	19	0
70	e	1762	1767	1767	41	0
71	f	1149	1165	1165	9	0
72	g	1097	1086	1085	16	0
73	h	882	866	867	13	0
74	i	827	857	857	15	0
75	j	689	678	678	9	0
76	k	732	745	745	7	0
77	l	673	654	653	9	0
78	m	500	525	525	11	0
79	o	797	804	804	16	0
80	p	1058	1083	1083	11	0
81	q	1379	1359	1359	11	0
82	r	1247	1267	1267	21	0
83	r1	252	0	169	12	0
84	r2	1486	0	835	42	0
85	r3	1459	0	829	47	0
86	s	3036	3023	3022	34	0
87	t1	354	378	374	1	0
87	t2	237	265	265	0	0
87	t3	238	268	270	1	0
87	t4	229	255	257	1	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
88	r	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	9	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	XI	1	0	0	0	0
89	XM	2	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	1	0
All	All	170697	143060	144817	1615	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 (1615) 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)
70:e:84:TYR:CE1	70:e:84:TYR:CD1	1.86	1.60
70:e:84:TYR:CD2	70:e:84:TYR:CE2	1.87	1.55
9:8:99:ARG:CD	70:e:84:TYR:CD1	2.24	1.20
9:8:99:ARG:CD	70:e:84:TYR:CE1	2.28	1.16
9:8:99:ARG:CD	70:e:84:TYR:CD2	2.28	1.16
9:8:99:ARG:CG	70:e:84:TYR:CD1	2.29	1.16
9:8:99:ARG:CG	70:e:84:TYR:CE2	2.28	1.16
9:8:99:ARG:CD	70:e:84:TYR:CE2	2.30	1.15
9:8:99:ARG:CG	70:e:84:TYR:CE1	2.29	1.15
9:8:99:ARG:CG	70:e:84:TYR:CD2	2.30	1.14
9:8:99:ARG:CD	70:e:84:TYR:CZ	2.31	1.13
9:8:99:ARG:CD	70:e:84:TYR:CG	2.32	1.12
9:8:99:ARG:CG	70:e:84:TYR:CZ	2.34	1.11
9:8:99:ARG:CG	70:e:84:TYR:CG	2.35	1.09
9:8:99:ARG:HD2	70:e:84:TYR:CE1	1.98	0.99
9:8:99:ARG:HD3	70:e:84:TYR:CG	1.97	0.99
11:XA:1881:A:OP2	72:g:111:ARG:NH2	1.95	0.98
48:XI:51:THR:O	53:XN:250:ARG:NH1	1.96	0.98
9:8:99:ARG:HG3	70:e:84:TYR:CZ	1.99	0.96
9:8:99:ARG:HG2	70:e:84:TYR:CD2	2.00	0.95
58:XS:138:ALA:O	67:b:127:GLN:NE2	2.01	0.94
38:AV:316:GLN:NE2	38:AV:317:LEU:O	2.02	0.93
67:b:107:GLN:NE2	67:b:108:SER:O	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:113:ARG:NH2	11:XA:1750:G:OP2	2.04	0.91
11:XA:1844:A:OP2	57:XR:48:ARG:NH2	2.04	0.90
18:AB:103:GLU:OE2	35:AS:52:ARG:NH2	2.06	0.89
38:AV:316:GLN:NE2	38:AV:320:GLU:O	2.05	0.89
11:XA:1777:A:N6	11:XA:1780:U:OP2	2.05	0.89
11:XA:1680:A:OP1	64:XY:230:LYS:NZ	2.05	0.89
4:3:113:ARG:NH1	52:XM:75:TYR:O	2.05	0.88
9:8:87:ASP:O	78:m:45:ARG:NH1	2.07	0.88
9:8:99:ARG:CB	70:e:84:TYR:CD1	2.56	0.87
17:AA:826:A:OP1	26:AJ:55:ARG:NH1	2.07	0.87
11:XA:2864:U:O5'	62:XW:50:ARG:NH1	2.07	0.86
11:XA:2125:C:OP2	58:XS:178:LYS:NZ	2.08	0.86
67:b:9:ARG:NH1	67:b:111:ASP:O	2.07	0.86
24:AH:107:LYS:NZ	24:AH:146:GLU:OE2	2.09	0.86
1:0:139:ARG:NH2	11:XA:2322:C:OP1	2.09	0.85
9:8:99:ARG:NE	70:e:84:TYR:CE2	2.43	0.85
11:XA:2275:U:O3'	68:c:33:LYS:NZ	2.10	0.85
13:A1:154:THR:OG1	24:AH:171:GLU:OE2	1.93	0.85
31:AO:185:SER:O	34:AR:183:LYS:NZ	2.09	0.85
52:XM:53:HIS:O	52:XM:58:GLN:NE2	2.10	0.85
11:XA:2537:G:O2'	11:XA:2634:U:OP2	1.93	0.85
11:XA:2064:A:OP1	62:XW:101:LYS:NZ	2.09	0.85
25:AI:71:SER:O	25:AI:74:ARG:NH1	2.10	0.84
34:AR:305:HIS:HD2	34:AR:314:ALA:HB2	1.42	0.84
17:AA:1396:C:O3'	78:m:89:ARG:NH1	2.09	0.84
1:0:95:ARG:NH1	11:XA:1821:A:OP2	2.10	0.84
11:XA:2191:A:N6	11:XA:2198:A:OP2	2.09	0.84
52:XM:146:ASP:OD2	80:p:143:GLN:NE2	2.11	0.84
11:XA:2954:C:O2	53:XN:182:LYS:NZ	2.10	0.83
23:AG:198:ARG:N	23:AG:246:ARG:O	2.11	0.83
68:c:139:GLN:NE2	68:c:143:ASP:OD2	2.11	0.83
29:AM:93:LEU:O	34:AR:175:ARG:NH2	2.11	0.83
11:XA:2146:A:N6	67:b:116:ARG:O	2.11	0.83
37:AU:126:GLN:OE1	37:AU:129:ARG:NH2	2.12	0.83
84:r2:45:Y5P:O2'	84:r2:46:P5P:OP1	1.95	0.83
14:A2:9:ARG:NH2	17:AA:1021:U:OP2	2.11	0.83
71:f:176:SER:O	78:m:35:SER:N	2.12	0.82
22:AF:126:TYR:O	22:AF:134:GLN:NE2	2.13	0.82
19:AC:88:GLU:OE2	19:AC:112:ARG:NH1	2.13	0.82
53:XN:85:GLY:O	53:XN:192:ARG:NH2	2.13	0.81
74:i:95:ARG:NH1	74:i:111:ASN:OD1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:164:ARG:NH1	71:f:84:THR:O	2.13	0.81
17:AA:701:G:N2	17:AA:841:A:O2'	2.13	0.81
27:AK:90:ARG:NH2	27:AK:95:SER:O	2.13	0.81
51:XL:35:MET:SD	51:XL:56:ARG:NH1	2.54	0.81
11:XA:1958:G:OP2	59:XT:160:GLY:N	2.14	0.81
52:XM:30:ASN:OD1	79:o:86:ARG:NH1	2.13	0.81
26:AJ:84:ARG:NH1	26:AJ:85:LEU:O	2.14	0.81
70:e:264:LEU:O	70:e:273:ARG:NH2	2.14	0.80
9:8:164:ARG:NH1	71:f:87:GLU:O	2.15	0.80
29:AM:20:ARG:NH1	29:AM:42:PRO:O	2.14	0.80
86:s:279:GLU:OE2	86:s:281:HIS:NE2	2.15	0.80
11:XA:1689:C:OP2	63:XX:5:LYS:NZ	2.15	0.80
14:A2:42:GLU:N	22:AF:241:TRP:O	2.14	0.80
51:XL:31:ALA:N	51:XL:91:MET:SD	2.55	0.80
23:AG:312:GLN:OE1	23:AG:345:ARG:NH2	2.16	0.79
7:6:360:ARG:NH2	11:XA:2869:A:N7	2.30	0.79
11:XA:2822:C:O2'	11:XA:2915:C:OP2	2.00	0.79
11:XA:3063:G:O2'	11:XA:3066:C:OP2	1.99	0.79
17:AA:1530:A:OP1	38:AV:64:LYS:NZ	2.16	0.79
11:XA:3068:G:N2	11:XA:3068:G:OP2	2.15	0.79
7:6:117:VAL:O	7:6:121:ARG:NH2	2.16	0.79
22:AF:52:ARG:NH2	23:AG:360:GLU:OE1	2.16	0.78
27:AK:60:ASN:O	27:AK:68:GLN:NE2	2.17	0.78
44:XD:128:GLN:NE2	44:XD:129:VAL:O	2.16	0.78
63:XX:150:LYS:HG3	63:XX:159:MET:HE2	1.66	0.78
17:AA:897:C:OP1	26:AJ:114:ARG:NH2	2.15	0.78
40:AX:53:GLU:N	40:AX:67:HIS:O	2.17	0.78
23:AG:136:ARG:NH1	23:AG:210:VAL:O	2.18	0.77
69:d:288:LYS:O	69:d:290:GLU:N	2.16	0.77
11:XA:2063:G:N2	62:XW:56:MET:SD	2.58	0.77
70:e:177:GLU:O	70:e:190:ARG:NH2	2.18	0.77
11:XA:2052:A:OP1	72:g:150:LYS:NZ	2.17	0.77
30:AN:62:ASP:OD1	30:AN:88:VAL:N	2.17	0.77
85:r3:25:Y5P:H2'	85:r3:26:P5P:H8	1.67	0.77
17:AA:668:U:O2'	31:AO:83:GLY:O	2.02	0.77
19:AC:89:ASP:OD1	19:AC:90:VAL:N	2.17	0.77
41:AY:340:SER:OG	41:AY:377:ARG:NH2	2.18	0.77
63:XX:150:LYS:HG3	63:XX:159:MET:CE	2.13	0.77
58:XS:194:ARG:NH2	67:b:13:SER:OG	2.18	0.77
67:b:45:GLU:OE2	67:b:49:ARG:NH2	2.16	0.76
11:XA:2166:C:O2	11:XA:2214:A:N6	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2351:U:O2	11:XA:2362:A:N6	2.17	0.76
10:9:54:LYS:NZ	11:XA:2415:C:O3'	2.18	0.76
71:f:92:ASN:ND2	71:f:193:ASP:OD2	2.18	0.76
11:XA:1700:U:O4	64:XY:193:ARG:NH2	2.19	0.76
2:1:53:ARG:NH2	11:XA:2879:A:O2'	2.18	0.76
9:8:99:ARG:HD2	70:e:84:TYR:CD1	2.18	0.76
32:AP:140:TYR:O	32:AP:141:ARG:NE	2.18	0.76
2:1:34:ARG:NH2	2:1:38:ARG:O	2.19	0.76
11:XA:2167:A:N6	11:XA:2212:C:OP2	2.18	0.76
9:8:99:ARG:HG2	70:e:84:TYR:CE2	2.18	0.76
12:A0:49:ARG:NH2	37:AU:41:ARG:O	2.18	0.76
17:AA:825:U:N3	17:AA:827:A:OP1	2.19	0.76
86:s:51:MET:O	86:s:62:ARG:NH2	2.19	0.76
9:8:99:ARG:HB3	70:e:84:TYR:CD1	2.21	0.75
61:XV:49:ILE:O	61:XV:81:ARG:NH1	2.18	0.75
36:AT:89:ASP:OD2	37:AU:120:ARG:NH2	2.19	0.75
64:XY:151:ASP:OD1	64:XY:154:ARG:NH2	2.20	0.75
6:5:30:ALA:N	44:XD:201:GLY:O	2.20	0.75
9:8:110:GLU:OE2	9:8:114:ARG:NE	2.19	0.75
22:AF:79:ALA:O	23:AG:312:GLN:NE2	2.20	0.75
84:r2:17:Y5P:O2'	84:r2:19:P5P:OP2	2.03	0.75
43:XB:1635:C:OP1	71:f:108:GLN:NE2	2.20	0.75
34:AR:176:GLU:OE2	34:AR:182:ARG:NE	2.20	0.75
38:AV:321:GLU:O	38:AV:326:LYS:NZ	2.19	0.75
14:A2:44:THR:O	22:AF:240:ARG:NH2	2.20	0.74
15:A3:187:GLU:O	28:AL:212:ARG:NH2	2.19	0.74
48:XI:224:HIS:O	48:XI:228:GLN:N	2.21	0.74
68:c:60:ARG:NH2	68:c:64:PRO:O	2.20	0.74
71:f:101:THR:OG1	78:m:67:ARG:NH1	2.20	0.74
20:AD:178:GLU:OE2	20:AD:181:ARG:NH2	2.20	0.74
54:XO:82:GLU:N	54:XO:82:GLU:OE1	2.20	0.74
16:A4:269:HIS:O	16:A4:270:ARG:NE	2.20	0.74
66:a:126:HIS:O	66:a:131:ARG:NH2	2.21	0.74
40:AX:174:ASN:OD1	40:AX:177:ARG:NH1	2.19	0.74
42:AZ:66:ARG:NH1	42:AZ:80:ASP:OD2	2.21	0.74
11:XA:2248:U:OP1	57:XR:99:ARG:NH2	2.21	0.74
42:AZ:26:THR:OG1	42:AZ:30:SER:OG	2.00	0.74
11:XA:3082:G:N2	11:XA:3085:A:OP2	2.21	0.73
14:A2:12:ARG:NH2	17:AA:1125:A:O4'	2.21	0.73
4:3:104:ARG:NH1	4:3:160:LYS:O	2.21	0.73
49:XJ:25:ARG:NH2	77:l:57:LYS:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AC:75:ASN:O	27:AK:103:ARG:NH2	2.22	0.73
53:XN:201:ASP:OD1	53:XN:202:GLN:N	2.22	0.73
42:AZ:26:THR:HG1	42:AZ:30:SER:HG	1.29	0.73
60:XU:71:ARG:NH2	60:XU:73:GLN:OE1	2.22	0.73
63:XX:118:ILE:O	63:XX:168:ARG:NH1	2.22	0.73
4:3:168:ARG:NH2	4:3:170:ASN:OD1	2.21	0.73
50:XK:61:ASN:ND2	50:XK:131:GLU:OE2	2.20	0.73
47:XH:103:GLU:OE1	47:XH:104:ASN:ND2	2.21	0.73
61:XV:181:ASP:O	64:XY:93:LYS:NZ	2.21	0.73
10:9:22:THR:OG1	10:9:36:ARG:NH1	2.22	0.73
38:AV:96:ARG:NH1	38:AV:101:CYS:SG	2.62	0.73
44:XD:132:ASP:OD2	44:XD:135:ARG:NH1	2.22	0.73
4:3:179:LYS:O	7:6:370:ARG:NH2	2.22	0.72
86:s:228:ASP:O	86:s:230:ARG:NH1	2.22	0.72
17:AA:996:A:OP2	25:AI:119:ASN:ND2	2.22	0.72
34:AR:133:GLU:N	34:AR:133:GLU:OE1	2.21	0.72
35:AS:6:LEU:O	35:AS:15:ARG:NH1	2.22	0.72
37:AU:77:GLU:OE1	37:AU:81:LYS:NZ	2.21	0.72
49:XJ:154:ARG:NH1	49:XJ:155:VAL:O	2.22	0.72
45:XE:69:ASP:OD1	45:XE:154:ARG:NH1	2.21	0.72
52:XM:238:ARG:NH1	80:p:70:ASP:OD1	2.22	0.72
75:j:63:GLN:OE1	75:j:66:ARG:NH1	2.23	0.72
17:AA:659:U:OP1	20:AD:226:ARG:NH2	2.22	0.72
22:AF:119:LYS:NZ	40:AX:398:LEU:O	2.23	0.72
67:b:132:PRO:O	67:b:136:LYS:NZ	2.22	0.72
17:AA:1143:C:N4	17:AA:1576:G:OP1	2.22	0.72
40:AX:111:TYR:O	40:AX:115:THR:OG1	2.07	0.72
9:8:99:ARG:HD3	70:e:84:TYR:CD2	2.20	0.71
13:A1:169:ARG:O	13:A1:218:ASN:ND2	2.23	0.71
3:2:49:ARG:NH2	11:XA:2500:A:N1	2.39	0.71
16:A4:479:GLU:HA	16:A4:482:ILE:HD12	1.71	0.71
23:AG:276:ARG:NH1	23:AG:373:ASP:OD2	2.24	0.71
22:AF:122:GLN:NE2	22:AF:138:GLU:O	2.23	0.71
5:4:84:ARG:NE	11:XA:3188:U:OP2	2.24	0.71
7:6:160:ASP:OD2	7:6:267:ARG:NH1	2.23	0.71
10:9:28:ARG:NH1	11:XA:2376:A:O2'	2.23	0.71
17:AA:752:C:O2'	17:AA:793:C:N4	2.23	0.71
17:AA:868:C:OP2	17:AA:870:C:N4	2.22	0.71
23:AG:220:GLN:OE1	23:AG:223:ARG:NH1	2.23	0.71
24:AH:74:LYS:N	24:AH:175:THR:O	2.23	0.71
39:AW:132:GLU:O	39:AW:135:GLN:NE2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:XV:150:SER:O	61:XV:152:ARG:NH1	2.23	0.71
6:5:72:ARG:NH2	11:XA:1712:A:OP2	2.24	0.70
34:AR:308:HIS:C	34:AR:310:ASP:H	1.95	0.70
11:XA:2111:C:OP1	48:XI:35:ARG:NH1	2.24	0.70
25:AI:81:GLU:O	25:AI:148:ARG:NH1	2.25	0.70
37:AU:138:GLU:OE2	37:AU:141:ARG:NH2	2.24	0.70
1:0:181:ARG:NH1	1:0:186:THR:O	2.25	0.70
17:AA:906:C:OP1	20:AD:117:ARG:NE	2.24	0.70
50:XK:73:GLU:OE2	82:r:149:ARG:NH2	2.24	0.70
11:XA:2082:G:OP1	79:o:66:ARG:NH2	2.24	0.70
38:AV:132:LYS:O	38:AV:136:GLY:N	2.24	0.70
76:k:19:GLN:OE1	76:k:56:ARG:NH1	2.25	0.70
35:AS:18:ASP:OD1	35:AS:19:LEU:N	2.24	0.70
16:A4:470:GLN:OE1	16:A4:472:ASP:N	2.25	0.70
17:AA:1589:C:OP1	25:AI:187:ARG:NH1	2.24	0.70
28:AL:149:ASP:OD2	28:AL:152:HIS:ND1	2.25	0.70
38:AV:132:LYS:NZ	38:AV:166:GLU:OE1	2.25	0.70
14:A2:17:ARG:NH2	17:AA:1022:A:OP2	2.25	0.69
33:AQ:55:GLU:OE2	33:AQ:59:ARG:NE	2.25	0.69
18:AB:111:LEU:O	18:AB:113:HIS:ND1	2.26	0.69
17:AA:949:U:O3'	30:AN:29:ARG:NH1	2.26	0.69
9:8:99:ARG:HG3	70:e:84:TYR:CE1	2.22	0.69
17:AA:893:G:OP2	26:AJ:79:LYS:NZ	2.25	0.69
54:XO:58:LYS:NZ	56:XQ:269:MET:O	2.26	0.69
85:r3:56:Y5P:O2'	85:r3:58:Y5P:OP2	2.07	0.69
17:AA:780:C:N3	28:AL:197:ARG:NH2	2.40	0.69
69:d:65:GLN:N	69:d:65:GLN:OE1	2.25	0.69
7:6:308:GLN:NE2	7:6:311:MET:SD	2.65	0.69
40:AX:56:PRO:O	40:AX:59:HIS:NE2	2.24	0.69
11:XA:2151:A:O3'	79:o:38:ARG:NH1	2.26	0.69
52:XM:203:ARG:NH2	52:XM:261:ASP:O	2.25	0.69
63:XX:144:TYR:O	63:XX:148:THR:HB	1.93	0.69
46:XF:75:GLU:OE2	46:XF:210:ARG:NE	2.25	0.68
60:XU:54:ARG:NH1	86:s:314:GLN:OE1	2.26	0.68
40:AX:121:ALA:N	40:AX:299:ASN:OD1	2.26	0.68
46:XF:167:MET:SD	46:XF:279:ARG:NH1	2.66	0.68
67:b:48:GLU:OE2	73:h:139:LYS:NZ	2.26	0.68
49:XJ:85:PRO:O	49:XJ:124:LYS:NZ	2.26	0.68
68:c:42:GLN:NE2	74:i:36:LEU:O	2.24	0.68
52:XM:148:PHE:O	52:XM:170:ASN:ND2	2.26	0.68
63:XX:80:TRP:O	63:XX:131:THR:OG1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:74:VAL:O	64:XY:83:ALA:N	2.27	0.68
44:XD:136:SER:O	44:XD:249:ASN:ND2	2.27	0.68
58:XS:72:GLU:O	58:XS:76:HIS:ND1	2.26	0.68
11:XA:1761:A:O2'	11:XA:1762:A:O5'	2.12	0.68
11:XA:2187:C:O3'	49:XJ:106:LYS:NZ	2.26	0.68
22:AF:129:ALA:O	22:AF:134:GLN:NE2	2.26	0.68
38:AV:173:PHE:O	38:AV:178:THR:OG1	2.12	0.68
6:5:334:LYS:N	6:5:362:THR:OG1	2.25	0.67
74:i:67:GLU:O	81:q:33:ARG:NH1	2.27	0.67
11:XA:3012:U:O4'	11:XA:3173:G:N2	2.27	0.67
67:b:64:TYR:OH	68:c:67:ASP:N	2.26	0.67
85:r3:54:Y5P:HC	85:r3:56:Y5P:H5	1.76	0.67
40:AX:206:GLU:OE1	40:AX:249:ARG:NH1	2.28	0.67
18:AB:60:ASP:OD1	18:AB:64:ASN:ND2	2.27	0.67
38:AV:213:LEU:O	38:AV:215:GLN:NE2	2.28	0.67
60:XU:9:LEU:N	64:XY:183:GLN:OE1	2.27	0.67
17:AA:1411:G:O3'	40:AX:279:LYS:NZ	2.26	0.67
21:AE:42:LEU:O	37:AU:184:ARG:NE	2.27	0.67
7:6:368:ARG:NH2	11:XA:2859:A:OP2	2.28	0.67
11:XA:2581:A:O2'	11:XA:2583:C:N4	2.27	0.67
12:A0:90:ASP:OD1	31:AO:215:ARG:NH1	2.28	0.67
61:XV:184:GLU:O	64:XY:93:LYS:NZ	2.28	0.67
26:AJ:107:ILE:N	26:AJ:131:ASP:OD2	2.28	0.67
56:XQ:118:ARG:NH2	56:XQ:202:VAL:O	2.27	0.67
11:XA:3217:A:O4'	56:XQ:86:ARG:NH2	2.27	0.66
84:r2:39:Y5P:C5	84:r2:40:Y5P:H5	2.25	0.66
86:s:381:THR:O	86:s:385:GLN:NE2	2.27	0.66
85:r3:69:Y5P:H4A	85:r3:70:Y5P:H4	1.78	0.66
19:AC:52:THR:OG1	19:AC:55:GLU:OE1	2.13	0.66
6:5:381:LEU:O	6:5:407:LYS:NZ	2.28	0.66
17:AA:947:U:OP1	28:AL:162:GLN:NE2	2.29	0.66
40:AX:266:ASN:ND2	40:AX:311:SER:O	2.29	0.66
56:XQ:71:PRO:O	56:XQ:73:ARG:NH1	2.29	0.66
1:0:136:GLU:OE1	1:0:177:ARG:NH2	2.27	0.66
22:AF:176:ASP:OD1	22:AF:179:ARG:NH2	2.29	0.66
29:AM:55:ASP:OD2	36:AT:146:GLN:NE2	2.29	0.66
84:r2:74:Y5P:H4A	84:r2:75:Y5P:HC	1.77	0.66
8:7:279:GLU:N	8:7:279:GLU:OE1	2.29	0.66
13:A1:74:ALA:O	13:A1:110:ASN:ND2	2.28	0.66
16:A4:478:TYR:CE2	16:A4:482:ILE:HD11	2.31	0.66
17:AA:661:C:OP1	20:AD:339:SER:OG	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AE:5:GLU:OE2	21:AE:96:HIS:ND1	2.29	0.65
21:AE:105:CYS:SG	32:AP:64:LYS:NZ	2.67	0.65
46:XF:223:HIS:O	81:q:26:ARG:NH2	2.29	0.65
19:AC:113:ARG:NH2	24:AH:166:GLU:OE2	2.28	0.65
17:AA:1195:U:OP1	22:AF:185:LYS:NZ	2.29	0.65
6:5:141:ASP:O	6:5:142:ASP:N	2.29	0.65
11:XA:1805:A:OP2	61:XV:94:HIS:NE2	2.30	0.65
14:A2:38:ARG:NH2	17:AA:1184:U:OP1	2.30	0.65
44:XD:111:ARG:NE	44:XD:165:ASN:OD1	2.30	0.65
11:XA:3127:G:O2'	11:XA:3130:A:N6	2.28	0.65
16:A4:198:TYR:O	16:A4:239:ARG:NH1	2.28	0.65
25:AI:79:LYS:N	25:AI:82:GLU:OE2	2.27	0.65
84:r2:58:P5P:O2'	84:r2:60:Y5P:H5	1.97	0.65
13:A1:163:VAL:O	41:AY:317:ASN:ND2	2.29	0.65
11:XA:2279:U:OP2	74:i:46:ARG:NH2	2.29	0.65
17:AA:826:A:N7	26:AJ:55:ARG:NE	2.45	0.64
84:r2:34:P5P:O2'	84:r2:35:P5P:OP1	2.13	0.64
11:XA:2558:A:O5'	17:AA:1001:C:N4	2.30	0.64
60:XU:16:GLN:NE2	60:XU:17:LEU:O	2.29	0.64
74:i:105:ASP:OD1	74:i:106:ASP:N	2.30	0.64
20:AD:307:LYS:NZ	34:AR:103:TYR:OH	2.31	0.64
11:XA:2195:A:OP1	77:l:119:ARG:NE	2.31	0.64
81:q:111:GLU:OE2	81:q:114:ARG:NH1	2.31	0.64
61:XV:54:TRP:NE1	61:XV:56:LEU:O	2.30	0.64
16:A4:478:TYR:CD2	16:A4:482:ILE:HD11	2.32	0.64
7:6:355:LYS:NZ	7:6:357:PHE:O	2.31	0.64
17:AA:860:A:N7	17:AA:919:A:O2'	2.30	0.64
34:AR:308:HIS:C	34:AR:310:ASP:N	2.56	0.64
11:XA:2458:A:OP2	54:XO:9:ILE:N	2.30	0.63
11:XA:2515:U:O2'	44:XD:282:ALA:O	2.15	0.63
51:XL:43:ASN:ND2	51:XL:117:THR:OG1	2.31	0.63
12:A0:132:GLU:OE1	12:A0:205:ALA:N	2.31	0.63
24:AH:75:ARG:N	24:AH:175:THR:OG1	2.31	0.63
11:XA:1962:A:OP2	11:XA:2501:C:N4	2.31	0.63
11:XA:2082:G:N2	65:XZ:88:MET:SD	2.71	0.63
17:AA:1130:G:OP1	20:AD:405:LYS:NZ	2.31	0.63
23:AG:272:SER:OG	23:AG:347:ALA:O	2.16	0.63
13:A1:256:SER:O	13:A1:260:ARG:NH1	2.31	0.63
70:e:198:ASN:ND2	70:e:242:ASP:OD1	2.32	0.63
36:AT:109:ASN:ND2	36:AT:111:GLU:OE2	2.32	0.63
48:XI:101:ASN:OD1	48:XI:151:ASN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2192:A:OP1	49:XJ:142:ARG:NE	2.32	0.63
20:AD:257:SER:OG	20:AD:271:ALA:O	2.16	0.62
34:AR:305:HIS:HD2	34:AR:314:ALA:CB	2.09	0.62
86:s:191:HIS:O	86:s:428:ARG:NH2	2.33	0.62
16:A4:455:ASN:O	16:A4:486:TYR:OH	2.17	0.62
17:AA:1320:G:OP1	19:AC:41:ARG:NH1	2.32	0.62
17:AA:1423:A:HO2'	85:r3:40:Y5P:HD	1.46	0.62
38:AV:141:ASN:ND2	38:AV:371:ASP:OD1	2.32	0.62
4:3:136:LYS:O	4:3:141:LYS:NZ	2.33	0.62
75:j:50:SER:OG	75:j:55:ARG:O	2.18	0.62
84:r2:9:P5P:O2'	84:r2:46:P5P:H5'2	2.00	0.62
86:s:321:GLU:OE2	86:s:398:SER:N	2.32	0.62
11:XA:2011:G:O6	74:i:113:ARG:NH1	2.30	0.62
11:XA:2416:U:OP1	86:s:313:ARG:NH1	2.31	0.62
84:r2:66:Y5P:H4A	84:r2:67:Y5P:H4	1.82	0.62
12:A0:87:TRP:O	31:A0:215:ARG:NH2	2.33	0.62
11:XA:3178:U:O2'	82:r:134:ARG:NH1	2.33	0.62
49:XJ:138:SER:OG	49:XJ:142:ARG:NH1	2.33	0.62
14:A2:24:ASN:ND2	17:AA:1597:C:OP2	2.33	0.61
45:XE:54:SER:OG	45:XE:57:ASN:OD1	2.17	0.61
11:XA:1939:G:O5'	44:XD:259:LYS:NZ	2.33	0.61
52:XM:100:ARG:NE	52:XM:126:GLY:O	2.31	0.61
11:XA:1905:C:OP1	46:XF:117:ARG:NH1	2.33	0.61
11:XA:3175:A:OP2	11:XA:3187:C:N4	2.34	0.61
13:A1:62:VAL:O	23:AG:90:ASN:ND2	2.31	0.61
20:AD:134:GLU:N	20:AD:134:GLU:OE1	2.33	0.61
49:XJ:115:LYS:N	77:l:92:TYR:OH	2.33	0.61
12:A0:96:ARG:N	12:A0:117:ILE:O	2.33	0.61
17:AA:1454:G:OP2	23:AG:377:ARG:NH2	2.33	0.61
22:AF:70:LYS:O	23:AG:365:ARG:NH1	2.34	0.61
46:XF:167:MET:SD	46:XF:276:GLN:NE2	2.73	0.61
52:XM:72:THR:OG1	52:XM:77:ARG:NH2	2.34	0.61
2:1:23:GLU:N	2:1:23:GLU:OE1	2.34	0.61
34:AR:89:LYS:O	34:AR:92:LYS:NZ	2.32	0.61
36:AT:97:GLU:N	36:AT:97:GLU:OE1	2.33	0.61
44:XD:124:GLU:OE2	44:XD:144:GLY:N	2.34	0.61
32:AP:49:ASP:OD2	39:AW:82:SER:N	2.34	0.61
11:XA:1864:A:OP1	57:XR:17:ARG:NH1	2.34	0.60
85:r3:21:P5P:H6	85:r3:46:P5P:O2'	2.01	0.60
5:4:73:LYS:NZ	11:XA:2954:C:OP1	2.34	0.60
19:AC:103:CYS:O	19:AC:124:LEU:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AG:382:PRO:O	24:AH:131:ARG:NH1	2.34	0.60
67:b:32:SER:OG	67:b:68:ARG:NH1	2.34	0.60
7:6:198:ALA:O	7:6:254:TYR:OH	2.19	0.60
11:XA:1672:C:OP1	59:XT:50:LYS:N	2.35	0.60
9:8:99:ARG:NE	70:e:84:TYR:CZ	2.69	0.60
11:XA:1955:G:O2'	11:XA:1958:G:O2'	2.17	0.60
11:XA:2145:G:N3	58:XS:104:ARG:NH2	2.49	0.60
17:AA:827:A:N7	26:AJ:55:ARG:NH2	2.48	0.60
20:AD:254:ALA:O	20:AD:280:HIS:N	2.33	0.60
30:AN:12:TRP:NE1	36:AT:81:ASP:O	2.34	0.60
60:XU:13:GLY:O	61:XV:211:LYS:NZ	2.33	0.60
11:XA:3078:C:N4	11:XA:3079:G:O6	2.34	0.60
20:AD:410:ASP:OD1	20:AD:411:VAL:N	2.35	0.60
50:XK:24:LYS:O	50:XK:26:GLN:NE2	2.35	0.60
63:XX:160:ASP:OD1	63:XX:161:LEU:N	2.34	0.60
7:6:286:ARG:NE	7:6:295:GLN:O	2.33	0.60
84:r2:45:Y5P:HA	84:r2:46:P5P:OP2	2.02	0.60
22:AF:153:GLU:OE1	22:AF:153:GLU:N	2.34	0.60
29:AM:59:ASN:ND2	29:AM:63:GLU:OE2	2.35	0.60
38:AV:34:TYR:OH	38:AV:371:ASP:OD2	2.20	0.60
11:XA:2192:A:OP2	77:l:119:ARG:NH1	2.35	0.60
23:AG:379:ARG:NH2	24:AH:133:GLN:OE1	2.35	0.60
77:l:112:PRO:O	77:l:118:TRP:NE1	2.34	0.60
80:p:113:GLU:OE1	80:p:116:ARG:NH2	2.34	0.60
11:XA:2755:A:O2'	63:XX:112:ARG:NH2	2.35	0.59
17:AA:722:C:N3	17:AA:798:C:O2'	2.33	0.59
22:AF:231:GLU:O	22:AF:234:ARG:NE	2.35	0.59
36:AT:130:GLY:N	36:AT:135:CYS:SG	2.75	0.59
56:XQ:226:PRO:O	56:XQ:229:TRP:NE1	2.35	0.59
59:XT:69:ARG:NH1	69:d:228:PHE:O	2.35	0.59
85:r3:23:P5P:H2'	85:r3:24:Y5P:H6	1.83	0.59
7:6:106:ARG:NH1	43:XB:1621:A:OP2	2.35	0.59
16:A4:99:SER:N	16:A4:102:GLU:OE2	2.33	0.59
17:AA:1423:A:O2'	85:r3:40:Y5P:O2'	2.18	0.59
41:AY:292:GLN:OE1	41:AY:292:GLN:N	2.35	0.59
44:XD:113:ARG:O	44:XD:147:ARG:NH1	2.34	0.59
65:XZ:149:TRP:NE1	75:j:45:GLU:OE1	2.33	0.59
43:XB:1630:A:OP1	78:m:42:ARG:NE	2.35	0.59
63:XX:147:LYS:O	63:XX:147:LYS:HG2	2.02	0.59
75:j:103:ARG:NE	75:j:106:GLU:OE2	2.35	0.59
84:r2:8:Y5P:O2'	84:r2:48:Y5P:HC	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:r2:70:P5P:H2'	84:r2:71:P5P:H8	1.85	0.59
73:h:78:PHE:O	73:h:80:SER:C	2.46	0.59
13:A1:118:ALA:O	13:A1:122:HIS:ND1	2.35	0.59
46:XF:121:ARG:O	46:XF:142:ARG:NE	2.34	0.59
52:XM:225:ASP:OD2	52:XM:228:LYS:NZ	2.35	0.59
7:6:239:ASN:OD1	7:6:275:GLN:NE2	2.36	0.59
11:XA:2028:G:N1	11:XA:2264:A:OP2	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:1347:G:OP1	27:AK:36:ARG:NH1	2.31	0.59
9:8:178:TYR:N	78:m:63:THR:O	2.35	0.59
17:AA:1048:C:O2'	17:AA:1049:A:OP1	2.21	0.59
66:a:104:GLU:OE1	66:a:104:GLU:N	2.36	0.59
85:r3:50:Y5P:H6	85:r3:50:Y5P:OP2	2.03	0.59
9:8:99:ARG:CB	70:e:84:TYR:CG	2.85	0.59
51:XL:131:GLU:N	51:XL:131:GLU:OE1	2.33	0.59
11:XA:1832:A:N6	11:XA:1837:C:OP2	2.36	0.58
57:XR:38:CYS:SG	57:XR:39:TYR:N	2.76	0.58
11:XA:1787:G:N2	11:XA:1790:A:OP2	2.32	0.58
14:A2:56:TRP:CD1	14:A2:66:CYS:HG	2.22	0.58
14:A2:95:GLU:OE2	14:A2:96:SER:N	2.36	0.58
21:AE:53:ALA:N	21:AE:56:GLN:O	2.32	0.58
85:r3:28:Y5P:H2'	85:r3:29:P5P:H8	1.85	0.58
85:r3:53:Y5P:H4	85:r3:59:Y5P:N3	2.16	0.58
36:AT:95:ASN:OD1	36:AT:96:LYS:N	2.36	0.58
11:XA:1868:G:N7	52:XM:51:ARG:NH2	2.47	0.58
16:A4:133:ALA:HB2	19:AC:148:LYS:HB2	1.83	0.58
11:XA:2195:A:O2'	11:XA:2196:A:O5'	2.19	0.58
43:XB:1626:C:N4	55:XP:86:GLN:OE1	2.35	0.58
17:AA:1179:G:N2	83:r1:46:Y5P:OP2	2.31	0.58
55:XP:107:ARG:O	55:XP:112:LYS:NZ	2.36	0.58
8:7:238:ASP:OD1	8:7:239:PHE:N	2.36	0.58
84:r2:41:Y5P:H2'	84:r2:42:Y5P:H6	1.85	0.58
9:8:99:ARG:HB3	70:e:84:TYR:CG	2.39	0.58
11:XA:2511:C:O2'	44:XD:257:ILE:O	2.19	0.58
34:AR:68:PRO:O	34:AR:69:THR:OG1	2.20	0.58
68:c:170:ALA:HB3	68:c:191:LEU:HD21	1.85	0.58
11:XA:2457:A:N3	54:XO:17:ARG:NH2	2.52	0.58
14:A2:102:ASN:OD1	14:A2:103:LYS:N	2.34	0.58
16:A4:64:THR:HG22	24:AH:64:THR:HG23	1.85	0.58
34:AR:299:ASN:OD1	34:AR:300:LEU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:XE:334:ASP:OD1	45:XE:335:GLU:N	2.37	0.58
63:XX:51:LYS:O	63:XX:60:GLU:N	2.37	0.58
85:r3:23:P5P:N1	85:r3:24:Y5P:H4	2.18	0.58
6:5:149:ASN:ND2	6:5:152:GLU:OE2	2.35	0.57
11:XA:2387:U:O2'	11:XA:2406:A:N6	2.37	0.57
11:XA:2724:G:OP1	46:XF:131:LYS:NZ	2.35	0.57
85:r3:62:Y5P:H4A	85:r3:63:Y5P:H4	1.84	0.57
11:XA:3059:A:OP1	11:XA:3061:G:O2'	2.21	0.57
12:A0:101:ARG:NH1	17:AA:1528:A:OP1	2.37	0.57
6:5:32:GLU:OE1	6:5:39:ARG:NH2	2.37	0.57
6:5:306:PRO:O	6:5:310:ARG:NE	2.32	0.57
11:XA:2599:U:OP2	11:XA:2625:C:N4	2.37	0.57
11:XA:2928:C:OP2	11:XA:3073:C:O2'	2.22	0.57
17:AA:1198:A:N6	17:AA:1199:G:O6	2.37	0.57
35:AS:7:GLU:N	35:AS:7:GLU:OE1	2.37	0.57
36:AT:91:GLU:OE2	37:AU:123:ARG:NH1	2.37	0.57
21:AE:48:PRO:O	32:AP:124:TYR:OH	2.21	0.57
25:AI:94:ASN:OD1	25:AI:95:THR:N	2.36	0.57
85:r3:29:P5P:H2'	85:r3:30:P5P:H8	1.85	0.57
17:AA:650:U:OP1	20:AD:427:ARG:NH1	2.38	0.57
56:XQ:79:GLU:OE2	56:XQ:167:TYR:OH	2.23	0.57
85:r3:62:Y5P:C4	85:r3:63:Y5P:H4	2.34	0.57
6:5:141:ASP:OD1	6:5:142:ASP:N	2.38	0.57
11:XA:1773:A:OP2	68:c:31:VAL:N	2.37	0.57
11:XA:2182:G:O2'	11:XA:2183:C:O4'	2.21	0.57
38:AV:120:ASP:OD1	38:AV:122:GLN:NE2	2.33	0.57
9:8:100:GLU:N	9:8:100:GLU:OE1	2.35	0.57
11:XA:2689:C:O3'	79:o:9:ARG:N	2.37	0.57
35:AS:27:GLU:N	35:AS:27:GLU:OE1	2.37	0.57
47:XH:108:ARG:NH1	47:XH:143:GLU:OE2	2.35	0.57
62:XW:62:HIS:N	62:XW:65:ASN:OD1	2.38	0.57
8:7:83:LYS:NZ	8:7:120:THR:O	2.34	0.57
11:XA:2756:C:OP1	47:XH:121:ASN:ND2	2.34	0.57
17:AA:989:U:OP1	25:AI:94:ASN:ND2	2.34	0.57
34:AR:305:HIS:CD2	34:AR:314:ALA:HB2	2.32	0.57
84:r2:29:P5P:H2'	84:r2:30:P5P:H8	1.86	0.57
85:r3:1:Y5P:C5	85:r3:2:Y5P:H4	2.35	0.57
11:XA:2096:U:O4	52:XM:57:ARG:NH1	2.31	0.56
27:AK:41:ARG:NH2	27:AK:88:ARG:O	2.38	0.56
82:r:65:ASN:ND2	82:r:73:CYS:O	2.37	0.56
11:XA:1755:A:O2'	47:XH:64:LEU:O	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2960:U:OP1	11:XA:3016:G:N2	2.37	0.56
2:1:47:ASP:O	2:1:51:LYS:N	2.37	0.56
11:XA:1689:C:O2	64:XY:213:ARG:NH2	2.39	0.56
11:XA:2643:G:O2'	11:XA:2645:G:OP2	2.22	0.56
16:A4:108:LEU:HD23	20:AD:148:LEU:HD21	1.87	0.56
17:AA:945:G:O2'	28:AL:154:ARG:NH2	2.37	0.56
17:AA:1428:G:OP1	23:AG:390:LYS:NZ	2.33	0.56
47:XH:136:ASN:OD1	47:XH:137:LYS:N	2.38	0.56
68:c:86:ASP:OD1	68:c:87:LEU:N	2.38	0.56
74:i:125:GLY:O	74:i:128:ARG:NH1	2.38	0.56
7:6:114:ARG:NH1	43:XB:1643:A:OP1	2.36	0.56
11:XA:2154:A:N7	79:o:30:ARG:NH2	2.54	0.56
46:XF:257:GLN:OE1	52:XM:21:ARG:NH1	2.35	0.56
48:XI:38:ARG:O	53:XN:242:TRP:NE1	2.34	0.56
53:XN:134:LYS:NZ	53:XN:138:HIS:O	2.39	0.56
54:XO:41:ARG:NE	54:XO:124:GLU:OE1	2.34	0.56
55:XP:59:SER:OG	80:p:177:ARG:NH1	2.38	0.56
11:XA:1884:G:N3	11:XA:1895:C:O2'	2.38	0.56
11:XA:2051:A:N3	72:g:104:ASN:ND2	2.53	0.56
11:XA:2190:C:OP2	77:l:120:ARG:NH2	2.37	0.56
68:c:80:GLN:O	68:c:210:ARG:NH2	2.39	0.56
76:k:24:GLU:OE2	76:k:26:ASN:N	2.38	0.56
6:5:280:GLN:OE1	86:s:158:ARG:NH1	2.39	0.56
11:XA:1737:A:O2'	74:i:93:ARG:NH1	2.39	0.56
13:A1:54:PRO:HD2	16:A4:518:GLU:OE2	2.06	0.56
13:A1:216:ARG:NH1	41:AY:326:SER:O	2.38	0.56
18:AB:197:HIS:NE2	18:AB:240:ASP:O	2.39	0.56
17:AA:710:U:OP2	29:AM:13:ARG:NH1	2.39	0.56
32:AP:111:ILE:O	32:AP:115:GLN:NE2	2.38	0.56
17:AA:1287:A:OP2	20:AD:260:LYS:NZ	2.35	0.56
68:c:78:ARG:O	68:c:80:GLN:NE2	2.38	0.56
70:e:83:LEU:N	78:m:48:TYR:O	2.38	0.56
6:5:174:GLU:OE1	6:5:298:ASN:ND2	2.38	0.56
23:AG:117:PHE:O	23:AG:122:ARG:NH1	2.39	0.56
7:6:119:GLU:N	7:6:119:GLU:OE1	2.38	0.56
11:XA:2182:G:N2	11:XA:2199:A:N3	2.53	0.56
11:XA:2990:A:O2'	11:XA:2992:G:OP2	2.21	0.56
83:r1:46:Y5P:OP1	83:r1:46:Y5P:HA	2.05	0.56
8:7:247:ASN:ND2	8:7:251:ILE:O	2.37	0.55
40:AX:161:TRP:NE1	40:AX:183:GLU:OE2	2.40	0.55
63:XX:83:GLU:N	63:XX:83:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:j:101:GLU:OE2	75:j:102:GLN:NE2	2.39	0.55
11:XA:1800:G:N1	11:XA:1803:A:OP2	2.40	0.55
11:XA:2931:A:OP2	46:XF:131:LYS:NZ	2.36	0.55
14:A2:24:ASN:OD1	14:A2:25:LYS:N	2.39	0.55
17:AA:1014:A:O2'	17:AA:1031:G:O4'	2.18	0.55
34:AR:70:PHE:O	34:AR:76:GLN:NE2	2.39	0.55
47:XH:95:GLU:OE2	47:XH:112:VAL:N	2.39	0.55
86:s:148:ASP:OD1	86:s:149:CYS:N	2.39	0.55
86:s:103:ASP:OD1	86:s:104:ARG:N	2.39	0.55
7:6:282:SER:OG	7:6:283:GLU:OE1	2.24	0.55
11:XA:2858:A:O2'	11:XA:2874:A:N6	2.39	0.55
16:A4:175:GLN:O	16:A4:180:GLY:N	2.40	0.55
85:r3:56:Y5P:H4A	85:r3:59:Y5P:C2	2.36	0.55
16:A4:264:ARG:HE	16:A4:293:THR:HG22	1.72	0.55
11:XA:3070:G:H21	84:r2:76:P5P:H8	1.72	0.55
20:AD:250:GLY:N	20:AD:326:LEU:O	2.40	0.55
85:r3:63:Y5P:C5	85:r3:64:Y5P:H5	2.37	0.55
11:XA:1681:G:OP2	64:XY:230:LYS:NZ	2.38	0.55
11:XA:1784:A:O2'	60:XU:84:ASN:ND2	2.39	0.55
38:AV:222:SER:OG	38:AV:277:ARG:NH1	2.38	0.55
40:AX:214:GLU:OE2	40:AX:232:ARG:NH2	2.40	0.55
86:s:62:ARG:O	86:s:65:ARG:HG2	2.06	0.55
13:A1:50:ARG:HD3	16:A4:94:TYR:CZ	2.41	0.55
17:AA:798:C:OP1	29:AM:10:LYS:N	2.40	0.55
52:XM:14:ASP:OD1	73:h:119:GLN:NE2	2.40	0.55
84:r2:68:Y5P:H2'	84:r2:69:P5P:C8	2.37	0.55
11:XA:2634:U:OP1	44:XD:278:LYS:NZ	2.40	0.54
11:XA:3220:A:OP1	45:XE:260:LYS:NZ	2.38	0.54
17:AA:1199:G:O6	17:AA:1424:U:O4	2.25	0.54
17:AA:1233:C:OP1	17:AA:1353:A:N6	2.41	0.54
17:AA:1236:C:OP2	27:AK:33:ARG:NH2	2.40	0.54
63:XX:207:THR:N	63:XX:210:GLU:OE2	2.36	0.54
46:XF:126:LYS:NZ	46:XF:130:GLN:OE1	2.36	0.54
57:XR:149:HIS:O	65:XZ:151:LEU:N	2.39	0.54
6:5:160:HIS:HA	6:5:164:TRP:HB2	1.90	0.54
11:XA:1876:U:OP1	72:g:105:ARG:NH1	2.40	0.54
32:AP:65:CYS:SG	32:AP:68:CYS:N	2.81	0.54
46:XF:191:ASP:OD1	46:XF:192:SER:N	2.41	0.54
50:XK:176:TYR:OH	82:r:94:ARG:NH2	2.40	0.54
11:XA:1672:C:O2'	59:XT:149:ARG:O	2.24	0.54
11:XA:2016:C:O2	11:XA:2931:A:O2'	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2457:A:O2'	54:XO:17:ARG:NH2	2.40	0.54
12:A0:103:ASP:OD2	12:A0:105:THR:OG1	2.25	0.54
56:XQ:227:LYS:O	56:XQ:229:TRP:N	2.41	0.54
69:d:158:ASP:OD1	69:d:159:ARG:N	2.39	0.54
83:r1:53:Y5P:H6	83:r1:53:Y5P:O5'	2.08	0.54
17:AA:1264:C:O3'	27:AK:112:ARG:NH2	2.36	0.54
34:AR:202:ARG:NE	34:AR:233:ALA:O	2.37	0.54
85:r3:40:Y5P:H5	85:r3:41:Y5P:C5	2.38	0.54
6:5:122:TRP:O	6:5:215:ARG:NE	2.37	0.54
67:b:9:ARG:NH1	67:b:111:ASP:OD1	2.41	0.54
7:6:183:ASP:OD2	80:p:189:ARG:NH1	2.41	0.54
83:r1:56:Y5P:O2'	83:r1:57:Y5P:O5'	2.26	0.54
46:XF:86:VAL:O	46:XF:179:THR:OG1	2.26	0.54
85:r3:2:Y5P:O3'	85:r3:3:P5P:O4'	2.26	0.54
46:XF:209:TYR:OH	73:h:56:ARG:NH2	2.42	0.53
61:XV:66:GLU:N	61:XV:66:GLU:OE1	2.41	0.53
6:5:337:GLU:N	6:5:337:GLU:OE1	2.41	0.53
8:7:262:ASP:OD1	8:7:263:VAL:N	2.41	0.53
11:XA:2472:A:OP1	51:XL:37:ARG:NH2	2.35	0.53
11:XA:2826:G:OP1	62:XW:49:ARG:NH1	2.39	0.53
11:XA:3219:G:O3'	45:XE:260:LYS:NZ	2.41	0.53
17:AA:864:U:O4	17:AA:865:A:N6	2.42	0.53
28:AL:169:ASN:OD1	28:AL:170:LEU:N	2.42	0.53
33:AQ:23:TYR:O	33:AQ:27:ASN:ND2	2.40	0.53
38:AV:235:GLU:O	38:AV:239:GLY:N	2.41	0.53
68:c:276:CYS:O	68:c:279:LYS:N	2.41	0.53
2:1:23:GLU:OE2	2:1:57:VAL:N	2.41	0.53
11:XA:1694:U:O4'	64:XY:162:ARG:NH2	2.42	0.53
84:r2:30:P5P:H2'	84:r2:31:P5P:H8	1.90	0.53
85:r3:40:Y5P:H5	85:r3:41:Y5P:C4	2.39	0.53
7:6:282:SER:O	7:6:283:GLU:N	2.41	0.53
17:AA:894:C:N4	26:AJ:117:ASP:OD2	2.40	0.53
22:AF:151:ASN:O	22:AF:223:LYS:NZ	2.38	0.53
57:XR:96:GLU:O	58:XS:105:GLN:NE2	2.34	0.53
47:XH:58:ARG:NH1	47:XH:77:HIS:O	2.41	0.53
50:XK:10:GLN:NE2	59:XT:203:LEU:O	2.34	0.53
72:g:154:ASP:OD1	72:g:155:GLN:N	2.41	0.53
84:r2:32:Y5P:O5'	84:r2:32:Y5P:H6	2.08	0.53
84:r2:68:Y5P:H2'	84:r2:69:P5P:H8	1.89	0.53
17:AA:869:C:OP2	31:AO:97:ARG:NH2	2.42	0.53
17:AA:1314:C:N3	22:AF:36:ARG:NH2	2.53	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:361:THR:OG1	6:5:363:ASP:OD1	2.24	0.53
11:XA:2499:U:OP2	11:XA:2504:A:N6	2.28	0.53
17:AA:703:A:OP2	37:AU:43:ASN:ND2	2.39	0.53
17:AA:939:A:O2'	17:AA:940:A:O4'	2.24	0.53
61:XV:147:SER:OG	61:XV:152:ARG:N	2.40	0.53
11:XA:1874:A:O2'	11:XA:2090:A:O2'	2.26	0.53
11:XA:2268:G:N7	52:XM:44:ARG:NH1	2.50	0.53
24:AH:161:GLN:HA	24:AH:164:LEU:CD1	2.39	0.53
86:s:375:ASN:N	86:s:391:ASN:OD1	2.40	0.53
12:A0:82:ARG:NH2	12:A0:138:ASP:O	2.42	0.53
23:AG:295:VAL:N	23:AG:298:ILE:O	2.41	0.53
1:0:99:LYS:NZ	11:XA:2709:A:O2'	2.42	0.53
83:r1:53:Y5P:H6	83:r1:53:Y5P:P	2.49	0.53
9:8:101:ARG:NH1	70:e:82:SER:O	2.43	0.52
17:AA:1225:C:O2'	17:AA:1449:G:O2'	2.19	0.52
46:XF:292:ASP:OD1	46:XF:293:PHE:N	2.42	0.52
85:r3:17:Y5P:OP1	85:r3:58:Y5P:O2'	2.18	0.52
63:XX:150:LYS:HG3	63:XX:159:MET:SD	2.49	0.52
64:XY:218:ARG:NH2	74:i:105:ASP:OD2	2.43	0.52
11:XA:2139:U:O4	65:XZ:77:ARG:NH1	2.41	0.52
37:AU:110:GLN:O	37:AU:114:ARG:NE	2.40	0.52
11:XA:3035:C:O2'	51:XL:34:LYS:NZ	2.42	0.52
17:AA:1106:C:O2'	17:AA:1108:C:OP2	2.23	0.52
11:XA:2237:A:OP1	82:r:168:ARG:NH1	2.43	0.52
11:XA:2813:U:N3	11:XA:2817:G:OP2	2.40	0.52
13:A1:50:ARG:HG2	16:A4:94:TYR:CE1	2.45	0.52
85:r3:73:Y5P:H2'	85:r3:74:P5P:C2	2.40	0.52
82:r:84:ASP:OD1	82:r:85:ASP:N	2.43	0.52
11:XA:2529:U:OP2	44:XD:208:ARG:NH1	2.43	0.52
41:AY:377:ARG:O	41:AY:381:ASN:ND2	2.43	0.52
50:XK:85:GLY:O	50:XK:88:ARG:NH1	2.42	0.52
11:XA:2262:C:OP1	58:XS:173:ARG:NH1	2.41	0.52
35:AS:75:TYR:OH	39:AW:91:GLN:O	2.27	0.52
39:AW:103:ARG:O	39:AW:115:ASP:N	2.43	0.52
45:XE:316:PHE:HB3	45:XE:317:PRO:HD3	1.92	0.52
11:XA:1671:G:C6	11:XA:1818:A:N1	2.79	0.51
11:XA:1746:A:O4'	47:XH:61:LYS:NZ	2.42	0.51
40:AX:157:ASP:OD1	40:AX:158:ALA:N	2.43	0.51
53:XN:234:ASP:O	53:XN:238:LYS:HA	2.10	0.51
56:XQ:103:ARG:NH2	56:XQ:167:TYR:OH	2.43	0.51
59:XT:133:ASN:O	69:d:230:ARG:NH2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:371:ASP:OD1	7:6:371:ASP:N	2.43	0.51
53:XN:123:ARG:O	53:XN:158:ARG:NH2	2.44	0.51
80:p:113:GLU:O	80:p:117:GLN:OE1	2.28	0.51
84:r2:67:Y5P:OP2	84:r2:67:Y5P:H6	2.10	0.51
6:5:189:LYS:NZ	86:s:182:SER:OG	2.43	0.51
11:XA:1770:G:OP2	57:XR:11:ARG:NH1	2.39	0.51
11:XA:3160:A:OP1	45:XE:213:LYS:NZ	2.37	0.51
16:A4:71:LEU:HB3	41:AY:302:ILE:CG2	2.40	0.51
34:AR:140:ASP:OD1	34:AR:141:VAL:N	2.43	0.51
64:XY:161:GLU:OE1	64:XY:161:GLU:N	2.43	0.51
11:XA:1708:A:O5'	64:XY:192:LYS:NZ	2.44	0.51
11:XA:2384:A:N1	11:XA:2409:A:N6	2.58	0.51
20:AD:281:TYR:OH	35:AS:21:ARG:NH2	2.43	0.51
78:m:52:TYR:N	78:m:68:TYR:O	2.37	0.51
82:r:153:ARG:NH1	82:r:176:VAL:O	2.40	0.51
86:s:403:GLU:N	86:s:403:GLU:OE1	2.44	0.51
16:A4:478:TYR:O	16:A4:482:ILE:HG13	2.11	0.51
18:AB:82:ARG:NH2	18:AB:86:ASP:OD1	2.40	0.51
48:XI:181:ILE:O	48:XI:184:THR:N	2.42	0.51
85:r3:53:Y5P:HB	85:r3:54:Y5P:H6	1.92	0.51
60:XU:58:GLU:OE2	60:XU:65:VAL:N	2.44	0.51
6:5:47:ASP:OD1	6:5:48:ARG:N	2.43	0.51
13:A1:255:ASN:OD1	13:A1:256:SER:N	2.44	0.51
16:A4:98:ALA:N	16:A4:102:GLU:OE2	2.44	0.51
17:AA:1526:U:O2	17:AA:1526:U:O2'	2.27	0.51
73:h:114:ASN:HA	73:h:117:LEU:HD22	1.92	0.51
83:r1:54:Y5P:C5	83:r1:55:Y5P:HC	2.40	0.51
85:r3:52:P5P:C4	85:r3:53:Y5P:H5	2.40	0.51
46:XF:102:TRP:NE1	46:XF:163:TYR:O	2.43	0.51
12:A0:50:LEU:O	12:A0:55:TRP:NE1	2.42	0.51
17:AA:1053:A:N1	17:AA:1100:C:O2'	2.43	0.51
47:XH:120:ARG:NH2	63:XX:136:ASP:OD2	2.39	0.51
58:XS:126:GLU:N	58:XS:126:GLU:OE1	2.44	0.51
17:AA:1234:C:O2'	17:AA:1235:U:OP1	2.24	0.51
46:XF:277:ASP:O	72:g:90:ARG:NH2	2.44	0.51
51:XL:35:MET:N	51:XL:57:CYS:O	2.43	0.51
6:5:310:ARG:NH1	6:5:378:SER:OG	2.44	0.50
8:7:159:LYS:HG3	66:a:91:HIS:HA	1.92	0.50
11:XA:2623:A:HO2'	17:AA:1549:G:HO2'	1.57	0.50
17:AA:1369:U:C6	22:AF:201:MET:HE1	2.46	0.50
84:r2:39:Y5P:C6	84:r2:40:Y5P:H5	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2155:A:N6	82:r:169:TRP:O	2.44	0.50
11:XA:2173:G:N3	49:XJ:150:SER:OG	2.44	0.50
17:AA:1486:C:H2'	17:AA:1487:C:O4'	2.11	0.50
38:AV:123:ASP:OD1	38:AV:124:LYS:N	2.43	0.50
38:AV:159:ASP:OD1	38:AV:160:ALA:N	2.42	0.50
55:XP:90:GLU:OE2	55:XP:107:ARG:NH2	2.44	0.50
68:c:248:ARG:O	68:c:249:ASN:OD1	2.29	0.50
69:d:157:HIS:O	69:d:161:HIS:ND1	2.44	0.50
85:r3:23:P5P:C6	85:r3:24:Y5P:H4	2.41	0.50
85:r3:73:Y5P:OP2	85:r3:74:P5P:H3'	2.12	0.50
16:A4:73:ALA:HB2	24:AH:61:PRO:HG2	1.94	0.50
18:AB:258:THR:O	18:AB:262:GLU:OE1	2.29	0.50
19:AC:89:ASP:OD1	19:AC:89:ASP:C	2.54	0.50
75:j:98:LEU:O	75:j:101:GLU:HG3	2.11	0.50
6:5:307:ASP:OD1	6:5:310:ARG:NH2	2.45	0.50
13:A1:152:ASP:N	13:A1:152:ASP:OD1	2.44	0.50
85:r3:13:Y5P:H2	85:r3:14:P5P:H6	1.94	0.50
85:r3:34:Y5P:H4A	85:r3:35:P5P:C6	2.42	0.50
10:9:134:ASN:OD1	10:9:135:PHE:N	2.43	0.50
13:A1:81:VAL:O	13:A1:99:LYS:NZ	2.43	0.50
17:AA:766:G:OP2	30:AN:76:HIS:NE2	2.37	0.50
17:AA:845:A:O2'	17:AA:846:A:O4'	2.27	0.50
22:AF:138:GLU:N	22:AF:138:GLU:OE1	2.45	0.50
46:XF:185:ASP:OD1	46:XF:185:ASP:C	2.55	0.50
3:2:87:ARG:NH2	11:XA:1792:G:N7	2.56	0.50
38:AV:47:HIS:O	38:AV:47:HIS:ND1	2.45	0.50
56:XQ:268:ASP:OD1	56:XQ:269:MET:N	2.45	0.50
61:XV:69:ASP:OD1	61:XV:72:LYS:NZ	2.41	0.50
68:c:258:THR:N	68:c:271:PHE:O	2.44	0.50
84:r2:60:Y5P:OP2	84:r2:61:Y5P:H5	2.12	0.50
20:AD:283:GLU:O	20:AD:356:GLN:NE2	2.45	0.50
56:XQ:102:ARG:NH1	56:XQ:167:TYR:O	2.44	0.50
85:r3:40:Y5P:H5	85:r3:41:Y5P:H4	1.94	0.50
11:XA:3151:A:N6	11:XA:3163:G:O2'	2.44	0.50
22:AF:35:SER:OG	22:AF:36:ARG:N	2.44	0.50
42:AZ:27:ASN:O	42:AZ:30:SER:OG	2.30	0.50
11:XA:2453:G:O6	11:XA:2672:A:N6	2.45	0.49
16:A4:247:ILE:O	16:A4:254:LYS:NZ	2.39	0.49
17:AA:1485:G:P	83:r1:48:Y5P:H2'	2.52	0.49
23:AG:276:ARG:HG3	23:AG:277:LYS:H	1.76	0.49
34:AR:176:GLU:N	34:AR:176:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:AV:201:GLU:OE1	38:AV:233:LYS:NZ	2.44	0.49
62:XW:115:ASP:C	62:XW:119:ARG:HE	2.20	0.49
11:XA:2029:A:O2'	11:XA:2030:U:OP1	2.27	0.49
11:XA:2066:C:O2'	11:XA:2067:C:OP1	2.30	0.49
11:XA:2187:C:O2'	49:XJ:106:LYS:NZ	2.43	0.49
38:AV:108:THR:O	38:AV:111:THR:OG1	2.26	0.49
46:XF:97:HIS:NE2	46:XF:101:MET:SD	2.85	0.49
82:r:94:ARG:N	82:r:98:GLY:O	2.40	0.49
84:r2:74:Y5P:C4	84:r2:75:Y5P:HC	2.42	0.49
6:5:214:ASN:OD1	6:5:214:ASN:N	2.44	0.49
8:7:203:THR:O	8:7:207:HIS:ND1	2.45	0.49
11:XA:2104:A:OP1	53:XN:73:ARG:NH1	2.43	0.49
13:A1:50:ARG:CG	16:A4:94:TYR:CE1	2.95	0.49
13:A1:154:THR:OG1	24:AH:172:VAL:O	2.30	0.49
17:AA:1048:C:O2'	28:AL:196:TYR:O	2.27	0.49
17:AA:1369:U:O4	22:AF:192:ARG:NH2	2.44	0.49
37:AU:52:GLU:N	37:AU:52:GLU:OE1	2.43	0.49
69:d:116:MET:SD	69:d:116:MET:N	2.85	0.49
8:7:51:GLU:OE2	8:7:54:ARG:NH2	2.44	0.49
15:A3:173:LEU:O	15:A3:176:ILE:HG22	2.11	0.49
11:XA:3096:U:C5	90:XA:5144:H8Q:O42	2.64	0.49
17:AA:881:A:O2'	17:AA:882:A:O4'	2.25	0.49
21:AE:38:ASP:OD1	21:AE:39:LEU:N	2.43	0.49
70:e:269:LEU:O	70:e:273:ARG:HD3	2.12	0.49
85:r3:32:Y5P:O5'	85:r3:32:Y5P:H6	2.13	0.49
11:XA:2381:A:N6	11:XA:2412:A:N1	2.60	0.49
11:XA:3070:G:N2	84:r2:76:P5P:O2'	2.45	0.49
28:AL:75:ASP:OD2	37:AU:153:LYS:NZ	2.39	0.49
28:AL:188:GLU:OE1	28:AL:188:GLU:N	2.45	0.49
36:AT:9:ILE:O	36:AT:12:THR:OG1	2.29	0.49
38:AV:131:ASN:ND2	38:AV:134:GLN:OE1	2.46	0.49
38:AV:192:LYS:NZ	38:AV:194:THR:O	2.45	0.49
43:XB:1632:U:N3	43:XB:1635:C:OP2	2.42	0.49
50:XK:9:GLN:NE2	50:XK:13:THR:OG1	2.46	0.49
82:r:40:GLU:OE2	82:r:47:THR:OG1	2.27	0.49
7:6:105:GLU:O	7:6:108:GLN:NE2	2.44	0.49
11:XA:2520:C:OP2	44:XD:295:TYR:OH	2.29	0.49
13:A1:153:SER:OG	13:A1:154:THR:N	2.46	0.49
17:AA:975:A:OP1	21:AE:90:ARG:NH1	2.40	0.49
85:r3:16:Y5P:HA1	85:r3:17(A):P5P:H5'1	1.93	0.49
11:XA:1885:A:OP2	46:XF:168:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2139:U:OP2	65:XZ:74:SER:N	2.34	0.49
11:XA:2400:C:O2'	11:XA:2401:A:O5'	2.29	0.49
11:XA:3008:C:C2	11:XA:3032:G:N2	2.81	0.49
38:AV:82:ARG:NH2	38:AV:119:TYR:O	2.46	0.49
41:AY:344:GLN:N	41:AY:344:GLN:OE1	2.46	0.49
45:XE:327:GLU:OE1	45:XE:327:GLU:N	2.45	0.49
11:XA:1796:A:OP1	46:XF:147:ARG:NH2	2.43	0.49
11:XA:3218:A:OP2	45:XE:212:GLY:N	2.46	0.49
13:A1:83:LEU:O	13:A1:99:LYS:NZ	2.45	0.49
16:A4:90:GLN:CG	19:AC:133:TYR:HE1	2.26	0.49
11:XA:2833:A:OP1	62:XW:74:ARG:NH1	2.36	0.49
25:AI:140:LYS:NZ	25:AI:168:GLY:O	2.42	0.49
63:XX:148:THR:HG23	63:XX:148:THR:O	2.12	0.49
15:A3:184:GLU:OE1	15:A3:184:GLU:N	2.46	0.48
69:d:235:GLN:OE1	69:d:235:GLN:N	2.46	0.48
75:j:76:ARG:O	75:j:80:LEU:HD23	2.13	0.48
84:r2:43:Y5P:H2'	84:r2:44:P5P:C8	2.43	0.48
86:s:294:TYR:OH	86:s:353:ARG:NH2	2.46	0.48
6:5:334:LYS:O	6:5:362:THR:OG1	2.28	0.48
11:XA:2525:C:OP2	11:XA:2526:C:O2'	2.28	0.48
13:A1:196:GLU:N	13:A1:196:GLU:OE1	2.46	0.48
17:AA:1200:G:N2	17:AA:1418:G:O2'	2.46	0.48
17:AA:1429:C:OP1	23:AG:388:ARG:NH2	2.44	0.48
33:AQ:37:GLU:OE2	33:AQ:41:HIS:NE2	2.41	0.48
49:XJ:149:ARG:NH2	77:l:101:LEU:O	2.43	0.48
8:7:94:HIS:NE2	59:XT:135:GLU:OE2	2.44	0.48
48:XI:163:GLU:O	48:XI:166:ARG:HG3	2.14	0.48
55:XP:125:GLU:OE1	55:XP:159:ARG:NH2	2.43	0.48
6:5:177:CYS:O	6:5:180:ILE:HG22	2.13	0.48
11:XA:1828:A:H4'	11:XA:1829:A:C8	2.49	0.48
11:XA:2138:U:O2'	11:XA:2151:A:N3	2.42	0.48
11:XA:2959:G:O2'	11:XA:2965:A:N6	2.47	0.48
43:XB:1644:G:O6	55:XP:87:HIS:NE2	2.44	0.48
46:XF:94:ASP:OD1	46:XF:95:ILE:N	2.44	0.48
46:XF:222:THR:OG1	46:XF:225:GLU:OE1	2.29	0.48
60:XU:16:GLN:N	61:XV:206:GLU:OE2	2.38	0.48
83:r1:56:Y5P:HD	83:r1:57:Y5P:P	2.36	0.48
7:6:283:GLU:OE1	7:6:283:GLU:N	2.46	0.48
17:AA:769:G:N2	17:AA:772:A:OP2	2.40	0.48
53:XN:204:GLU:OE1	53:XN:208:ASN:ND2	2.47	0.48
85:r3:52:P5P:N3	85:r3:53:Y5P:H5	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:180:CYS:SG	8:7:181:TYR:N	2.86	0.48
70:e:175:GLN:N	70:e:175:GLN:OE1	2.46	0.48
4:3:169:ARG:NH2	11:XA:1892:A:OP1	2.46	0.48
11:XA:2082:G:C2	65:XZ:88:MET:HE2	2.47	0.48
12:A0:19:ARG:O	12:A0:23:GLU:OE1	2.32	0.48
17:AA:1399:A:H2'	17:AA:1400:U:C6	2.49	0.48
21:AE:115:GLU:N	21:AE:115:GLU:OE1	2.46	0.48
29:AM:18:THR:N	29:AM:37:ALA:O	2.36	0.48
32:AP:108:THR:O	32:AP:111:ILE:HG22	2.13	0.48
37:AU:178:GLU:OE1	37:AU:178:GLU:N	2.43	0.48
41:AY:367:LYS:O	41:AY:371:GLU:OE1	2.31	0.48
62:XW:114:VAL:O	62:XW:117:ILE:HG22	2.13	0.48
11:XA:1859:A:OP1	11:XA:2299:U:O2'	2.31	0.48
11:XA:2083:U:H1'	65:XZ:88:MET:CE	2.43	0.48
52:XM:255:MET:O	52:XM:258:THR:OG1	2.29	0.48
59:XT:55:ASN:O	69:d:227:ARG:NH2	2.46	0.48
68:c:68:TYR:O	68:c:72:ILE:HD12	2.14	0.48
12:A0:61:GLU:OE2	12:A0:139:TRP:N	2.47	0.48
24:AH:154:ASP:O	24:AH:157:LEU:HG	2.13	0.48
36:AT:48:VAL:HA	36:AT:52:ILE:CD1	2.44	0.48
11:XA:2754:A:N3	63:XX:108:GLN:NE2	2.62	0.48
17:AA:917:C:OP2	31:AO:91:ARG:NH2	2.47	0.48
54:XO:129:CYS:SG	54:XO:130:LEU:N	2.87	0.48
65:XZ:81:TRP:O	65:XZ:84:ASP:OD1	2.32	0.48
84:r2:23:P5P:O2'	84:r2:24:P5P:O5'	2.31	0.48
11:XA:1883:G:N7	46:XF:281:ARG:NH1	2.62	0.47
11:XA:1953:A:O2'	11:XA:2463:A:OP1	2.32	0.47
11:XA:3119:C:C2	11:XA:3120:C:C5	3.02	0.47
12:A0:135:MET:SD	12:A0:135:MET:N	2.84	0.47
17:AA:812:A:O2'	17:AA:813:A:O4'	2.30	0.47
53:XN:78:GLU:OE2	53:XN:158:ARG:NE	2.46	0.47
57:XR:57:ARG:O	57:XR:61:LYS:HG2	2.14	0.47
3:2:56:SER:OG	11:XA:1980:A:OP1	2.29	0.47
8:7:314:ASP:OD2	45:XE:166:ARG:NH2	2.48	0.47
11:XA:1742:G:O2'	11:XA:1754:G:O6	2.32	0.47
52:XM:289:ASN:OD1	52:XM:290:LEU:N	2.45	0.47
70:e:201:GLU:N	70:e:201:GLU:OE1	2.47	0.47
23:AG:299:ASP:OD1	23:AG:300:TYR:N	2.47	0.47
80:p:81:CYS:SG	80:p:82:ARG:N	2.86	0.47
20:AD:95:ALA:N	42:AZ:74:GLU:OE1	2.47	0.47
56:XQ:118:ARG:NH2	56:XQ:204:MET:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:XW:38:SER:OG	62:XW:39:SER:N	2.47	0.47
65:XZ:43:GLU:OE1	65:XZ:43:GLU:N	2.47	0.47
68:c:121:SER:OG	68:c:122:ASN:N	2.45	0.47
85:r3:32:Y5P:H4A	85:r3:33:Y5P:N3	2.30	0.47
11:XA:2993:U:O2	84:r2:76:P5P:O2'	2.30	0.47
13:A1:142:LYS:O	13:A1:146:HIS:ND1	2.43	0.47
56:XQ:108:ILE:O	56:XQ:108:ILE:HG13	2.13	0.47
59:XT:115:LYS:O	59:XT:119:GLU:OE1	2.32	0.47
60:XU:49:THR:O	60:XU:52:ASP:OD1	2.32	0.47
63:XX:36:ARG:NH2	63:XX:151:GLU:OE1	2.48	0.47
65:XZ:80:TYR:HA	65:XZ:83:LYS:HG2	1.96	0.47
11:XA:1749:C:OP2	11:XA:2899:C:O2'	2.26	0.47
14:A2:105:ASN:O	14:A2:109:GLN:OE1	2.33	0.47
35:AS:105:GLU:OE2	35:AS:106:LEU:HD12	2.14	0.47
50:XK:74:GLN:HA	82:r:161:PRO:HA	1.96	0.47
51:XL:120:LYS:O	51:XL:143:ASN:ND2	2.46	0.47
52:XM:270:ALA:HB1	52:XM:271:PRO:HD2	1.97	0.47
70:e:65:PRO:O	70:e:69:GLU:OE1	2.32	0.47
73:h:139:LYS:HZ2	79:o:101:TRP:CD1	2.32	0.47
80:p:121:ILE:O	80:p:124:LYS:NZ	2.47	0.47
4:3:110:VAL:HG11	4:3:161:MET:SD	2.54	0.47
6:5:270:ILE:HG22	6:5:270:ILE:O	2.14	0.47
11:XA:1917:A:C8	11:XA:1983:U:C4	3.03	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
19:AC:84:GLU:OE1	19:AC:84:GLU:N	2.43	0.47
22:AF:116:GLU:O	22:AF:120:ARG:HG2	2.14	0.47
28:AL:86:ASP:OD1	28:AL:87:ASP:N	2.48	0.47
44:XD:118:LYS:NZ	44:XD:119:SER:O	2.42	0.47
46:XF:142:ARG:HA	46:XF:149:GLY:HA2	1.96	0.47
53:XN:214:THR:O	53:XN:218:ILE:HD12	2.15	0.47
82:r:99:MET:SD	82:r:99:MET:N	2.85	0.47
83:r1:47:Y5P:H4A	83:r1:48:Y5P:H4	1.96	0.47
86:s:92:MET:HG3	86:s:92:MET:O	2.14	0.47
11:XA:1851:G:O4'	11:XA:2134:A:N6	2.47	0.47
13:A1:129:PHE:O	16:A4:63:LYS:NZ	2.47	0.47
40:AX:171:SER:OG	40:AX:178:PHE:O	2.33	0.47
42:AZ:54:ASN:ND2	42:AZ:57:THR:OG1	2.48	0.47
86:s:242:ARG:NH2	86:s:290:ASP:OD2	2.48	0.47
11:XA:2574:G:O2'	11:XA:2575:U:P	2.72	0.47
11:XA:2752:C:C2	11:XA:2753:A:C8	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AG:203:GLU:O	23:AG:207:GLU:OE1	2.33	0.47
23:AG:359:ASP:OD2	23:AG:363:TRP:NE1	2.47	0.47
40:AX:272:THR:OG1	40:AX:282:ILE:O	2.31	0.47
8:7:237:VAL:O	8:7:241:GLU:OE1	2.33	0.47
14:A2:84:ARG:NH2	17:AA:1464:G:OP1	2.39	0.47
19:AC:75:ASN:OD1	19:AC:76:LEU:N	2.47	0.47
55:XP:46:GLU:OE1	55:XP:48:THR:OG1	2.33	0.47
70:e:203:LYS:N	70:e:237:LEU:O	2.48	0.47
84:r2:39:Y5P:H2'	84:r2:40:Y5P:H6	1.97	0.47
7:6:146:TYR:O	7:6:149:GLN:NE2	2.48	0.46
7:6:364:ARG:NE	11:XA:2859:A:OP2	2.32	0.46
11:XA:2939:C:H2'	11:XA:2940:A:O4'	2.14	0.46
46:XF:215:SER:OG	46:XF:257:GLN:N	2.36	0.46
73:h:97:LYS:NZ	73:h:120:MET:O	2.48	0.46
9:8:186:GLN:N	9:8:186:GLN:OE1	2.47	0.46
40:AX:346:SER:OG	40:AX:347:ASN:N	2.47	0.46
52:XM:153:ASN:ND2	52:XM:256:LEU:O	2.48	0.46
54:XO:86:ILE:HB	54:XO:87:PRO:HD3	1.97	0.46
8:7:64:LYS:NZ	69:d:278:LYS:O	2.48	0.46
17:AA:1067:A:H2'	17:AA:1068:A:O4'	2.15	0.46
22:AF:201:MET:N	22:AF:202:PRO:HD2	2.31	0.46
41:AY:299:GLU:HA	41:AY:302:ILE:HG12	1.97	0.46
54:XO:16:ARG:NE	54:XO:51:GLU:OE2	2.40	0.46
38:AV:328:PRO:O	38:AV:332:GLU:OE1	2.33	0.46
49:XJ:50:CYS:O	49:XJ:54:ASN:ND2	2.48	0.46
11:XA:2525:C:O2'	11:XA:2533:A:O2'	2.34	0.46
21:AE:56:GLN:OE1	21:AE:56:GLN:N	2.48	0.46
44:XD:251:ASP:OD1	44:XD:251:ASP:C	2.57	0.46
64:XY:134:LYS:O	64:XY:137:ASP:OD1	2.34	0.46
69:d:249:GLU:OE2	69:d:262:HIS:ND1	2.48	0.46
7:6:58:ARG:O	7:6:62:GLU:OE1	2.34	0.46
11:XA:1990:G:OP1	44:XD:269:ARG:NH2	2.46	0.46
36:AT:114:ARG:O	36:AT:118:GLU:OE1	2.33	0.46
43:XB:1620:A:N3	43:XB:1620:A:H2'	2.30	0.46
57:XR:122:ARG:NH2	57:XR:126:GLU:OE2	2.48	0.46
59:XT:88:TRP:CH2	59:XT:92:LYS:HD2	2.50	0.46
2:1:42:THR:O	81:q:135:TRP:NE1	2.49	0.46
20:AD:108:ALA:O	20:AD:114:ARG:NH1	2.48	0.46
31:AO:196:GLY:O	34:AR:146:LYS:NZ	2.48	0.46
68:c:290:LEU:O	68:c:294:GLU:OE1	2.34	0.46
71:f:138:GLN:HG3	71:f:144:MET:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:1799:U:H2'	11:XA:1800:G:O4'	2.16	0.46
13:A1:199:CYS:O	13:A1:203:ASP:N	2.49	0.46
15:A3:138:MET:HE2	17:AA:1489:G:H4'	1.97	0.46
63:XX:213:GLU:OE2	63:XX:216:ARG:NH1	2.46	0.46
63:XX:226:LEU:HA	63:XX:229:ILE:HG22	1.97	0.46
1:O:91:ARG:HG3	1:O:95:ARG:HE	1.80	0.46
7:6:57:TYR:CE2	62:XW:117:ILE:HD11	2.51	0.46
11:XA:1882:A:N6	11:XA:1893:A:O4'	2.49	0.46
11:XA:2521:A:N6	44:XD:202:ARG:O	2.47	0.46
11:XA:2538:C:H2'	11:XA:2539:A:O4'	2.15	0.46
13:A1:52:ALA:HB2	16:A4:94:TYR:HB2	1.98	0.46
16:A4:64:THR:CG2	24:AH:64:THR:CG2	2.94	0.46
16:A4:643:GLU:O	16:A4:646:THR:OG1	2.34	0.46
17:AA:819:A:O2'	17:AA:831:U:O2'	2.30	0.46
37:AU:114:ARG:O	37:AU:118:GLU:OE1	2.34	0.46
41:AY:367:LYS:O	41:AY:370:VAL:HG12	2.15	0.46
51:XL:99:ARG:HH12	56:XQ:191:ARG:HE	1.62	0.46
66:a:70:GLU:O	67:b:141:ARG:N	2.44	0.46
69:d:90:GLY:O	69:d:262:HIS:NE2	2.47	0.46
8:7:306:LEU:O	8:7:306:LEU:HG	2.15	0.46
11:XA:2292:G:C6	57:XR:10:LEU:N	2.84	0.46
11:XA:3066:C:C2'	11:XA:3067:U:H5'	2.45	0.46
16:A4:64:THR:HG22	24:AH:64:THR:CG2	2.46	0.46
24:AH:154:ASP:O	24:AH:158:GLU:OE1	2.34	0.46
61:XV:216:TYR:OH	64:XY:186:ILE:O	2.27	0.46
67:b:53:ASP:OD1	67:b:54:PHE:N	2.48	0.46
72:g:104:ASN:OD1	72:g:105:ARG:N	2.49	0.46
81:q:169:ASP:N	81:q:170:PRO:CD	2.78	0.46
82:r:112:HIS:O	82:r:116:GLU:OE1	2.34	0.46
84:r2:16:Y5P:C4	84:r2:60:Y5P:H2'	2.46	0.46
84:r2:48:Y5P:HA	84:r2:49:Y5P:OP2	2.16	0.46
11:XA:1744:A:OP1	52:XM:87:HIS:NE2	2.41	0.45
11:XA:2531:U:O4	44:XD:246:ARG:NH2	2.49	0.45
53:XN:201:ASP:OD1	53:XN:201:ASP:C	2.59	0.45
56:XQ:107:HIS:O	56:XQ:108:ILE:HG13	2.16	0.45
73:h:75:LYS:O	73:h:80:SER:HA	2.16	0.45
80:p:128:ASN:OD1	80:p:129:ARG:N	2.46	0.45
11:XA:2347:C:O3'	69:d:69:LYS:NZ	2.47	0.45
16:A4:66:ASP:OD1	16:A4:67:LYS:N	2.49	0.45
23:AG:321:ASP:C	23:AG:321:ASP:OD1	2.58	0.45
40:AX:100:MET:HB3	92:AX:500:GTP:HN1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:AX:130:LYS:O	40:AX:130:LYS:HG3	2.15	0.45
45:XE:310:LEU:HG	45:XE:310:LEU:O	2.15	0.45
60:XU:52:ASP:OD1	60:XU:53:LEU:N	2.49	0.45
11:XA:2083:U:H1'	65:XZ:88:MET:HE3	1.99	0.45
16:A4:164:ARG:H	16:A4:167:LYS:HE3	1.82	0.45
17:AA:1289:G:O2'	17:AA:1297:G:OP2	2.35	0.45
17:AA:1433:A:N3	17:AA:1458:A:N6	2.64	0.45
23:AG:140:TRP:HA	23:AG:146:PRO:HA	1.99	0.45
35:AS:67:GLU:OE2	39:AW:85:ARG:NE	2.48	0.45
40:AX:51:THR:O	40:AX:67:HIS:N	2.48	0.45
46:XF:220:ASP:O	46:XF:245:ALA:N	2.50	0.45
63:XX:160:ASP:OD1	63:XX:160:ASP:C	2.59	0.45
7:6:288:SER:O	7:6:289:PRO:C	2.60	0.45
11:XA:1769:C:O2'	57:XR:11:ARG:NH2	2.50	0.45
11:XA:2386:C:OP2	44:XD:71:LYS:NZ	2.44	0.45
11:XA:3148:C:OP1	45:XE:211:ILE:HD12	2.16	0.45
13:A1:91:VAL:O	13:A1:94:GLY:N	2.49	0.45
17:AA:1161:A:C2	17:AA:1162:A:C8	3.05	0.45
34:AR:69:THR:OG1	34:AR:71:MET:SD	2.74	0.45
38:AV:233:LYS:O	38:AV:288:LYS:NZ	2.48	0.45
40:AX:337:LEU:HG	40:AX:337:LEU:O	2.16	0.45
41:AY:277:LEU:O	41:AY:281:GLU:OE1	2.34	0.45
84:r2:19:P5P:N7	84:r2:59:Y5P:H4	2.31	0.45
85:r3:13:Y5P:HC	85:r3:14:P5P:N7	2.31	0.45
86:s:296:HIS:NE2	86:s:427:ASN:O	2.49	0.45
11:XA:1939:G:O4'	44:XD:259:LYS:NZ	2.45	0.45
11:XA:2658:U:OP1	45:XE:225:LYS:NZ	2.44	0.45
16:A4:71:LEU:CB	41:AY:302:ILE:HG22	2.46	0.45
44:XD:113:ARG:O	44:XD:147:ARG:NH2	2.47	0.45
53:XN:203:GLU:O	53:XN:206:GLU:HG3	2.17	0.45
75:j:102:GLN:O	75:j:106:GLU:OE1	2.35	0.45
79:o:40:GLU:O	79:o:44:GLU:OE1	2.34	0.45
81:q:159:GLU:HG2	81:q:160:ALA:H	1.81	0.45
86:s:222:ARG:NH1	86:s:227:ASP:OD2	2.49	0.45
4:3:182:ASP:OD1	4:3:183:ARG:N	2.48	0.45
11:XA:2934:G:C2'	11:XA:2987:U:OP2	2.65	0.45
13:A1:50:ARG:HB3	16:A4:94:TYR:CE1	2.52	0.45
14:A2:113:ASN:OD1	14:A2:114:LYS:N	2.50	0.45
17:AA:1199:G:N1	17:AA:1424:U:C4	2.85	0.45
17:AA:1235:U:H5''	17:AA:1236:C:OP2	2.16	0.45
23:AG:158:TYR:CD2	23:AG:162:MET:HE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AG:340:GLN:O	23:AG:344:ILE:HG12	2.17	0.45
25:AI:181:ILE:O	25:AI:181:ILE:HG13	2.16	0.45
36:AT:52:ILE:N	36:AT:53:PRO:CD	2.80	0.45
41:AY:339:GLU:OE1	41:AY:339:GLU:N	2.50	0.45
55:XP:71:PHE:HB3	55:XP:72:PRO:HD3	1.99	0.45
63:XX:180:ASP:N	63:XX:181:PRO:HD3	2.32	0.45
81:q:134:ASN:O	81:q:137:GLN:NE2	2.50	0.45
90:XA:5144:H8Q:O57	90:XA:5144:H8Q:O58	2.33	0.45
52:XM:44:ARG:HD3	52:XM:45:ARG:HG3	1.97	0.45
55:XP:109:TRP:HA	55:XP:112:LYS:HG2	1.98	0.45
61:XV:148:THR:HG22	61:XV:149:ARG:H	1.80	0.45
61:XV:196:GLU:O	61:XV:200:GLU:OE1	2.34	0.45
65:XZ:117:ILE:O	79:o:45:ASN:ND2	2.49	0.45
8:7:38:THR:O	8:7:42:GLU:OE1	2.35	0.45
10:9:72:PRO:O	64:XY:85:TRP:NE1	2.50	0.45
11:XA:3219:G:O2'	11:XA:3221:A:OP2	2.32	0.45
28:AL:140:GLU:O	28:AL:144:GLU:OE1	2.35	0.45
43:XB:1631:C:OP2	78:m:42:ARG:NH2	2.50	0.45
57:XR:51:VAL:O	57:XR:54:THR:OG1	2.32	0.45
7:6:124:ARG:NH2	9:8:112:GLU:OE1	2.39	0.45
11:XA:2239:A:OP2	50:XK:75:LYS:NZ	2.45	0.45
25:AI:151:VAL:O	25:AI:178:ASN:N	2.50	0.45
36:AT:31:THR:OG1	36:AT:65:MET:SD	2.61	0.45
36:AT:45:ARG:HA	36:AT:48:VAL:HG12	1.98	0.45
40:AX:170:GLN:OE1	40:AX:175:LYS:NZ	2.41	0.45
46:XF:280:TYR:CE2	52:XM:125:ARG:HD3	2.52	0.45
57:XR:36:ASN:OD1	57:XR:37:ARG:N	2.50	0.45
61:XV:148:THR:HG22	61:XV:149:ARG:HD3	1.98	0.45
64:XY:231:ALA:HA	64:XY:234:LEU:CD2	2.47	0.45
76:k:57:HIS:O	76:k:57:HIS:ND1	2.50	0.45
86:s:350:ASP:OD1	86:s:351:VAL:N	2.49	0.45
10:9:127:LEU:O	10:9:134:ASN:ND2	2.40	0.45
10:9:137:ARG:NE	60:XU:21:ARG:O	2.49	0.45
11:XA:2079:C:O2	79:o:60:ARG:NH1	2.48	0.45
11:XA:2552:U:C2	11:XA:2553:G:C8	3.04	0.45
13:A1:156:TYR:O	13:A1:167:ARG:NH1	2.50	0.45
17:AA:662:U:H2'	17:AA:663:A:O4'	2.17	0.45
17:AA:762:G:OP1	28:AL:206:LYS:NZ	2.40	0.45
23:AG:244:PHE:O	23:AG:246:ARG:NH1	2.50	0.45
28:AL:176:ASP:N	28:AL:176:ASP:OD1	2.50	0.45
48:XI:198:PRO:O	48:XI:199:SER:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:XR:17:ARG:HA	57:XR:20:ARG:HG2	1.98	0.45
62:XW:115:ASP:O	62:XW:119:ARG:NE	2.49	0.45
73:h:65:ASP:OD1	73:h:65:ASP:C	2.60	0.45
3:2:70:LEU:O	64:XY:198:ARG:NH2	2.50	0.44
11:XA:2080:U:O2'	79:o:60:ARG:O	2.25	0.44
11:XA:2216:A:N3	48:XI:150:HIS:NE2	2.62	0.44
13:A1:216:ARG:NH2	41:AY:326:SER:O	2.47	0.44
20:AD:198:TRP:HA	20:AD:201:ILE:HD13	1.99	0.44
52:XM:238:ARG:O	80:p:155:ARG:NH2	2.44	0.44
57:XR:65:ARG:O	57:XR:69:ILE:HG12	2.16	0.44
79:o:68:ARG:O	79:o:72:GLU:OE1	2.35	0.44
82:r:167:PRO:O	82:r:171:ARG:N	2.50	0.44
4:3:113:ARG:HH12	52:XM:76:ILE:HA	1.82	0.44
7:6:39:ASP:OD1	7:6:40:ILE:N	2.50	0.44
11:XA:2665:U:OP2	54:XO:17:ARG:HD2	2.16	0.44
16:A4:482:ILE:CG2	16:A4:519:TYR:HE2	2.30	0.44
17:AA:918:A:O2'	17:AA:919:A:O4'	2.35	0.44
17:AA:1281:U:OP1	18:AB:210:ARG:NH2	2.50	0.44
73:h:135:GLN:N	73:h:135:GLN:OE1	2.51	0.44
75:j:98:LEU:O	75:j:102:GLN:OE1	2.35	0.44
36:AT:48:VAL:HA	36:AT:52:ILE:HD13	1.99	0.44
37:AU:102:HIS:O	37:AU:106:MET:SD	2.75	0.44
53:XN:59:VAL:HG13	53:XN:59:VAL:O	2.18	0.44
54:XO:94:ALA:HB3	54:XO:95:PRO:HD3	1.99	0.44
61:XV:188:VAL:O	61:XV:190:CYS:N	2.50	0.44
82:r:37:GLU:OE1	82:r:37:GLU:N	2.51	0.44
5:4:88:TRP:NE1	11:XA:2160:A:OP2	2.36	0.44
8:7:143:TRP:HE3	8:7:179:PHE:HB3	1.82	0.44
10:9:122:THR:OG1	10:9:124:GLU:OE1	2.34	0.44
11:XA:2093:U:O2	11:XA:2266:U:O2'	2.35	0.44
50:XK:130:ASP:OD1	50:XK:131:GLU:N	2.45	0.44
11:XA:2182:G:H2'	11:XA:2183:C:C6	2.52	0.44
11:XA:2355:A:H2'	11:XA:2356:A:H5'	1.98	0.44
13:A1:49:ARG:O	13:A1:51:LYS:NZ	2.48	0.44
17:AA:798:C:H2'	17:AA:799:A:C8	2.52	0.44
26:AJ:49:LEU:HD23	26:AJ:50:GLY:N	2.33	0.44
31:AO:120:VAL:HG23	31:AO:121:LYS:N	2.33	0.44
46:XF:77:VAL:O	46:XF:77:VAL:HG13	2.18	0.44
56:XQ:278:ILE:O	56:XQ:282:ILE:HG12	2.18	0.44
70:e:265:LYS:N	70:e:266:PRO:HD3	2.32	0.44
72:g:118:TRP:O	72:g:121:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:i:80:LEU:HD12	74:i:80:LEU:O	2.18	0.44
84:r2:1:P5P:H2'	84:r2:2:Y5P:H6	1.99	0.44
11:XA:3096:U:C6	90:XA:5144:H8Q:O42	2.71	0.44
30:AN:66:LEU:HD13	30:AN:79:HIS:HB3	2.00	0.44
31:AO:163:LEU:HD23	31:AO:163:LEU:H	1.81	0.44
48:XI:66:PRO:O	48:XI:67:SER:OG	2.32	0.44
68:c:290:LEU:O	68:c:293:GLU:HG2	2.17	0.44
83:r1:52:Y5P:HB	83:r1:53:Y5P:H6	2.00	0.44
4:3:116:ARG:NH2	4:3:159:ASP:OD1	2.50	0.44
6:5:362:THR:O	6:5:364:LEU:N	2.51	0.44
8:7:235:TYR:O	8:7:238:ASP:OD1	2.36	0.44
11:XA:1939:G:O2'	11:XA:1973:G:H4'	2.17	0.44
18:AB:162:CYS:O	18:AB:261:LYS:NZ	2.47	0.44
20:AD:127:ASN:O	42:AZ:72:ARG:NH1	2.48	0.44
26:AJ:49:LEU:HD23	26:AJ:50:GLY:H	1.83	0.44
35:AS:15:ARG:O	35:AS:18:ASP:OD1	2.36	0.44
49:XJ:45:SER:OG	49:XJ:47:ASN:OD1	2.36	0.44
53:XN:72:ILE:HD11	53:XN:96:TYR:CE1	2.53	0.44
63:XX:82:GLY:N	63:XX:83:GLU:OE1	2.51	0.44
67:b:66:ASN:O	73:h:155:THR:OG1	2.34	0.44
69:d:80:ASP:N	69:d:80:ASP:OD1	2.50	0.44
72:g:38:PHE:O	72:g:38:PHE:CG	2.70	0.44
86:s:243:ILE:HG22	86:s:244:SER:N	2.32	0.44
4:3:154:GLN:O	4:3:158:LEU:HD23	2.18	0.44
6:5:201:ARG:NH1	6:5:418:TYR:O	2.48	0.44
7:6:206:TYR:OH	7:6:242:GLY:O	2.28	0.44
9:8:104:VAL:HG23	9:8:104:VAL:O	2.18	0.44
13:A1:270:LYS:NZ	40:AX:118:ALA:O	2.45	0.44
17:AA:940:A:O2'	17:AA:1135:C:O2'	2.35	0.44
19:AC:108:LEU:HD23	19:AC:108:LEU:H	1.82	0.44
52:XM:61:THR:O	52:XM:61:THR:HG22	2.17	0.44
52:XM:231:GLU:O	52:XM:235:GLU:OE1	2.35	0.44
55:XP:177:ILE:O	55:XP:178:TYR:C	2.61	0.44
56:XQ:199:THR:O	56:XQ:199:THR:HG23	2.17	0.44
7:6:27:ARG:N	11:XA:2073:A:OP2	2.51	0.44
11:XA:2574:G:HO2'	11:XA:2575:U:P	2.41	0.44
11:XA:3195:A:OP2	11:XA:3196:G:O2'	2.27	0.44
12:A0:107:GLN:O	38:AV:97:HIS:NE2	2.48	0.44
22:AF:196:HIS:HB3	22:AF:204:LYS:HD3	2.00	0.44
27:AK:69:ASP:O	27:AK:73:GLU:OE1	2.36	0.44
43:XB:1615:A:O2'	43:XB:1616:A:O4'	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:XS:48:PRO:O	82:r:76:ASN:ND2	2.51	0.44
63:XX:53:ASN:ND2	63:XX:56:ASN:OD1	2.51	0.44
63:XX:144:TYR:O	63:XX:148:THR:CB	2.62	0.44
72:g:38:PHE:O	72:g:38:PHE:CD2	2.70	0.44
86:s:271:LEU:O	86:s:273:LEU:N	2.47	0.44
17:AA:805:C:O2	17:AA:805:C:O4'	2.35	0.43
17:AA:1052:C:OP1	28:AL:150:LYS:NZ	2.40	0.43
48:XI:181:ILE:O	48:XI:182:ASP:OD1	2.36	0.43
7:6:374:GLU:OE2	80:p:140:SER:OG	2.34	0.43
9:8:138:ALA:O	9:8:141:GLU:HG3	2.17	0.43
11:XA:2349:G:H2'	11:XA:2350:A:C8	2.54	0.43
11:XA:2600:A:O2'	11:XA:2602:U:O2	2.36	0.43
17:AA:1211:G:N1	17:AA:1354:A:C6	2.86	0.43
18:AB:153:TYR:O	18:AB:157:ASN:ND2	2.50	0.43
20:AD:412:LYS:HB3	20:AD:418:LYS:HB2	1.99	0.43
22:AF:88:ASP:OD1	22:AF:91:ILE:HG12	2.18	0.43
32:AP:127:PRO:HA	32:AP:130:LEU:HD23	2.00	0.43
34:AR:292:ASP:OD1	34:AR:292:ASP:N	2.50	0.43
35:AS:90:PRO:O	35:AS:91:ASN:OD1	2.36	0.43
37:AU:80:ARG:HA	37:AU:83:HIS:CD2	2.52	0.43
53:XN:106:ARG:NH1	84:r2:54:Y5P:OP1	2.52	0.43
65:XZ:75:THR:HG22	65:XZ:83:LYS:HB3	1.98	0.43
85:r3:1:Y5P:C4	85:r3:71:P5P:H2	2.49	0.43
11:XA:2692:G:N1	11:XA:2696:A:OP2	2.43	0.43
16:A4:108:LEU:HD21	20:AD:154:VAL:CG1	2.48	0.43
44:XD:207:ILE:O	44:XD:212:THR:OG1	2.26	0.43
46:XF:93:LEU:HD21	79:o:91:GLN:HG2	2.01	0.43
59:XT:59:TYR:N	69:d:227:ARG:O	2.51	0.43
68:c:151:GLU:HG2	68:c:152:GLY:N	2.33	0.43
79:o:38:ARG:O	79:o:41:ILE:HG22	2.18	0.43
83:r1:52:Y5P:N1	83:r1:53:Y5P:H5	2.33	0.43
84:r2:24:P5P:N3	84:r2:24:P5P:H2'	2.32	0.43
85:r3:2:Y5P:HB	85:r3:2:Y5P:H6	2.00	0.43
85:r3:8:P5P:OP2	85:r3:13:Y5P:H5	2.18	0.43
87:t3:4:GLN:OE1	87:t3:4:GLN:N	2.48	0.43
7:6:228:PRO:O	7:6:229:ASP:OD1	2.37	0.43
9:8:165:ASP:OD1	9:8:165:ASP:N	2.48	0.43
11:XA:1849:C:OP2	52:XM:53:HIS:NE2	2.52	0.43
11:XA:2289:G:H5'	46:XF:101:MET:HE1	2.00	0.43
11:XA:2328:C:N4	86:s:52:THR:O	2.48	0.43
17:AA:1447:G:C6	17:AA:1449:G:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AB:202:ILE:O	18:AB:202:ILE:HG22	2.18	0.43
35:AS:61:GLN:OE1	35:AS:61:GLN:N	2.51	0.43
38:AV:144:PHE:CZ	38:AV:167:VAL:HG21	2.52	0.43
46:XF:250:VAL:HA	46:XF:253:MET:HG2	2.00	0.43
53:XN:71:ASP:OD1	53:XN:72:ILE:HD12	2.19	0.43
63:XX:36:ARG:NE	63:XX:151:GLU:OE2	2.49	0.43
66:a:104:GLU:HG2	66:a:107:PRO:HD2	2.00	0.43
84:r2:5:P5P:H2'	84:r2:6:P5P:H8	1.99	0.43
11:XA:1759:U:H2'	11:XA:1760:G:O4'	2.17	0.43
11:XA:2459:A:C4	11:XA:2460:A:C8	3.06	0.43
13:A1:50:ARG:HD3	16:A4:94:TYR:CE1	2.54	0.43
16:A4:256:GLU:O	16:A4:257:HIS:C	2.61	0.43
17:AA:681:U:H2'	17:AA:682:A:C8	2.53	0.43
17:AA:1213:A:H2'	17:AA:1214:A:C4	2.54	0.43
20:AD:94:THR:O	20:AD:98:LEU:HD13	2.18	0.43
42:AZ:64:THR:O	42:AZ:68:LEU:HD23	2.18	0.43
58:XS:106:TRP:CD2	58:XS:114:ILE:HD11	2.54	0.43
3:2:55:PRO:HB2	11:XA:2339:G:H4'	2.01	0.43
11:XA:1837:C:O2	11:XA:1837:C:O4'	2.37	0.43
17:AA:865:A:H2'	17:AA:866:A:N9	2.34	0.43
17:AA:1309:A:O2'	24:AH:137:ARG:NH2	2.47	0.43
38:AV:76:ILE:O	38:AV:115:GLN:NE2	2.50	0.43
38:AV:79:ILE:HD11	38:AV:88:ALA:HB2	1.99	0.43
40:AX:350:PRO:O	40:AX:354:GLU:OE1	2.36	0.43
41:AY:295:GLN:N	41:AY:295:GLN:OE1	2.52	0.43
44:XD:127:ILE:HD11	44:XD:143:ALA:HB3	2.01	0.43
66:a:95:LEU:H	66:a:95:LEU:HD12	1.82	0.43
68:c:227:GLU:OE2	68:c:230:GLU:N	2.51	0.43
69:d:244:GLU:N	69:d:244:GLU:OE1	2.51	0.43
76:k:55:VAL:HG12	76:k:55:VAL:O	2.19	0.43
85:r3:22:P5P:H2'	85:r3:23:P5P:H8	2.01	0.43
11:XA:2401:A:OP1	44:XD:262:ARG:NH1	2.52	0.43
11:XA:2455:U:C2	11:XA:2456:U:C5	3.06	0.43
11:XA:2472:A:O2'	11:XA:2478:G:N7	2.37	0.43
15:A3:161:ARG:NH1	17:AA:1146:C:OP1	2.43	0.43
15:A3:174:ARG:HA	15:A3:177:TRP:CE2	2.53	0.43
16:A4:634:ALA:HB3	16:A4:641:ILE:HG21	2.01	0.43
17:AA:1476:G:H2'	17:AA:1477:U:O4'	2.19	0.43
18:AB:194:ILE:HA	18:AB:220:VAL:O	2.19	0.43
34:AR:295:ASP:OD1	34:AR:296:ASP:N	2.52	0.43
37:AU:123:ARG:O	37:AU:127:GLU:OE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:XD:216:LEU:HD23	44:XD:216:LEU:H	1.84	0.43
45:XE:145:LEU:HD13	45:XE:181:ILE:HG21	2.00	0.43
57:XR:134:ASP:OD1	57:XR:134:ASP:N	2.51	0.43
58:XS:92:TYR:O	68:c:312:ARG:NE	2.52	0.43
84:r2:54:Y5P:H4A	84:r2:55:Y5P:H4	2.00	0.43
11:XA:2470:G:O2'	51:XL:36:THR:HG22	2.19	0.43
26:AJ:57:GLN:HB3	26:AJ:109:LEU:HD21	2.00	0.43
34:AR:165:ILE:O	34:AR:170:ARG:NH2	2.52	0.43
38:AV:107:TRP:HB3	38:AV:382:TRP:CD2	2.54	0.43
42:AZ:77:ASP:O	42:AZ:81:GLU:OE1	2.36	0.43
49:XJ:59:ASP:N	49:XJ:59:ASP:OD1	2.51	0.43
50:XK:9:GLN:NE2	67:b:129:GLN:HG2	2.33	0.43
58:XS:110:SER:OG	58:XS:111:GLU:OE1	2.36	0.43
69:d:197:VAL:O	69:d:198:ARG:NE	2.51	0.43
74:i:64:GLY:O	74:i:65:ASN:OD1	2.36	0.43
82:r:162:ILE:HG13	82:r:162:ILE:O	2.19	0.43
86:s:145:VAL:O	86:s:148:ASP:OD1	2.35	0.43
6:5:300:ARG:HA	6:5:303:ARG:HE	1.84	0.43
11:XA:2151:A:OP2	11:XA:2249:G:N1	2.40	0.43
13:A1:103:LEU:HD23	13:A1:103:LEU:H	1.84	0.43
24:AH:51:HIS:NE2	24:AH:53:ASP:O	2.51	0.43
40:AX:72:PRO:O	40:AX:76:GLU:OE1	2.37	0.43
45:XE:57:ASN:O	45:XE:61:ILE:HD12	2.19	0.43
46:XF:218:LEU:HD13	46:XF:260:VAL:HB	2.01	0.43
52:XM:156:VAL:HG22	52:XM:157:GLN:H	1.84	0.43
52:XM:168:GLU:OE2	52:XM:220:ARG:NH2	2.52	0.43
78:m:87:GLU:OE1	78:m:91:ARG:NH2	2.52	0.43
11:XA:1737:A:N6	11:XA:1760:G:O2'	2.45	0.43
11:XA:2239:A:O2'	50:XK:29:GLY:HA3	2.18	0.43
11:XA:2667:U:C4	11:XA:2668:A:C8	3.07	0.43
11:XA:2694:A:O2'	11:XA:2941:G:N2	2.49	0.43
17:AA:682:A:N6	17:AA:865:A:H61	2.17	0.43
17:AA:796:G:H4'	29:AM:46:ARG:HB3	2.01	0.43
20:AD:410:ASP:OD1	20:AD:410:ASP:C	2.62	0.43
31:AO:81:HIS:ND1	31:AO:82:LYS:O	2.51	0.43
35:AS:18:ASP:OD1	35:AS:18:ASP:C	2.61	0.43
47:XH:131:TYR:O	47:XH:136:ASN:ND2	2.40	0.43
82:r:50:GLU:O	82:r:52:ARG:NH1	2.52	0.43
86:s:233:ILE:HD11	86:s:334:ALA:CB	2.49	0.43
4:3:140:ARG:O	4:3:144:LEU:HG	2.19	0.42
8:7:225:VAL:O	8:7:229:ILE:HG12	2.19	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	2.52	0.42
11:XA:2939:C:O2'	11:XA:2940:A:H5'	2.18	0.42
29:AM:82:HIS:C	29:AM:83:LEU:HD22	2.43	0.42
44:XD:194:ASN:ND2	44:XD:245:GLY:O	2.52	0.42
86:s:243:ILE:HD13	86:s:296:HIS:HB2	1.99	0.42
6:5:311:ALA:O	6:5:315:LEU:HD23	2.18	0.42
9:8:99:ARG:O	9:8:100:GLU:C	2.62	0.42
11:XA:3212:C:O4'	11:XA:3212:C:O2	2.35	0.42
12:A0:130:GLU:OE1	12:A0:130:GLU:N	2.51	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
31:AO:106:PRO:HA	31:AO:109:ARG:HG2	2.01	0.42
40:AX:63:HIS:O	40:AX:63:HIS:ND1	2.51	0.42
49:XJ:30:MET:HB2	49:XJ:31:PRO:HD3	2.01	0.42
57:XR:76:SER:O	57:XR:80:GLY:N	2.53	0.42
66:a:107:PRO:O	66:a:110:GLU:HG3	2.19	0.42
85:r3:8:P5P:H1'	85:r3:15:P5P:H6	2.01	0.42
8:7:259:ASP:OD1	8:7:260:PHE:N	2.52	0.42
11:XA:2082:G:N3	65:XZ:88:MET:HE2	2.34	0.42
11:XA:3118:U:C2	11:XA:3119:C:C5	3.07	0.42
13:A1:73:ALA:HA	13:A1:113:HIS:CD2	2.54	0.42
17:AA:995:A:P	25:AI:120:ALA:HB2	2.59	0.42
32:AP:80:LEU:HB3	32:AP:111:ILE:CD1	2.49	0.42
32:AP:87:PHE:O	33:AQ:10:ARG:N	2.50	0.42
34:AR:247:HIS:O	34:AR:251:GLU:OE1	2.38	0.42
40:AX:268:LEU:HD21	40:AX:294:ARG:HE	1.83	0.42
41:AY:382:GLU:OE1	41:AY:382:GLU:N	2.52	0.42
43:XB:1629:A:C2	43:XB:1630:A:C8	3.07	0.42
48:XI:181:ILE:O	48:XI:184:THR:OG1	2.32	0.42
50:XK:35:ALA:O	50:XK:39:LEU:HB2	2.19	0.42
52:XM:133:LYS:C	52:XM:134:ARG:HG2	2.43	0.42
64:XY:208:PHE:O	64:XY:212:GLU:OE1	2.37	0.42
70:e:257:LYS:NZ	70:e:273:ARG:O	2.38	0.42
11:XA:2044:A:C4	11:XA:2045:A:C8	3.08	0.42
11:XA:2564:A:O2'	11:XA:2565:A:OP1	2.34	0.42
11:XA:3220:A:P	45:XE:260:LYS:NZ	2.92	0.42
20:AD:400:GLU:N	20:AD:400:GLU:OE1	2.53	0.42
23:AG:208:MET:SD	23:AG:246:ARG:NH2	2.89	0.42
53:XN:216:GLU:HG3	53:XN:238:LYS:CD	2.49	0.42
55:XP:93:VAL:O	55:XP:101:VAL:HG12	2.20	0.42
56:XQ:84:ARG:NH1	56:XQ:271:ARG:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:XV:132:GLU:O	61:XV:148:THR:OG1	2.37	0.42
72:g:123:ASP:O	72:g:126:ASP:OD1	2.38	0.42
86:s:93:VAL:HB	86:s:233:ILE:HG22	2.01	0.42
6:5:409:GLU:OE1	6:5:409:GLU:N	2.51	0.42
11:XA:2146:A:C4	57:XR:64:MET:HE1	2.54	0.42
15:A3:153:LEU:O	15:A3:156:LYS:HG2	2.20	0.42
27:AK:49:ASP:OD1	27:AK:50:GLU:N	2.49	0.42
28:AL:141:GLU:HA	28:AL:144:GLU:CD	2.44	0.42
40:AX:297:MET:O	40:AX:297:MET:HG2	2.19	0.42
53:XN:198:MET:O	53:XN:201:ASP:OD1	2.37	0.42
76:k:65:ASP:OD1	76:k:66:VAL:N	2.52	0.42
85:r3:42:P5P:H2'	85:r3:43:P5P:O4'	2.19	0.42
9:8:60:LYS:N	9:8:63:GLU:OE2	2.52	0.42
11:XA:1697:A:N3	11:XA:1703:C:O2'	2.51	0.42
11:XA:1825:A:N7	11:XA:2704:A:N6	2.67	0.42
14:A2:62:ARG:HG2	14:A2:64:ASP:OD1	2.20	0.42
16:A4:638:SER:OG	16:A4:640:PRO:HD2	2.20	0.42
23:AG:200:LEU:O	23:AG:218:TYR:OH	2.36	0.42
23:AG:227:LYS:O	23:AG:230:THR:OG1	2.37	0.42
38:AV:47:HIS:N	38:AV:78:ASN:OD1	2.53	0.42
68:c:85:LEU:HB3	68:c:89:LYS:NZ	2.34	0.42
68:c:169:VAL:O	68:c:172:ASN:OD1	2.37	0.42
68:c:216:ARG:O	68:c:217:ASP:C	2.62	0.42
73:h:84:SER:OG	73:h:85:ASN:N	2.52	0.42
74:i:111:ASN:HA	74:i:114:ILE:HG12	2.01	0.42
76:k:8:LEU:HD12	76:k:10:LEU:H	1.85	0.42
81:q:80:GLU:O	81:q:84:GLU:OE1	2.38	0.42
84:r2:4:Y5P:H2'	84:r2:5:P5P:H8	2.02	0.42
86:s:63:ILE:HA	86:s:66:TRP:CD1	2.55	0.42
4:3:108:LYS:NZ	11:XA:1744:A:OP2	2.48	0.42
11:XA:2060:A:O2'	11:XA:2061:C:OP2	2.33	0.42
11:XA:2551:G:C2	11:XA:2552:U:C6	3.08	0.42
13:A1:69:VAL:HA	16:A4:81:ASP:OD2	2.19	0.42
16:A4:319:LEU:HA	16:A4:322:HIS:CD2	2.55	0.42
17:AA:692:C:N3	17:AA:823:A:N1	2.67	0.42
23:AG:320:VAL:O	23:AG:321:ASP:OD1	2.37	0.42
6:5:189:LYS:NZ	86:s:182:SER:O	2.49	0.42
11:XA:1868:G:OP2	11:XA:1868:G:N2	2.43	0.42
11:XA:2091:A:H2'	11:XA:2092:C:O4'	2.20	0.42
23:AG:362:GLU:OE2	23:AG:365:ARG:NH1	2.51	0.42
30:AN:85:VAL:HG13	30:AN:86:PHE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:AQ:82:ASP:OD1	33:AQ:82:ASP:N	2.53	0.42
38:AV:82:ARG:CZ	38:AV:121:ALA:HB2	2.50	0.42
49:XJ:149:ARG:NH2	77:l:102:GLY:O	2.53	0.42
63:XX:157:PHE:O	63:XX:160:ASP:OD1	2.37	0.42
71:f:202:PRO:O	71:f:206:GLU:OE1	2.37	0.42
85:r3:41:Y5P:H2'	85:r3:42:P5P:H8	2.02	0.42
4:3:151:ASN:OD1	4:3:154:GLN:NE2	2.53	0.42
6:5:216:GLU:O	6:5:218:LEU:HD22	2.20	0.42
11:XA:2278:A:H2'	11:XA:2279:U:O4'	2.20	0.42
11:XA:2338:A:C4	11:XA:2339:G:C8	3.08	0.42
11:XA:2723:A:OP1	46:XF:131:LYS:O	2.38	0.42
11:XA:3169:C:O2'	11:XA:3170:C:O4'	2.33	0.42
11:XA:3180:A:C4	11:XA:3190:A:C6	3.08	0.42
13:A1:189:LYS:O	13:A1:193:LEU:HD23	2.20	0.42
13:A1:264:GLU:CD	40:AX:339:PRO:HG3	2.45	0.42
16:A4:335:PHE:HA	16:A4:338:ILE:HG22	2.01	0.42
17:AA:1210:U:H2'	17:AA:1211:G:C8	2.55	0.42
36:AT:116:GLU:O	36:AT:119:GLU:HG3	2.19	0.42
46:XF:175:LYS:O	46:XF:178:LEU:HD23	2.20	0.42
50:XK:21:LEU:HD21	50:XK:31:LEU:HD22	2.01	0.42
79:o:55:THR:HG22	79:o:56:ARG:N	2.35	0.42
84:r2:46:P5P:H2'	84:r2:46:P5P:H8	1.83	0.42
7:6:50:LYS:HA	62:XW:121:PRO:HA	2.02	0.42
11:XA:2558:A:C4'	11:XA:2559:U:OP2	2.68	0.42
16:A4:640:PRO:O	16:A4:643:GLU:HG2	2.20	0.42
20:AD:120:LYS:HD2	83:r1:56:Y5P:H4A	2.02	0.42
20:AD:407:ASP:O	20:AD:410:ASP:OD1	2.38	0.42
23:AG:107:ALA:O	23:AG:111:LEU:HD23	2.20	0.42
23:AG:310:ARG:NH1	40:AX:383:LEU:O	2.53	0.42
25:AI:186:CYS:SG	25:AI:187:ARG:N	2.92	0.42
65:XZ:56:TYR:CE1	79:o:44:GLU:HG3	2.54	0.42
85:r3:17:Y5P:OP2	85:r3:17(A):P5P:H5'2	2.20	0.42
1:0:94:ARG:NH2	11:XA:2310:G:OP2	2.37	0.41
13:A1:52:ALA:HB1	16:A4:93:PRO:HG2	2.01	0.41
13:A1:165:ASN:HB2	13:A1:167:ARG:CZ	2.50	0.41
17:AA:826:A:N7	26:AJ:55:ARG:CZ	2.82	0.41
17:AA:942:A:N6	17:AA:1047:A:OP1	2.53	0.41
17:AA:1390:A:H1'	17:AA:1392:A:N7	2.34	0.41
29:AM:73:ILE:O	29:AM:77:ILE:HG12	2.20	0.41
48:XI:197:LEU:O	48:XI:198:PRO:C	2.63	0.41
81:q:159:GLU:HG2	81:q:160:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:138:ARG:HA	1:0:141:ILE:HG12	2.02	0.41
4:3:138:PRO:HA	4:3:141:LYS:HG2	2.02	0.41
10:9:61:VAL:O	64:XY:103:TYR:OH	2.38	0.41
11:XA:1723:A:N6	11:XA:1726:C:OP2	2.52	0.41
11:XA:1821:A:H2'	11:XA:1822:U:O4'	2.20	0.41
11:XA:2738:U:H2'	11:XA:2740:A:OP2	2.20	0.41
17:AA:1048:C:O2	28:AL:196:TYR:N	2.53	0.41
22:AF:114:THR:HG22	22:AF:202:PRO:HA	2.03	0.41
46:XF:145:LEU:N	46:XF:145:LEU:HD12	2.35	0.41
54:XO:18:MET:SD	54:XO:48:ARG:NE	2.94	0.41
54:XO:149:LEU:HA	54:XO:152:LEU:CD2	2.50	0.41
56:XQ:96:ARG:NH1	56:XQ:285:GLU:OE2	2.53	0.41
59:XT:197:LYS:HA	59:XT:200:ILE:HG12	2.01	0.41
63:XX:46:HIS:ND1	63:XX:64:ASP:OD1	2.53	0.41
67:b:133:PHE:CD1	68:c:259:ARG:HD3	2.56	0.41
8:7:207:HIS:HA	8:7:210:ILE:HG12	2.01	0.41
11:XA:1839:C:O3'	50:XK:115:ASN:ND2	2.54	0.41
11:XA:1861:U:H2'	11:XA:1862:U:C6	2.56	0.41
11:XA:2718:C:H2'	11:XA:2991:U:H4'	2.02	0.41
14:A2:89:ILE:O	14:A2:92:THR:OG1	2.31	0.41
16:A4:455:ASN:HA	16:A4:486:TYR:CE1	2.55	0.41
17:AA:950:A:OP2	30:AN:16:LYS:NZ	2.51	0.41
19:AC:138:TYR:CZ	19:AC:142:LEU:HD11	2.55	0.41
20:AD:96:ASP:OD1	20:AD:97:GLU:N	2.53	0.41
20:AD:362:LEU:O	20:AD:365:LYS:HG2	2.20	0.41
31:AO:58:TYR:O	31:AO:61:SER:OG	2.31	0.41
38:AV:156:ASN:OD1	38:AV:157:TYR:N	2.53	0.41
58:XS:76:HIS:CD2	66:a:50:ALA:HA	2.55	0.41
60:XU:47:GLU:OE1	60:XU:47:GLU:N	2.53	0.41
61:XV:148:THR:O	61:XV:149:ARG:C	2.63	0.41
63:XX:141:LEU:O	63:XX:145:ILE:HD12	2.20	0.41
86:s:407:ASP:O	86:s:408:ASN:OD1	2.38	0.41
6:5:215:ARG:O	6:5:216:GLU:HG3	2.21	0.41
6:5:291:LEU:HG	6:5:344:SER:HB3	2.03	0.41
11:XA:1846:C:OP2	58:XS:177:ARG:N	2.36	0.41
11:XA:2498:U:H2'	11:XA:2499:U:C2	2.55	0.41
11:XA:3121:C:OP2	11:XA:3122:U:H2'	2.21	0.41
21:AE:21:THR:O	21:AE:24:ARG:HG2	2.20	0.41
28:AL:175:TYR:O	28:AL:179:GLU:OE1	2.38	0.41
34:AR:135:ARG:NH1	34:AR:236:GLU:OE2	2.53	0.41
44:XD:194:ASN:HA	44:XD:207:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:XI:200:LEU:HB3	48:XI:201:PRO:HD3	2.01	0.41
50:XK:109:TYR:OH	50:XK:118:ARG:NH1	2.53	0.41
53:XN:200:LYS:O	53:XN:203:GLU:HG3	2.20	0.41
73:h:103:HIS:O	73:h:106:ASP:OD1	2.38	0.41
76:k:9:GLY:C	76:k:10:LEU:HD23	2.45	0.41
81:q:147:GLN:HA	81:q:150:LYS:HG2	2.02	0.41
5:4:99:LYS:NZ	11:XA:3013:G:O2'	2.46	0.41
7:6:89:ASP:OD1	7:6:89:ASP:N	2.53	0.41
10:9:23:SER:O	10:9:31:ARG:HG2	2.19	0.41
11:XA:2492:G:N2	11:XA:2494:C:H5''	2.35	0.41
11:XA:2877:C:H2'	11:XA:2878:G:O4'	2.21	0.41
16:A4:95:LEU:HD13	19:AC:129:PRO:HB3	2.03	0.41
34:AR:67:LYS:N	34:AR:68:PRO:CD	2.83	0.41
38:AV:106:ASN:ND2	38:AV:140:ASP:OD2	2.53	0.41
38:AV:338:HIS:ND1	38:AV:342:GLN:OE1	2.52	0.41
40:AX:371:ALA:O	40:AX:373:THR:N	2.53	0.41
48:XI:112:MET:O	48:XI:116:LEU:HD23	2.20	0.41
71:f:138:GLN:CG	71:f:144:MET:H	2.33	0.41
85:r3:8:P5P:N9	85:r3:15:P5P:H6	2.36	0.41
6:5:178:PRO:HA	6:5:181:VAL:HG22	2.02	0.41
7:6:57:TYR:CD2	62:XW:117:ILE:HD11	2.55	0.41
7:6:118:GLU:OE1	7:6:121:ARG:NH1	2.53	0.41
9:8:116:LEU:O	9:8:119:LYS:HG3	2.21	0.41
11:XA:1851:G:H2'	11:XA:2693:A:N7	2.35	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:807:A:O2'	17:AA:809:G:O6	2.34	0.41
24:AH:135:GLU:OE2	27:AK:124:GLN:NE2	2.54	0.41
49:XJ:108:VAL:HG12	49:XJ:108:VAL:O	2.21	0.41
54:XO:22:PRO:O	54:XO:25:ARG:HG2	2.21	0.41
67:b:112:VAL:O	67:b:112:VAL:HG23	2.21	0.41
74:i:59:ASN:O	74:i:63:LEU:HD23	2.20	0.41
86:s:427:ASN:OD1	86:s:428:ARG:N	2.52	0.41
87:t1:11:ALA:O	87:t4:14:THR:OG1	2.38	0.41
11:XA:1935:A:N6	11:XA:1936:A:N3	2.69	0.41
11:XA:2370:A:OP1	60:XU:41:GLN:NE2	2.37	0.41
11:XA:3126:C:H2'	11:XA:3127:G:O4'	2.21	0.41
13:A1:189:LYS:NZ	13:A1:235:ASN:O	2.48	0.41
17:AA:1033:U:O2'	21:AE:93:ILE:O	2.39	0.41
17:AA:1332:A:C4	17:AA:1333:G:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:1449:G:C2	17:AA:1450:C:C6	3.08	0.41
23:AG:201:ILE:HG22	23:AG:202:LYS:N	2.36	0.41
53:XN:65:GLU:HB2	53:XN:66:PRO:HD2	2.02	0.41
61:XV:103:ASP:OD1	61:XV:104:TYR:N	2.53	0.41
62:XW:141:THR:OG1	62:XW:143:LYS:NZ	2.53	0.41
68:c:150:THR:O	68:c:153:ILE:HG22	2.20	0.41
82:r:149:ARG:HD3	82:r:152:THR:HG21	2.03	0.41
84:r2:8:Y5P:H2	84:r2:15:P5P:H6	2.03	0.41
84:r2:33:Y5P:H6	84:r2:33:Y5P:H2'	1.74	0.41
85:r3:53:Y5P:OP2	85:r3:54:Y5P:H5	2.21	0.41
6:5:242:ARG:HA	6:5:245:ILE:HG12	2.01	0.41
11:XA:3181:U:OP2	11:XA:3182:A:O2'	2.33	0.41
12:A0:110:ASP:OD1	12:A0:111:HIS:ND1	2.52	0.41
17:AA:949:U:O2'	30:AN:29:ARG:NH1	2.53	0.41
18:AB:227:CYS:SG	18:AB:228:ASN:N	2.94	0.41
21:AE:14:GLN:N	21:AE:17:GLU:OE2	2.41	0.41
31:AO:105:CYS:HB2	31:AO:106:PRO:HD2	2.03	0.41
33:AQ:49:CYS:SG	33:AQ:50:ARG:N	2.94	0.41
38:AV:353:LEU:O	38:AV:356:THR:OG1	2.35	0.41
46:XF:220:ASP:OD1	46:XF:221:LEU:N	2.52	0.41
49:XJ:27:GLY:O	49:XJ:58:LYS:NZ	2.53	0.41
50:XK:39:LEU:O	50:XK:54:GLY:HA2	2.20	0.41
54:XO:41:ARG:NH2	54:XO:131:PRO:O	2.52	0.41
56:XQ:201:ASP:OD2	56:XQ:204:MET:N	2.54	0.41
56:XQ:225:LYS:CG	56:XQ:226:PRO:HD2	2.51	0.41
58:XS:172:MET:SD	58:XS:183:LYS:HG3	2.61	0.41
59:XT:135:GLU:OE2	69:d:279:THR:OG1	2.30	0.41
6:5:201:ARG:NH2	6:5:420:HIS:O	2.54	0.41
6:5:363:ASP:OD1	6:5:363:ASP:N	2.52	0.41
7:6:210:GLU:CD	7:6:210:GLU:H	2.29	0.41
11:XA:1883:G:O5'	72:g:91:MET:HG3	2.21	0.41
11:XA:2233:U:C2	45:XE:248:ILE:HD12	2.56	0.41
11:XA:2307:U:H2'	11:XA:2308:A:O4'	2.21	0.41
11:XA:2574:G:O2'	11:XA:2575:U:OP1	2.33	0.41
11:XA:3124:U:C2	11:XA:3125:A:C8	3.09	0.41
16:A4:416:PHE:CE2	16:A4:457:TYR:CG	3.09	0.41
16:A4:491:GLN:O	16:A4:495:HIS:ND1	2.45	0.41
17:AA:1516:G:C6	17:AA:1517:A:N6	2.89	0.41
17:AA:1526:U:O2	17:AA:1526:U:C2'	2.69	0.41
18:AB:59:ASN:O	18:AB:63:LEU:HD23	2.20	0.41
18:AB:162:CYS:SG	18:AB:254:GLN:HA	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AE:15:ARG:HA	21:AE:18:THR:OG1	2.21	0.41
23:AG:115:GLY:N	24:AH:84:ASP:OD2	2.54	0.41
24:AH:126:ILE:O	24:AH:127:TYR:CG	2.73	0.41
40:AX:374:GLU:HG2	40:AX:375:GLU:N	2.35	0.41
41:AY:379:TYR:O	41:AY:383:LYS:HG2	2.21	0.41
41:AY:387:LEU:O	41:AY:388:LYS:HE2	2.21	0.41
43:XB:1623:G:OP2	55:XP:87:HIS:HB2	2.21	0.41
46:XF:93:LEU:H	46:XF:93:LEU:HD23	1.86	0.41
48:XI:40:MET:SD	48:XI:44:ARG:NH1	2.92	0.41
52:XM:247:ILE:HG22	52:XM:247:ILE:O	2.20	0.41
56:XQ:168:ASN:O	56:XQ:171:VAL:HG22	2.20	0.41
63:XX:72:PRO:O	63:XX:75:SER:OG	2.35	0.41
63:XX:146:LEU:CD2	63:XX:165:MET:SD	3.09	0.41
67:b:126:ILE:O	67:b:127:GLN:HB2	2.21	0.41
68:c:276:CYS:O	68:c:277:ASP:C	2.64	0.41
72:g:41:SER:OG	72:g:43:ASP:OD1	2.39	0.41
82:r:124:ARG:HE	82:r:155:ALA:HA	1.85	0.41
7:6:228:PRO:O	7:6:229:ASP:C	2.64	0.41
8:7:64:LYS:NZ	69:d:276:ILE:O	2.47	0.41
11:XA:2079:C:C4	11:XA:2080:U:C6	3.09	0.41
11:XA:2292:G:N1	57:XR:10:LEU:N	2.69	0.41
11:XA:2350:A:H2'	11:XA:2351:U:O4'	2.21	0.41
11:XA:2356:A:N1	11:XA:2357:C:H1'	2.36	0.41
11:XA:2682:A:H2'	11:XA:2683:C:C5'	2.50	0.41
18:AB:180:ARG:HG3	18:AB:185:PRO:HA	2.03	0.41
19:AC:109:VAL:CG2	19:AC:120:CYS:HB3	2.51	0.41
28:AL:166:MET:O	28:AL:169:ASN:OD1	2.39	0.41
40:AX:378:LYS:HA	40:AX:381:LEU:CD2	2.51	0.41
43:XB:1642:G:H2'	43:XB:1643:A:C8	2.56	0.41
49:XJ:107:GLU:OE1	49:XJ:109:ALA:N	2.51	0.41
78:m:54:VAL:HG12	78:m:55:LEU:N	2.36	0.41
84:r2:9:P5P:O2'	84:r2:45:Y5P:O2'	2.35	0.41
84:r2:38:P5P:O5'	84:r2:38:P5P:H8	2.20	0.41
6:5:232:THR:OG1	6:5:234:ASP:O	2.37	0.40
11:XA:2086:A:H2'	11:XA:2087:U:C6	2.56	0.40
11:XA:2123:C:OP1	65:XZ:76:ARG:NH2	2.54	0.40
11:XA:2287:U:C4	11:XA:2288:A:N7	2.89	0.40
11:XA:3189:C:C2'	11:XA:3190:A:OP2	2.69	0.40
16:A4:108:LEU:CD2	20:AD:154:VAL:CG1	2.99	0.40
23:AG:302:LEU:HD23	23:AG:302:LEU:H	1.85	0.40
24:AH:170:MET:SD	24:AH:172:VAL:HG13	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AS:18:ASP:HA	35:AS:21:ARG:HG2	2.03	0.40
40:AX:353:PHE:CE2	40:AX:357:ILE:HD11	2.56	0.40
40:AX:393:ARG:O	40:AX:397:TYR:CD2	2.74	0.40
46:XF:284:TYR:O	46:XF:290:TYR:OH	2.35	0.40
68:c:195:PHE:O	68:c:198:VAL:HG12	2.20	0.40
81:q:44:ASP:O	81:q:47:THR:OG1	2.29	0.40
82:r:117:GLU:O	82:r:121:MET:HG2	2.21	0.40
4:3:124:ARG:NH2	11:XA:2868:C:OP1	2.53	0.40
6:5:381:LEU:O	6:5:381:LEU:HD23	2.21	0.40
7:6:144:GLY:N	7:6:145:PRO:CD	2.84	0.40
7:6:289:PRO:O	7:6:290:CYS:SG	2.80	0.40
11:XA:1765:C:O3'	74:i:75:ARG:NH1	2.54	0.40
11:XA:2002:G:C8	11:XA:2927:C:O2	2.74	0.40
11:XA:2275:U:H2'	11:XA:2276:C:C6	2.56	0.40
15:A3:156:LYS:O	15:A3:159:GLU:HG3	2.21	0.40
17:AA:1227:G:OP1	24:AH:128:LYS:NZ	2.48	0.40
17:AA:1524:A:H4'	38:AV:103:TYR:OH	2.21	0.40
28:AL:137:ARG:O	28:AL:140:GLU:HG3	2.21	0.40
40:AX:181:PRO:HB2	40:AX:233:VAL:HG22	2.03	0.40
46:XF:91:PRO:O	46:XF:176:VAL:HG21	2.20	0.40
48:XI:116:LEU:HD12	48:XI:121:ILE:HG21	2.03	0.40
56:XQ:227:LYS:N	56:XQ:228:PRO:CD	2.85	0.40
62:XW:95:GLY:HA3	62:XW:134:VAL:O	2.22	0.40
66:a:69:TYR:O	66:a:72:THR:OG1	2.32	0.40
1:0:90:ASN:OD1	1:0:93:ARG:NH1	2.46	0.40
11:XA:2576:A:N6	17:AA:1491:C:O2'	2.54	0.40
11:XA:2727:C:H2'	11:XA:2728:C:H6	1.86	0.40
11:XA:3203:A:OP2	45:XE:141:LYS:NZ	2.54	0.40
16:A4:71:LEU:HB2	41:AY:302:ILE:HG22	2.03	0.40
17:AA:701:G:O6	17:AA:709:G:N1	2.55	0.40
21:AE:85:ASP:OD1	44:XD:171:ARG:NH1	2.44	0.40
22:AF:147:GLN:OE1	22:AF:151:ASN:ND2	2.54	0.40
29:AM:59:ASN:OD1	29:AM:62:GLY:N	2.55	0.40
43:XB:1607:U:O2'	43:XB:1608:G:H5'	2.21	0.40
52:XM:100:ARG:O	52:XM:104:LEU:HG	2.20	0.40
55:XP:124:CYS:O	55:XP:160:LEU:HD21	2.21	0.40
61:XV:45:VAL:HG21	64:XY:237:LYS:HE2	2.02	0.40
72:g:106:GLN:O	72:g:151:GLY:N	2.49	0.40
77:l:106:THR:N	77:l:109:GLU:OE2	2.44	0.40
85:r3:21:P5P:C8	85:r3:47:Y5P:H4	2.52	0.40
85:r3:32:Y5P:H4A	85:r3:33:Y5P:C4	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:1880:C:OP2	72:g:111:ARG:NH1	2.55	0.40
11:XA:2262:C:O2'	58:XS:175:ARG:NH2	2.54	0.40
11:XA:2802:A:H2'	11:XA:2803:A:O4'	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:1460:C:O3'	22:AF:177:ARG:NH2	2.54	0.40
33:AQ:26:LEU:O	33:AQ:29:ILE:HG22	2.21	0.40
38:AV:317:LEU:HD23	38:AV:319:ILE:H	1.86	0.40
52:XM:252:LEU:H	52:XM:252:LEU:HD23	1.86	0.40
66:a:112:LEU:CD1	66:a:123:TRP:CE2	3.04	0.40
68:c:164:GLU:HG2	68:c:165:VAL:N	2.36	0.40
72:g:47:PHE:O	72:g:51:LEU:HD23	2.21	0.40
84:r:2:34:P5P:HO2'	84:r:2:35:P5P:P	2.40	0.40
11:XA:1696:C:OP2	64:XY:180:LYS:NZ	2.48	0.40
11:XA:2135:A:H2'	11:XA:2135:A:N3	2.36	0.40
11:XA:2379:C:O2	11:XA:2379:C:O4'	2.39	0.40
11:XA:2546:G:C2	11:XA:2547:C:C5	3.10	0.40
11:XA:2955:U:C5	11:XA:2963:A:N1	2.90	0.40
11:XA:3067:U:H2'	11:XA:3068:G:O4'	2.21	0.40
11:XA:3096:U:H5	90:XA:5144:H8Q:O42	2.05	0.40
14:A2:53:MET:SD	22:AF:234:ARG:HD2	2.61	0.40
17:AA:920:G:C2	17:AA:921:U:C4	3.10	0.40
17:AA:1464:G:O2'	17:AA:1465:C:O4'	2.39	0.40
32:AP:81:SER:O	32:AP:84:VAL:HG12	2.22	0.40
34:AR:305:HIS:HD2	34:AR:314:ALA:CA	2.34	0.40
48:XI:50:VAL:HG21	79:o:35:MET:SD	2.61	0.40
50:XK:7:ALA:HB3	50:XK:8:PRO:HD3	2.04	0.40
55:XP:178:TYR:O	55:XP:179:GLU:C	2.65	0.40
57:XR:28:ALA:HB2	57:XR:46:VAL:CG2	2.52	0.40
68:c:43:LYS:O	68:c:46:GLU:HG3	2.21	0.40
70:e:158:VAL:O	70:e:255:VAL:N	2.45	0.40
74:i:79:TRP:HA	74:i:97:MET:SD	2.62	0.40
86:s:168:GLU:O	86:s:172:ILE:HG12	2.21	0.40
86:s:295:GLY:HA3	86:s:335:TRP:HZ2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
2	1	51/65 (78%)	49 (96%)	2 (4%)	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	93 (100%)	0	0	100	100
5	4	36/103 (35%)	34 (94%)	2 (6%)	0	100	100
6	5	389/423 (92%)	364 (94%)	25 (6%)	0	100	100
7	6	348/380 (92%)	319 (92%)	29 (8%)	0	100	100
8	7	283/338 (84%)	265 (94%)	18 (6%)	0	100	100
9	8	137/206 (66%)	131 (96%)	6 (4%)	0	100	100
10	9	122/137 (89%)	116 (95%)	6 (5%)	0	100	100
12	A0	197/218 (90%)	191 (97%)	6 (3%)	0	100	100
13	A1	273/323 (84%)	262 (96%)	11 (4%)	0	100	100
14	A2	114/118 (97%)	107 (94%)	7 (6%)	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%)	211 (98%)	5 (2%)	0	100	100
19	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
20	AD	341/430 (79%)	320 (94%)	21 (6%)	0	100	100
21	AE	120/125 (96%)	115 (96%)	5 (4%)	0	100	100
22	AF	197/242 (81%)	191 (97%)	6 (3%)	0	100	100
23	AG	300/396 (76%)	285 (95%)	15 (5%)	0	100	100
24	AH	133/201 (66%)	125 (94%)	8 (6%)	0	100	100
25	AI	134/194 (69%)	131 (98%)	3 (2%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	AL	162/257 (63%)	157 (97%)	5 (3%)	0	100	100
29	AM	114/137 (83%)	113 (99%)	1 (1%)	0	100	100
30	AN	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
31	AO	183/258 (71%)	179 (98%)	4 (2%)	0	100	100
32	AP	93/142 (66%)	86 (92%)	7 (8%)	0	100	100
33	AQ	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
34	AR	248/360 (69%)	237 (96%)	11 (4%)	0	100	100
35	AS	131/190 (69%)	122 (93%)	9 (7%)	0	100	100
36	AT	160/173 (92%)	150 (94%)	10 (6%)	0	100	100
37	AU	171/205 (83%)	169 (99%)	2 (1%)	0	100	100
38	AV	341/414 (82%)	322 (94%)	19 (6%)	0	100	100
39	AW	95/187 (51%)	90 (95%)	5 (5%)	0	100	100
40	AX	346/398 (87%)	327 (94%)	19 (6%)	0	100	100
41	AY	111/395 (28%)	102 (92%)	9 (8%)	0	100	100
42	AZ	84/106 (79%)	83 (99%)	1 (1%)	0	100	100
44	XD	234/305 (77%)	221 (94%)	11 (5%)	2 (1%)	14	48
45	XE	302/348 (87%)	291 (96%)	11 (4%)	0	100	100
46	XF	248/311 (80%)	241 (97%)	7 (3%)	0	100	100
47	XH	93/267 (35%)	85 (91%)	8 (9%)	0	100	100
48	XI	209/261 (80%)	193 (92%)	16 (8%)	0	100	100
49	XJ	168/192 (88%)	156 (93%)	12 (7%)	0	100	100
50	XK	175/178 (98%)	167 (95%)	8 (5%)	0	100	100
51	XL	113/145 (78%)	105 (93%)	8 (7%)	0	100	100
52	XM	285/296 (96%)	274 (96%)	11 (4%)	0	100	100
53	XN	219/251 (87%)	207 (94%)	12 (6%)	0	100	100
54	XO	150/175 (86%)	145 (97%)	5 (3%)	0	100	100
55	XP	141/180 (78%)	133 (94%)	8 (6%)	0	100	100
56	XQ	236/292 (81%)	227 (96%)	9 (4%)	0	100	100
57	XR	138/149 (93%)	134 (97%)	4 (3%)	0	100	100
58	XS	158/205 (77%)	155 (98%)	3 (2%)	0	100	100
59	XT	164/206 (80%)	159 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	XU	137/153 (90%)	131 (96%)	6 (4%)	0	100	100
61	XV	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
62	XW	109/148 (74%)	104 (95%)	5 (5%)	0	100	100
63	XX	241/256 (94%)	234 (97%)	7 (3%)	0	100	100
64	XY	176/250 (70%)	170 (97%)	6 (3%)	0	100	100
65	XZ	118/161 (73%)	116 (98%)	2 (2%)	0	100	100
66	a	93/142 (66%)	89 (96%)	4 (4%)	0	100	100
67	b	146/215 (68%)	133 (91%)	13 (9%)	0	100	100
68	c	271/332 (82%)	262 (97%)	9 (3%)	0	100	100
69	d	212/306 (69%)	200 (94%)	11 (5%)	1 (0%)	24	60
70	e	211/279 (76%)	205 (97%)	6 (3%)	0	100	100
71	f	139/212 (66%)	133 (96%)	6 (4%)	0	100	100
72	g	130/166 (78%)	123 (95%)	6 (5%)	1 (1%)	16	52
73	h	106/158 (67%)	100 (94%)	6 (6%)	0	100	100
74	i	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
75	j	84/123 (68%)	83 (99%)	1 (1%)	0	100	100
76	k	93/112 (83%)	87 (94%)	6 (6%)	0	100	100
77	l	78/138 (56%)	72 (92%)	6 (8%)	0	100	100
78	m	58/128 (45%)	52 (90%)	6 (10%)	0	100	100
79	o	92/102 (90%)	87 (95%)	5 (5%)	0	100	100
80	p	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
81	q	162/222 (73%)	156 (96%)	6 (4%)	0	100	100
82	r	144/196 (74%)	138 (96%)	6 (4%)	0	100	100
86	s	366/439 (83%)	353 (96%)	13 (4%)	0	100	100
87	t1	44/198 (22%)	41 (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	13781/19160 (72%)	13145 (95%)	632 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
72	g	38	PHE
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
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	267/303 (88%)	267 (100%)	0	100	100
9	8	128/190 (67%)	128 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
12	A0	176/190 (93%)	176 (100%)	0	100	100
13	A1	253/291 (87%)	253 (100%)	0	100	100
14	A2	99/101 (98%)	99 (100%)	0	100	100
15	A3	63/166 (38%)	63 (100%)	0	100	100
16	A4	494/609 (81%)	494 (100%)	0	100	100
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%)	283 (100%)	0	100	100
21	AE	104/107 (97%)	104 (100%)	0	100	100
22	AF	178/209 (85%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AG	264/342 (77%)	263 (100%)	1 (0%)	84	84
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%)	229 (100%)	0	100	100
35	AS	115/164 (70%)	115 (100%)	0	100	100
36	AT	150/157 (96%)	150 (100%)	0	100	100
37	AU	149/174 (86%)	149 (100%)	0	100	100
38	AV	315/364 (86%)	315 (100%)	0	100	100
39	AW	84/158 (53%)	84 (100%)	0	100	100
40	AX	307/351 (88%)	307 (100%)	0	100	100
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%)	133 (100%)	0	100	100
50	XK	155/156 (99%)	155 (100%)	0	100	100
51	XL	98/124 (79%)	98 (100%)	0	100	100
52	XM	245/249 (98%)	245 (100%)	0	100	100
53	XN	188/211 (89%)	188 (100%)	0	100	100
54	XO	133/150 (89%)	133 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	146 (100%)	0	100	100
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%)	91 (100%)	0	100	100
63	XX	219/229 (96%)	219 (100%)	0	100	100
64	XY	161/223 (72%)	161 (100%)	0	100	100
65	XZ	111/147 (76%)	111 (100%)	0	100	100
66	a	93/133 (70%)	93 (100%)	0	100	100
67	b	130/186 (70%)	130 (100%)	0	100	100
68	c	241/288 (84%)	241 (100%)	0	100	100
69	d	196/274 (72%)	196 (100%)	0	100	100
70	e	188/236 (80%)	187 (100%)	1 (0%)	81	82
71	f	128/188 (68%)	128 (100%)	0	100	100
72	g	122/148 (82%)	121 (99%)	1 (1%)	73	77
73	h	103/148 (70%)	103 (100%)	0	100	100
74	i	86/110 (78%)	86 (100%)	0	100	100
75	j	68/97 (70%)	68 (100%)	0	100	100
76	k	80/90 (89%)	80 (100%)	0	100	100
77	l	74/116 (64%)	74 (100%)	0	100	100
78	m	54/113 (48%)	54 (100%)	0	100	100
79	o	80/87 (92%)	80 (100%)	0	100	100
80	p	117/181 (65%)	117 (100%)	0	100	100
81	q	141/178 (79%)	141 (100%)	0	100	100
82	r	138/169 (82%)	138 (100%)	0	100	100
86	s	326/381 (86%)	326 (100%)	0	100	100
87	t1	40/158 (25%)	40 (100%)	0	100	100
87	t2	28/158 (18%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	12395/16507 (75%)	12392 (100%)	3 (0%)	100	100

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

Mol	Chain	Res	Type
23	AG	207	GLU
70	e	278	ASP
72	g	38	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	106	ASN
1	0	120	HIS
5	4	95	HIS
6	5	195	HIS
6	5	384	GLN
7	6	249	GLN
7	6	307	HIS
8	7	69	HIS
9	8	144	GLN
13	A1	165	ASN
15	A3	140	HIS
16	A4	129	GLN
16	A4	590	GLN
19	AC	81	HIS
20	AD	165	GLN
20	AD	292	HIS
20	AD	347	GLN
22	AF	127	HIS
22	AF	196	HIS
23	AG	77	GLN
23	AG	326	HIS
23	AG	384	GLN
24	AH	130	HIS
24	AH	183	HIS

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Mol	Chain	Res	Type
27	AK	117	HIS
28	AL	146	HIS
29	AM	39	ASN
29	AM	61	HIS
31	AO	80	ASN
31	AO	147	HIS
31	AO	155	GLN
31	AO	221	GLN
34	AR	86	ASN
34	AR	278	ASN
38	AV	106	ASN
38	AV	342	GLN
40	AX	140	HIS
40	AX	394	HIS
41	AY	285	GLN
44	XD	156	ASN
45	XE	52	HIS
45	XE	117	HIS
48	XI	189	GLN
50	XK	9	GLN
50	XK	126	HIS
50	XK	160	GLN
52	XM	71	GLN
52	XM	264	GLN
55	XP	54	ASN
55	XP	114	HIS
57	XR	77	GLN
57	XR	94	GLN
58	XS	75	HIS
58	XS	100	HIS
62	XW	72	HIS
62	XW	110	ASN
64	XY	99	HIS
67	b	16	HIS
67	b	102	GLN
68	c	123	GLN
69	d	66	HIS
69	d	131	ASN
69	d	157	HIS
70	e	251	HIS
71	f	54	HIS
71	f	158	GLN

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Mol	Chain	Res	Type
72	g	93	ASN
72	g	155	GLN
73	h	85	ASN
74	i	108	HIS
74	i	120	HIS
76	k	15	GLN
76	k	80	HIS
80	p	146	ASN
86	s	191	HIS
87	t1	5	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	XA	1490/1559 (95%)	269 (18%)	8 (0%)
17	AA	916/954 (96%)	163 (17%)	4 (0%)
43	XB	56/72 (77%)	13 (23%)	0
83	r1	13/14 (92%)	7 (53%)	0
84	r2	75/76 (98%)	30 (40%)	0
85	r3	74/75 (98%)	22 (29%)	0
All	All	2624/2750 (95%)	504 (19%)	12 (0%)

All (504) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	XA	1681	G
11	XA	1685	C
11	XA	1689	C
11	XA	1692	A
11	XA	1693	C
11	XA	1695	C
11	XA	1699	C
11	XA	1700	U
11	XA	1704	U
11	XA	1707	C
11	XA	1708	A
11	XA	1709	G
11	XA	1710	A
11	XA	1711	C
11	XA	1712	A
11	XA	1713	A

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Mol	Chain	Res	Type
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	1781	A
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	1887	A
11	XA	1893	A
11	XA	1902	C
11	XA	1903	C
11	XA	1909	A
11	XA	1918	G
11	XA	1919	C

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Mol	Chain	Res	Type
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	1986	A
11	XA	1992	C
11	XA	1993	A
11	XA	1994	A
11	XA	2000	C
11	XA	2001	C
11	XA	2002	G
11	XA	2003	A
11	XA	2010	U
11	XA	2015	G
11	XA	2022	G
11	XA	2030	U
11	XA	2036	C
11	XA	2037	U
11	XA	2039	A
11	XA	2055	U
11	XA	2060	A
11	XA	2067	C
11	XA	2079	C
11	XA	2083	U
11	XA	2099	U
11	XA	2105	G
11	XA	2111	C
11	XA	2113	G
11	XA	2125	C
11	XA	2126	U
11	XA	2134	A
11	XA	2135	A
11	XA	2138	U
11	XA	2147	G
11	XA	2159	U
11	XA	2168	U
11	XA	2169	A
11	XA	2176	C

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Mol	Chain	Res	Type
11	XA	2177	U
11	XA	2178	A
11	XA	2179	A
11	XA	2180	A
11	XA	2181	A
11	XA	2182	G
11	XA	2188	A
11	XA	2195	A
11	XA	2196	A
11	XA	2198	A
11	XA	2200	A
11	XA	2237	A
11	XA	2241	A
11	XA	2243	A
11	XA	2244	U
11	XA	2245	A
11	XA	2251	A
11	XA	2260	A
11	XA	2262	C
11	XA	2283	C
11	XA	2284	C
11	XA	2285	U
11	XA	2297	A
11	XA	2299	U
11	XA	2300	G
11	XA	2316	U
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
11	XA	2446	A
11	XA	2451	A

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Mol	Chain	Res	Type
11	XA	2458	A
11	XA	2476	C
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	2602	U
11	XA	2603	C
11	XA	2618	U
11	XA	2626	U
11	XA	2627	G
11	XA	2628	U
11	XA	2630	U
11	XA	2633	A
11	XA	2635	G
11	XA	2654	U
11	XA	2656	U
11	XA	2659	C
11	XA	2683	C
11	XA	2686	G
11	XA	2694	A
11	XA	2695	G
11	XA	2696	A
11	XA	2706	A
11	XA	2715	A
11	XA	2718	C
11	XA	2719	G

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Mol	Chain	Res	Type
11	XA	2723	A
11	XA	2724	G
11	XA	2725	A
11	XA	2732	G
11	XA	2733	G
11	XA	2740	A
11	XA	2745	A
11	XA	2758	G
11	XA	2788	C
11	XA	2789	C
11	XA	2791	A
11	XA	2810	G
11	XA	2832	A
11	XA	2833	A
11	XA	2847	C
11	XA	2854	U
11	XA	2859	A
11	XA	2864	U
11	XA	2865	C
11	XA	2869	A
11	XA	2871	U
11	XA	2879	A
11	XA	2893	A
11	XA	2906	C
11	XA	2910	A
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	2956	A
11	XA	2962	C
11	XA	2963	A
11	XA	2985	C
11	XA	2989	G
11	XA	2992	G
11	XA	3000	A
11	XA	3005	A

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Mol	Chain	Res	Type
11	XA	3007	C
11	XA	3016	G
11	XA	3021	C
11	XA	3038	U
11	XA	3041	U
11	XA	3049	U
11	XA	3053	A
11	XA	3054	G
11	XA	3067	U
11	XA	3069	A
11	XA	3073	C
11	XA	3089	A
11	XA	3090	G
11	XA	3096	U
11	XA	3100	U
11	XA	3122	U
11	XA	3124	U
11	XA	3129	A
11	XA	3150	U
11	XA	3151	A
11	XA	3154	U
11	XA	3157	C
11	XA	3158	A
11	XA	3160	A
11	XA	3162	C
11	XA	3168	C
11	XA	3169	C
11	XA	3172	C
11	XA	3177	A
11	XA	3182	A
11	XA	3184	C
11	XA	3189	C
11	XA	3190	A
11	XA	3194	U
11	XA	3196	G
11	XA	3208	C
11	XA	3209	A
11	XA	3210	C
11	XA	3212	C
11	XA	3217	A
11	XA	3218	A
11	XA	3219	G

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Mol	Chain	Res	Type
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	831	U
17	AA	832	U
17	AA	835	C
17	AA	836	A
17	AA	844	A
17	AA	851	A
17	AA	856	A
17	AA	860	A
17	AA	861	U
17	AA	865	A
17	AA	866	A
17	AA	868	C
17	AA	869	C
17	AA	880	C
17	AA	881	A
17	AA	890	C
17	AA	893	G
17	AA	897	C

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Mol	Chain	Res	Type
17	AA	899	G
17	AA	903	U
17	AA	905	A
17	AA	909	G
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	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	1126	A
17	AA	1128	C
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	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	1331	A
17	AA	1341	C
17	AA	1342	C
17	AA	1343	A
17	AA	1344	U
17	AA	1349	U
17	AA	1353	A
17	AA	1354	A
17	AA	1356	A
17	AA	1365	A
17	AA	1369	U

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Mol	Chain	Res	Type
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	1423	A
17	AA	1430	A
17	AA	1432	U
17	AA	1448	U
17	AA	1459	A
17	AA	1461	A
17	AA	1462	G
17	AA	1463	G
17	AA	1478	A
17	AA	1481	C
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	1558	A
17	AA	1559	G
17	AA	1568	U
17	AA	1571	U
17	AA	1582	G
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

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Mol	Chain	Res	Type
43	XB	1619	C
43	XB	1620	A
43	XB	1621	A
43	XB	1641	G
43	XB	1646	U
43	XB	1648	U
43	XB	1649	C
43	XB	1659	U
43	XB	1663	C
83	r1	46	Y5P
83	r1	49	Y5P
83	r1	53	Y5P
83	r1	54	Y5P
83	r1	55	Y5P
83	r1	56	Y5P
83	r1	57	Y5P
84	r2	8	Y5P
84	r2	9	P5P
84	r2	10	P5P
84	r2	13	Y5P
84	r2	14	P5P
84	r2	15	P5P
84	r2	18	P5P
84	r2	21	P5P
84	r2	23	P5P
84	r2	24	P5P
84	r2	25	Y5P
84	r2	33	Y5P
84	r2	35	P5P
84	r2	36	P5P
84	r2	45	Y5P
84	r2	46	P5P
84	r2	47	Y5P
84	r2	48	Y5P
84	r2	49	Y5P
84	r2	50	Y5P
84	r2	59	Y5P
84	r2	66	Y5P
84	r2	67	Y5P
84	r2	68	Y5P
84	r2	69	P5P
84	r2	70	P5P

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Mol	Chain	Res	Type
84	r2	73	P5P
84	r2	74	Y5P
84	r2	75	Y5P
84	r2	76	P5P
85	r3	3	P5P
85	r3	4	P5P
85	r3	13	Y5P
85	r3	14	P5P
85	r3	16	Y5P
85	r3	17(A)	P5P
85	r3	18	P5P
85	r3	19	P5P
85	r3	20	Y5P
85	r3	21	P5P
85	r3	34	Y5P
85	r3	43	P5P
85	r3	46	P5P
85	r3	47	Y5P
85	r3	48	P5P
85	r3	50	Y5P
85	r3	53	Y5P
85	r3	55	P5P
85	r3	56	Y5P
85	r3	59	Y5P
85	r3	63	Y5P
85	r3	74	P5P

All (12) 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	2602	U
11	XA	2961	C
11	XA	2962	C
17	AA	770	C
17	AA	1048	C
17	AA	1234	C
17	AA	1558	A

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

165 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	P5P	r2	53	84	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	10	84	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
85	P5P	r3	18	85	20,23,24	1.26	3 (15%)	27,33,36	2.48	11 (40%)
84	P5P	r2	69	84	20,23,24	1.29	3 (15%)	27,33,36	2.46	10 (37%)
85	P5P	r3	23	85	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	36	84	20,23,24	1.30	3 (15%)	27,33,36	2.52	11 (40%)
85	P5P	r3	6	85	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	15	84	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
85	Y5P	r3	7	85	14,19,20	7.38	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	40	84	14,19,20	7.39	3 (21%)	18,26,29	0.57	0
85	P5P	r3	11	85	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	9	84	20,23,24	1.28	3 (15%)	27,33,36	2.50	11 (40%)
85	P5P	r3	8	85	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	35	85	20,23,24	1.30	3 (15%)	27,33,36	2.49	11 (40%)
84	Y5P	r2	67	84	14,19,20	7.36	3 (21%)	18,26,29	0.53	0
84	Y5P	r2	45	84	14,19,20	7.35	3 (21%)	18,26,29	0.54	0
84	P5P	r2	18	84	20,23,24	1.26	3 (15%)	27,33,36	2.50	11 (40%)
85	P5P	r3	14	85	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
84	Y5P	r2	3	84	14,19,20	7.37	3 (21%)	18,26,29	0.54	0
85	Y5P	r3	41	85	14,19,20	7.36	3 (21%)	18,26,29	0.57	0
84	P5P	r2	38	84	20,23,24	1.30	3 (15%)	27,33,36	2.50	11 (40%)
85	Y5P	r3	2	85	14,19,20	7.32	3 (21%)	18,26,29	0.53	0
84	Y5P	r2	20	84	14,19,20	7.40	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	53	85	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	48	84	14,19,20	7.36	3 (21%)	18,26,29	0.61	0
84	Y5P	r2	8	84	14,19,20	7.37	3 (21%)	18,26,29	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	P5P	r2	6	84	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	22	84	20,23,24	1.27	3 (15%)	27,33,36	2.51	11 (40%)
85	Y5P	r3	39	85	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	54	85	14,19,20	7.41	3 (21%)	18,26,29	0.57	0
84	P5P	r2	64	84	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
84	Y5P	r2	61	84	14,19,20	7.35	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	54	83	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
85	P5P	r3	55	85	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
83	Y5P	r1	44	83	14,19,20	7.42	3 (21%)	18,26,29	0.57	0
85	P5P	r3	44	85	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
84	P5P	r2	19	84	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
85	Y5P	r3	56	85	14,19,20	7.38	3 (21%)	18,26,29	0.60	0
85	Y5P	r3	25	85	14,19,20	7.39	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	74	84	14,19,20	7.44	3 (21%)	18,26,29	0.56	0
84	Y5P	r2	17	84	14,19,20	7.40	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	55	84	14,19,20	7.42	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	54	84	14,19,20	7.39	3 (21%)	18,26,29	0.55	0
84	P5P	r2	34	84	20,23,24	1.28	3 (15%)	27,33,36	2.50	11 (40%)
85	Y5P	r3	64	85	14,19,20	7.34	3 (21%)	18,26,29	0.56	0
84	P5P	r2	35	84	20,23,24	1.31	3 (15%)	27,33,36	2.50	11 (40%)
83	Y5P	r1	57	83	14,19,20	7.36	3 (21%)	18,26,29	0.57	0
85	P5P	r3	57	85	20,23,24	1.27	3 (15%)	27,33,36	2.51	11 (40%)
85	Y5P	r3	20	85	14,19,20	7.39	3 (21%)	18,26,29	0.55	0
83	Y5P	r1	47	83	14,19,20	7.30	3 (21%)	18,26,29	0.58	0
84	P5P	r2	14	84	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
85	P5P	r3	3	85	20,23,24	1.30	3 (15%)	27,33,36	2.48	11 (40%)
84	Y5P	r2	41	84	14,19,20	7.34	3 (21%)	18,26,29	0.59	0
84	Y5P	r2	16	84	14,19,20	7.37	3 (21%)	18,26,29	0.56	0
84	P5P	r2	52	84	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
85	Y5P	r3	69	85	14,19,20	7.34	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	60	84	14,19,20	7.37	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	12	84	14,19,20	7.39	3 (21%)	18,26,29	0.59	0
84	Y5P	r2	56	84	14,19,20	7.36	3 (21%)	18,26,29	0.55	0
85	P5P	r3	30	85	20,23,24	1.30	3 (15%)	27,33,36	2.47	11 (40%)
85	Y5P	r3	58	85	14,19,20	7.41	3 (21%)	18,26,29	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	Y5P	r2	39	84	14,19,20	7.33	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	59	85	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
84	P5P	r2	29	84	20,23,24	1.29	3 (15%)	27,33,36	2.50	11 (40%)
84	P5P	r2	24	84	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
84	P5P	r2	28	84	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
85	P5P	r3	43	85	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	65	84	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
85	Y5P	r3	60	85	14,19,20	7.39	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	13	85	14,19,20	7.44	3 (21%)	18,26,29	0.61	0
84	P5P	r2	44	84	20,23,24	1.29	3 (15%)	27,33,36	2.47	11 (40%)
85	Y5P	r3	65	85	14,19,20	7.42	3 (21%)	18,26,29	0.60	0
84	Y5P	r2	25	84	14,19,20	7.38	3 (21%)	18,26,29	0.54	0
85	P5P	r3	42	85	20,23,24	1.29	3 (15%)	27,33,36	2.47	10 (37%)
84	Y5P	r2	43	84	14,19,20	7.35	3 (21%)	18,26,29	0.57	0
84	P5P	r2	71	84	20,23,24	1.26	3 (15%)	27,33,36	2.48	11 (40%)
84	P5P	r2	21	84	20,23,24	1.29	3 (15%)	27,33,36	2.46	11 (40%)
84	Y5P	r2	11	84	14,19,20	7.37	3 (21%)	18,26,29	0.59	0
85	P5P	r3	68	85	20,23,24	1.30	3 (15%)	27,33,36	2.48	11 (40%)
83	Y5P	r1	51	83	14,19,20	7.33	3 (21%)	18,26,29	0.59	0
85	P5P	r3	46	85	20,23,24	1.27	3 (15%)	27,33,36	2.46	11 (40%)
84	P5P	r2	1	84	20,23,24	1.27	3 (15%)	27,33,36	2.46	10 (37%)
85	Y5P	r3	63	85	14,19,20	7.40	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	52	83	14,19,20	7.35	3 (21%)	18,26,29	0.57	0
85	P5P	r3	17(A)	85	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)
85	Y5P	r3	50	85	14,19,20	7.38	3 (21%)	18,26,29	0.54	0
84	P5P	r2	76	84	20,23,24	1.27	3 (15%)	27,33,36	2.45	11 (40%)
85	P5P	r3	48	85	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)
85	Y5P	r3	67	85	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	32	85	14,19,20	7.35	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	42	84	14,19,20	7.36	3 (21%)	18,26,29	0.57	0
85	P5P	r3	15	85	20,23,24	1.28	3 (15%)	27,33,36	2.52	11 (40%)
85	P5P	r3	21	85	20,23,24	1.30	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	5	85	20,23,24	1.30	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	45	85	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
85	P5P	r3	4	85	20,23,24	1.29	3 (15%)	27,33,36	2.51	11 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	Y5P	r1	53	83	14,19,20	7.39	3 (21%)	18,26,29	0.60	0
84	Y5P	r2	59	84	14,19,20	7.35	3 (21%)	18,26,29	0.56	0
84	P5P	r2	57	84	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
85	P5P	r3	22	85	20,23,24	1.28	3 (15%)	27,33,36	2.46	11 (40%)
85	P5P	r3	52	85	20,23,24	1.28	3 (15%)	27,33,36	2.48	10 (37%)
84	P5P	r2	27	84	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
85	Y5P	r3	73	85	14,19,20	7.33	3 (21%)	18,26,29	0.52	0
85	Y5P	r3	17	85	14,19,20	7.36	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	4	84	14,19,20	7.37	3 (21%)	18,26,29	0.57	0
83	Y5P	r1	45	83	14,19,20	7.44	3 (21%)	18,26,29	0.59	0
83	Y5P	r1	55	83	14,19,20	7.42	3 (21%)	18,26,29	0.53	0
83	Y5P	r1	56	83	14,19,20	7.37	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	62	85	14,19,20	7.42	3 (21%)	18,26,29	0.60	0
85	P5P	r3	71	85	20,23,24	1.27	3 (15%)	27,33,36	2.47	11 (40%)
84	P5P	r2	73	84	20,23,24	1.28	3 (15%)	27,33,36	2.50	11 (40%)
84	P5P	r2	23	84	20,23,24	1.28	3 (15%)	27,33,36	2.47	10 (37%)
85	P5P	r3	26	85	20,23,24	1.29	3 (15%)	27,33,36	2.47	11 (40%)
84	P5P	r2	46	84	20,23,24	1.28	3 (15%)	27,33,36	2.50	11 (40%)
84	Y5P	r2	72	84	14,19,20	7.39	3 (21%)	18,26,29	0.58	0
84	P5P	r2	58	84	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
85	Y5P	r3	47	85	14,19,20	7.38	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	24	85	14,19,20	7.34	3 (21%)	18,26,29	0.59	0
84	Y5P	r2	2	84	14,19,20	7.39	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	61	85	14,19,20	7.37	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	48	83	14,19,20	7.30	3 (21%)	18,26,29	0.58	0
85	P5P	r3	66	85	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	37	85	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)
85	Y5P	r3	40	85	14,19,20	7.36	3 (21%)	18,26,29	0.60	0
84	Y5P	r2	62	84	14,19,20	7.37	3 (21%)	18,26,29	0.57	0
85	P5P	r3	19	85	20,23,24	1.27	3 (15%)	27,33,36	2.47	11 (40%)
84	Y5P	r2	68	84	14,19,20	7.39	3 (21%)	18,26,29	0.53	0
84	Y5P	r2	49	84	14,19,20	7.40	3 (21%)	18,26,29	0.58	0
85	P5P	r3	10	85	20,23,24	1.29	3 (15%)	27,33,36	2.47	11 (40%)
85	Y5P	r3	49	85	14,19,20	7.40	3 (21%)	18,26,29	0.55	0
84	P5P	r2	31	84	20,23,24	1.30	3 (15%)	27,33,36	2.48	11 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	Y5P	r2	66	84	14,19,20	7.41	3 (21%)	18,26,29	0.58	0
83	Y5P	r1	49	83	14,19,20	7.33	3 (21%)	18,26,29	0.55	0
85	P5P	r3	29	85	20,23,24	1.30	3 (15%)	27,33,36	2.49	11 (40%)
85	Y5P	r3	36	85	14,19,20	7.37	3 (21%)	18,26,29	0.58	0
85	Y5P	r3	16	85	14,19,20	7.41	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	50	84	14,19,20	7.41	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	51	84	14,19,20	7.35	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	1	85	18,20,20	6.57	3 (16%)	25,29,29	0.68	0
85	Y5P	r3	12	85	14,19,20	7.36	3 (21%)	18,26,29	0.55	0
85	P5P	r3	31	85	20,23,24	1.30	3 (15%)	27,33,36	2.46	11 (40%)
85	Y5P	r3	38	85	14,19,20	7.34	3 (21%)	18,26,29	0.54	0
85	P5P	r3	74	85	20,23,24	1.30	3 (15%)	27,33,36	2.51	11 (40%)
84	P5P	r2	63	84	20,23,24	1.30	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	5	84	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
85	Y5P	r3	72	85	14,19,20	7.37	3 (21%)	18,26,29	0.56	0
84	P5P	r2	26	84	20,23,24	1.29	3 (15%)	27,33,36	2.47	11 (40%)
85	P5P	r3	9	85	20,23,24	1.29	3 (15%)	27,33,36	2.51	11 (40%)
84	Y5P	r2	32	84	14,19,20	7.39	3 (21%)	18,26,29	0.58	0
83	Y5P	r1	46	83	14,19,20	7.34	3 (21%)	18,26,29	0.63	0
84	Y5P	r2	13	84	14,19,20	7.43	3 (21%)	18,26,29	0.58	0
83	Y5P	r1	50	83	14,19,20	7.34	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	47	84	14,19,20	7.38	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	27	85	14,19,20	7.36	3 (21%)	18,26,29	0.53	0
84	P5P	r2	37	84	24,24,24	1.20	3 (12%)	34,36,36	3.01	17 (50%)
85	Y5P	r3	70	85	14,19,20	7.36	3 (21%)	18,26,29	0.53	0
85	Y5P	r3	33	85	14,19,20	7.34	3 (21%)	18,26,29	0.56	0
84	Y5P	r2	75	84	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	28	85	14,19,20	7.41	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	34	85	14,19,20	7.36	3 (21%)	18,26,29	0.53	0
84	P5P	r2	7	84	20,23,24	1.26	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	30	84	20,23,24	1.29	3 (15%)	27,33,36	2.47	11 (40%)
84	Y5P	r2	33	84	14,19,20	7.43	3 (21%)	18,26,29	0.65	0
84	P5P	r2	70	84	20,23,24	1.28	3 (15%)	27,33,36	2.46	10 (37%)
85	P5P	r3	51	85	20,23,24	1.29	3 (15%)	27,33,36	2.47	10 (37%)

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	P5P	r2	53	84	-	0/7/25/26	0/3/3/3
84	P5P	r2	10	84	-	0/7/25/26	0/3/3/3
85	P5P	r3	18	85	-	3/7/25/26	0/3/3/3
84	P5P	r2	69	84	-	2/7/25/26	0/3/3/3
85	P5P	r3	23	85	-	0/7/25/26	0/3/3/3
84	P5P	r2	36	84	-	3/7/25/26	0/3/3/3
85	P5P	r3	6	85	-	0/7/25/26	0/3/3/3
84	P5P	r2	15	84	-	4/7/25/26	0/3/3/3
85	Y5P	r3	7	85	-	3/7/33/34	0/2/2/2
84	Y5P	r2	40	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	11	85	-	0/7/25/26	0/3/3/3
84	P5P	r2	9	84	-	5/7/25/26	0/3/3/3
85	P5P	r3	8	85	-	0/7/25/26	0/3/3/3
85	P5P	r3	35	85	-	0/7/25/26	0/3/3/3
84	Y5P	r2	67	84	-	3/7/33/34	0/2/2/2
84	Y5P	r2	45	84	-	4/7/33/34	0/2/2/2
84	P5P	r2	18	84	-	0/7/25/26	0/3/3/3
85	P5P	r3	14	85	-	1/7/25/26	0/3/3/3
84	Y5P	r2	3	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	41	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	38	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	2	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	20	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	53	85	-	3/7/33/34	0/2/2/2
84	Y5P	r2	48	84	-	2/7/33/34	0/2/2/2
84	Y5P	r2	8	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	6	84	-	0/7/25/26	0/3/3/3
84	P5P	r2	22	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	39	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	54	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	64	84	-	0/7/25/26	0/3/3/3
84	Y5P	r2	61	84	-	2/7/33/34	0/2/2/2
83	Y5P	r1	54	83	-	1/7/33/34	0/2/2/2
85	P5P	r3	55	85	-	2/7/25/26	0/3/3/3
83	Y5P	r1	44	83	-	3/7/33/34	0/2/2/2
85	P5P	r3	44	85	-	1/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	P5P	r2	19	84	-	3/7/25/26	0/3/3/3
85	Y5P	r3	56	85	-	3/7/33/34	0/2/2/2
85	Y5P	r3	25	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	74	84	-	2/7/33/34	0/2/2/2
84	Y5P	r2	17	84	-	4/7/33/34	0/2/2/2
84	Y5P	r2	55	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	54	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	34	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	64	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	35	84	-	2/7/25/26	0/3/3/3
83	Y5P	r1	57	83	-	1/7/33/34	0/2/2/2
85	P5P	r3	57	85	-	0/7/25/26	0/3/3/3
85	Y5P	r3	20	85	-	1/7/33/34	0/2/2/2
83	Y5P	r1	47	83	-	4/7/33/34	0/2/2/2
84	P5P	r2	14	84	-	2/7/25/26	0/3/3/3
85	P5P	r3	3	85	-	3/7/25/26	0/3/3/3
84	Y5P	r2	41	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	16	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	52	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	69	85	-	4/7/33/34	0/2/2/2
84	Y5P	r2	60	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	12	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	56	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	30	85	-	0/7/25/26	0/3/3/3
85	Y5P	r3	58	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	39	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	59	85	-	2/7/33/34	0/2/2/2
84	P5P	r2	29	84	-	0/7/25/26	0/3/3/3
84	P5P	r2	24	84	-	2/7/25/26	0/3/3/3
84	P5P	r2	28	84	-	0/7/25/26	0/3/3/3
85	P5P	r3	43	85	-	1/7/25/26	0/3/3/3
84	P5P	r2	65	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	60	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	13	85	-	5/7/33/34	0/2/2/2
84	P5P	r2	44	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	65	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	25	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	42	85	-	2/7/25/26	0/3/3/3
84	Y5P	r2	43	84	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	P5P	r2	71	84	-	0/7/25/26	0/3/3/3
84	P5P	r2	21	84	-	2/7/25/26	0/3/3/3
84	Y5P	r2	11	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	68	85	-	0/7/25/26	0/3/3/3
83	Y5P	r1	51	83	-	1/7/33/34	0/2/2/2
85	P5P	r3	46	85	-	1/7/25/26	0/3/3/3
84	P5P	r2	1	84	-	2/7/25/26	0/3/3/3
85	Y5P	r3	63	85	-	3/7/33/34	0/2/2/2
83	Y5P	r1	52	83	-	3/7/33/34	0/2/2/2
85	P5P	r3	17(A)	85	-	5/7/25/26	0/3/3/3
85	Y5P	r3	50	85	-	4/7/33/34	0/2/2/2
84	P5P	r2	76	84	-	3/7/25/26	0/3/3/3
85	P5P	r3	48	85	-	0/7/25/26	0/3/3/3
85	Y5P	r3	67	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	32	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	42	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	15	85	-	0/7/25/26	0/3/3/3
85	P5P	r3	21	85	-	3/7/25/26	0/3/3/3
85	P5P	r3	5	85	-	2/7/25/26	0/3/3/3
85	P5P	r3	45	85	-	0/7/25/26	0/3/3/3
85	P5P	r3	4	85	-	3/7/25/26	0/3/3/3
83	Y5P	r1	53	83	-	3/7/33/34	0/2/2/2
84	Y5P	r2	59	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	57	84	-	0/7/25/26	0/3/3/3
85	P5P	r3	22	85	-	0/7/25/26	0/3/3/3
85	P5P	r3	52	85	-	0/7/25/26	0/3/3/3
84	P5P	r2	27	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	73	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	17	85	-	4/7/33/34	0/2/2/2
84	Y5P	r2	4	84	-	1/7/33/34	0/2/2/2
83	Y5P	r1	45	83	-	1/7/33/34	0/2/2/2
83	Y5P	r1	55	83	-	4/7/33/34	0/2/2/2
83	Y5P	r1	56	83	-	1/7/33/34	0/2/2/2
85	Y5P	r3	62	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	71	85	-	0/7/25/26	0/3/3/3
84	P5P	r2	73	84	-	3/7/25/26	0/3/3/3
84	P5P	r2	23	84	-	1/7/25/26	0/3/3/3
85	P5P	r3	26	85	-	0/7/25/26	0/3/3/3
84	P5P	r2	46	84	-	6/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	Y5P	r2	72	84	-	3/7/33/34	0/2/2/2
84	P5P	r2	58	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	47	85	-	4/7/33/34	0/2/2/2
85	Y5P	r3	24	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	2	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	61	85	-	3/7/33/34	0/2/2/2
83	Y5P	r1	48	83	-	1/7/33/34	0/2/2/2
85	P5P	r3	66	85	-	0/7/25/26	0/3/3/3
85	P5P	r3	37	85	-	0/7/25/26	0/3/3/3
85	Y5P	r3	40	85	-	3/7/33/34	0/2/2/2
84	Y5P	r2	62	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	19	85	-	1/7/25/26	0/3/3/3
84	Y5P	r2	68	84	-	3/7/33/34	0/2/2/2
84	Y5P	r2	49	84	-	3/7/33/34	0/2/2/2
85	P5P	r3	10	85	-	0/7/25/26	0/3/3/3
85	Y5P	r3	49	85	-	3/7/33/34	0/2/2/2
84	P5P	r2	31	84	-	0/7/25/26	0/3/3/3
84	Y5P	r2	66	84	-	3/7/33/34	0/2/2/2
83	Y5P	r1	49	83	-	2/7/33/34	0/2/2/2
85	P5P	r3	29	85	-	2/7/25/26	0/3/3/3
85	Y5P	r3	36	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	16	85	-	2/7/33/34	0/2/2/2
84	Y5P	r2	50	84	-	3/7/33/34	0/2/2/2
84	Y5P	r2	51	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	1	85	-	4/10/34/34	0/2/2/2
85	Y5P	r3	12	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	31	85	-	0/7/25/26	0/3/3/3
85	Y5P	r3	38	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	74	85	-	2/7/25/26	0/3/3/3
84	P5P	r2	63	84	-	0/7/25/26	0/3/3/3
84	P5P	r2	5	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	72	85	-	2/7/33/34	0/2/2/2
84	P5P	r2	26	84	-	0/7/25/26	0/3/3/3
85	P5P	r3	9	85	-	0/7/25/26	0/3/3/3
84	Y5P	r2	32	84	-	1/7/33/34	0/2/2/2
83	Y5P	r1	46	83	-	4/7/33/34	0/2/2/2
84	Y5P	r2	13	84	-	3/7/33/34	0/2/2/2
83	Y5P	r1	50	83	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	Y5P	r2	47	84	-	3/7/33/34	0/2/2/2
85	Y5P	r3	27	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	37	84	-	3/10/26/26	0/3/3/3
85	Y5P	r3	70	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	33	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	75	84	-	4/7/33/34	0/2/2/2
85	Y5P	r3	28	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	34	85	-	3/7/33/34	0/2/2/2
84	P5P	r2	7	84	-	2/7/25/26	0/3/3/3
84	P5P	r2	30	84	-	0/7/25/26	0/3/3/3
84	Y5P	r2	33	84	-	6/7/33/34	0/2/2/2
84	P5P	r2	70	84	-	3/7/25/26	0/3/3/3
85	P5P	r3	51	85	-	2/7/25/26	0/3/3/3

All (495) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r3	1	Y5P	C2-N3	26.93	1.48	1.27
84	r2	74	Y5P	C2-N3	26.92	1.48	1.27
84	r2	33	Y5P	C2-N3	26.92	1.48	1.27
83	r1	45	Y5P	C2-N3	26.91	1.48	1.27
85	r3	13	Y5P	C2-N3	26.91	1.48	1.27
84	r2	13	Y5P	C2-N3	26.90	1.48	1.27
85	r3	65	Y5P	C2-N3	26.85	1.48	1.27
83	r1	55	Y5P	C2-N3	26.85	1.48	1.27
85	r3	62	Y5P	C2-N3	26.84	1.48	1.27
85	r3	58	Y5P	C2-N3	26.84	1.48	1.27
83	r1	44	Y5P	C2-N3	26.84	1.48	1.27
84	r2	55	Y5P	C2-N3	26.83	1.48	1.27
84	r2	50	Y5P	C2-N3	26.82	1.48	1.27
85	r3	16	Y5P	C2-N3	26.82	1.48	1.27
85	r3	28	Y5P	C2-N3	26.82	1.48	1.27
84	r2	66	Y5P	C2-N3	26.81	1.48	1.27
85	r3	54	Y5P	C2-N3	26.80	1.48	1.27
84	r2	17	Y5P	C2-N3	26.79	1.48	1.27
84	r2	49	Y5P	C2-N3	26.79	1.48	1.27
85	r3	49	Y5P	C2-N3	26.79	1.48	1.27
84	r2	20	Y5P	C2-N3	26.77	1.48	1.27
85	r3	63	Y5P	C2-N3	26.77	1.48	1.27
85	r3	60	Y5P	C2-N3	26.75	1.48	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r1	53	Y5P	C2-N3	26.75	1.48	1.27
84	r2	32	Y5P	C2-N3	26.75	1.48	1.27
85	r3	20	Y5P	C2-N3	26.74	1.48	1.27
84	r2	54	Y5P	C2-N3	26.74	1.48	1.27
84	r2	40	Y5P	C2-N3	26.74	1.48	1.27
85	r3	25	Y5P	C2-N3	26.73	1.48	1.27
84	r2	2	Y5P	C2-N3	26.73	1.48	1.27
84	r2	72	Y5P	C2-N3	26.73	1.48	1.27
84	r2	68	Y5P	C2-N3	26.72	1.48	1.27
85	r3	56	Y5P	C2-N3	26.72	1.48	1.27
85	r3	7	Y5P	C2-N3	26.72	1.48	1.27
84	r2	12	Y5P	C2-N3	26.72	1.48	1.27
85	r3	50	Y5P	C2-N3	26.70	1.48	1.27
84	r2	47	Y5P	C2-N3	26.70	1.48	1.27
85	r3	47	Y5P	C2-N3	26.70	1.48	1.27
84	r2	25	Y5P	C2-N3	26.70	1.48	1.27
85	r3	36	Y5P	C2-N3	26.68	1.48	1.27
84	r2	60	Y5P	C2-N3	26.67	1.48	1.27
84	r2	75	Y5P	C2-N3	26.67	1.48	1.27
85	r3	72	Y5P	C2-N3	26.67	1.48	1.27
84	r2	62	Y5P	C2-N3	26.67	1.48	1.27
84	r2	8	Y5P	C2-N3	26.67	1.48	1.27
84	r2	3	Y5P	C2-N3	26.66	1.48	1.27
85	r3	53	Y5P	C2-N3	26.66	1.48	1.27
83	r1	56	Y5P	C2-N3	26.65	1.48	1.27
84	r2	11	Y5P	C2-N3	26.65	1.48	1.27
84	r2	16	Y5P	C2-N3	26.65	1.48	1.27
84	r2	4	Y5P	C2-N3	26.65	1.48	1.27
85	r3	40	Y5P	C2-N3	26.65	1.48	1.27
85	r3	70	Y5P	C2-N3	26.64	1.48	1.27
85	r3	61	Y5P	C2-N3	26.64	1.48	1.27
85	r3	12	Y5P	C2-N3	26.64	1.48	1.27
83	r1	57	Y5P	C2-N3	26.64	1.48	1.27
85	r3	39	Y5P	C2-N3	26.63	1.48	1.27
83	r1	54	Y5P	C2-N3	26.63	1.48	1.27
85	r3	41	Y5P	C2-N3	26.62	1.48	1.27
85	r3	67	Y5P	C2-N3	26.61	1.47	1.27
85	r3	17	Y5P	C2-N3	26.61	1.47	1.27
84	r2	42	Y5P	C2-N3	26.61	1.47	1.27
85	r3	27	Y5P	C2-N3	26.61	1.47	1.27
84	r2	56	Y5P	C2-N3	26.61	1.47	1.27
84	r2	67	Y5P	C2-N3	26.60	1.47	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r2	48	Y5P	C2-N3	26.60	1.47	1.27
85	r3	59	Y5P	C2-N3	26.60	1.47	1.27
85	r3	34	Y5P	C2-N3	26.60	1.47	1.27
85	r3	32	Y5P	C2-N3	26.59	1.47	1.27
84	r2	45	Y5P	C2-N3	26.59	1.47	1.27
84	r2	59	Y5P	C2-N3	26.59	1.47	1.27
84	r2	51	Y5P	C2-N3	26.58	1.47	1.27
83	r1	52	Y5P	C2-N3	26.58	1.47	1.27
84	r2	61	Y5P	C2-N3	26.58	1.47	1.27
84	r2	43	Y5P	C2-N3	26.57	1.47	1.27
83	r1	46	Y5P	C2-N3	26.57	1.47	1.27
85	r3	24	Y5P	C2-N3	26.56	1.47	1.27
85	r3	33	Y5P	C2-N3	26.56	1.47	1.27
84	r2	41	Y5P	C2-N3	26.56	1.47	1.27
85	r3	38	Y5P	C2-N3	26.55	1.47	1.27
85	r3	69	Y5P	C2-N3	26.55	1.47	1.27
85	r3	73	Y5P	C2-N3	26.54	1.47	1.27
83	r1	50	Y5P	C2-N3	26.54	1.47	1.27
85	r3	64	Y5P	C2-N3	26.54	1.47	1.27
83	r1	51	Y5P	C2-N3	26.52	1.47	1.27
83	r1	49	Y5P	C2-N3	26.51	1.47	1.27
84	r2	39	Y5P	C2-N3	26.51	1.47	1.27
85	r3	2	Y5P	C2-N3	26.50	1.47	1.27
83	r1	48	Y5P	C2-N3	26.43	1.47	1.27
83	r1	47	Y5P	C2-N3	26.39	1.47	1.27
84	r2	47	Y5P	C6-C5	6.22	1.52	1.33
85	r3	27	Y5P	C6-C5	6.22	1.52	1.33
85	r3	38	Y5P	C6-C5	6.21	1.52	1.33
85	r3	69	Y5P	C6-C5	6.21	1.52	1.33
85	r3	16	Y5P	C6-C5	6.21	1.52	1.33
84	r2	48	Y5P	C6-C5	6.21	1.52	1.33
84	r2	39	Y5P	C6-C5	6.21	1.52	1.33
84	r2	67	Y5P	C6-C5	6.21	1.52	1.33
84	r2	56	Y5P	C6-C5	6.20	1.52	1.33
84	r2	59	Y5P	C6-C5	6.20	1.52	1.33
84	r2	51	Y5P	C6-C5	6.20	1.52	1.33
85	r3	41	Y5P	C6-C5	6.20	1.52	1.33
84	r2	75	Y5P	C6-C5	6.20	1.52	1.33
85	r3	34	Y5P	C6-C5	6.20	1.52	1.33
83	r1	57	Y5P	C6-C5	6.20	1.52	1.33
85	r3	17	Y5P	C6-C5	6.20	1.52	1.33
84	r2	20	Y5P	C6-C5	6.20	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r3	61	Y5P	C6-C5	6.20	1.52	1.33
84	r2	32	Y5P	C6-C5	6.20	1.52	1.33
84	r2	12	Y5P	C6-C5	6.19	1.52	1.33
84	r2	43	Y5P	C6-C5	6.19	1.52	1.33
84	r2	11	Y5P	C6-C5	6.19	1.52	1.33
84	r2	16	Y5P	C6-C5	6.19	1.52	1.33
85	r3	59	Y5P	C6-C5	6.19	1.52	1.33
84	r2	45	Y5P	C6-C5	6.19	1.52	1.33
84	r2	61	Y5P	C6-C5	6.19	1.52	1.33
84	r2	42	Y5P	C6-C5	6.19	1.52	1.33
85	r3	12	Y5P	C6-C5	6.19	1.52	1.33
84	r2	25	Y5P	C6-C5	6.19	1.52	1.33
85	r3	60	Y5P	C6-C5	6.19	1.52	1.33
84	r2	62	Y5P	C6-C5	6.19	1.52	1.33
84	r2	68	Y5P	C6-C5	6.19	1.52	1.33
84	r2	2	Y5P	C6-C5	6.18	1.52	1.33
83	r1	54	Y5P	C6-C5	6.18	1.52	1.33
84	r2	17	Y5P	C6-C5	6.18	1.52	1.33
84	r2	4	Y5P	C6-C5	6.18	1.52	1.33
84	r2	74	Y5P	C6-C5	6.18	1.52	1.33
85	r3	50	Y5P	C6-C5	6.18	1.52	1.33
85	r3	20	Y5P	C6-C5	6.18	1.52	1.33
84	r2	72	Y5P	C6-C5	6.18	1.52	1.33
85	r3	54	Y5P	C6-C5	6.18	1.52	1.33
84	r2	54	Y5P	C6-C5	6.18	1.52	1.33
85	r3	2	Y5P	C6-C5	6.18	1.52	1.33
84	r2	3	Y5P	C6-C5	6.18	1.52	1.33
83	r1	44	Y5P	C6-C5	6.18	1.52	1.33
84	r2	8	Y5P	C6-C5	6.18	1.52	1.33
84	r2	55	Y5P	C6-C5	6.18	1.52	1.33
85	r3	39	Y5P	C6-C5	6.18	1.52	1.33
85	r3	70	Y5P	C6-C5	6.18	1.52	1.33
85	r3	72	Y5P	C6-C5	6.18	1.52	1.33
84	r2	66	Y5P	C6-C5	6.18	1.52	1.33
85	r3	67	Y5P	C6-C5	6.18	1.52	1.33
84	r2	50	Y5P	C6-C5	6.17	1.52	1.33
85	r3	13	Y5P	C6-C5	6.17	1.52	1.33
85	r3	62	Y5P	C6-C5	6.17	1.52	1.33
85	r3	33	Y5P	C6-C5	6.17	1.52	1.33
85	r3	64	Y5P	C6-C5	6.17	1.52	1.33
85	r3	58	Y5P	C6-C5	6.16	1.52	1.33
85	r3	28	Y5P	C6-C5	6.16	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r3	73	Y5P	C6-C5	6.16	1.52	1.33
85	r3	25	Y5P	C6-C5	6.16	1.52	1.33
85	r3	63	Y5P	C6-C5	6.16	1.52	1.33
85	r3	36	Y5P	C6-C5	6.16	1.52	1.33
83	r1	56	Y5P	C6-C5	6.16	1.52	1.33
84	r2	13	Y5P	C6-C5	6.16	1.52	1.33
83	r1	52	Y5P	C6-C5	6.16	1.52	1.33
83	r1	55	Y5P	C6-C5	6.16	1.52	1.33
83	r1	45	Y5P	C6-C5	6.16	1.52	1.33
85	r3	49	Y5P	C6-C5	6.16	1.52	1.33
85	r3	47	Y5P	C6-C5	6.15	1.52	1.33
83	r1	50	Y5P	C6-C5	6.15	1.52	1.33
85	r3	32	Y5P	C6-C5	6.15	1.52	1.33
84	r2	40	Y5P	C6-C5	6.15	1.52	1.33
85	r3	53	Y5P	C6-C5	6.15	1.52	1.33
83	r1	49	Y5P	C6-C5	6.15	1.52	1.33
84	r2	60	Y5P	C6-C5	6.15	1.52	1.33
85	r3	56	Y5P	C6-C5	6.15	1.52	1.33
83	r1	46	Y5P	C6-C5	6.15	1.52	1.33
83	r1	47	Y5P	C6-C5	6.15	1.52	1.33
83	r1	48	Y5P	C6-C5	6.15	1.52	1.33
84	r2	41	Y5P	C6-C5	6.15	1.52	1.33
84	r2	49	Y5P	C6-C5	6.15	1.52	1.33
85	r3	24	Y5P	C6-C5	6.14	1.52	1.33
83	r1	51	Y5P	C6-C5	6.14	1.52	1.33
84	r2	33	Y5P	C6-C5	6.14	1.52	1.33
85	r3	7	Y5P	C6-C5	6.14	1.52	1.33
85	r3	1	Y5P	C6-C5	6.13	1.51	1.33
85	r3	65	Y5P	C6-C5	6.11	1.51	1.33
85	r3	40	Y5P	C6-C5	6.10	1.51	1.33
83	r1	53	Y5P	C6-C5	6.10	1.51	1.33
85	r3	29	P5P	C5-C4	-3.31	1.35	1.40
85	r3	68	P5P	C5-C4	-3.30	1.35	1.40
84	r2	73	P5P	C5-C4	-3.30	1.35	1.40
85	r3	5	P5P	C5-C4	-3.29	1.35	1.40
84	r2	31	P5P	C5-C4	-3.29	1.35	1.40
85	r3	30	P5P	C5-C4	-3.29	1.35	1.40
84	r2	37	P5P	C5-C4	-3.29	1.35	1.40
85	r3	4	P5P	C5-C4	-3.28	1.35	1.40
85	r3	42	P5P	C5-C4	-3.27	1.35	1.40
85	r3	51	P5P	C5-C4	-3.27	1.35	1.40
84	r2	52	P5P	C5-C4	-3.27	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r3	6	P5P	C5-C4	-3.27	1.35	1.40
84	r2	57	P5P	C5-C4	-3.26	1.35	1.40
85	r3	48	P5P	C5-C4	-3.26	1.35	1.40
85	r3	31	P5P	C5-C4	-3.26	1.35	1.40
84	r2	35	P5P	C5-C4	-3.26	1.35	1.40
84	r2	53	P5P	C5-C4	-3.26	1.35	1.40
85	r3	10	P5P	C5-C4	-3.26	1.35	1.40
84	r2	38	P5P	C5-C4	-3.25	1.35	1.40
84	r2	70	P5P	C5-C4	-3.25	1.35	1.40
85	r3	44	P5P	C5-C4	-3.25	1.35	1.40
84	r2	5	P5P	C5-C4	-3.25	1.35	1.40
84	r2	30	P5P	C5-C4	-3.25	1.35	1.40
84	r2	23	P5P	C5-C4	-3.25	1.35	1.40
84	r2	21	P5P	C5-C4	-3.25	1.35	1.40
84	r2	26	P5P	C5-C4	-3.24	1.35	1.40
84	r2	63	P5P	C5-C4	-3.24	1.35	1.40
85	r3	35	P5P	C5-C4	-3.24	1.35	1.40
85	r3	21	P5P	C5-C4	-3.24	1.35	1.40
85	r3	26	P5P	C5-C4	-3.24	1.35	1.40
84	r2	24	P5P	C5-C4	-3.24	1.35	1.40
85	r3	43	P5P	C5-C4	-3.24	1.35	1.40
85	r3	9	P5P	C5-C4	-3.24	1.35	1.40
84	r2	27	P5P	C5-C4	-3.24	1.35	1.40
85	r3	37	P5P	C5-C4	-3.23	1.35	1.40
84	r2	69	P5P	C5-C4	-3.23	1.35	1.40
85	r3	19	P5P	C5-C4	-3.23	1.35	1.40
84	r2	28	P5P	C5-C4	-3.23	1.35	1.40
84	r2	1	P5P	C5-C4	-3.23	1.35	1.40
84	r2	19	P5P	C5-C4	-3.23	1.35	1.40
85	r3	8	P5P	C5-C4	-3.23	1.35	1.40
85	r3	11	P5P	C5-C4	-3.23	1.35	1.40
84	r2	44	P5P	C5-C4	-3.22	1.35	1.40
84	r2	58	P5P	C5-C4	-3.22	1.35	1.40
85	r3	22	P5P	C5-C4	-3.22	1.35	1.40
84	r2	46	P5P	C5-C4	-3.22	1.35	1.40
85	r3	3	P5P	C5-C4	-3.22	1.35	1.40
84	r2	29	P5P	C5-C4	-3.22	1.35	1.40
84	r2	65	P5P	C5-C4	-3.22	1.35	1.40
84	r2	64	P5P	C5-C4	-3.22	1.35	1.40
84	r2	6	P5P	C5-C4	-3.22	1.35	1.40
85	r3	71	P5P	C5-C4	-3.21	1.35	1.40
84	r2	14	P5P	C5-C4	-3.21	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r3	14	P5P	C5-C4	-3.21	1.35	1.40
84	r2	15	P5P	C5-C4	-3.21	1.35	1.40
85	r3	23	P5P	C5-C4	-3.21	1.35	1.40
85	r3	46	P5P	C5-C4	-3.21	1.35	1.40
85	r3	45	P5P	C5-C4	-3.21	1.35	1.40
84	r2	36	P5P	C5-C4	-3.20	1.35	1.40
85	r3	15	P5P	C5-C4	-3.20	1.35	1.40
84	r2	34	P5P	C5-C4	-3.20	1.35	1.40
85	r3	52	P5P	C5-C4	-3.20	1.35	1.40
85	r3	66	P5P	C5-C4	-3.19	1.35	1.40
85	r3	55	P5P	C5-C4	-3.19	1.35	1.40
84	r2	71	P5P	C5-C4	-3.19	1.35	1.40
85	r3	18	P5P	C5-C4	-3.18	1.35	1.40
84	r2	76	P5P	C5-C4	-3.18	1.35	1.40
84	r2	10	P5P	C5-C4	-3.17	1.35	1.40
84	r2	22	P5P	C5-C4	-3.16	1.35	1.40
84	r2	18	P5P	C5-C4	-3.16	1.35	1.40
85	r3	57	P5P	C5-C4	-3.16	1.35	1.40
84	r2	7	P5P	C5-C4	-3.16	1.35	1.40
85	r3	17(A)	P5P	C5-C4	-3.15	1.35	1.40
84	r2	9	P5P	C5-C4	-3.14	1.35	1.40
85	r3	74	P5P	C5-C4	-3.13	1.35	1.40
85	r3	74	P5P	C5-N7	-2.83	1.34	1.39
83	r1	44	Y5P	C6-N1	2.79	1.44	1.37
85	r3	1	Y5P	C6-N1	2.78	1.44	1.37
85	r3	3	P5P	C5-N7	-2.78	1.34	1.39
84	r2	55	Y5P	C6-N1	2.77	1.44	1.37
84	r2	3	Y5P	C6-N1	2.77	1.44	1.37
84	r2	20	Y5P	C6-N1	2.77	1.44	1.37
84	r2	68	Y5P	C6-N1	2.77	1.44	1.37
84	r2	74	Y5P	C6-N1	2.77	1.44	1.37
84	r2	47	Y5P	C6-N1	2.77	1.44	1.37
84	r2	42	Y5P	C6-N1	2.77	1.44	1.37
83	r1	45	Y5P	C6-N1	2.77	1.44	1.37
84	r2	59	Y5P	C6-N1	2.77	1.44	1.37
84	r2	54	Y5P	C6-N1	2.76	1.44	1.37
84	r2	17	Y5P	C6-N1	2.76	1.44	1.37
84	r2	25	Y5P	C6-N1	2.76	1.44	1.37
85	r3	54	Y5P	C6-N1	2.76	1.44	1.37
84	r2	2	Y5P	C6-N1	2.76	1.43	1.37
84	r2	13	Y5P	C6-N1	2.76	1.43	1.37
83	r1	54	Y5P	C6-N1	2.75	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r2	45	Y5P	C6-N1	2.75	1.43	1.37
84	r2	75	Y5P	C6-N1	2.75	1.43	1.37
85	r3	12	Y5P	C6-N1	2.75	1.43	1.37
83	r1	56	Y5P	C6-N1	2.75	1.43	1.37
85	r3	7	Y5P	C6-N1	2.75	1.43	1.37
85	r3	20	Y5P	C6-N1	2.75	1.43	1.37
84	r2	72	Y5P	C6-N1	2.75	1.43	1.37
85	r3	53	Y5P	C6-N1	2.75	1.43	1.37
85	r3	49	Y5P	C6-N1	2.75	1.43	1.37
85	r3	62	Y5P	C6-N1	2.75	1.43	1.37
83	r1	55	Y5P	C6-N1	2.75	1.43	1.37
85	r3	47	Y5P	C6-N1	2.75	1.43	1.37
85	r3	60	Y5P	C6-N1	2.75	1.43	1.37
85	r3	25	Y5P	C6-N1	2.74	1.43	1.37
84	r2	66	Y5P	C6-N1	2.74	1.43	1.37
85	r3	27	Y5P	C6-N1	2.74	1.43	1.37
84	r2	56	Y5P	C6-N1	2.74	1.43	1.37
84	r2	51	Y5P	C6-N1	2.74	1.43	1.37
84	r2	61	Y5P	C6-N1	2.74	1.43	1.37
84	r2	60	Y5P	C6-N1	2.74	1.43	1.37
84	r2	8	Y5P	C6-N1	2.74	1.43	1.37
85	r3	24	Y5P	C6-N1	2.74	1.43	1.37
84	r2	4	Y5P	C6-N1	2.74	1.43	1.37
85	r3	16	Y5P	C6-N1	2.74	1.43	1.37
83	r1	57	Y5P	C6-N1	2.74	1.43	1.37
85	r3	39	Y5P	C6-N1	2.73	1.43	1.37
85	r3	59	Y5P	C6-N1	2.73	1.43	1.37
85	r3	50	Y5P	C6-N1	2.73	1.43	1.37
84	r2	12	Y5P	C6-N1	2.73	1.43	1.37
85	r3	34	Y5P	C6-N1	2.73	1.43	1.37
84	r2	62	Y5P	C6-N1	2.73	1.43	1.37
84	r2	11	Y5P	C6-N1	2.73	1.43	1.37
84	r2	41	Y5P	C6-N1	2.73	1.43	1.37
85	r3	58	Y5P	C6-N1	2.72	1.43	1.37
84	r2	32	Y5P	C6-N1	2.72	1.43	1.37
84	r2	31	P5P	C5-N7	-2.72	1.34	1.39
85	r3	17	Y5P	C6-N1	2.72	1.43	1.37
85	r3	35	P5P	C5-N7	-2.72	1.34	1.39
85	r3	4	P5P	C5-N7	-2.72	1.34	1.39
85	r3	65	Y5P	C6-N1	2.72	1.43	1.37
84	r2	50	Y5P	C6-N1	2.72	1.43	1.37
84	r2	43	Y5P	C6-N1	2.72	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r3	36	Y5P	C6-N1	2.72	1.43	1.37
85	r3	13	Y5P	C6-N1	2.72	1.43	1.37
85	r3	63	Y5P	C6-N1	2.72	1.43	1.37
85	r3	10	P5P	C5-N7	-2.71	1.34	1.39
85	r3	56	Y5P	C6-N1	2.71	1.43	1.37
84	r2	67	Y5P	C6-N1	2.71	1.43	1.37
85	r3	64	Y5P	C6-N1	2.71	1.43	1.37
84	r2	35	P5P	C5-N7	-2.71	1.34	1.39
85	r3	69	Y5P	C6-N1	2.71	1.43	1.37
84	r2	16	Y5P	C6-N1	2.71	1.43	1.37
83	r1	53	Y5P	C6-N1	2.71	1.43	1.37
84	r2	36	P5P	C5-N7	-2.71	1.34	1.39
85	r3	21	P5P	C5-N7	-2.70	1.34	1.39
84	r2	29	P5P	C5-N7	-2.70	1.34	1.39
83	r1	49	Y5P	C6-N1	2.70	1.43	1.37
84	r2	49	Y5P	C6-N1	2.70	1.43	1.37
85	r3	28	Y5P	C6-N1	2.70	1.43	1.37
84	r2	48	Y5P	C6-N1	2.70	1.43	1.37
84	r2	34	P5P	C5-N7	-2.70	1.34	1.39
85	r3	26	P5P	C5-N7	-2.70	1.34	1.39
85	r3	22	P5P	C5-N7	-2.70	1.34	1.39
84	r2	5	P5P	C5-N7	-2.70	1.34	1.39
83	r1	52	Y5P	C6-N1	2.70	1.43	1.37
85	r3	41	Y5P	C6-N1	2.70	1.43	1.37
84	r2	38	P5P	C5-N7	-2.69	1.34	1.39
85	r3	15	P5P	C5-N7	-2.69	1.34	1.39
85	r3	32	Y5P	C6-N1	2.69	1.43	1.37
84	r2	69	P5P	C5-N7	-2.69	1.34	1.39
85	r3	37	P5P	C5-N7	-2.69	1.34	1.39
84	r2	27	P5P	C5-N7	-2.69	1.34	1.39
85	r3	33	Y5P	C6-N1	2.69	1.43	1.37
85	r3	61	Y5P	C6-N1	2.69	1.43	1.37
84	r2	39	Y5P	C6-N1	2.69	1.43	1.37
83	r1	47	Y5P	C6-N1	2.69	1.43	1.37
84	r2	40	Y5P	C6-N1	2.69	1.43	1.37
85	r3	38	Y5P	C6-N1	2.69	1.43	1.37
85	r3	5	P5P	C5-N7	-2.69	1.34	1.39
85	r3	23	P5P	C5-N7	-2.69	1.34	1.39
84	r2	33	Y5P	C6-N1	2.69	1.43	1.37
85	r3	2	Y5P	C6-N1	2.69	1.43	1.37
85	r3	70	Y5P	C6-N1	2.68	1.43	1.37
84	r2	30	P5P	C5-N7	-2.68	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r3	43	P5P	C5-N7	-2.68	1.34	1.39
85	r3	9	P5P	C5-N7	-2.68	1.34	1.39
84	r2	21	P5P	C5-N7	-2.68	1.34	1.39
85	r3	66	P5P	C5-N7	-2.68	1.34	1.39
85	r3	40	Y5P	C6-N1	2.68	1.43	1.37
84	r2	7	P5P	C5-N7	-2.68	1.34	1.39
85	r3	31	P5P	C5-N7	-2.68	1.34	1.39
84	r2	22	P5P	C5-N7	-2.68	1.34	1.39
84	r2	76	P5P	C5-N7	-2.68	1.34	1.39
83	r1	51	Y5P	C6-N1	2.68	1.43	1.37
85	r3	30	P5P	C5-N7	-2.67	1.34	1.39
85	r3	67	Y5P	C6-N1	2.67	1.43	1.37
85	r3	17(A)	P5P	C5-N7	-2.67	1.34	1.39
84	r2	37	P5P	C5-N7	-2.67	1.34	1.39
83	r1	50	Y5P	C6-N1	2.67	1.43	1.37
84	r2	58	P5P	C5-N7	-2.66	1.34	1.39
84	r2	63	P5P	C5-N7	-2.66	1.34	1.39
85	r3	51	P5P	C5-N7	-2.66	1.34	1.39
85	r3	14	P5P	C5-N7	-2.66	1.34	1.39
85	r3	44	P5P	C5-N7	-2.66	1.34	1.39
84	r2	46	P5P	C5-N7	-2.66	1.34	1.39
84	r2	18	P5P	C5-N7	-2.66	1.34	1.39
84	r2	26	P5P	C5-N7	-2.66	1.34	1.39
83	r1	48	Y5P	C6-N1	2.66	1.43	1.37
84	r2	44	P5P	C5-N7	-2.65	1.34	1.39
84	r2	14	P5P	C5-N7	-2.65	1.34	1.39
85	r3	29	P5P	C5-N7	-2.65	1.34	1.39
84	r2	10	P5P	C5-N7	-2.65	1.34	1.39
85	r3	45	P5P	C5-N7	-2.65	1.34	1.39
84	r2	73	P5P	C5-N7	-2.65	1.34	1.39
85	r3	68	P5P	C5-N7	-2.65	1.34	1.39
84	r2	9	P5P	C5-N7	-2.65	1.34	1.39
84	r2	52	P5P	C5-N7	-2.65	1.34	1.39
85	r3	57	P5P	C5-N7	-2.65	1.34	1.39
85	r3	42	P5P	C5-N7	-2.65	1.34	1.39
83	r1	46	Y5P	C6-N1	2.65	1.43	1.37
85	r3	46	P5P	C5-N7	-2.65	1.34	1.39
85	r3	11	P5P	C5-N7	-2.64	1.34	1.39
85	r3	73	Y5P	C6-N1	2.64	1.43	1.37
85	r3	19	P5P	C5-N7	-2.64	1.34	1.39
84	r2	6	P5P	C5-N7	-2.64	1.34	1.39
84	r2	53	P5P	C5-N7	-2.64	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r2	28	P5P	C5-N7	-2.64	1.34	1.39
85	r3	8	P5P	C5-N7	-2.64	1.34	1.39
85	r3	52	P5P	C5-N7	-2.64	1.34	1.39
85	r3	72	Y5P	C6-N1	2.63	1.43	1.37
84	r2	19	P5P	C5-N7	-2.63	1.34	1.39
84	r2	23	P5P	C5-N7	-2.63	1.34	1.39
85	r3	48	P5P	C5-N7	-2.63	1.34	1.39
84	r2	1	P5P	C5-N7	-2.63	1.34	1.39
84	r2	15	P5P	C5-N7	-2.63	1.34	1.39
84	r2	57	P5P	C5-N7	-2.63	1.34	1.39
85	r3	71	P5P	C5-N7	-2.62	1.34	1.39
84	r2	24	P5P	C5-N7	-2.62	1.34	1.39
84	r2	64	P5P	C5-N7	-2.62	1.34	1.39
85	r3	55	P5P	C5-N7	-2.62	1.34	1.39
85	r3	18	P5P	C5-N7	-2.61	1.34	1.39
85	r3	6	P5P	C5-N7	-2.61	1.34	1.39
84	r2	65	P5P	C5-N7	-2.60	1.34	1.39
84	r2	70	P5P	C5-N7	-2.60	1.34	1.39
84	r2	71	P5P	C5-N7	-2.57	1.35	1.39
84	r2	35	P5P	C4-N9	-2.36	1.32	1.37
84	r2	36	P5P	C4-N9	-2.33	1.32	1.37
85	r3	9	P5P	C4-N9	-2.32	1.32	1.37
85	r3	3	P5P	C4-N9	-2.32	1.32	1.37
85	r3	35	P5P	C4-N9	-2.31	1.32	1.37
84	r2	26	P5P	C4-N9	-2.31	1.32	1.37
84	r2	63	P5P	C4-N9	-2.30	1.32	1.37
84	r2	44	P5P	C4-N9	-2.30	1.32	1.37
85	r3	29	P5P	C4-N9	-2.30	1.32	1.37
84	r2	38	P5P	C4-N9	-2.30	1.32	1.37
85	r3	51	P5P	C4-N9	-2.30	1.32	1.37
84	r2	15	P5P	C4-N9	-2.30	1.32	1.37
85	r3	31	P5P	C4-N9	-2.29	1.32	1.37
84	r2	30	P5P	C4-N9	-2.29	1.32	1.37
85	r3	21	P5P	C4-N9	-2.29	1.32	1.37
85	r3	30	P5P	C4-N9	-2.29	1.32	1.37
85	r3	5	P5P	C4-N9	-2.29	1.32	1.37
84	r2	27	P5P	C4-N9	-2.29	1.32	1.37
85	r3	26	P5P	C4-N9	-2.29	1.32	1.37
84	r2	28	P5P	C4-N9	-2.28	1.32	1.37
85	r3	37	P5P	C4-N9	-2.28	1.32	1.37
84	r2	21	P5P	C4-N9	-2.28	1.32	1.37
85	r3	11	P5P	C4-N9	-2.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r2	31	P5P	C4-N9	-2.28	1.32	1.37
84	r2	23	P5P	C4-N9	-2.28	1.32	1.37
85	r3	57	P5P	C4-N9	-2.28	1.33	1.37
85	r3	43	P5P	C4-N9	-2.27	1.33	1.37
85	r3	42	P5P	C4-N9	-2.27	1.33	1.37
84	r2	46	P5P	C4-N9	-2.27	1.33	1.37
85	r3	6	P5P	C4-N9	-2.26	1.33	1.37
84	r2	22	P5P	C4-N9	-2.26	1.33	1.37
84	r2	6	P5P	C4-N9	-2.26	1.33	1.37
84	r2	52	P5P	C4-N9	-2.26	1.33	1.37
84	r2	69	P5P	C4-N9	-2.26	1.33	1.37
85	r3	68	P5P	C4-N9	-2.26	1.33	1.37
84	r2	65	P5P	C4-N9	-2.26	1.33	1.37
85	r3	74	P5P	C4-N9	-2.26	1.33	1.37
85	r3	71	P5P	C4-N9	-2.25	1.33	1.37
84	r2	1	P5P	C4-N9	-2.25	1.33	1.37
84	r2	5	P5P	C4-N9	-2.25	1.33	1.37
84	r2	29	P5P	C4-N9	-2.25	1.33	1.37
85	r3	46	P5P	C4-N9	-2.25	1.33	1.37
84	r2	37	P5P	C4-N9	-2.25	1.33	1.37
84	r2	9	P5P	C4-N9	-2.24	1.33	1.37
84	r2	58	P5P	C4-N9	-2.24	1.33	1.37
85	r3	48	P5P	C4-N9	-2.24	1.33	1.37
85	r3	52	P5P	C4-N9	-2.24	1.33	1.37
85	r3	45	P5P	C4-N9	-2.24	1.33	1.37
85	r3	15	P5P	C4-N9	-2.24	1.33	1.37
85	r3	44	P5P	C4-N9	-2.24	1.33	1.37
85	r3	8	P5P	C4-N9	-2.24	1.33	1.37
84	r2	70	P5P	C4-N9	-2.23	1.33	1.37
84	r2	53	P5P	C4-N9	-2.23	1.33	1.37
84	r2	19	P5P	C4-N9	-2.23	1.33	1.37
85	r3	23	P5P	C4-N9	-2.23	1.33	1.37
85	r3	4	P5P	C4-N9	-2.23	1.33	1.37
84	r2	73	P5P	C4-N9	-2.23	1.33	1.37
84	r2	64	P5P	C4-N9	-2.23	1.33	1.37
84	r2	14	P5P	C4-N9	-2.22	1.33	1.37
84	r2	71	P5P	C4-N9	-2.22	1.33	1.37
85	r3	55	P5P	C4-N9	-2.22	1.33	1.37
84	r2	57	P5P	C4-N9	-2.22	1.33	1.37
85	r3	18	P5P	C4-N9	-2.22	1.33	1.37
85	r3	10	P5P	C4-N9	-2.22	1.33	1.37
84	r2	76	P5P	C4-N9	-2.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	r3	22	P5P	C4-N9	-2.22	1.33	1.37
84	r2	10	P5P	C4-N9	-2.21	1.33	1.37
85	r3	17(A)	P5P	C4-N9	-2.20	1.33	1.37
85	r3	14	P5P	C4-N9	-2.20	1.33	1.37
84	r2	34	P5P	C4-N9	-2.19	1.33	1.37
84	r2	18	P5P	C4-N9	-2.19	1.33	1.37
84	r2	24	P5P	C4-N9	-2.18	1.33	1.37
85	r3	66	P5P	C4-N9	-2.18	1.33	1.37
85	r3	19	P5P	C4-N9	-2.16	1.33	1.37
84	r2	7	P5P	C4-N9	-2.15	1.33	1.37

All (824) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	37	P5P	OP3-P-OP1	-6.03	87.34	110.83
84	r2	37	P5P	OP3-P-O5'	-5.82	91.48	106.67
85	r3	42	P5P	N9-C8-N7	-5.35	106.34	113.94
85	r3	4	P5P	N9-C8-N7	-5.33	106.37	113.94
84	r2	29	P5P	N9-C8-N7	-5.30	106.42	113.94
84	r2	28	P5P	N9-C8-N7	-5.30	106.42	113.94
84	r2	58	P5P	N9-C8-N7	-5.29	106.43	113.94
85	r3	6	P5P	N9-C8-N7	-5.29	106.43	113.94
84	r2	38	P5P	N9-C8-N7	-5.29	106.43	113.94
84	r2	63	P5P	N9-C8-N7	-5.29	106.44	113.94
84	r2	65	P5P	N9-C8-N7	-5.28	106.44	113.94
85	r3	43	P5P	N9-C8-N7	-5.28	106.45	113.94
84	r2	73	P5P	N9-C8-N7	-5.28	106.45	113.94
85	r3	9	P5P	N9-C8-N7	-5.27	106.45	113.94
84	r2	21	P5P	N9-C8-N7	-5.27	106.46	113.94
85	r3	30	P5P	N9-C8-N7	-5.27	106.47	113.94
84	r2	19	P5P	N9-C8-N7	-5.26	106.47	113.94
84	r2	27	P5P	N9-C8-N7	-5.26	106.48	113.94
84	r2	44	P5P	N9-C8-N7	-5.25	106.48	113.94
84	r2	71	P5P	N9-C8-N7	-5.25	106.49	113.94
84	r2	69	P5P	N9-C8-N7	-5.25	106.49	113.94
84	r2	37	P5P	OP3-P-OP2	-5.25	88.12	107.80
85	r3	21	P5P	N9-C8-N7	-5.25	106.49	113.94
84	r2	15	P5P	N9-C8-N7	-5.25	106.49	113.94
84	r2	30	P5P	N9-C8-N7	-5.25	106.49	113.94
85	r3	29	P5P	N9-C8-N7	-5.25	106.49	113.94
85	r3	11	P5P	N9-C8-N7	-5.24	106.50	113.94
84	r2	1	P5P	N9-C8-N7	-5.24	106.50	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r3	44	P5P	N9-C8-N7	-5.24	106.50	113.94
84	r2	5	P5P	N9-C8-N7	-5.24	106.50	113.94
84	r2	26	P5P	N9-C8-N7	-5.24	106.50	113.94
85	r3	51	P5P	N9-C8-N7	-5.24	106.50	113.94
84	r2	70	P5P	N9-C8-N7	-5.24	106.51	113.94
85	r3	52	P5P	N9-C8-N7	-5.24	106.51	113.94
84	r2	57	P5P	N9-C8-N7	-5.23	106.51	113.94
84	r2	52	P5P	N9-C8-N7	-5.23	106.52	113.94
84	r2	14	P5P	N9-C8-N7	-5.23	106.52	113.94
85	r3	10	P5P	N9-C8-N7	-5.23	106.52	113.94
85	r3	31	P5P	N9-C8-N7	-5.23	106.52	113.94
84	r2	22	P5P	N9-C8-N7	-5.23	106.52	113.94
85	r3	8	P5P	N9-C8-N7	-5.23	106.52	113.94
85	r3	15	P5P	N9-C8-N7	-5.23	106.52	113.94
85	r3	19	P5P	N9-C8-N7	-5.23	106.52	113.94
84	r2	24	P5P	N9-C8-N7	-5.22	106.53	113.94
85	r3	5	P5P	N9-C8-N7	-5.22	106.53	113.94
85	r3	66	P5P	N9-C8-N7	-5.22	106.53	113.94
84	r2	6	P5P	N9-C8-N7	-5.22	106.53	113.94
84	r2	23	P5P	N9-C8-N7	-5.22	106.53	113.94
84	r2	46	P5P	N9-C8-N7	-5.22	106.53	113.94
84	r2	31	P5P	N9-C8-N7	-5.22	106.54	113.94
85	r3	68	P5P	N9-C8-N7	-5.22	106.54	113.94
85	r3	23	P5P	N9-C8-N7	-5.21	106.54	113.94
85	r3	48	P5P	N9-C8-N7	-5.21	106.54	113.94
85	r3	71	P5P	N9-C8-N7	-5.21	106.54	113.94
84	r2	37	P5P	N9-C8-N7	-5.21	106.55	113.94
84	r2	53	P5P	N9-C8-N7	-5.20	106.55	113.94
85	r3	45	P5P	N9-C8-N7	-5.20	106.55	113.94
85	r3	57	P5P	N9-C8-N7	-5.20	106.56	113.94
84	r2	9	P5P	N9-C8-N7	-5.20	106.56	113.94
85	r3	22	P5P	N9-C8-N7	-5.20	106.56	113.94
85	r3	55	P5P	N9-C8-N7	-5.20	106.56	113.94
85	r3	35	P5P	N9-C8-N7	-5.20	106.56	113.94
85	r3	18	P5P	N9-C8-N7	-5.19	106.57	113.94
84	r2	10	P5P	N9-C8-N7	-5.19	106.57	113.94
85	r3	26	P5P	N9-C8-N7	-5.19	106.57	113.94
84	r2	35	P5P	N9-C8-N7	-5.19	106.58	113.94
85	r3	46	P5P	N9-C8-N7	-5.19	106.58	113.94
84	r2	64	P5P	N9-C8-N7	-5.18	106.58	113.94
84	r2	7	P5P	N9-C8-N7	-5.17	106.60	113.94
85	r3	3	P5P	N9-C8-N7	-5.17	106.61	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	18	P5P	N9-C8-N7	-5.16	106.62	113.94
84	r2	34	P5P	C5-C4-N3	-5.15	120.10	127.18
85	r3	37	P5P	N9-C8-N7	-5.14	106.64	113.94
85	r3	14	P5P	N9-C8-N7	-5.14	106.65	113.94
85	r3	17(A)	P5P	N9-C8-N7	-5.13	106.65	113.94
84	r2	36	P5P	N9-C8-N7	-5.10	106.70	113.94
84	r2	34	P5P	N9-C8-N7	-5.10	106.70	113.94
84	r2	76	P5P	C5-C4-N3	-5.08	120.20	127.18
85	r3	37	P5P	C5-C4-N3	-5.07	120.21	127.18
85	r3	66	P5P	C5-C4-N3	-5.06	120.23	127.18
84	r2	7	P5P	C5-C4-N3	-5.05	120.24	127.18
85	r3	15	P5P	C5-C4-N3	-5.05	120.24	127.18
84	r2	18	P5P	C5-C4-N3	-5.05	120.25	127.18
84	r2	36	P5P	C5-C4-N3	-5.04	120.25	127.18
84	r2	46	P5P	C5-C4-N3	-5.04	120.26	127.18
85	r3	11	P5P	C5-C4-N3	-5.03	120.27	127.18
85	r3	4	P5P	C5-C4-N3	-5.02	120.28	127.18
84	r2	53	P5P	C5-C4-N3	-5.02	120.29	127.18
85	r3	17(A)	P5P	C5-C4-N3	-5.01	120.30	127.18
85	r3	52	P5P	C5-C4-N3	-5.01	120.31	127.18
85	r3	68	P5P	C5-C4-N3	-5.00	120.31	127.18
85	r3	55	P5P	C5-C4-N3	-5.00	120.31	127.18
85	r3	5	P5P	C5-C4-N3	-5.00	120.31	127.18
85	r3	18	P5P	C5-C4-N3	-5.00	120.32	127.18
84	r2	73	P5P	C5-C4-N3	-5.00	120.32	127.18
85	r3	23	P5P	C5-C4-N3	-5.00	120.32	127.18
85	r3	74	P5P	N9-C8-N7	-5.00	106.85	113.94
85	r3	74	P5P	C5-C4-N3	-4.99	120.32	127.18
85	r3	22	P5P	C5-C4-N3	-4.99	120.33	127.18
85	r3	71	P5P	C5-C4-N3	-4.99	120.33	127.18
84	r2	6	P5P	C5-C4-N3	-4.99	120.33	127.18
84	r2	71	P5P	C5-C4-N3	-4.98	120.34	127.18
84	r2	57	P5P	C5-C4-N3	-4.98	120.34	127.18
85	r3	48	P5P	C5-C4-N3	-4.98	120.34	127.18
84	r2	24	P5P	C5-C4-N3	-4.98	120.34	127.18
85	r3	57	P5P	C5-C4-N3	-4.98	120.34	127.18
84	r2	37	P5P	C5-C4-N3	-4.98	120.34	127.18
84	r2	65	P5P	C5-C4-N3	-4.98	120.35	127.18
84	r2	1	P5P	C5-C4-N3	-4.98	120.35	127.18
84	r2	9	P5P	C5-C4-N3	-4.98	120.35	127.18
85	r3	19	P5P	C5-C4-N3	-4.97	120.35	127.18
85	r3	29	P5P	C5-C4-N3	-4.97	120.35	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r3	45	P5P	C5-C4-N3	-4.97	120.36	127.18
85	r3	9	P5P	C5-C4-N3	-4.97	120.36	127.18
85	r3	21	P5P	C5-C4-N3	-4.96	120.36	127.18
85	r3	43	P5P	C5-C4-N3	-4.96	120.36	127.18
85	r3	14	P5P	C5-C4-N3	-4.96	120.37	127.18
84	r2	64	P5P	C5-C4-N3	-4.96	120.37	127.18
84	r2	76	P5P	N9-C8-N7	-4.96	106.90	113.94
84	r2	19	P5P	C5-C4-N3	-4.96	120.37	127.18
84	r2	10	P5P	C5-C4-N3	-4.95	120.38	127.18
84	r2	52	P5P	C5-C4-N3	-4.95	120.38	127.18
84	r2	63	P5P	C5-C4-N3	-4.95	120.39	127.18
85	r3	8	P5P	C5-C4-N3	-4.95	120.39	127.18
85	r3	6	P5P	C5-C4-N3	-4.95	120.39	127.18
84	r2	37	P5P	OP2-P-OP1	4.95	130.10	110.83
84	r2	22	P5P	C5-C4-N3	-4.94	120.39	127.18
85	r3	10	P5P	C5-C4-N3	-4.94	120.39	127.18
84	r2	58	P5P	C5-C4-N3	-4.94	120.39	127.18
85	r3	30	P5P	C5-C4-N3	-4.94	120.40	127.18
85	r3	35	P5P	C5-C4-N3	-4.94	120.40	127.18
85	r3	3	P5P	C5-C4-N3	-4.94	120.40	127.18
84	r2	15	P5P	C5-C4-N3	-4.93	120.41	127.18
84	r2	27	P5P	C5-C4-N3	-4.93	120.41	127.18
84	r2	38	P5P	C5-C4-N3	-4.93	120.41	127.18
85	r3	26	P5P	C5-C4-N3	-4.93	120.41	127.18
84	r2	23	P5P	C5-C4-N3	-4.93	120.42	127.18
84	r2	29	P5P	C5-C4-N3	-4.93	120.42	127.18
84	r2	35	P5P	C5-C4-N3	-4.92	120.42	127.18
84	r2	5	P5P	C5-C4-N3	-4.92	120.42	127.18
84	r2	31	P5P	C5-C4-N3	-4.92	120.42	127.18
84	r2	26	P5P	C5-C4-N3	-4.92	120.42	127.18
84	r2	44	P5P	C5-C4-N3	-4.92	120.42	127.18
85	r3	44	P5P	C5-C4-N3	-4.92	120.43	127.18
84	r2	28	P5P	C5-C4-N3	-4.92	120.43	127.18
84	r2	14	P5P	C5-C4-N3	-4.91	120.44	127.18
84	r2	70	P5P	C5-C4-N3	-4.91	120.44	127.18
85	r3	31	P5P	C5-C4-N3	-4.91	120.44	127.18
84	r2	30	P5P	C5-C4-N3	-4.90	120.45	127.18
85	r3	46	P5P	C5-C4-N3	-4.90	120.45	127.18
85	r3	51	P5P	C5-C4-N3	-4.88	120.48	127.18
85	r3	42	P5P	C5-C4-N3	-4.86	120.51	127.18
84	r2	69	P5P	C5-C4-N3	-4.86	120.51	127.18
84	r2	21	P5P	C5-C4-N3	-4.84	120.53	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r3	74	P5P	C1'-N9-C8	-4.40	117.33	127.09
84	r2	70	P5P	N1-C2-N3	-4.33	119.97	127.33
85	r3	3	P5P	N1-C2-N3	-4.33	119.97	127.33
85	r3	48	P5P	N1-C2-N3	-4.33	119.98	127.33
85	r3	42	P5P	N1-C2-N3	-4.32	119.99	127.33
84	r2	63	P5P	N1-C2-N3	-4.32	119.99	127.33
84	r2	69	P5P	N1-C2-N3	-4.32	119.99	127.33
84	r2	21	P5P	N1-C2-N3	-4.32	120.00	127.33
85	r3	51	P5P	N1-C2-N3	-4.31	120.00	127.33
84	r2	65	P5P	N1-C2-N3	-4.31	120.00	127.33
84	r2	28	P5P	N1-C2-N3	-4.31	120.00	127.33
84	r2	27	P5P	N1-C2-N3	-4.31	120.01	127.33
84	r2	35	P5P	N1-C2-N3	-4.30	120.02	127.33
84	r2	29	P5P	N1-C2-N3	-4.30	120.02	127.33
84	r2	36	P5P	C1'-N9-C8	-4.30	117.56	127.09
84	r2	6	P5P	N1-C2-N3	-4.29	120.03	127.33
85	r3	68	P5P	N1-C2-N3	-4.29	120.04	127.33
84	r2	46	P5P	N1-C2-N3	-4.29	120.04	127.33
84	r2	5	P5P	N1-C2-N3	-4.29	120.04	127.33
84	r2	36	P5P	N1-C2-N3	-4.29	120.04	127.33
84	r2	23	P5P	N1-C2-N3	-4.29	120.05	127.33
84	r2	24	P5P	N1-C2-N3	-4.29	120.05	127.33
85	r3	19	P5P	N1-C2-N3	-4.29	120.05	127.33
85	r3	14	P5P	N1-C2-N3	-4.28	120.05	127.33
84	r2	26	P5P	N1-C2-N3	-4.28	120.05	127.33
85	r3	18	P5P	N1-C2-N3	-4.28	120.06	127.33
84	r2	38	P5P	N1-C2-N3	-4.27	120.07	127.33
84	r2	52	P5P	N1-C2-N3	-4.27	120.07	127.33
85	r3	29	P5P	N1-C2-N3	-4.27	120.07	127.33
85	r3	6	P5P	N1-C2-N3	-4.27	120.07	127.33
85	r3	17(A)	P5P	N1-C2-N3	-4.27	120.07	127.33
85	r3	30	P5P	N1-C2-N3	-4.27	120.07	127.33
84	r2	7	P5P	N1-C2-N3	-4.27	120.07	127.33
85	r3	37	P5P	N1-C2-N3	-4.27	120.07	127.33
85	r3	52	P5P	N1-C2-N3	-4.27	120.07	127.33
85	r3	35	P5P	N1-C2-N3	-4.27	120.08	127.33
84	r2	15	P5P	N1-C2-N3	-4.27	120.08	127.33
84	r2	14	P5P	N1-C2-N3	-4.27	120.08	127.33
85	r3	23	P5P	N1-C2-N3	-4.27	120.08	127.33
85	r3	66	P5P	N1-C2-N3	-4.27	120.08	127.33
85	r3	5	P5P	N1-C2-N3	-4.27	120.08	127.33
85	r3	11	P5P	N1-C2-N3	-4.27	120.08	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	31	P5P	N1-C2-N3	-4.27	120.08	127.33
85	r3	8	P5P	N1-C2-N3	-4.27	120.08	127.33
85	r3	55	P5P	N1-C2-N3	-4.27	120.08	127.33
84	r2	30	P5P	N1-C2-N3	-4.26	120.08	127.33
84	r2	57	P5P	N1-C2-N3	-4.26	120.08	127.33
85	r3	22	P5P	N1-C2-N3	-4.26	120.09	127.33
84	r2	19	P5P	N1-C2-N3	-4.26	120.09	127.33
85	r3	4	P5P	N1-C2-N3	-4.26	120.09	127.33
84	r2	9	P5P	N1-C2-N3	-4.26	120.09	127.33
84	r2	53	P5P	N1-C2-N3	-4.26	120.09	127.33
84	r2	10	P5P	N1-C2-N3	-4.26	120.10	127.33
84	r2	37	P5P	N1-C2-N3	-4.26	120.10	127.33
84	r2	44	P5P	N1-C2-N3	-4.25	120.11	127.33
85	r3	43	P5P	N1-C2-N3	-4.25	120.11	127.33
84	r2	18	P5P	N1-C2-N3	-4.25	120.11	127.33
85	r3	26	P5P	N1-C2-N3	-4.25	120.11	127.33
85	r3	9	P5P	N1-C2-N3	-4.24	120.13	127.33
85	r3	21	P5P	N1-C2-N3	-4.24	120.13	127.33
84	r2	22	P5P	N1-C2-N3	-4.24	120.13	127.33
85	r3	10	P5P	N1-C2-N3	-4.23	120.14	127.33
84	r2	73	P5P	N1-C2-N3	-4.23	120.14	127.33
84	r2	58	P5P	N1-C2-N3	-4.23	120.15	127.33
85	r3	44	P5P	N1-C2-N3	-4.23	120.15	127.33
85	r3	15	P5P	C1'-N9-C8	-4.23	117.72	127.09
84	r2	64	P5P	N1-C2-N3	-4.23	120.15	127.33
85	r3	31	P5P	N1-C2-N3	-4.22	120.16	127.33
84	r2	1	P5P	N1-C2-N3	-4.21	120.18	127.33
84	r2	76	P5P	N1-C2-N3	-4.20	120.19	127.33
84	r2	34	P5P	N1-C2-N3	-4.20	120.19	127.33
85	r3	15	P5P	N1-C2-N3	-4.20	120.19	127.33
84	r2	71	P5P	N1-C2-N3	-4.20	120.20	127.33
85	r3	57	P5P	C1'-N9-C8	-4.20	117.78	127.09
85	r3	57	P5P	N1-C2-N3	-4.20	120.20	127.33
85	r3	71	P5P	N1-C2-N3	-4.17	120.25	127.33
84	r2	34	P5P	C1'-N9-C8	-4.16	117.87	127.09
85	r3	45	P5P	N1-C2-N3	-4.15	120.28	127.33
85	r3	46	P5P	N1-C2-N3	-4.15	120.28	127.33
84	r2	22	P5P	C1'-N9-C8	-4.15	117.89	127.09
85	r3	9	P5P	C1'-N9-C8	-4.13	117.93	127.09
85	r3	42	P5P	C4-N9-C8	4.12	110.07	105.74
85	r3	74	P5P	N1-C2-N3	-4.12	120.33	127.33
84	r2	38	P5P	C4-N9-C8	4.12	110.07	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	28	P5P	C4-N9-C8	4.11	110.05	105.74
85	r3	8	P5P	C1'-N9-C8	-4.11	117.98	127.09
85	r3	6	P5P	C4-N9-C8	4.10	110.05	105.74
84	r2	9	P5P	C1'-N9-C8	-4.10	117.98	127.09
85	r3	9	P5P	C4-N9-C8	4.10	110.05	105.74
85	r3	17(A)	P5P	C1'-N9-C8	-4.10	117.99	127.09
84	r2	29	P5P	C4-N9-C8	4.10	110.05	105.74
84	r2	35	P5P	C1'-N9-C8	-4.10	118.00	127.09
84	r2	63	P5P	C4-N9-C8	4.10	110.04	105.74
84	r2	65	P5P	C4-N9-C8	4.08	110.03	105.74
84	r2	27	P5P	C4-N9-C8	4.08	110.03	105.74
84	r2	18	P5P	C1'-N9-C8	-4.08	118.04	127.09
85	r3	57	P5P	C4-N9-C8	4.07	110.01	105.74
84	r2	21	P5P	C4-N9-C8	4.07	110.01	105.74
84	r2	52	P5P	C4-N9-C8	4.05	109.99	105.74
85	r3	43	P5P	C4-N9-C8	4.05	109.99	105.74
84	r2	5	P5P	C4-N9-C8	4.05	109.99	105.74
84	r2	9	P5P	C4-N9-C8	4.05	109.99	105.74
85	r3	8	P5P	C4-N9-C8	4.05	109.99	105.74
85	r3	29	P5P	C4-N9-C8	4.05	109.99	105.74
84	r2	22	P5P	C4-N9-C8	4.05	109.99	105.74
84	r2	15	P5P	C4-N9-C8	4.04	109.98	105.74
84	r2	73	P5P	C4-N9-C8	4.04	109.98	105.74
85	r3	31	P5P	C4-N9-C8	4.04	109.98	105.74
85	r3	14	P5P	C1'-N9-C8	-4.04	118.13	127.09
84	r2	35	P5P	C4-N9-C8	4.04	109.97	105.74
85	r3	44	P5P	C4-N9-C8	4.03	109.97	105.74
85	r3	11	P5P	C4-N9-C8	4.03	109.97	105.74
84	r2	30	P5P	C4-N9-C8	4.03	109.97	105.74
84	r2	58	P5P	C4-N9-C8	4.03	109.97	105.74
85	r3	21	P5P	C4-N9-C8	4.02	109.96	105.74
84	r2	14	P5P	C4-N9-C8	4.02	109.96	105.74
84	r2	44	P5P	C4-N9-C8	4.02	109.96	105.74
85	r3	52	P5P	C4-N9-C8	4.02	109.96	105.74
84	r2	71	P5P	C4-N9-C8	4.02	109.96	105.74
85	r3	51	P5P	C4-N9-C8	4.02	109.95	105.74
84	r2	69	P5P	C4-N9-C8	4.01	109.95	105.74
84	r2	70	P5P	C4-N9-C8	4.01	109.95	105.74
85	r3	21	P5P	C1'-N9-C8	-4.01	118.20	127.09
85	r3	30	P5P	C4-N9-C8	4.01	109.94	105.74
84	r2	19	P5P	C4-N9-C8	4.01	109.94	105.74
84	r2	1	P5P	C4-N9-C8	4.00	109.94	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r3	35	P5P	C4-N9-C8	4.00	109.94	105.74
85	r3	45	P5P	C4-N9-C8	4.00	109.94	105.74
84	r2	53	P5P	C1'-N9-C8	-4.00	118.21	127.09
85	r3	46	P5P	C4-N9-C8	4.00	109.94	105.74
84	r2	26	P5P	C4-N9-C8	4.00	109.94	105.74
85	r3	4	P5P	C4-N9-C8	4.00	109.94	105.74
84	r2	57	P5P	C4-N9-C8	4.00	109.93	105.74
84	r2	38	P5P	C1'-N9-C8	-4.00	118.23	127.09
85	r3	45	P5P	C1'-N9-C8	-3.99	118.23	127.09
85	r3	23	P5P	C4-N9-C8	3.99	109.93	105.74
85	r3	15	P5P	C4-N9-C8	3.99	109.93	105.74
84	r2	46	P5P	C4-N9-C8	3.99	109.93	105.74
84	r2	24	P5P	C4-N9-C8	3.99	109.93	105.74
84	r2	10	P5P	C1'-N9-C8	-3.99	118.24	127.09
84	r2	52	P5P	C1'-N9-C8	-3.99	118.24	127.09
84	r2	6	P5P	C4-N9-C8	3.99	109.92	105.74
85	r3	71	P5P	C4-N9-C8	3.99	109.92	105.74
85	r3	55	P5P	C4-N9-C8	3.98	109.92	105.74
84	r2	31	P5P	C1'-N9-C8	-3.98	118.26	127.09
85	r3	10	P5P	C4-N9-C8	3.98	109.91	105.74
85	r3	5	P5P	C4-N9-C8	3.98	109.91	105.74
84	r2	73	P5P	C1'-N9-C8	-3.98	118.27	127.09
85	r3	18	P5P	C4-N9-C8	3.98	109.91	105.74
85	r3	5	P5P	C1'-N9-C8	-3.98	118.27	127.09
84	r2	46	P5P	C1'-N9-C8	-3.97	118.28	127.09
85	r3	35	P5P	C1'-N9-C8	-3.97	118.28	127.09
84	r2	64	P5P	C4-N9-C8	3.97	109.91	105.74
84	r2	64	P5P	C1'-N9-C8	-3.97	118.28	127.09
84	r2	36	P5P	C4-N9-C8	3.97	109.90	105.74
85	r3	48	P5P	C4-N9-C8	3.97	109.90	105.74
85	r3	55	P5P	C1'-N9-C8	-3.97	118.29	127.09
84	r2	76	P5P	C1'-N9-C8	-3.97	118.29	127.09
85	r3	66	P5P	C4-N9-C8	3.97	109.90	105.74
84	r2	10	P5P	C4-N9-C8	3.97	109.90	105.74
85	r3	46	P5P	C1'-N9-C8	-3.97	118.29	127.09
85	r3	3	P5P	C4-N9-C8	3.96	109.90	105.74
85	r3	26	P5P	C1'-N9-C8	-3.96	118.30	127.09
85	r3	19	P5P	C4-N9-C8	3.96	109.89	105.74
85	r3	68	P5P	C4-N9-C8	3.96	109.89	105.74
84	r2	23	P5P	C4-N9-C8	3.95	109.89	105.74
84	r2	27	P5P	C1'-N9-C8	-3.95	118.32	127.09
84	r2	6	P5P	C1'-N9-C8	-3.95	118.33	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	53	P5P	C4-N9-C8	3.95	109.88	105.74
85	r3	14	P5P	C4-N9-C8	3.95	109.88	105.74
85	r3	26	P5P	C4-N9-C8	3.95	109.88	105.74
84	r2	18	P5P	C4-N9-C8	3.95	109.88	105.74
84	r2	37	P5P	C4-N9-C8	3.95	109.88	105.74
84	r2	7	P5P	C1'-N9-C8	-3.95	118.34	127.09
84	r2	37	P5P	C1'-N9-C8	-3.95	118.34	127.09
84	r2	31	P5P	C4-N9-C8	3.94	109.87	105.74
85	r3	66	P5P	C1'-N9-C8	-3.94	118.35	127.09
85	r3	18	P5P	C1'-N9-C8	-3.93	118.37	127.09
85	r3	10	P5P	C1'-N9-C8	-3.93	118.37	127.09
84	r2	5	P5P	C1'-N9-C8	-3.92	118.39	127.09
85	r3	11	P5P	C1'-N9-C8	-3.92	118.39	127.09
85	r3	29	P5P	C1'-N9-C8	-3.92	118.39	127.09
85	r3	3	P5P	C6-N1-C2	3.92	120.43	115.80
85	r3	22	P5P	C4-N9-C8	3.92	109.85	105.74
85	r3	23	P5P	C1'-N9-C8	-3.92	118.40	127.09
84	r2	29	P5P	C1'-N9-C8	-3.91	118.41	127.09
85	r3	43	P5P	C1'-N9-C8	-3.91	118.42	127.09
85	r3	37	P5P	C4-N9-C8	3.90	109.84	105.74
85	r3	71	P5P	C1'-N9-C8	-3.90	118.43	127.09
85	r3	51	P5P	C6-N1-C2	3.89	120.39	115.80
85	r3	3	P5P	C1'-N9-C8	-3.89	118.46	127.09
85	r3	37	P5P	C1'-N9-C8	-3.89	118.46	127.09
84	r2	63	P5P	C1'-N9-C8	-3.89	118.47	127.09
85	r3	17(A)	P5P	C4-N9-C8	3.89	109.82	105.74
84	r2	26	P5P	C1'-N9-C8	-3.88	118.48	127.09
84	r2	14	P5P	C1'-N9-C8	-3.88	118.49	127.09
85	r3	31	P5P	C1'-N9-C8	-3.88	118.49	127.09
85	r3	44	P5P	C1'-N9-C8	-3.88	118.49	127.09
84	r2	7	P5P	C4-N9-C8	3.87	109.80	105.74
85	r3	6	P5P	C1'-N9-C8	-3.87	118.51	127.09
84	r2	69	P5P	C6-N1-C2	3.86	120.36	115.80
84	r2	15	P5P	C1'-N9-C8	-3.86	118.53	127.09
85	r3	68	P5P	C1'-N9-C8	-3.86	118.53	127.09
84	r2	19	P5P	C1'-N9-C8	-3.86	118.53	127.09
84	r2	70	P5P	C6-N1-C2	3.86	120.35	115.80
85	r3	48	P5P	C1'-N9-C8	-3.85	118.56	127.09
84	r2	44	P5P	C1'-N9-C8	-3.85	118.56	127.09
84	r2	30	P5P	C1'-N9-C8	-3.85	118.56	127.09
84	r2	71	P5P	C1'-N9-C8	-3.84	118.57	127.09
84	r2	36	P5P	C6-N1-C2	3.84	120.33	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	28	P5P	C1'-N9-C8	-3.84	118.57	127.09
85	r3	35	P5P	C6-N1-C2	3.84	120.33	115.80
84	r2	27	P5P	C6-N1-C2	3.84	120.33	115.80
84	r2	57	P5P	C1'-N9-C8	-3.84	118.58	127.09
84	r2	65	P5P	C1'-N9-C8	-3.84	118.58	127.09
84	r2	35	P5P	C6-N1-C2	3.84	120.33	115.80
84	r2	22	P5P	C6-N1-C2	3.83	120.32	115.80
85	r3	4	P5P	C1'-N9-C8	-3.83	118.60	127.09
84	r2	6	P5P	C6-N1-C2	3.83	120.32	115.80
84	r2	58	P5P	C1'-N9-C8	-3.82	118.61	127.09
85	r3	22	P5P	C1'-N9-C8	-3.82	118.62	127.09
84	r2	34	P5P	C4-N9-C8	3.80	109.73	105.74
84	r2	38	P5P	C6-N1-C2	3.80	120.28	115.80
84	r2	15	P5P	C6-N1-C2	3.80	120.28	115.80
85	r3	48	P5P	C6-N1-C2	3.80	120.28	115.80
84	r2	29	P5P	C6-N1-C2	3.80	120.28	115.80
84	r2	21	P5P	C6-N1-C2	3.80	120.28	115.80
84	r2	21	P5P	C1'-N9-C8	-3.79	118.68	127.09
84	r2	26	P5P	C6-N1-C2	3.79	120.27	115.80
84	r2	63	P5P	C6-N1-C2	3.79	120.27	115.80
84	r2	24	P5P	C1'-N9-C8	-3.79	118.69	127.09
85	r3	42	P5P	C6-N1-C2	3.78	120.27	115.80
84	r2	5	P5P	C6-N1-C2	3.78	120.27	115.80
84	r2	23	P5P	C6-N1-C2	3.78	120.27	115.80
85	r3	30	P5P	C1'-N9-C8	-3.78	118.71	127.09
84	r2	10	P5P	C6-N1-C2	3.78	120.26	115.80
85	r3	57	P5P	C6-N1-C2	3.78	120.26	115.80
85	r3	19	P5P	C1'-N9-C8	-3.78	118.72	127.09
85	r3	29	P5P	C6-N1-C2	3.77	120.26	115.80
84	r2	30	P5P	C6-N1-C2	3.77	120.25	115.80
84	r2	31	P5P	C6-N1-C2	3.77	120.25	115.80
85	r3	52	P5P	C1'-N9-C8	-3.77	118.73	127.09
84	r2	28	P5P	C6-N1-C2	3.76	120.24	115.80
85	r3	74	P5P	C4-N9-C8	3.76	109.69	105.74
85	r3	18	P5P	C6-N1-C2	3.76	120.24	115.80
84	r2	65	P5P	C6-N1-C2	3.76	120.23	115.80
84	r2	19	P5P	C6-N1-C2	3.76	120.23	115.80
85	r3	51	P5P	C1'-N9-C8	-3.75	118.77	127.09
84	r2	52	P5P	C6-N1-C2	3.74	120.22	115.80
85	r3	74	P5P	C6-N1-C2	3.74	120.22	115.80
85	r3	9	P5P	C6-N1-C2	3.74	120.21	115.80
85	r3	17(A)	P5P	C6-N1-C2	3.74	120.21	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	46	P5P	C6-N1-C2	3.74	120.21	115.80
85	r3	21	P5P	C6-N1-C2	3.73	120.21	115.80
85	r3	30	P5P	C6-N1-C2	3.73	120.21	115.80
84	r2	76	P5P	C4-N9-C8	3.73	109.66	105.74
85	r3	5	P5P	C6-N1-C2	3.73	120.21	115.80
84	r2	1	P5P	C1'-N9-C8	-3.73	118.81	127.09
84	r2	24	P5P	C6-N1-C2	3.73	120.20	115.80
84	r2	44	P5P	C6-N1-C2	3.73	120.20	115.80
84	r2	23	P5P	C1'-N9-C8	-3.73	118.82	127.09
84	r2	9	P5P	C6-N1-C2	3.73	120.20	115.80
84	r2	37	P5P	C6-N1-C2	3.73	120.20	115.80
85	r3	26	P5P	C6-N1-C2	3.73	120.20	115.80
84	r2	57	P5P	C6-N1-C2	3.73	120.20	115.80
85	r3	19	P5P	C6-N1-C2	3.73	120.20	115.80
85	r3	46	P5P	C6-N1-C2	3.72	120.20	115.80
85	r3	14	P5P	C6-N1-C2	3.72	120.19	115.80
85	r3	43	P5P	C6-N1-C2	3.72	120.19	115.80
84	r2	14	P5P	C6-N1-C2	3.72	120.19	115.80
84	r2	53	P5P	C6-N1-C2	3.72	120.19	115.80
85	r3	52	P5P	C6-N1-C2	3.72	120.19	115.80
85	r3	4	P5P	C6-N1-C2	3.71	120.18	115.80
85	r3	23	P5P	C6-N1-C2	3.71	120.18	115.80
85	r3	6	P5P	C6-N1-C2	3.71	120.18	115.80
85	r3	68	P5P	C6-N1-C2	3.71	120.18	115.80
84	r2	7	P5P	C6-N1-C2	3.70	120.17	115.80
84	r2	64	P5P	C6-N1-C2	3.70	120.16	115.80
85	r3	42	P5P	C1'-N9-C8	-3.69	118.89	127.09
85	r3	55	P5P	C6-N1-C2	3.69	120.16	115.80
85	r3	8	P5P	C6-N1-C2	3.69	120.16	115.80
85	r3	22	P5P	C6-N1-C2	3.69	120.15	115.80
84	r2	71	P5P	C6-N1-C2	3.69	120.15	115.80
85	r3	66	P5P	C6-N1-C2	3.69	120.15	115.80
84	r2	18	P5P	C6-N1-C2	3.69	120.15	115.80
85	r3	10	P5P	C6-N1-C2	3.68	120.15	115.80
85	r3	44	P5P	C6-N1-C2	3.68	120.14	115.80
84	r2	69	P5P	C1'-N9-C8	-3.67	118.94	127.09
84	r2	73	P5P	C6-N1-C2	3.67	120.14	115.80
84	r2	58	P5P	C6-N1-C2	3.67	120.13	115.80
85	r3	31	P5P	C6-N1-C2	3.66	120.13	115.80
85	r3	71	P5P	C6-N1-C2	3.66	120.12	115.80
85	r3	15	P5P	C6-N1-C2	3.66	120.12	115.80
85	r3	45	P5P	C6-N1-C2	3.65	120.11	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r3	37	P5P	C6-N1-C2	3.64	120.10	115.80
84	r2	76	P5P	C6-N1-C2	3.63	120.09	115.80
84	r2	1	P5P	C6-N1-C2	3.63	120.09	115.80
85	r3	11	P5P	C6-N1-C2	3.63	120.08	115.80
84	r2	70	P5P	C1'-N9-C8	-3.60	119.11	127.09
84	r2	34	P5P	C6-N1-C2	3.59	120.04	115.80
85	r3	4	P5P	C5-N7-C8	3.48	108.67	104.40
84	r2	34	P5P	N3-C4-N9	3.45	133.03	127.17
84	r2	18	P5P	N3-C4-N9	3.45	133.03	127.17
85	r3	15	P5P	N3-C4-N9	3.44	133.02	127.17
84	r2	36	P5P	N3-C4-N9	3.44	133.02	127.17
85	r3	57	P5P	N3-C4-N9	3.42	132.98	127.17
85	r3	66	P5P	N3-C4-N9	3.42	132.98	127.17
84	r2	76	P5P	N3-C4-N9	3.41	132.97	127.17
84	r2	7	P5P	N3-C4-N9	3.40	132.95	127.17
84	r2	9	P5P	N3-C4-N9	3.40	132.95	127.17
85	r3	37	P5P	N3-C4-N9	3.39	132.94	127.17
84	r2	46	P5P	N3-C4-N9	3.39	132.94	127.17
85	r3	74	P5P	N3-C4-N9	3.39	132.94	127.17
85	r3	11	P5P	N3-C4-N9	3.39	132.94	127.17
85	r3	9	P5P	N3-C4-N9	3.39	132.93	127.17
84	r2	22	P5P	N3-C4-N9	3.39	132.93	127.17
85	r3	55	P5P	N3-C4-N9	3.39	132.93	127.17
85	r3	23	P5P	N3-C4-N9	3.38	132.92	127.17
84	r2	73	P5P	N3-C4-N9	3.38	132.92	127.17
85	r3	14	P5P	N3-C4-N9	3.38	132.92	127.17
85	r3	17(A)	P5P	N3-C4-N9	3.38	132.91	127.17
85	r3	8	P5P	N3-C4-N9	3.38	132.91	127.17
85	r3	42	P5P	C5-N7-C8	3.37	108.54	104.40
84	r2	27	P5P	N3-C4-N9	3.37	132.91	127.17
85	r3	45	P5P	N3-C4-N9	3.37	132.90	127.17
84	r2	53	P5P	N3-C4-N9	3.36	132.89	127.17
85	r3	18	P5P	N3-C4-N9	3.36	132.89	127.17
84	r2	58	P5P	C5-N7-C8	3.36	108.52	104.40
85	r3	52	P5P	N3-C4-N9	3.36	132.88	127.17
84	r2	5	P5P	N3-C4-N9	3.36	132.88	127.17
85	r3	5	P5P	N3-C4-N9	3.36	132.88	127.17
84	r2	29	P5P	N3-C4-N9	3.36	132.87	127.17
84	r2	24	P5P	N3-C4-N9	3.35	132.87	127.17
84	r2	52	P5P	N3-C4-N9	3.35	132.87	127.17
84	r2	35	P5P	N3-C4-N9	3.35	132.87	127.17
85	r3	4	P5P	N3-C4-N9	3.35	132.87	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	r3	29	P5P	N3-C4-N9	3.35	132.87	127.17
84	r2	38	P5P	N3-C4-N9	3.35	132.87	127.17
84	r2	6	P5P	N3-C4-N9	3.35	132.87	127.17
84	r2	24	P5P	C5-N7-C8	3.35	108.51	104.40
85	r3	71	P5P	N3-C4-N9	3.35	132.86	127.17
85	r3	6	P5P	C5-N7-C8	3.35	108.51	104.40
84	r2	71	P5P	C5-N7-C8	3.35	108.51	104.40
84	r2	10	P5P	N3-C4-N9	3.35	132.86	127.17
85	r3	6	P5P	N3-C4-N9	3.35	132.86	127.17
85	r3	15	P5P	C5-N7-C8	3.35	108.51	104.40
85	r3	21	P5P	N3-C4-N9	3.35	132.86	127.17
84	r2	64	P5P	N3-C4-N9	3.35	132.86	127.17
84	r2	69	P5P	C5-N7-C8	3.34	108.51	104.40
85	r3	43	P5P	C5-N7-C8	3.34	108.51	104.40
85	r3	74	P5P	C6-C5-C4	3.34	119.90	116.24
84	r2	1	P5P	N3-C4-N9	3.34	132.85	127.17
84	r2	65	P5P	N3-C4-N9	3.34	132.85	127.17
85	r3	19	P5P	C5-N7-C8	3.34	108.50	104.40
84	r2	19	P5P	C5-N7-C8	3.34	108.50	104.40
85	r3	35	P5P	N3-C4-N9	3.34	132.85	127.17
84	r2	63	P5P	N3-C4-N9	3.34	132.85	127.17
84	r2	57	P5P	N3-C4-N9	3.34	132.84	127.17
85	r3	66	P5P	C5-N7-C8	3.34	108.50	104.40
85	r3	43	P5P	N3-C4-N9	3.34	132.84	127.17
85	r3	11	P5P	C5-N7-C8	3.34	108.49	104.40
85	r3	10	P5P	N3-C4-N9	3.33	132.84	127.17
84	r2	37	P5P	N3-C4-N9	3.33	132.84	127.17
85	r3	19	P5P	N3-C4-N9	3.33	132.84	127.17
85	r3	22	P5P	N3-C4-N9	3.33	132.84	127.17
84	r2	29	P5P	C5-N7-C8	3.33	108.49	104.40
84	r2	73	P5P	C5-N7-C8	3.33	108.49	104.40
84	r2	71	P5P	N3-C4-N9	3.33	132.83	127.17
84	r2	19	P5P	N3-C4-N9	3.33	132.83	127.17
85	r3	48	P5P	N3-C4-N9	3.33	132.83	127.17
84	r2	28	P5P	N3-C4-N9	3.33	132.83	127.17
85	r3	68	P5P	N3-C4-N9	3.33	132.83	127.17
85	r3	44	P5P	N3-C4-N9	3.33	132.82	127.17
84	r2	38	P5P	C5-N7-C8	3.32	108.48	104.40
84	r2	15	P5P	N3-C4-N9	3.32	132.81	127.17
85	r3	3	P5P	N3-C4-N9	3.32	132.81	127.17
84	r2	7	P5P	C5-N7-C8	3.32	108.47	104.40
85	r3	30	P5P	C5-N7-C8	3.32	108.47	104.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	14	P5P	N3-C4-N9	3.32	132.81	127.17
85	r3	21	P5P	C5-N7-C8	3.32	108.47	104.40
84	r2	1	P5P	C5-N7-C8	3.32	108.47	104.40
84	r2	57	P5P	C5-N7-C8	3.32	108.47	104.40
84	r2	14	P5P	C5-N7-C8	3.31	108.47	104.40
84	r2	70	P5P	C5-N7-C8	3.31	108.47	104.40
85	r3	46	P5P	N3-C4-N9	3.31	132.80	127.17
84	r2	28	P5P	C5-N7-C8	3.31	108.46	104.40
84	r2	23	P5P	C5-N7-C8	3.31	108.46	104.40
84	r2	37	P5P	C5-N7-C8	3.31	108.46	104.40
84	r2	44	P5P	C5-N7-C8	3.31	108.46	104.40
85	r3	44	P5P	C5-N7-C8	3.31	108.46	104.40
85	r3	10	P5P	C5-N7-C8	3.31	108.46	104.40
85	r3	52	P5P	C5-N7-C8	3.31	108.46	104.40
85	r3	31	P5P	N3-C4-N9	3.30	132.79	127.17
84	r2	58	P5P	N3-C4-N9	3.30	132.79	127.17
84	r2	6	P5P	C5-N7-C8	3.30	108.45	104.40
84	r2	15	P5P	C5-N7-C8	3.30	108.45	104.40
84	r2	52	P5P	C5-N7-C8	3.30	108.45	104.40
85	r3	26	P5P	N3-C4-N9	3.30	132.78	127.17
84	r2	26	P5P	C5-N7-C8	3.30	108.45	104.40
85	r3	23	P5P	C5-N7-C8	3.30	108.45	104.40
84	r2	5	P5P	C5-N7-C8	3.30	108.45	104.40
84	r2	65	P5P	C5-N7-C8	3.30	108.45	104.40
85	r3	37	P5P	C2-N3-C4	3.30	119.88	111.83
85	r3	8	P5P	C5-N7-C8	3.29	108.44	104.40
84	r2	10	P5P	C5-N7-C8	3.29	108.44	104.40
85	r3	71	P5P	C5-N7-C8	3.29	108.44	104.40
84	r2	30	P5P	N3-C4-N9	3.29	132.77	127.17
84	r2	31	P5P	N3-C4-N9	3.29	132.77	127.17
85	r3	22	P5P	C5-N7-C8	3.29	108.44	104.40
85	r3	66	P5P	C2-N3-C4	3.29	119.87	111.83
84	r2	7	P5P	C2-N3-C4	3.29	119.86	111.83
84	r2	46	P5P	C2-N3-C4	3.29	119.86	111.83
84	r2	46	P5P	C5-N7-C8	3.29	108.44	104.40
84	r2	63	P5P	C5-N7-C8	3.29	108.44	104.40
85	r3	55	P5P	C5-N7-C8	3.29	108.44	104.40
84	r2	34	P5P	C2-N3-C4	3.29	119.86	111.83
84	r2	64	P5P	C5-N7-C8	3.29	108.43	104.40
84	r2	44	P5P	N3-C4-N9	3.29	132.75	127.17
85	r3	51	P5P	C5-N7-C8	3.28	108.43	104.40
84	r2	26	P5P	N3-C4-N9	3.28	132.75	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	21	P5P	N3-C4-N9	3.28	132.75	127.17
84	r2	53	P5P	C5-N7-C8	3.28	108.43	104.40
84	r2	22	P5P	C5-N7-C8	3.28	108.43	104.40
85	r3	11	P5P	C2-N3-C4	3.28	119.84	111.83
85	r3	17(A)	P5P	C5-N7-C8	3.28	108.42	104.40
85	r3	30	P5P	N3-C4-N9	3.28	132.74	127.17
85	r3	45	P5P	C5-N7-C8	3.28	108.42	104.40
84	r2	9	P5P	C5-N7-C8	3.28	108.42	104.40
84	r2	18	P5P	C5-N7-C8	3.28	108.42	104.40
85	r3	9	P5P	C5-N7-C8	3.28	108.42	104.40
85	r3	29	P5P	C5-N7-C8	3.28	108.42	104.40
85	r3	52	P5P	C2-N3-C4	3.27	119.83	111.83
84	r2	76	P5P	C2-N3-C4	3.27	119.82	111.83
84	r2	65	P5P	C2-N3-C4	3.27	119.82	111.83
85	r3	48	P5P	C2-N3-C4	3.27	119.82	111.83
84	r2	70	P5P	N3-C4-N9	3.27	132.73	127.17
84	r2	31	P5P	C5-N7-C8	3.27	108.41	104.40
85	r3	57	P5P	C5-N7-C8	3.27	108.41	104.40
85	r3	68	P5P	C5-N7-C8	3.27	108.41	104.40
85	r3	55	P5P	C2-N3-C4	3.27	119.81	111.83
85	r3	5	P5P	C5-N7-C8	3.26	108.41	104.40
84	r2	18	P5P	C2-N3-C4	3.26	119.80	111.83
85	r3	42	P5P	N3-C4-N9	3.26	132.72	127.17
84	r2	30	P5P	C5-N7-C8	3.26	108.41	104.40
85	r3	31	P5P	C5-N7-C8	3.26	108.41	104.40
85	r3	22	P5P	C2-N3-C4	3.26	119.80	111.83
85	r3	46	P5P	C5-N7-C8	3.26	108.40	104.40
85	r3	48	P5P	C5-N7-C8	3.26	108.40	104.40
84	r2	24	P5P	C2-N3-C4	3.26	119.80	111.83
85	r3	68	P5P	C2-N3-C4	3.26	119.80	111.83
84	r2	27	P5P	C5-N7-C8	3.26	108.40	104.40
84	r2	21	P5P	C5-N7-C8	3.26	108.40	104.40
85	r3	51	P5P	N3-C4-N9	3.26	132.71	127.17
84	r2	34	P5P	C5-N7-C8	3.26	108.40	104.40
85	r3	18	P5P	C5-N7-C8	3.26	108.40	104.40
85	r3	26	P5P	C5-N7-C8	3.26	108.40	104.40
84	r2	28	P5P	C2-N3-C4	3.26	119.78	111.83
84	r2	1	P5P	C2-N3-C4	3.26	119.78	111.83
85	r3	19	P5P	C2-N3-C4	3.26	119.78	111.83
85	r3	17(A)	P5P	C2-N3-C4	3.25	119.78	111.83
85	r3	18	P5P	C2-N3-C4	3.25	119.78	111.83
84	r2	23	P5P	N3-C4-N9	3.25	132.70	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	70	P5P	C2-N3-C4	3.25	119.78	111.83
85	r3	8	P5P	C2-N3-C4	3.25	119.77	111.83
84	r2	63	P5P	C2-N3-C4	3.25	119.77	111.83
85	r3	23	P5P	C2-N3-C4	3.25	119.77	111.83
84	r2	73	P5P	C2-N3-C4	3.25	119.77	111.83
84	r2	34	P5P	C6-C5-C4	3.25	119.79	116.24
85	r3	4	P5P	C2-N3-C4	3.25	119.76	111.83
84	r2	69	P5P	N3-C4-N9	3.25	132.69	127.17
84	r2	53	P5P	C2-N3-C4	3.25	119.76	111.83
85	r3	6	P5P	C2-N3-C4	3.24	119.76	111.83
84	r2	5	P5P	C2-N3-C4	3.24	119.75	111.83
84	r2	57	P5P	C2-N3-C4	3.24	119.75	111.83
85	r3	35	P5P	C5-N7-C8	3.24	108.38	104.40
85	r3	42	P5P	C2-N3-C4	3.24	119.75	111.83
85	r3	5	P5P	C2-N3-C4	3.24	119.75	111.83
84	r2	36	P5P	C6-C5-C4	3.24	119.78	116.24
84	r2	27	P5P	C2-N3-C4	3.24	119.74	111.83
85	r3	37	P5P	C5-N7-C8	3.24	108.38	104.40
84	r2	6	P5P	C2-N3-C4	3.24	119.74	111.83
84	r2	52	P5P	C2-N3-C4	3.24	119.74	111.83
85	r3	14	P5P	C2-N3-C4	3.24	119.74	111.83
84	r2	19	P5P	C2-N3-C4	3.24	119.74	111.83
84	r2	29	P5P	C2-N3-C4	3.24	119.74	111.83
84	r2	14	P5P	C2-N3-C4	3.23	119.73	111.83
84	r2	26	P5P	C2-N3-C4	3.23	119.73	111.83
84	r2	64	P5P	C2-N3-C4	3.23	119.73	111.83
85	r3	3	P5P	C2-N3-C4	3.23	119.73	111.83
85	r3	29	P5P	C2-N3-C4	3.23	119.72	111.83
84	r2	9	P5P	C2-N3-C4	3.23	119.72	111.83
84	r2	23	P5P	C2-N3-C4	3.23	119.72	111.83
84	r2	37	P5P	C2-N3-C4	3.23	119.72	111.83
85	r3	30	P5P	C2-N3-C4	3.23	119.72	111.83
84	r2	36	P5P	C2-N3-C4	3.23	119.72	111.83
85	r3	10	P5P	C2-N3-C4	3.23	119.72	111.83
85	r3	43	P5P	C2-N3-C4	3.23	119.72	111.83
85	r3	15	P5P	C2-N3-C4	3.23	119.72	111.83
84	r2	30	P5P	C2-N3-C4	3.23	119.71	111.83
84	r2	44	P5P	C2-N3-C4	3.23	119.71	111.83
85	r3	51	P5P	C2-N3-C4	3.22	119.71	111.83
84	r2	21	P5P	C2-N3-C4	3.22	119.70	111.83
84	r2	35	P5P	C2-N3-C4	3.22	119.70	111.83
84	r2	58	P5P	C2-N3-C4	3.22	119.70	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	38	P5P	C2-N3-C4	3.22	119.70	111.83
84	r2	69	P5P	C2-N3-C4	3.22	119.70	111.83
84	r2	71	P5P	C2-N3-C4	3.22	119.70	111.83
85	r3	44	P5P	C2-N3-C4	3.22	119.69	111.83
85	r3	3	P5P	C5-N7-C8	3.22	108.35	104.40
84	r2	31	P5P	C2-N3-C4	3.22	119.69	111.83
85	r3	26	P5P	C2-N3-C4	3.22	119.69	111.83
84	r2	10	P5P	C2-N3-C4	3.22	119.68	111.83
84	r2	15	P5P	C2-N3-C4	3.22	119.68	111.83
85	r3	35	P5P	C2-N3-C4	3.21	119.68	111.83
85	r3	9	P5P	C2-N3-C4	3.21	119.67	111.83
85	r3	31	P5P	C2-N3-C4	3.21	119.67	111.83
84	r2	35	P5P	C5-N7-C8	3.21	108.34	104.40
85	r3	14	P5P	C5-N7-C8	3.21	108.33	104.40
85	r3	57	P5P	C6-C5-C4	3.21	119.75	116.24
85	r3	71	P5P	C2-N3-C4	3.21	119.66	111.83
85	r3	21	P5P	C2-N3-C4	3.20	119.65	111.83
84	r2	22	P5P	C2-N3-C4	3.20	119.64	111.83
85	r3	45	P5P	C2-N3-C4	3.19	119.63	111.83
84	r2	37	P5P	O5'-P-OP1	3.19	115.07	106.44
85	r3	57	P5P	C2-N3-C4	3.18	119.61	111.83
84	r2	36	P5P	C5-N7-C8	3.17	108.29	104.40
85	r3	15	P5P	C6-C5-C4	3.16	119.70	116.24
85	r3	4	P5P	C6-C5-C4	3.16	119.70	116.24
84	r2	76	P5P	C6-C5-C4	3.16	119.69	116.24
84	r2	35	P5P	C6-C5-C4	3.16	119.69	116.24
85	r3	46	P5P	C2-N3-C4	3.16	119.54	111.83
84	r2	53	P5P	C6-C5-C4	3.15	119.69	116.24
85	r3	9	P5P	C6-C5-C4	3.15	119.68	116.24
84	r2	38	P5P	C6-C5-C4	3.14	119.67	116.24
85	r3	43	P5P	C6-C5-C4	3.14	119.67	116.24
85	r3	5	P5P	C6-C5-C4	3.14	119.67	116.24
85	r3	3	P5P	C6-C5-C4	3.13	119.67	116.24
85	r3	74	P5P	C5-N7-C8	3.13	108.25	104.40
85	r3	68	P5P	C6-C5-C4	3.13	119.67	116.24
84	r2	22	P5P	C6-C5-C4	3.13	119.66	116.24
85	r3	45	P5P	C6-C5-C4	3.13	119.66	116.24
85	r3	21	P5P	C6-C5-C4	3.13	119.66	116.24
85	r3	74	P5P	C2-N3-C4	3.13	119.47	111.83
84	r2	6	P5P	C6-C5-C4	3.12	119.66	116.24
84	r2	31	P5P	C6-C5-C4	3.12	119.65	116.24
84	r2	71	P5P	C6-C5-C4	3.12	119.65	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	46	P5P	C6-C5-C4	3.12	119.65	116.24
84	r2	57	P5P	C6-C5-C4	3.12	119.65	116.24
84	r2	9	P5P	C6-C5-C4	3.12	119.65	116.24
85	r3	17(A)	P5P	C6-C5-C4	3.12	119.65	116.24
84	r2	64	P5P	C6-C5-C4	3.11	119.64	116.24
85	r3	35	P5P	C6-C5-C4	3.11	119.64	116.24
84	r2	52	P5P	C6-C5-C4	3.11	119.64	116.24
85	r3	48	P5P	C6-C5-C4	3.11	119.64	116.24
85	r3	71	P5P	C6-C5-C4	3.11	119.64	116.24
84	r2	37	P5P	C6-C5-C4	3.10	119.63	116.24
84	r2	15	P5P	C6-C5-C4	3.10	119.63	116.24
84	r2	19	P5P	C6-C5-C4	3.10	119.63	116.24
85	r3	37	P5P	C6-C5-C4	3.10	119.63	116.24
84	r2	18	P5P	C6-C5-C4	3.10	119.63	116.24
84	r2	73	P5P	C6-C5-C4	3.10	119.63	116.24
85	r3	46	P5P	C6-C5-C4	3.10	119.63	116.24
84	r2	76	P5P	C5-N7-C8	3.09	108.20	104.40
84	r2	23	P5P	C6-C5-C4	3.09	119.62	116.24
85	r3	29	P5P	C6-C5-C4	3.09	119.62	116.24
84	r2	7	P5P	C6-C5-C4	3.09	119.62	116.24
84	r2	10	P5P	C6-C5-C4	3.09	119.62	116.24
85	r3	23	P5P	C6-C5-C4	3.09	119.62	116.24
84	r2	58	P5P	C6-C5-C4	3.08	119.61	116.24
84	r2	37	P5P	OP2-P-O5'	3.08	114.70	106.67
85	r3	10	P5P	C6-C5-C4	3.08	119.61	116.24
85	r3	55	P5P	C6-C5-C4	3.08	119.61	116.24
85	r3	18	P5P	C6-C5-C4	3.08	119.61	116.24
85	r3	52	P5P	C6-C5-C4	3.08	119.61	116.24
85	r3	26	P5P	C6-C5-C4	3.08	119.60	116.24
84	r2	44	P5P	C6-C5-C4	3.07	119.60	116.24
85	r3	66	P5P	C6-C5-C4	3.07	119.60	116.24
85	r3	11	P5P	C6-C5-C4	3.07	119.59	116.24
85	r3	14	P5P	C6-C5-C4	3.06	119.59	116.24
85	r3	31	P5P	C6-C5-C4	3.06	119.58	116.24
85	r3	8	P5P	C6-C5-C4	3.05	119.58	116.24
85	r3	22	P5P	C6-C5-C4	3.05	119.58	116.24
84	r2	5	P5P	C6-C5-C4	3.05	119.57	116.24
84	r2	27	P5P	C6-C5-C4	3.05	119.57	116.24
85	r3	19	P5P	C6-C5-C4	3.05	119.57	116.24
85	r3	30	P5P	C6-C5-C4	3.05	119.57	116.24
84	r2	1	P5P	C6-C5-C4	3.04	119.57	116.24
84	r2	29	P5P	C6-C5-C4	3.04	119.56	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	24	P5P	C6-C5-C4	3.04	119.56	116.24
84	r2	26	P5P	C6-C5-C4	3.04	119.56	116.24
85	r3	6	P5P	C6-C5-C4	3.03	119.56	116.24
84	r2	65	P5P	C6-C5-C4	3.03	119.56	116.24
85	r3	44	P5P	C6-C5-C4	3.03	119.56	116.24
84	r2	69	P5P	C6-C5-C4	3.03	119.55	116.24
84	r2	63	P5P	C6-C5-C4	3.02	119.55	116.24
85	r3	51	P5P	C6-C5-C4	3.02	119.54	116.24
84	r2	14	P5P	C6-C5-C4	3.01	119.54	116.24
84	r2	30	P5P	C6-C5-C4	3.01	119.53	116.24
84	r2	70	P5P	C6-C5-C4	3.00	119.53	116.24
84	r2	28	P5P	C6-C5-C4	2.96	119.48	116.24
85	r3	42	P5P	C6-C5-C4	2.95	119.46	116.24
84	r2	21	P5P	C6-C5-C4	2.90	119.41	116.24
85	r3	74	P5P	C4-N9-C1'	2.71	132.98	126.63
84	r2	36	P5P	C4-N9-C1'	2.52	132.53	126.63
84	r2	34	P5P	C4-N9-C1'	2.46	132.38	126.63
85	r3	15	P5P	C4-N9-C1'	2.45	132.35	126.63
85	r3	57	P5P	C4-N9-C1'	2.38	132.20	126.63
85	r3	17(A)	P5P	C4-N9-C1'	2.38	132.19	126.63
84	r2	22	P5P	C4-N9-C1'	2.35	132.12	126.63
84	r2	18	P5P	C4-N9-C1'	2.33	132.08	126.63
84	r2	76	P5P	C4-N9-C1'	2.31	132.05	126.63
84	r2	35	P5P	C4-N9-C1'	2.31	132.03	126.63
85	r3	8	P5P	C4-N9-C1'	2.31	132.03	126.63
84	r2	9	P5P	C4-N9-C1'	2.31	132.03	126.63
85	r3	9	P5P	C4-N9-C1'	2.31	132.02	126.63
85	r3	14	P5P	C4-N9-C1'	2.29	131.99	126.63
84	r2	53	P5P	C4-N9-C1'	2.25	131.90	126.63
84	r2	31	P5P	C4-N9-C1'	2.24	131.87	126.63
84	r2	7	P5P	C4-N9-C1'	2.24	131.86	126.63
84	r2	10	P5P	C4-N9-C1'	2.23	131.86	126.63
85	r3	21	P5P	C4-N9-C1'	2.23	131.84	126.63
85	r3	45	P5P	C4-N9-C1'	2.22	131.83	126.63
85	r3	5	P5P	C4-N9-C1'	2.22	131.81	126.63
85	r3	26	P5P	C4-N9-C1'	2.22	131.81	126.63
84	r2	64	P5P	C4-N9-C1'	2.21	131.81	126.63
84	r2	46	P5P	C4-N9-C1'	2.21	131.79	126.63
85	r3	55	P5P	C4-N9-C1'	2.21	131.79	126.63
85	r3	35	P5P	C4-N9-C1'	2.20	131.78	126.63
84	r2	37	P5P	C4-N9-C1'	2.20	131.78	126.63
85	r3	46	P5P	C4-N9-C1'	2.20	131.77	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	r2	52	P5P	C4-N9-C1'	2.19	131.76	126.63
84	r2	6	P5P	C4-N9-C1'	2.19	131.75	126.63
84	r2	73	P5P	C4-N9-C1'	2.19	131.74	126.63
85	r3	66	P5P	C4-N9-C1'	2.19	131.74	126.63
85	r3	18	P5P	C4-N9-C1'	2.18	131.72	126.63
85	r3	10	P5P	C4-N9-C1'	2.17	131.71	126.63
84	r2	38	P5P	C4-N9-C1'	2.17	131.71	126.63
85	r3	37	P5P	C4-N9-C1'	2.17	131.70	126.63
85	r3	23	P5P	C4-N9-C1'	2.15	131.66	126.63
84	r2	27	P5P	C4-N9-C1'	2.15	131.65	126.63
85	r3	11	P5P	C4-N9-C1'	2.14	131.64	126.63
85	r3	71	P5P	C4-N9-C1'	2.14	131.64	126.63
85	r3	3	P5P	C4-N9-C1'	2.14	131.64	126.63
85	r3	29	P5P	C4-N9-C1'	2.13	131.62	126.63
84	r2	5	P5P	C4-N9-C1'	2.13	131.62	126.63
85	r3	43	P5P	C4-N9-C1'	2.12	131.59	126.63
84	r2	26	P5P	C4-N9-C1'	2.12	131.58	126.63
85	r3	68	P5P	C4-N9-C1'	2.11	131.57	126.63
84	r2	14	P5P	C4-N9-C1'	2.10	131.55	126.63
84	r2	29	P5P	C4-N9-C1'	2.10	131.54	126.63
85	r3	48	P5P	C4-N9-C1'	2.10	131.54	126.63
85	r3	44	P5P	C4-N9-C1'	2.10	131.53	126.63
85	r3	22	P5P	C4-N9-C1'	2.09	131.53	126.63
84	r2	19	P5P	C4-N9-C1'	2.09	131.52	126.63
85	r3	31	P5P	C4-N9-C1'	2.09	131.52	126.63
84	r2	63	P5P	C4-N9-C1'	2.08	131.49	126.63
84	r2	57	P5P	C4-N9-C1'	2.08	131.49	126.63
84	r2	15	P5P	C4-N9-C1'	2.08	131.49	126.63
84	r2	44	P5P	C4-N9-C1'	2.07	131.48	126.63
84	r2	71	P5P	C4-N9-C1'	2.07	131.47	126.63
84	r2	30	P5P	C4-N9-C1'	2.07	131.47	126.63
85	r3	4	P5P	C4-N9-C1'	2.06	131.46	126.63
85	r3	6	P5P	C4-N9-C1'	2.06	131.44	126.63
84	r2	58	P5P	C4-N9-C1'	2.05	131.42	126.63
84	r2	65	P5P	C4-N9-C1'	2.04	131.39	126.63
85	r3	19	P5P	C4-N9-C1'	2.03	131.39	126.63
84	r2	24	P5P	C4-N9-C1'	2.03	131.38	126.63
84	r2	28	P5P	C4-N9-C1'	2.03	131.38	126.63
85	r3	30	P5P	C4-N9-C1'	2.02	131.35	126.63
84	r2	21	P5P	C4-N9-C1'	2.00	131.31	126.63

There are no chirality outliers.

All (259) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	r1	44	Y5P	O4'-C4'-C5'-O5'
83	r1	46	Y5P	C4'-C5'-O5'-P
83	r1	51	Y5P	O4'-C1'-N1-C2
84	r2	4	Y5P	O4'-C1'-N1-C2
84	r2	32	Y5P	O4'-C1'-N1-C2
84	r2	33	Y5P	C2'-C1'-N1-C6
84	r2	35	P5P	O4'-C4'-C5'-O5'
84	r2	37	P5P	C5'-O5'-P-OP3
84	r2	43	Y5P	O4'-C1'-N1-C2
84	r2	45	Y5P	O4'-C4'-C5'-O5'
84	r2	46	P5P	C2'-C1'-N9-C8
84	r2	50	Y5P	O4'-C4'-C5'-O5'
84	r2	54	Y5P	O4'-C1'-N1-C2
84	r2	55	Y5P	O4'-C1'-N1-C2
84	r2	60	Y5P	O4'-C1'-N1-C2
84	r2	67	Y5P	O4'-C4'-C5'-O5'
84	r2	73	P5P	O4'-C4'-C5'-O5'
84	r2	76	P5P	O4'-C1'-N9-C4
84	r2	76	P5P	O4'-C1'-N9-C8
85	r3	12	Y5P	O4'-C1'-N1-C2
85	r3	16	Y5P	C4'-C5'-O5'-P
85	r3	21	P5P	C3'-C4'-C5'-O5'
85	r3	21	P5P	O4'-C4'-C5'-O5'
85	r3	21	P5P	C4'-C5'-O5'-P
85	r3	25	Y5P	O4'-C1'-N1-C2
85	r3	27	Y5P	O4'-C1'-N1-C2
85	r3	28	Y5P	O4'-C1'-N1-C2
85	r3	32	Y5P	O4'-C1'-N1-C2
85	r3	34	Y5P	O4'-C4'-C5'-O5'
85	r3	34	Y5P	C3'-C4'-C5'-O5'
85	r3	36	Y5P	O4'-C1'-N1-C2
85	r3	38	Y5P	O4'-C1'-N1-C2
85	r3	41	Y5P	O4'-C1'-N1-C2
85	r3	59	Y5P	O4'-C1'-N1-C2
85	r3	63	Y5P	O4'-C4'-C5'-O5'
85	r3	63	Y5P	O4'-C1'-N1-C2
85	r3	65	Y5P	O4'-C1'-N1-C2
85	r3	67	Y5P	O4'-C1'-N1-C2
85	r3	69	Y5P	O4'-C1'-N1-C2
83	r1	44	Y5P	O4'-C1'-N1-C2
83	r1	47	Y5P	O4'-C1'-N1-C2
83	r1	48	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
83	r1	49	Y5P	O4'-C1'-N1-C2
83	r1	50	Y5P	O4'-C1'-N1-C2
83	r1	52	Y5P	O4'-C1'-N1-C2
83	r1	54	Y5P	O4'-C1'-N1-C2
83	r1	57	Y5P	O4'-C1'-N1-C2
84	r2	2	Y5P	O4'-C1'-N1-C2
84	r2	3	Y5P	O4'-C1'-N1-C2
84	r2	8	Y5P	O4'-C1'-N1-C2
84	r2	11	Y5P	O4'-C1'-N1-C2
84	r2	12	Y5P	O4'-C1'-N1-C2
84	r2	13	Y5P	O4'-C1'-N1-C2
84	r2	16	Y5P	O4'-C1'-N1-C2
84	r2	17	Y5P	O4'-C1'-N1-C2
84	r2	25	Y5P	O4'-C1'-N1-C2
84	r2	39	Y5P	O4'-C1'-N1-C2
84	r2	40	Y5P	O4'-C1'-N1-C2
84	r2	41	Y5P	O4'-C1'-N1-C2
84	r2	42	Y5P	O4'-C1'-N1-C2
84	r2	45	Y5P	O4'-C1'-N1-C2
84	r2	47	Y5P	O4'-C1'-N1-C2
84	r2	48	Y5P	O4'-C1'-N1-C2
84	r2	49	Y5P	O4'-C1'-N1-C2
84	r2	50	Y5P	O4'-C1'-N1-C2
84	r2	51	Y5P	O4'-C1'-N1-C2
84	r2	56	Y5P	O4'-C1'-N1-C2
84	r2	59	Y5P	O4'-C1'-N1-C2
84	r2	61	Y5P	O4'-C1'-N1-C2
84	r2	62	Y5P	O4'-C1'-N1-C2
84	r2	66	Y5P	O4'-C1'-N1-C2
84	r2	68	Y5P	O4'-C1'-N1-C2
84	r2	72	Y5P	O4'-C1'-N1-C2
84	r2	74	Y5P	O4'-C1'-N1-C2
84	r2	75	Y5P	O4'-C1'-N1-C2
85	r3	7	Y5P	O4'-C1'-N1-C2
85	r3	24	Y5P	O4'-C1'-N1-C2
85	r3	33	Y5P	O4'-C1'-N1-C2
85	r3	34	Y5P	O4'-C1'-N1-C2
85	r3	49	Y5P	O4'-C1'-N1-C2
85	r3	50	Y5P	O4'-C1'-N1-C2
85	r3	53	Y5P	O4'-C1'-N1-C2
85	r3	54	Y5P	O4'-C1'-N1-C2
85	r3	60	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
85	r3	61	Y5P	O4'-C1'-N1-C2
85	r3	62	Y5P	O4'-C1'-N1-C2
85	r3	64	Y5P	O4'-C1'-N1-C2
85	r3	70	Y5P	O4'-C1'-N1-C2
85	r3	72	Y5P	O4'-C1'-N1-C2
85	r3	73	Y5P	O4'-C1'-N1-C2
83	r1	46	Y5P	O4'-C1'-N1-C6
85	r3	40	Y5P	C2'-C1'-N1-C6
83	r1	53	Y5P	O4'-C4'-C5'-O5'
83	r1	55	Y5P	O4'-C4'-C5'-O5'
84	r2	9	P5P	O4'-C4'-C5'-O5'
84	r2	13	Y5P	O4'-C4'-C5'-O5'
84	r2	13	Y5P	C3'-C4'-C5'-O5'
84	r2	21	P5P	O4'-C4'-C5'-O5'
84	r2	35	P5P	C3'-C4'-C5'-O5'
84	r2	36	P5P	O4'-C4'-C5'-O5'
84	r2	45	Y5P	C3'-C4'-C5'-O5'
84	r2	50	Y5P	C3'-C4'-C5'-O5'
84	r2	66	Y5P	O4'-C4'-C5'-O5'
84	r2	66	Y5P	C3'-C4'-C5'-O5'
84	r2	68	Y5P	O4'-C4'-C5'-O5'
85	r3	3	P5P	O4'-C4'-C5'-O5'
85	r3	4	P5P	O4'-C4'-C5'-O5'
85	r3	50	Y5P	O4'-C4'-C5'-O5'
85	r3	55	P5P	C3'-C4'-C5'-O5'
85	r3	63	Y5P	C3'-C4'-C5'-O5'
84	r2	47	Y5P	C4'-C5'-O5'-P
85	r3	13	Y5P	C4'-C5'-O5'-P
85	r3	43	P5P	C4'-C5'-O5'-P
85	r3	47	Y5P	C4'-C5'-O5'-P
85	r3	74	P5P	O4'-C1'-N9-C8
83	r1	45	Y5P	O4'-C1'-N1-C2
85	r3	40	Y5P	O4'-C1'-N1-C6
84	r2	33	Y5P	C2'-C1'-N1-C2
85	r3	40	Y5P	C2'-C1'-N1-C2
83	r1	52	Y5P	O4'-C4'-C5'-O5'
84	r2	14	P5P	O4'-C4'-C5'-O5'
84	r2	21	P5P	C3'-C4'-C5'-O5'
84	r2	36	P5P	C3'-C4'-C5'-O5'
84	r2	67	Y5P	C3'-C4'-C5'-O5'
84	r2	70	P5P	C3'-C4'-C5'-O5'
84	r2	75	Y5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
85	r3	5	P5P	C3'-C4'-C5'-O5'
85	r3	7	Y5P	O4'-C4'-C5'-O5'
85	r3	17(A)	P5P	O4'-C4'-C5'-O5'
85	r3	50	Y5P	C3'-C4'-C5'-O5'
85	r3	53	Y5P	O4'-C4'-C5'-O5'
85	r3	53	Y5P	C3'-C4'-C5'-O5'
85	r3	55	P5P	O4'-C4'-C5'-O5'
85	r3	74	P5P	O4'-C1'-N9-C4
84	r2	46	P5P	C2'-C1'-N9-C4
85	r3	16	Y5P	O4'-C1'-N1-C2
85	r3	1	Y5P	C2'-C1'-N1-C2
85	r3	13	Y5P	C2'-C1'-N1-C2
85	r3	17	Y5P	C2'-C1'-N1-C2
85	r3	17	Y5P	C2'-C1'-N1-C6
83	r1	44	Y5P	C3'-C4'-C5'-O5'
84	r2	14	P5P	C3'-C4'-C5'-O5'
84	r2	70	P5P	O4'-C4'-C5'-O5'
85	r3	17(A)	P5P	C3'-C4'-C5'-O5'
84	r2	20	Y5P	O4'-C1'-N1-C2
84	r2	67	Y5P	O4'-C1'-N1-C2
85	r3	39	Y5P	O4'-C1'-N1-C2
85	r3	46	P5P	C4'-C5'-O5'-P
85	r3	1	Y5P	C2'-C1'-N1-C6
85	r3	13	Y5P	C2'-C1'-N1-C6
83	r1	53	Y5P	C3'-C4'-C5'-O5'
84	r2	1	P5P	O4'-C4'-C5'-O5'
84	r2	72	Y5P	C3'-C4'-C5'-O5'
84	r2	73	P5P	C3'-C4'-C5'-O5'
85	r3	18	P5P	O4'-C4'-C5'-O5'
85	r3	61	Y5P	C3'-C4'-C5'-O5'
83	r1	53	Y5P	O4'-C1'-N1-C2
85	r3	20	Y5P	O4'-C1'-N1-C2
83	r1	55	Y5P	C3'-C4'-C5'-O5'
84	r2	7	P5P	O4'-C4'-C5'-O5'
84	r2	68	Y5P	C3'-C4'-C5'-O5'
85	r3	4	P5P	C3'-C4'-C5'-O5'
85	r3	18	P5P	C3'-C4'-C5'-O5'
85	r3	42	P5P	O4'-C4'-C5'-O5'
85	r3	61	Y5P	O4'-C4'-C5'-O5'
83	r1	46	Y5P	C3'-C4'-C5'-O5'
84	r2	33	Y5P	O4'-C4'-C5'-O5'
85	r3	49	Y5P	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
84	r2	33	Y5P	C4'-C5'-O5'-P
84	r2	15	P5P	C2'-C1'-N9-C8
83	r1	47	Y5P	C3'-C4'-C5'-O5'
84	r2	49	Y5P	O4'-C4'-C5'-O5'
84	r2	72	Y5P	O4'-C4'-C5'-O5'
85	r3	59	Y5P	O4'-C4'-C5'-O5'
84	r2	48	Y5P	C4'-C5'-O5'-P
84	r2	33	Y5P	O4'-C1'-N1-C6
84	r2	9	P5P	C3'-C4'-C5'-O5'
84	r2	49	Y5P	C3'-C4'-C5'-O5'
84	r2	75	Y5P	C3'-C4'-C5'-O5'
85	r3	3	P5P	C3'-C4'-C5'-O5'
85	r3	5	P5P	O4'-C4'-C5'-O5'
85	r3	7	Y5P	C3'-C4'-C5'-O5'
85	r3	17(A)	P5P	C2'-C1'-N9-C4
83	r1	49	Y5P	O4'-C4'-C5'-O5'
84	r2	7	P5P	C3'-C4'-C5'-O5'
84	r2	15	P5P	O4'-C4'-C5'-O5'
84	r2	33	Y5P	C3'-C4'-C5'-O5'
83	r1	52	Y5P	C3'-C4'-C5'-O5'
85	r3	47	Y5P	C3'-C4'-C5'-O5'
85	r3	51	P5P	C3'-C4'-C5'-O5'
84	r2	19	P5P	O4'-C1'-N9-C4
84	r2	23	P5P	C4'-C5'-O5'-P
85	r3	3	P5P	C4'-C5'-O5'-P
85	r3	13	Y5P	O4'-C1'-N1-C2
84	r2	24	P5P	C2'-C1'-N9-C4
84	r2	19	P5P	O4'-C1'-N9-C8
85	r3	13	Y5P	O4'-C1'-N1-C6
84	r2	46	P5P	O4'-C4'-C5'-O5'
85	r3	47	Y5P	O4'-C4'-C5'-O5'
85	r3	1	Y5P	O4'-C1'-N1-C2
85	r3	47	Y5P	O4'-C1'-N1-C2
85	r3	69	Y5P	C3'-C4'-C5'-O5'
85	r3	17(A)	P5P	C2'-C1'-N9-C8
83	r1	56	Y5P	O4'-C1'-N1-C6
85	r3	1	Y5P	O4'-C1'-N1-C6
84	r2	15	P5P	C2'-C1'-N9-C4
85	r3	17	Y5P	O4'-C1'-N1-C2
85	r3	58	Y5P	O4'-C1'-N1-C2
85	r3	49	Y5P	O4'-C4'-C5'-O5'
84	r2	9	P5P	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
84	r2	76	P5P	C4'-C5'-O5'-P
84	r2	24	P5P	C2'-C1'-N9-C8
84	r2	47	Y5P	C3'-C4'-C5'-O5'
85	r3	17	Y5P	O4'-C1'-N1-C6
84	r2	1	P5P	C4'-C5'-O5'-P
84	r2	73	P5P	C4'-C5'-O5'-P
85	r3	14	P5P	C4'-C5'-O5'-P
85	r3	17(A)	P5P	C4'-C5'-O5'-P
84	r2	15	P5P	C3'-C4'-C5'-O5'
84	r2	46	P5P	C3'-C4'-C5'-O5'
85	r3	29	P5P	C3'-C4'-C5'-O5'
85	r3	29	P5P	O4'-C4'-C5'-O5'
84	r2	19	P5P	C2'-C1'-N9-C8
84	r2	36	P5P	C4'-C5'-O5'-P
84	r2	17	Y5P	O4'-C4'-C5'-O5'
85	r3	2	Y5P	O4'-C1'-N1-C2
84	r2	9	P5P	O4'-C1'-N9-C8
84	r2	9	P5P	O4'-C1'-N9-C4
85	r3	18	P5P	C4'-C5'-O5'-P
85	r3	50	Y5P	C4'-C5'-O5'-P
83	r1	55	Y5P	O4'-C1'-N1-C2
84	r2	70	P5P	C4'-C5'-O5'-P
83	r1	47	Y5P	O4'-C4'-C5'-O5'
85	r3	19	P5P	C3'-C4'-C5'-O5'
85	r3	42	P5P	C3'-C4'-C5'-O5'
85	r3	51	P5P	O4'-C4'-C5'-O5'
85	r3	56	Y5P	O4'-C1'-N1-C2
84	r2	69	P5P	C4'-C5'-O5'-P
84	r2	75	Y5P	C2'-C1'-N1-C6
84	r2	17	Y5P	C3'-C4'-C5'-O5'
84	r2	37	P5P	C5'-O5'-P-OP1
84	r2	37	P5P	C5'-O5'-P-OP2
84	r2	74	Y5P	O4'-C4'-C5'-O5'
85	r3	69	Y5P	O4'-C4'-C5'-O5'
83	r1	55	Y5P	C2'-C1'-N1-C2
85	r3	56	Y5P	C2'-C1'-N1-C2
84	r2	69	P5P	C3'-C4'-C5'-O5'
85	r3	56	Y5P	O4'-C4'-C5'-O5'
84	r2	17	Y5P	C4'-C5'-O5'-P
84	r2	46	P5P	C4'-C5'-O5'-P
85	r3	4	P5P	C4'-C5'-O5'-P
85	r3	44	P5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
84	r2	45	Y5P	C4'-C5'-O5'-P
85	r3	69	Y5P	C4'-C5'-O5'-P
85	r3	72	Y5P	C4'-C5'-O5'-P
83	r1	47	Y5P	C4'-C5'-O5'-P
84	r2	61	Y5P	C4'-C5'-O5'-P
84	r2	46	P5P	O4'-C1'-N9-C8
83	r1	46	Y5P	O4'-C4'-C5'-O5'

There are no ring outliers.

99 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	r2	69	P5P	2	0
85	r3	23	P5P	4	0
84	r2	15	P5P	1	0
84	r2	40	Y5P	3	0
84	r2	9	P5P	2	0
85	r3	8	P5P	3	0
85	r3	35	P5P	1	0
84	r2	67	Y5P	2	0
84	r2	45	Y5P	3	0
85	r3	14	P5P	2	0
85	r3	41	Y5P	4	0
84	r2	38	P5P	1	0
85	r3	2	Y5P	3	0
85	r3	53	Y5P	5	0
84	r2	48	Y5P	2	0
84	r2	8	Y5P	2	0
84	r2	6	P5P	1	0
85	r3	54	Y5P	3	0
84	r2	61	Y5P	1	0
83	r1	54	Y5P	1	0
84	r2	19	P5P	2	0
85	r3	56	Y5P	3	0
85	r3	25	Y5P	1	0
84	r2	74	Y5P	2	0
84	r2	17	Y5P	1	0
84	r2	55	Y5P	1	0
84	r2	54	Y5P	2	0
84	r2	34	P5P	2	0
85	r3	64	Y5P	1	0
84	r2	35	P5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	r1	57	Y5P	2	0
83	r1	47	Y5P	1	0
85	r3	3	P5P	1	0
84	r2	41	Y5P	1	0
84	r2	16	Y5P	1	0
85	r3	69	Y5P	1	0
84	r2	60	Y5P	3	0
85	r3	30	P5P	1	0
85	r3	58	Y5P	2	0
84	r2	39	Y5P	3	0
85	r3	59	Y5P	2	0
84	r2	29	P5P	1	0
84	r2	24	P5P	2	0
85	r3	43	P5P	1	0
85	r3	13	Y5P	3	0
84	r2	44	P5P	1	0
85	r3	42	P5P	2	0
84	r2	43	Y5P	1	0
84	r2	71	P5P	1	0
85	r3	46	P5P	1	0
84	r2	1	P5P	1	0
85	r3	63	Y5P	3	0
83	r1	52	Y5P	2	0
85	r3	17(A)	P5P	2	0
85	r3	50	Y5P	1	0
84	r2	76	P5P	3	0
85	r3	32	Y5P	3	0
84	r2	42	Y5P	1	0
85	r3	15	P5P	2	0
85	r3	21	P5P	2	0
83	r1	53	Y5P	4	0
84	r2	59	Y5P	1	0
85	r3	22	P5P	1	0
85	r3	52	P5P	2	0
85	r3	73	Y5P	2	0
85	r3	17	Y5P	2	0
84	r2	4	Y5P	1	0
83	r1	55	Y5P	1	0
83	r1	56	Y5P	3	0
85	r3	62	Y5P	2	0
85	r3	71	P5P	1	0
84	r2	23	P5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	r3	26	P5P	1	0
84	r2	46	P5P	4	0
84	r2	58	P5P	1	0
85	r3	47	Y5P	1	0
85	r3	24	Y5P	3	0
84	r2	2	Y5P	1	0
83	r1	48	Y5P	2	0
85	r3	40	Y5P	5	0
84	r2	68	Y5P	2	0
84	r2	49	Y5P	1	0
84	r2	31	P5P	1	0
84	r2	66	Y5P	1	0
85	r3	29	P5P	2	0
85	r3	16	Y5P	1	0
85	r3	1	Y5P	2	0
85	r3	74	P5P	2	0
84	r2	5	P5P	2	0
84	r2	32	Y5P	1	0
83	r1	46	Y5P	2	0
85	r3	70	Y5P	1	0
85	r3	33	Y5P	2	0
84	r2	75	Y5P	2	0
85	r3	28	Y5P	1	0
85	r3	34	Y5P	1	0
84	r2	30	P5P	2	0
84	r2	33	Y5P	1	0
84	r2	70	P5P	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
92	GTP	AX	500	-	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
90	H8Q	XA	5144	-	78,80,80	1.12	5 (6%)	102,115,115	1.40	15 (14%)
91	DOL	XA	5145	-	47,50,50	3.96	18 (38%)	57,70,70	2.91	14 (24%)

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
92	GTP	AX	500	-	-	7/22/38/38	0/3/3/3
90	H8Q	XA	5144	-	-	31/83/127/127	0/8/8/8
91	DOL	XA	5145	-	-	23/64/77/77	0/2/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	XA	5145	DOL	C28-C29	10.64	1.56	1.32
91	XA	5145	DOL	C6-N5	10.31	1.49	1.34
91	XA	5145	DOL	C22-C23	9.22	1.57	1.32
91	XA	5145	DOL	C10-N9	9.08	1.39	1.29
91	XA	5145	DOL	C19-C20	8.61	1.57	1.34
91	XA	5145	DOL	C26-N25	7.03	1.48	1.34
91	XA	5145	DOL	C22-C20	5.90	1.58	1.46
91	XA	5145	DOL	C13-C10	5.89	1.57	1.50
90	XA	5144	H8Q	C20-S21	-5.71	1.76	1.82
91	XA	5145	DOL	O36-C37	5.21	1.46	1.34
90	XA	5144	H8Q	O41-C34	5.08	1.45	1.34
91	XA	5145	DOL	C8-C6	4.38	1.56	1.49
91	XA	5145	DOL	C16-C14	4.13	1.57	1.51
91	XA	5145	DOL	C12-C8	4.04	1.39	1.34
91	XA	5145	DOL	C28-C26	3.73	1.56	1.48
90	XA	5144	H8Q	C22-S21	-3.48	1.76	1.82
91	XA	5145	DOL	O27-C26	-2.90	1.18	1.24
91	XA	5145	DOL	O18-C17	-2.81	1.38	1.43
90	XA	5144	H8Q	O41-C43	-2.47	1.42	1.46
91	XA	5145	DOL	C24-C23	2.36	1.58	1.49
91	XA	5145	DOL	C3-C2	-2.27	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	XA	5144	H8Q	C35-C33	-2.20	1.49	1.52
92	AX	500	GTP	C2-N3	2.19	1.38	1.33
91	XA	5145	DOL	O36-C32	-2.02	1.41	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	XA	5145	DOL	O40-S39-O41	-15.05	101.06	118.13
91	XA	5145	DOL	O11-C10-C13	8.20	125.28	117.70
91	XA	5145	DOL	C24-N25-C26	-6.09	112.29	122.17
91	XA	5145	DOL	O11-C10-N9	-5.43	108.22	114.09
92	AX	500	GTP	C5-C4-N3	-5.08	120.31	128.39
92	AX	500	GTP	C2-N3-C4	4.57	120.18	112.30
90	XA	5144	H8Q	O41-C34-C33	4.52	122.03	110.61
91	XA	5145	DOL	C32-O36-C37	-3.56	111.86	117.76
90	XA	5144	H8Q	C17-C16-C15	3.49	119.86	115.39
91	XA	5145	DOL	O40-S39-C2	3.48	111.86	108.50
90	XA	5144	H8Q	C50-C51-N52	3.42	121.92	115.81
91	XA	5145	DOL	C4-N5-C1	-3.41	108.50	112.51
90	XA	5144	H8Q	C3-C2-N71	-3.35	107.38	112.71
90	XA	5144	H8Q	C40-C35-C33	-3.31	115.48	120.78
92	AX	500	GTP	N9-C4-N3	3.28	132.52	125.95
90	XA	5144	H8Q	C43-O41-C34	-3.25	112.74	117.55
91	XA	5145	DOL	C23-C22-C20	-3.17	121.10	125.89
92	AX	500	GTP	C2-N1-C6	-3.11	119.48	125.11
90	XA	5144	H8Q	O41-C34-O42	-3.08	118.38	123.95
90	XA	5144	H8Q	C36-C35-C33	3.01	125.62	120.78
90	XA	5144	H8Q	C35-C33-N31	-2.88	105.49	112.75
92	AX	500	GTP	N9-C8-N7	-2.68	108.42	113.40
91	XA	5145	DOL	C21-C20-C22	2.64	122.12	118.09
90	XA	5144	H8Q	O58-C50-C51	-2.60	116.60	120.75
92	AX	500	GTP	C8-N7-C5	2.59	108.87	104.26
90	XA	5144	H8Q	C14-C15-C16	2.57	111.23	107.65
92	AX	500	GTP	C5-C6-N1	2.57	119.79	113.25
91	XA	5145	DOL	C37-C1-N5	-2.54	107.78	112.13
91	XA	5145	DOL	C3-C4-N5	2.50	105.96	103.22
90	XA	5144	H8Q	C34-C33-N31	2.43	114.46	109.60
92	AX	500	GTP	O6-C6-C5	-2.42	120.16	126.53
91	XA	5145	DOL	C17-C16-C14	-2.39	108.88	113.90
90	XA	5144	H8Q	C17-C18-N13	-2.35	107.50	109.90
90	XA	5144	H8Q	C53-N52-C51	2.29	121.26	116.80
91	XA	5145	DOL	C14-C13-C10	-2.17	108.08	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	XA	5144	H8Q	C2-C1-N13	2.03	122.76	117.71
91	XA	5145	DOL	C30-C29-C28	-2.00	121.00	126.30

There are no chirality outliers.

All (61) 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	C1-C2-S39-O40
91	XA	5145	DOL	C43-C42-S39-C2
91	XA	5145	DOL	C43-C42-S39-O41
91	XA	5145	DOL	C43-C42-S39-O40
91	XA	5145	DOL	C29-C30-C32-C33
91	XA	5145	DOL	C31-C30-C32-C33
91	XA	5145	DOL	O36-C32-C33-C34
92	AX	500	GTP	PB-O3B-PG-O3G
92	AX	500	GTP	C5'-O5'-PA-O3A
92	AX	500	GTP	C5'-O5'-PA-O2A
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	O36-C32-C33-C35
91	XA	5145	DOL	C28-C29-C30-C31
90	XA	5144	H8Q	C43-C45-C46-N49
91	XA	5145	DOL	C3-C2-S39-C42

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Mol	Chain	Res	Type	Atoms
91	XA	5145	DOL	C30-C32-C33-C34
90	XA	5144	H8Q	N48-C45-C46-O47
91	XA	5145	DOL	N9-C10-C13-C14
92	AX	500	GTP	O4'-C4'-C5'-O5'
91	XA	5145	DOL	C1-C2-S39-O41
90	XA	5144	H8Q	N48-C45-C46-N49
92	AX	500	GTP	C3'-C4'-C5'-O5'
91	XA	5145	DOL	O11-C10-C13-C14
91	XA	5145	DOL	C29-C30-C32-O36
91	XA	5145	DOL	C31-C30-C32-O36
91	XA	5145	DOL	C3-C2-S39-O41
91	XA	5145	DOL	C16-C17-C19-C20
91	XA	5145	DOL	O18-C17-C19-C20
90	XA	5144	H8Q	N31-C33-C34-O42
90	XA	5144	H8Q	N31-C33-C34-O41
90	XA	5144	H8Q	N13-C18-C30-N31
90	XA	5144	H8Q	N13-C18-C30-O32
90	XA	5144	H8Q	C34-C33-C35-C40
91	XA	5145	DOL	C28-C29-C30-C32
90	XA	5144	H8Q	N13-C1-C2-C3
91	XA	5145	DOL	C30-C32-C33-C35
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-C47
91	XA	5145	DOL	C42-C43-N44-C45

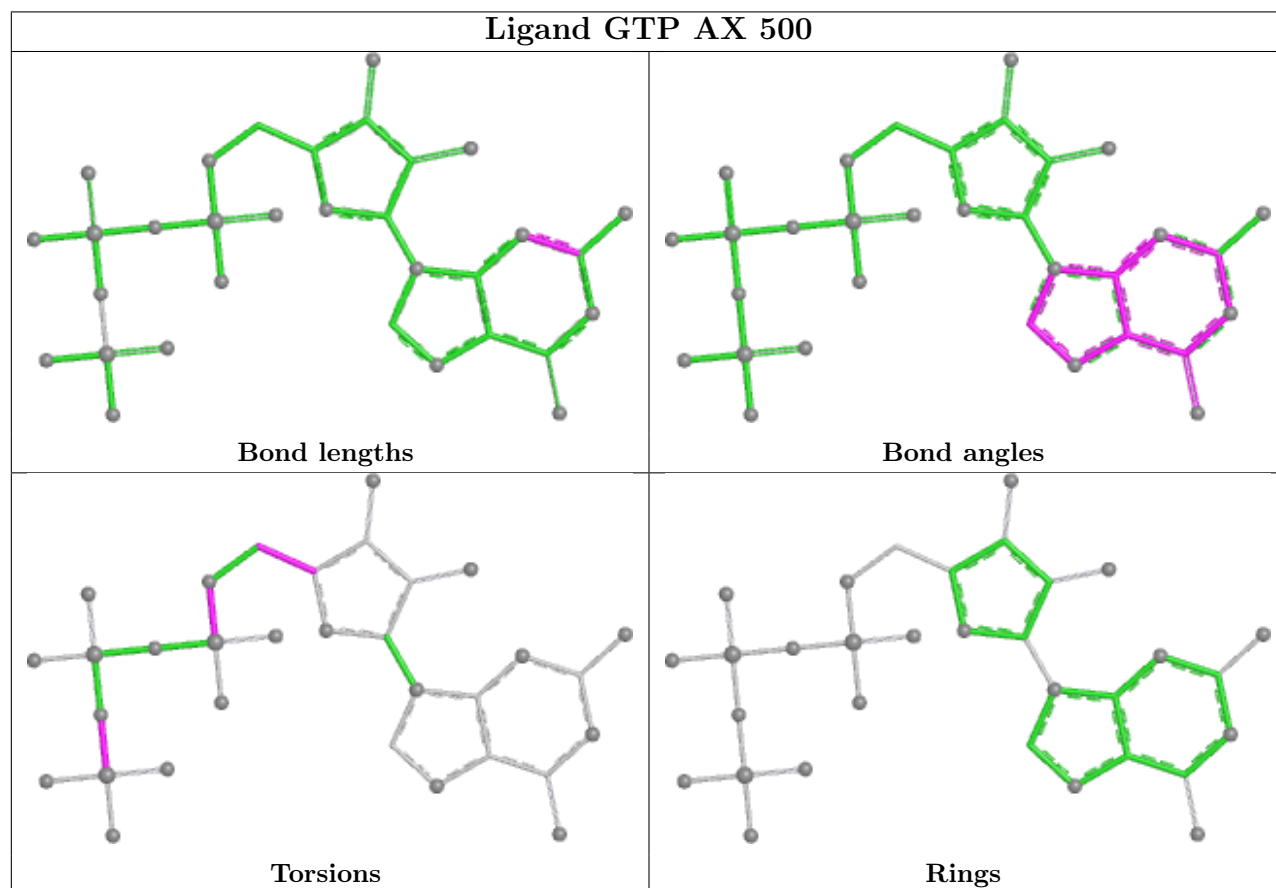
There are no ring outliers.

2 monomers are involved in 5 short contacts:

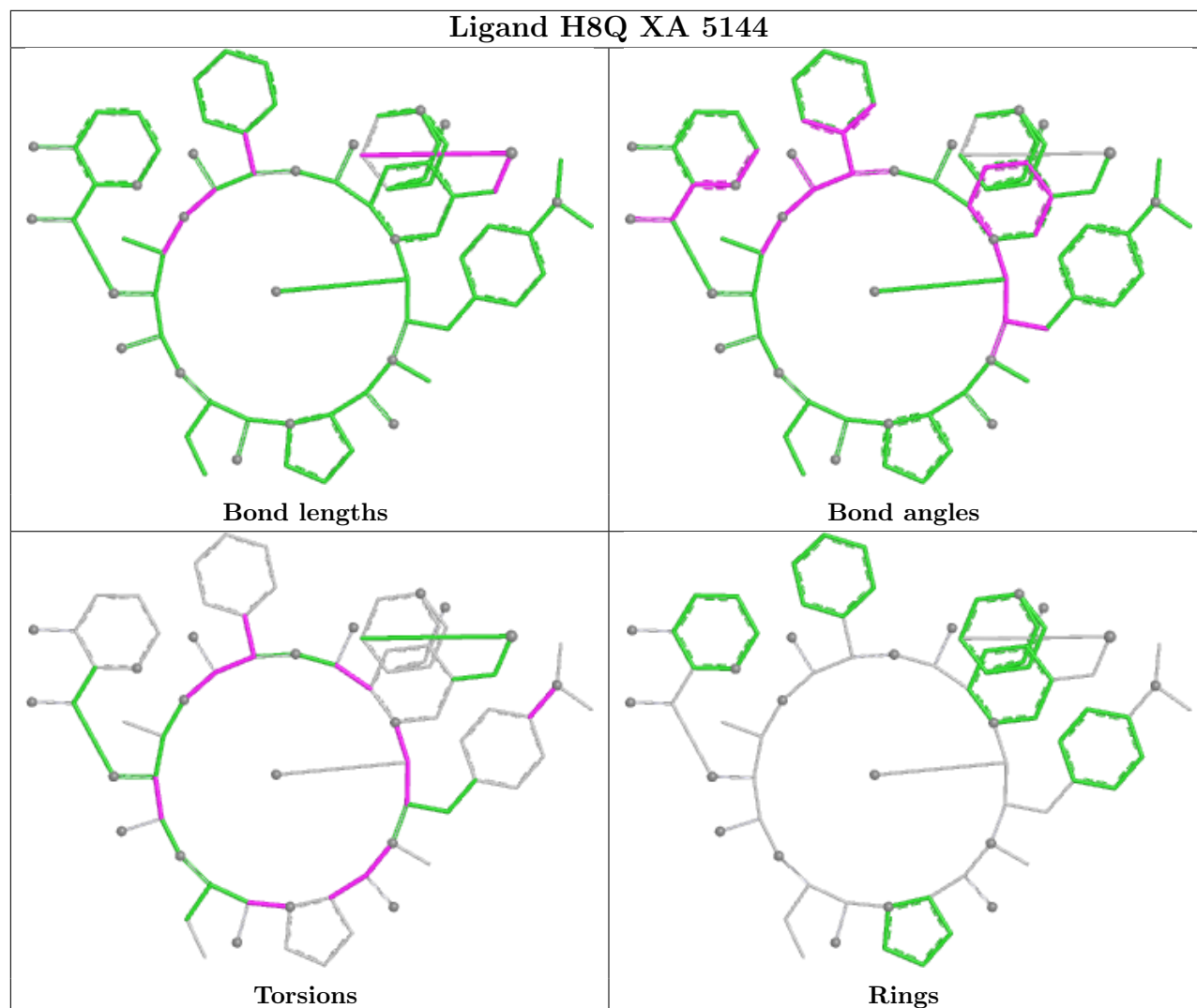
Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	AX	500	GTP	1	0
90	XA	5144	H8Q	4	0

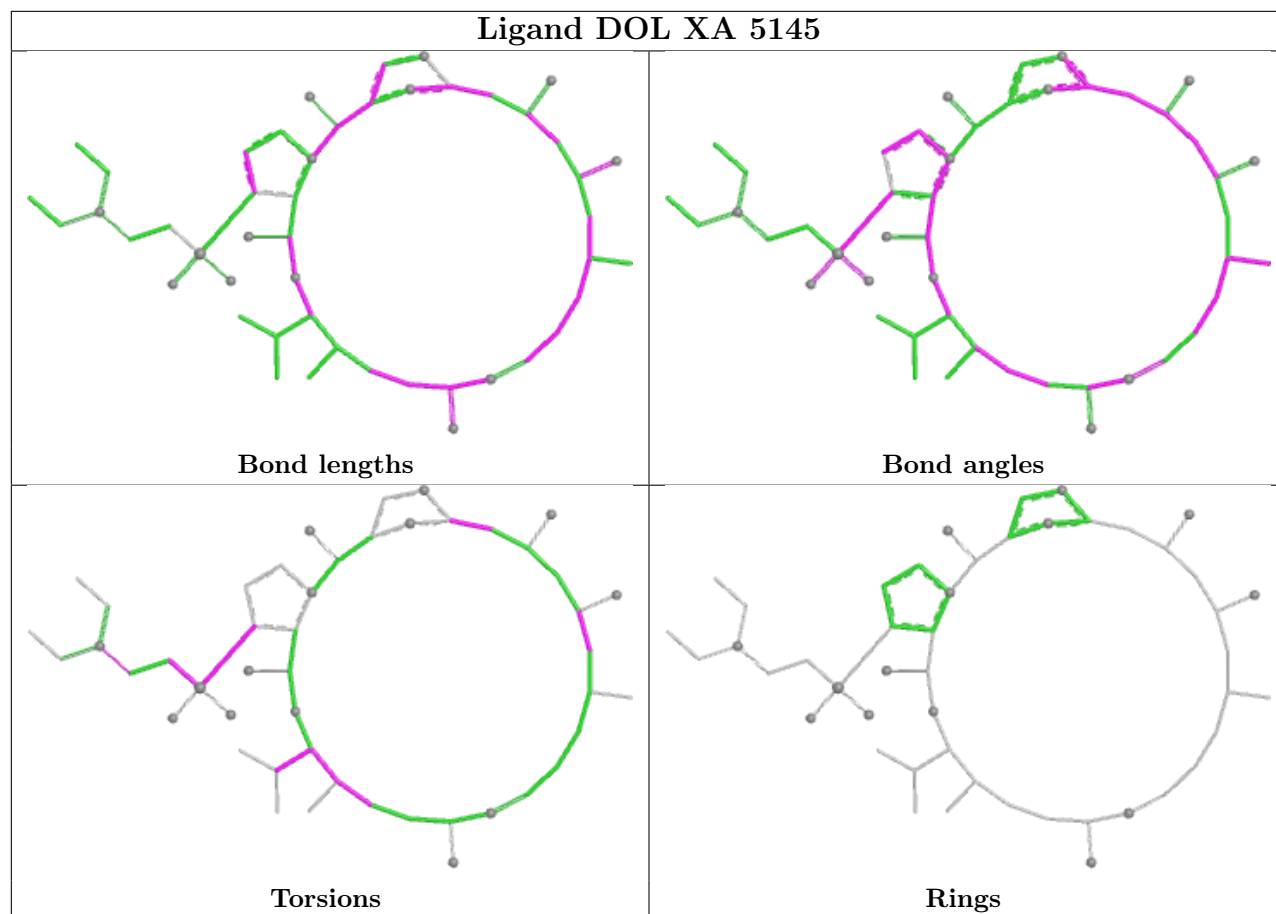
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	7	3
16	A4	2
7	6	2
82	r	1
38	AV	1
6	5	1
34	AR	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	285:ASN	C	286:LEU	N	6.42
1	A4	537:ARG	C	538:ASP	N	6.17
1	r	134:ARG	C	135:LEU	N	5.44
1	7	158:PHE	C	159:LYS	N	5.03
1	AV	269:SER	C	270:PRO	N	4.51
1	6	79:GLY	C	80:GLU	N	3.51
1	7	185:LEU	C	186:ASP	N	3.23
1	A4	143:GLU	C	144:TYR	N	3.07
1	6	282:SER	C	283:GLU	N	3.01
1	5	141:ASP	C	142:ASP	N	3.00
1	AR	308:HIS	C	309:PRO	N	1.62

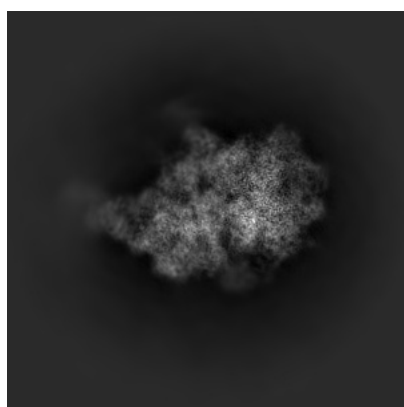
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11391. These allow visual inspection of the internal detail of the map and identification of artifacts.

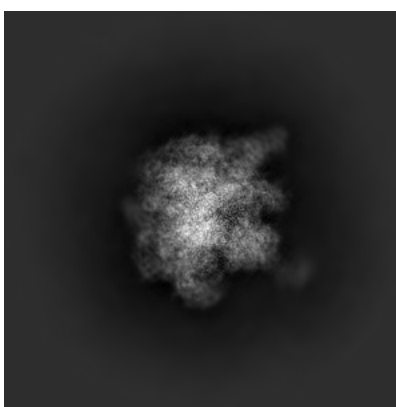
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

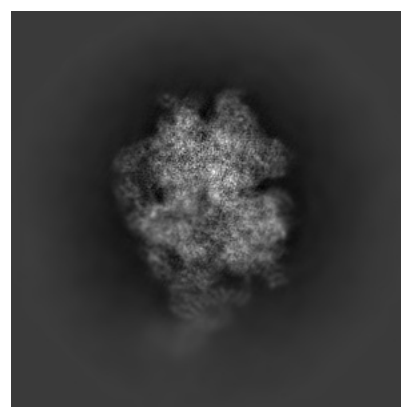
6.1.1 Primary map



X



Y

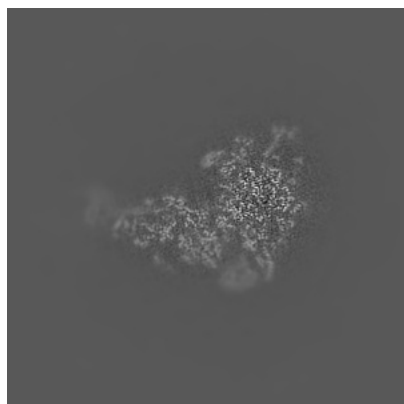


Z

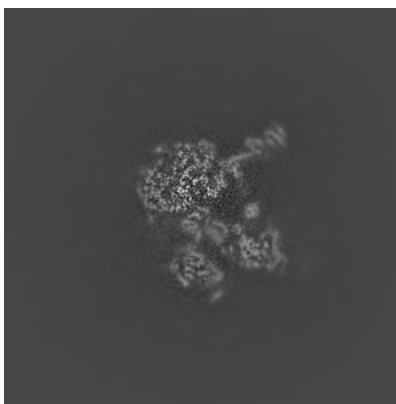
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

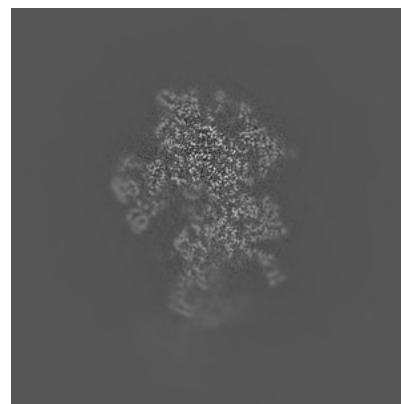
6.2.1 Primary map



X Index: 260



Y Index: 260

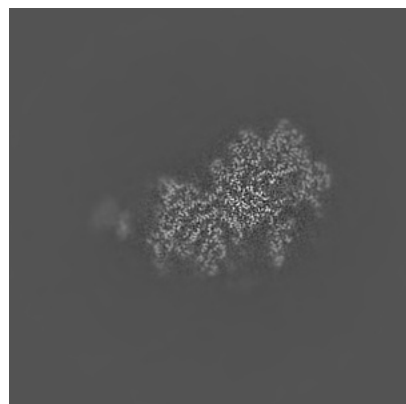


Z Index: 260

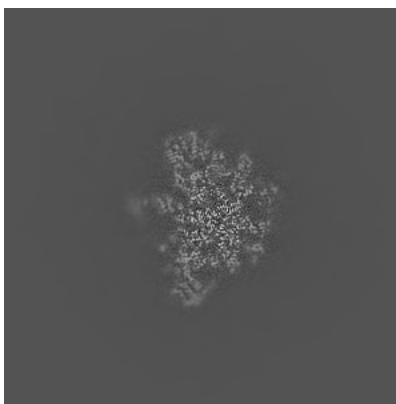
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

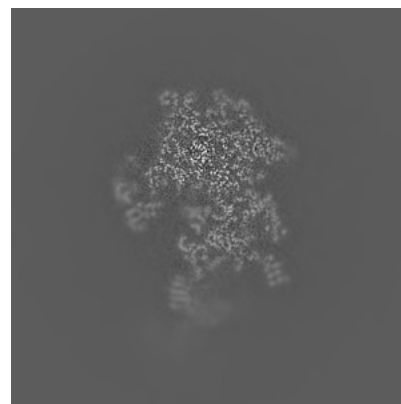
6.3.1 Primary map



X Index: 281



Y Index: 321

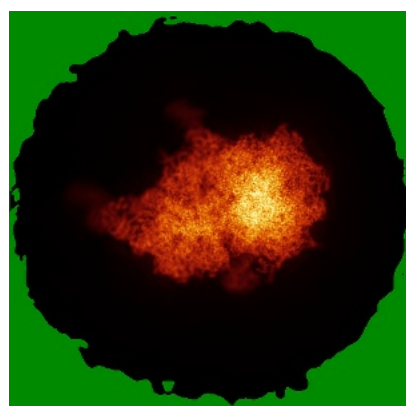


Z Index: 265

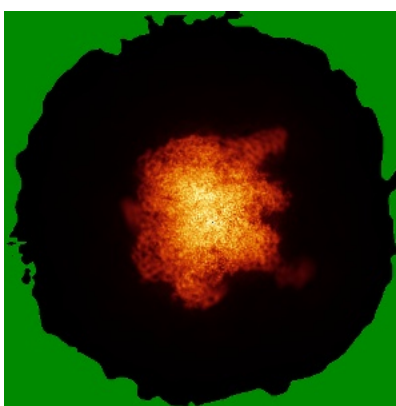
The images above show the largest variance slices of the map in three orthogonal directions.

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

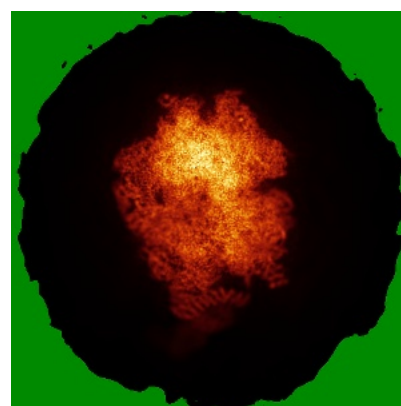
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

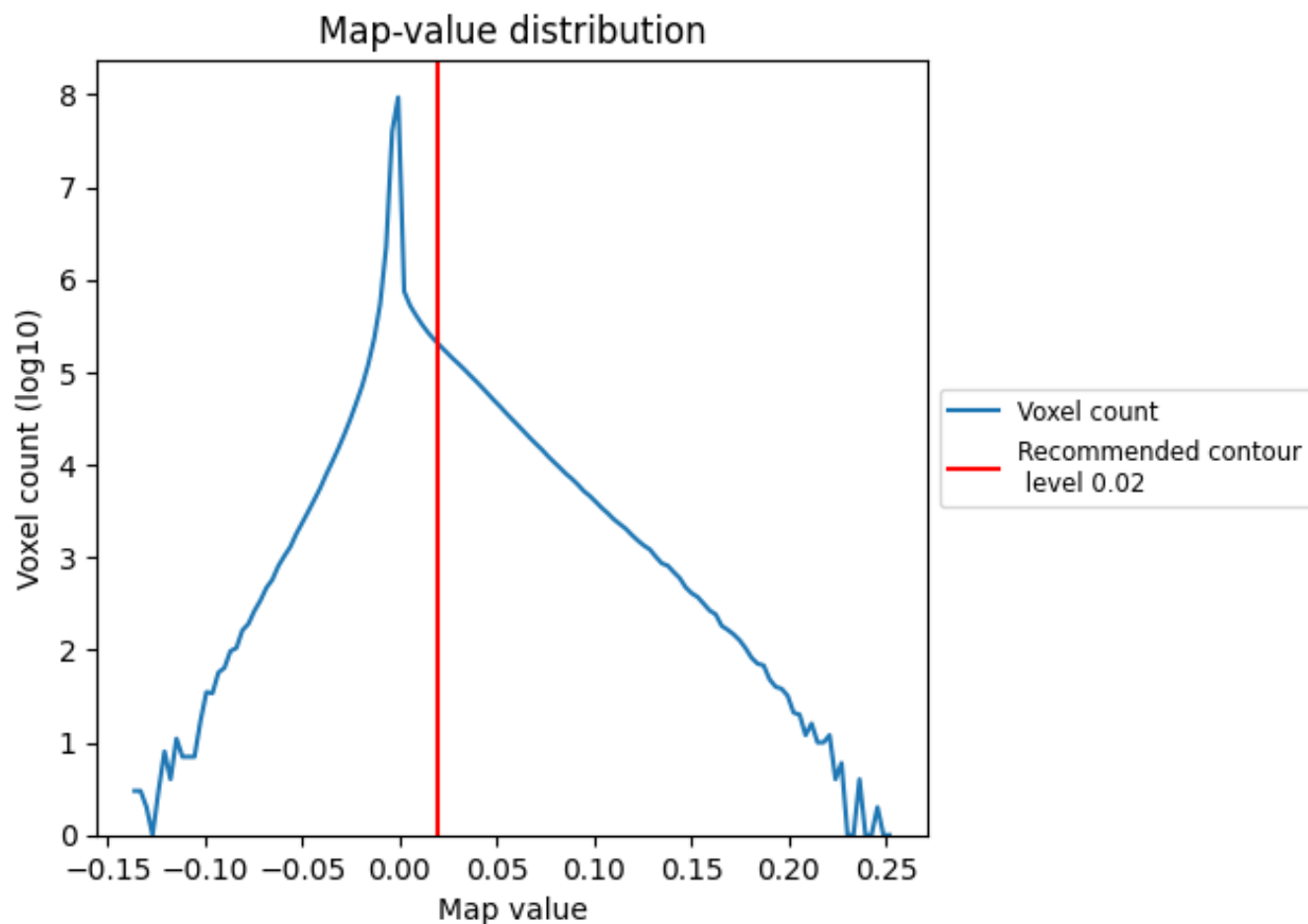
6.6 Mask visualisation

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

7 Map analysis [i](#)

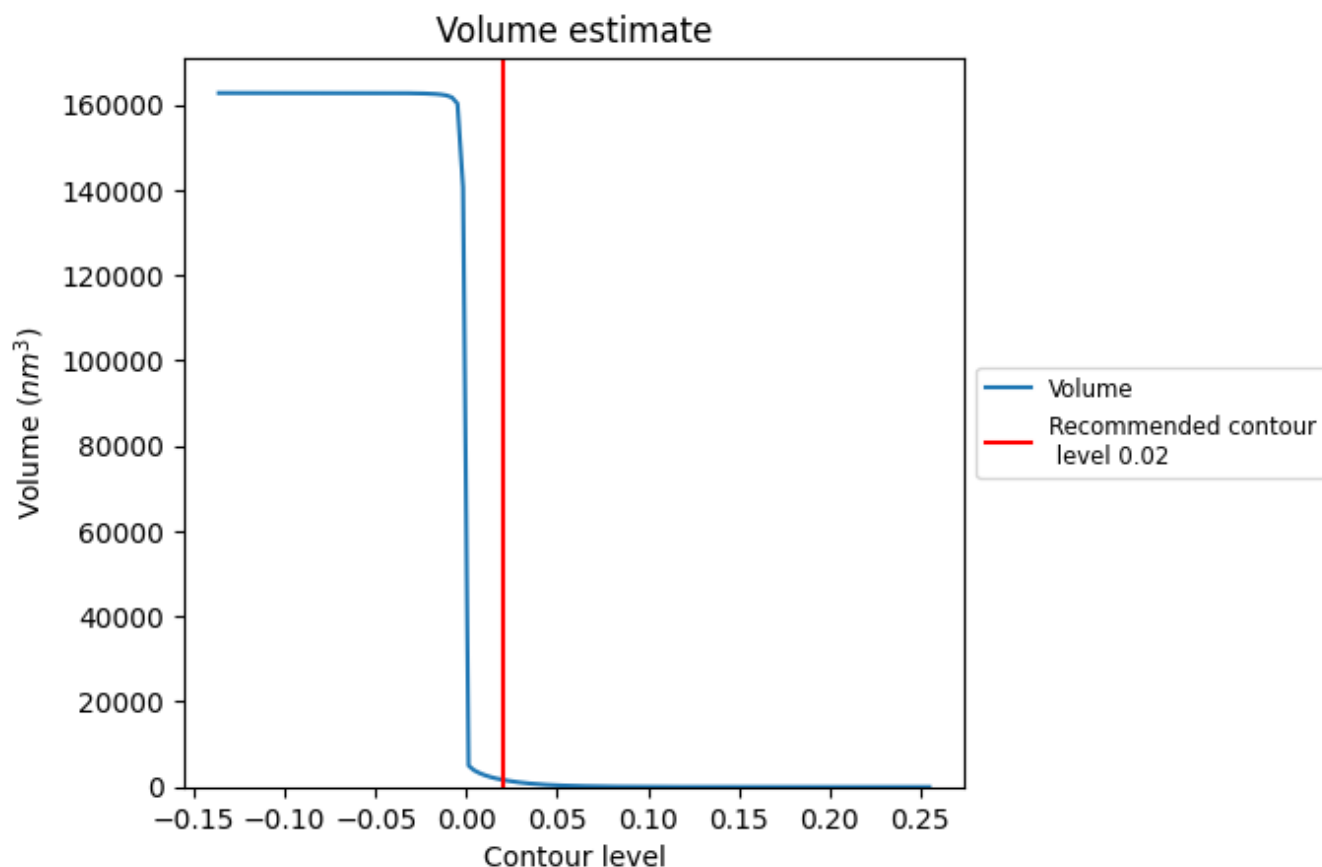
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

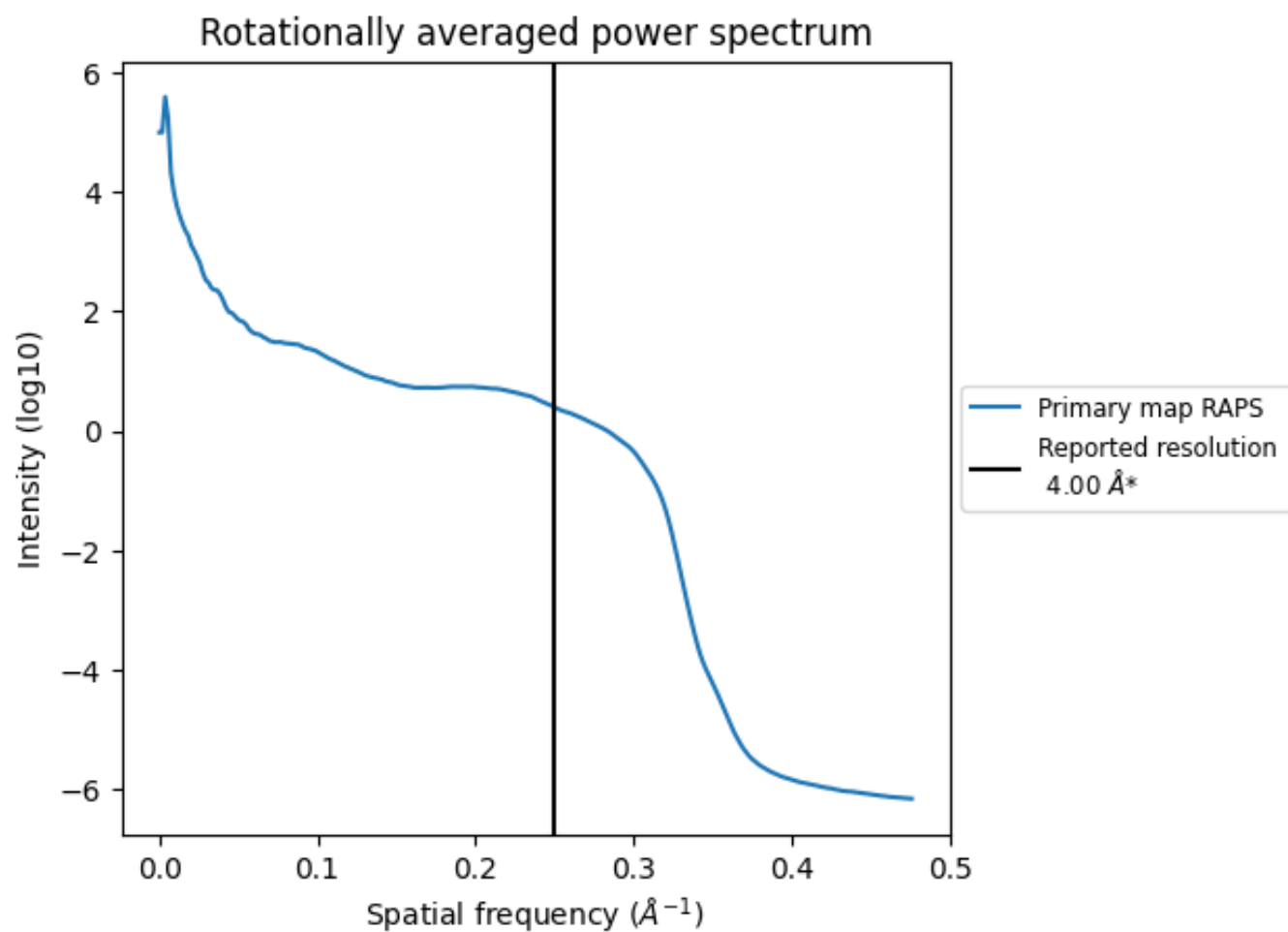
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1671 nm^3 ; this corresponds to an approximate mass of 1509 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



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

8 Fourier-Shell correlation

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

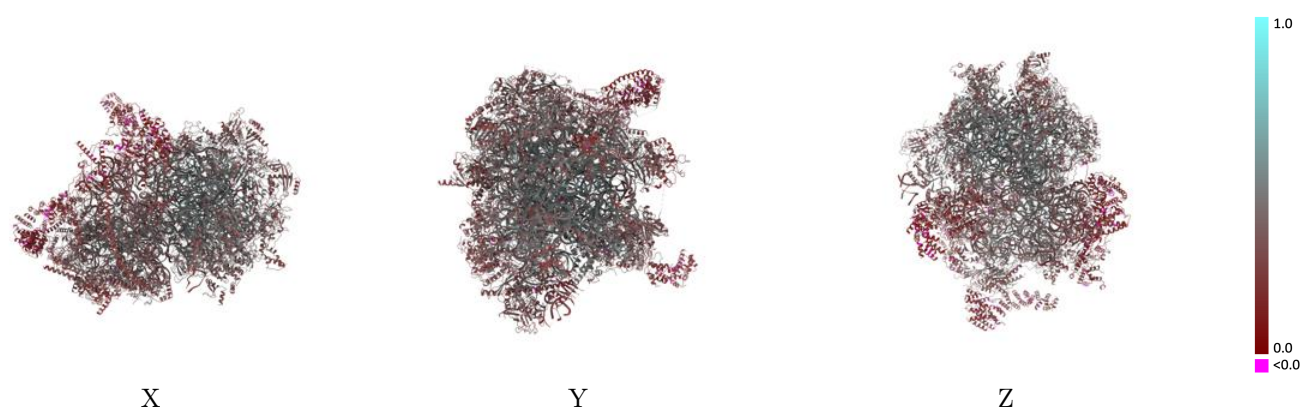
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11391 and PDB model 6ZSA. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)

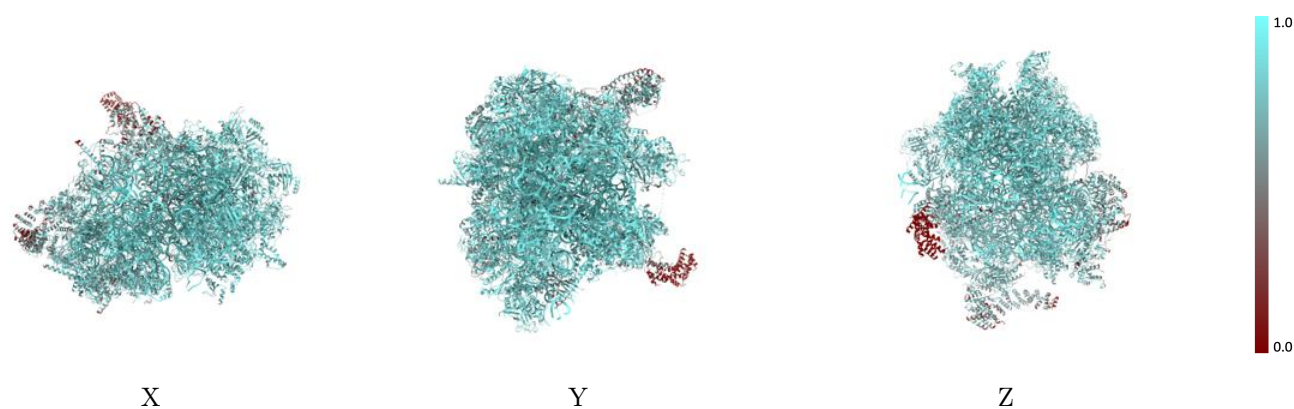
This section was not generated.

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



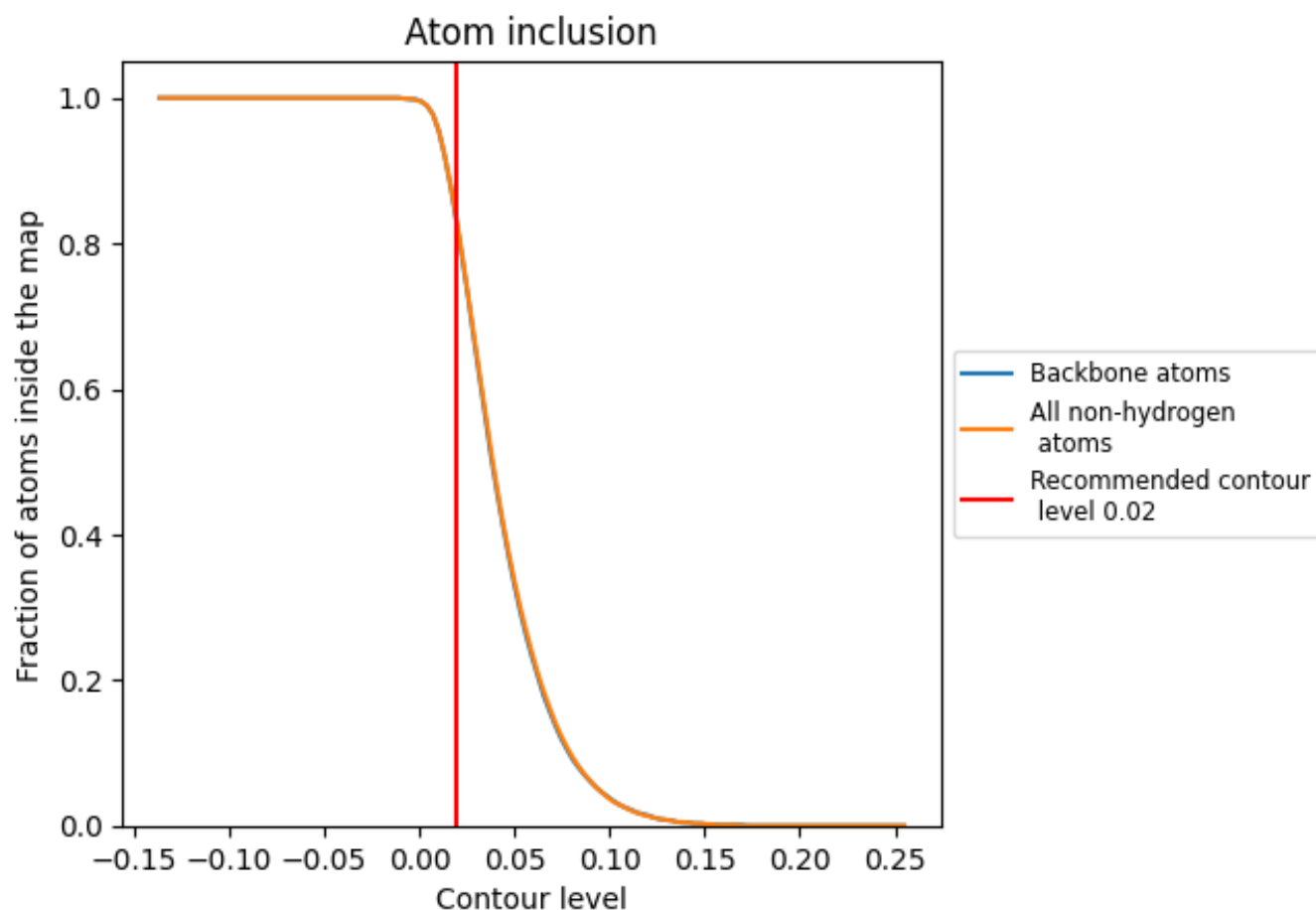
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.3730
0	 0.8570	 0.4160
1	 0.8170	 0.3960
2	 0.9080	 0.5060
3	 0.8900	 0.4920
4	 0.8930	 0.4490
5	 0.8440	 0.3870
6	 0.8210	 0.3550
7	 0.8010	 0.3460
8	 0.7000	 0.2570
9	 0.8240	 0.3910
A0	 0.6440	 0.2010
A1	 0.7000	 0.2660
A2	 0.7480	 0.3320
A3	 0.8490	 0.4250
A4	 0.5500	 0.1770
AA	 0.9520	 0.3990
AB	 0.7980	 0.3570
AC	 0.7800	 0.3830
AD	 0.7830	 0.3650
AE	 0.7870	 0.3770
AF	 0.7610	 0.3070
AG	 0.7640	 0.3210
AH	 0.7730	 0.3530
AI	 0.8170	 0.3650
AJ	 0.8140	 0.3810
AK	 0.8050	 0.3430
AL	 0.7850	 0.3370
AM	 0.7350	 0.2570
AN	 0.8240	 0.3780
AO	 0.7570	 0.2970
AP	 0.8190	 0.3740
AQ	 0.8200	 0.3980
AR	 0.6730	 0.2250
AS	 0.7280	 0.2900



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Chain	Atom inclusion	Q-score
AT	 0.7890	 0.3340
AU	 0.7160	 0.2470
AV	 0.5800	 0.1740
AW	 0.7830	 0.3380
AX	 0.6760	 0.2200
AY	 0.6810	 0.2510
AZ	 0.7700	 0.3010
XA	 0.9600	 0.4720
XB	 0.9600	 0.3310
XD	 0.8730	 0.4410
XE	 0.8570	 0.4270
XF	 0.8750	 0.4470
XH	 0.8100	 0.3720
XI	 0.5890	 0.2530
XJ	 0.6700	 0.2100
XK	 0.8690	 0.4400
XL	 0.8650	 0.4400
XM	 0.8560	 0.4280
XN	 0.8490	 0.4330
XO	 0.8620	 0.4220
XP	 0.8560	 0.3920
XQ	 0.7900	 0.3840
XR	 0.8740	 0.4590
XS	 0.8580	 0.4520
XT	 0.8800	 0.4590
XU	 0.8670	 0.4160
XV	 0.8200	 0.3710
XW	 0.8840	 0.4650
XX	 0.8390	 0.3900
XY	 0.8640	 0.4130
XZ	 0.8900	 0.4580
a	 0.8140	 0.3980
b	 0.8810	 0.4450
c	 0.8350	 0.3830
d	 0.7690	 0.3320
e	 0.6740	 0.2090
f	 0.7390	 0.2970
g	 0.8500	 0.4210
h	 0.8050	 0.3410
i	 0.8890	 0.4740
j	 0.8510	 0.4080
k	 0.7400	 0.2650

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Chain	Atom inclusion	Q-score
l	 0.7160	 0.2640
m	 0.7670	 0.2760
o	 0.9080	 0.4610
p	 0.8050	 0.3370
q	 0.7240	 0.2920
r	 0.8530	 0.4010
r1	 0.8570	 0.3870
r2	 0.8130	 0.2540
r3	 0.8600	 0.3070
s	 0.8550	 0.4030
t1	 0.2240	 0.2110
t2	 0.2400	 0.1750
t3	 0.0000	 0.1630
t4	 0.0000	 0.1450
t5	 0.0000	 0.1030
t6	 0.0000	 0.1260