



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 02:11 AM UTC

PDB ID : 6ZSC / pdb_00006zsc
EMDB ID : EMD-11393
Title : Human mitochondrial ribosome in complex with E-site tRNA
Authors : Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.
Deposited on : 2020-07-15
Resolution : 3.50 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

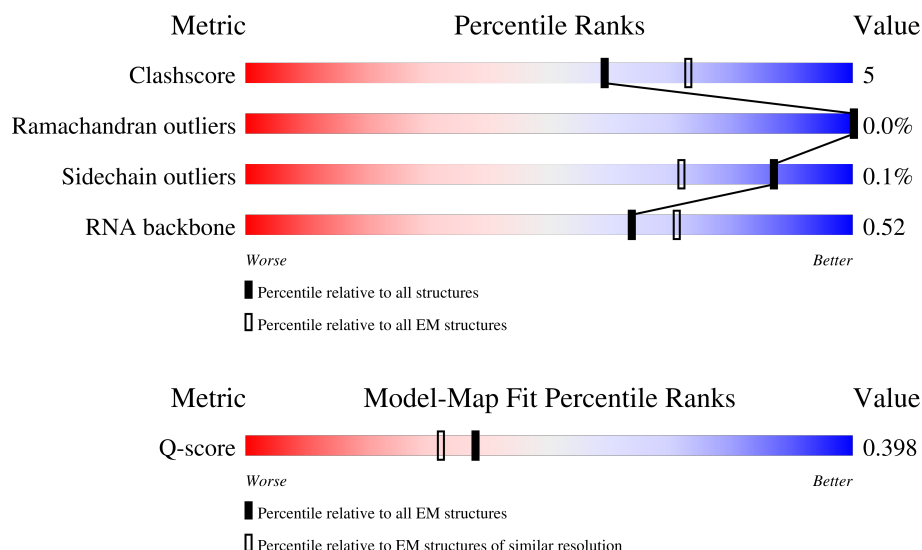
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	

Continued on next page...

Continued from previous page...

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	1561	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	AM	137	
30	AN	130	
31	AO	258	
32	AP	142	
33	AQ	85	
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	

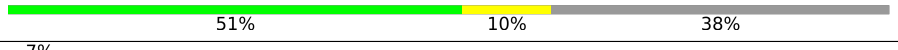
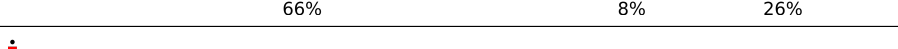
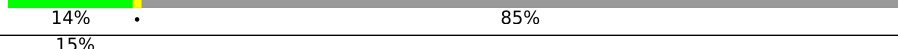
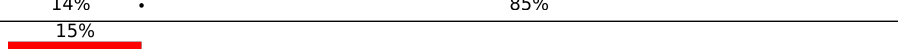
Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	o	102	
80	p	206	
81	q	222	
82	r	196	
83	r4	76	
84	s	439	
85	t1	198	
85	t2	198	
85	t3	198	
85	t4	198	
85	t5	198	
85	t6	198	
86	A	8	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 311612 atoms, of which 142812 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	291	Total	C	H	N	O	S	0	0
			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	123	Total	C	H	N	O	S	0	0
			2069	659	1036	177	195	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	1500	Total	C	H	N	O	P	0	0
			48025	14293	16172	5759	10301	1500		

- 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
			29592	8800	9964	3540	6364	924		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AF	201	Total	C	H	N	O	S	0	0
			3382	1069	1714	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
			4996	1593	2491	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	conflict	UNP P82921

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
45	XE	304	Total	C	H	N	O	S	0	0
			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
			2657	825	1366	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
			4682	1472	2377	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	
			2326	729	1162	223	207	5	
								0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
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
			1584	510	775	145	149	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	135	Total	C	H	N	O	S	0	0
			2172	694	1089	177	208	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	109	Total	C	H	N	O	S	0	0
			1756	562	870	155	166	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	0	0
			2514	792	1267	239	208	8		

- Molecule 83 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	r4	76	Total	C	N	O	P	0	0
			1485	723	230	456	76		

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

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

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

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

- Molecule 86 is a protein called Quinupristin.

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

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

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

Continued on next page...

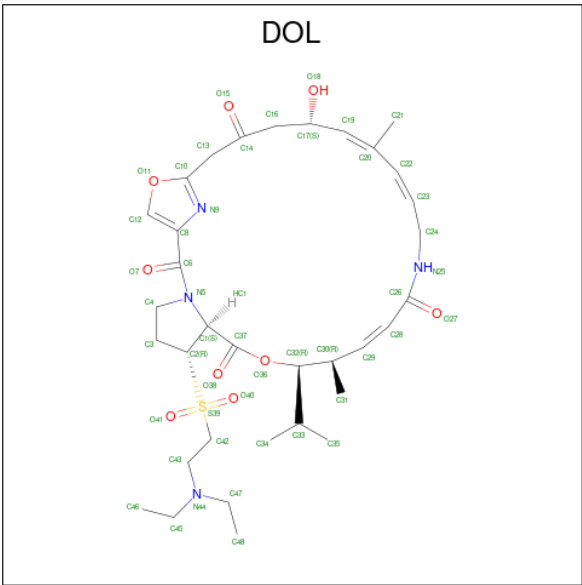
Continued from previous page...

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

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

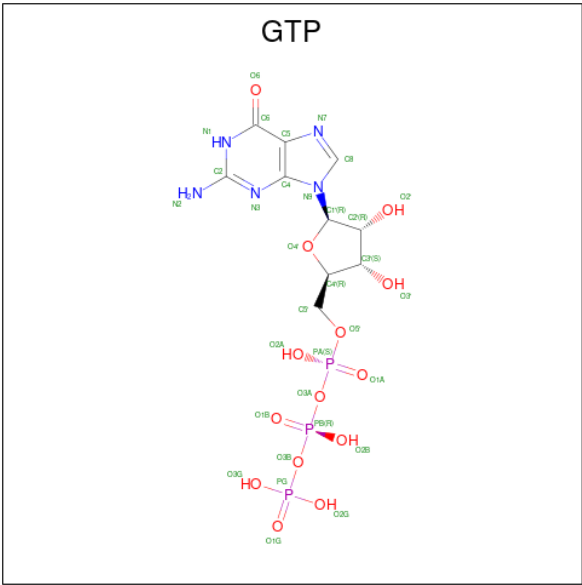
Mol	Chain	Residues	Atoms		AltConf
88	XA	143	Total 143	Mg 143	0
88	AA	46	Total 46	Mg 46	0
88	XD	1	Total 1	Mg 1	0
88	XE	1	Total 1	Mg 1	0
88	XI	1	Total 1	Mg 1	0
88	XM	2	Total 2	Mg 2	0
88	g	1	Total 1	Mg 1	0

- Molecule 89 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (CCD ID: DOL) (formula: C₃₄H₅₀N₄O₉S).



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

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

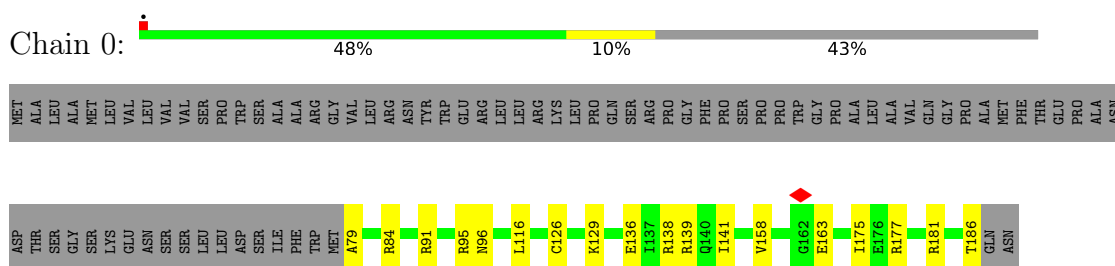


Mol	Chain	Residues	Atoms						AltConf
90	AX	1	Total	C	H	N	O	P	0
			42	10	10	5	14	3	

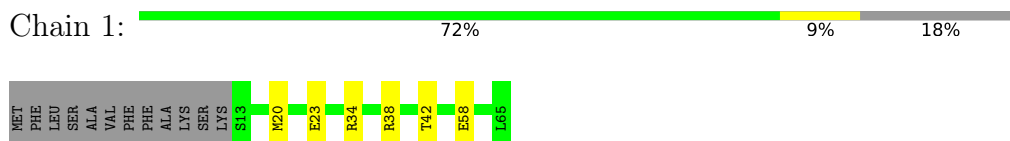
3 Residue-property plots [i](#)

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

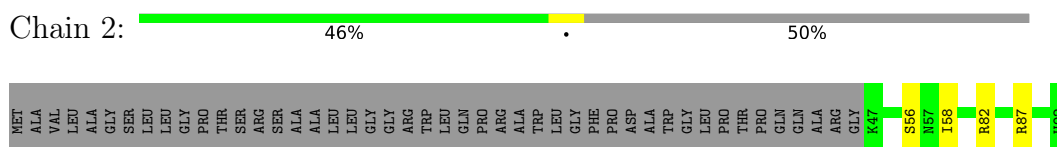
- Molecule 1: 39S ribosomal protein L32, mitochondrial



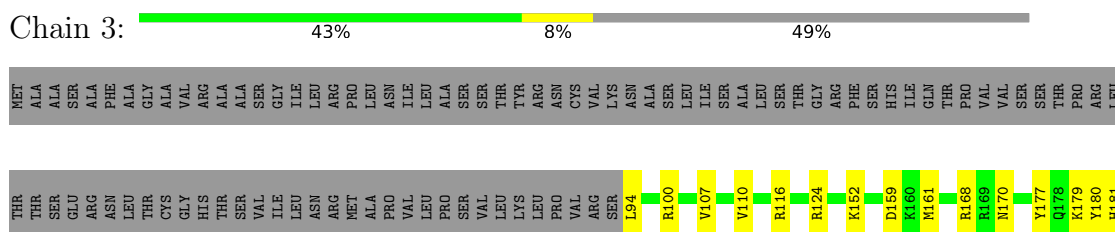
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial



- Molecule 4: 39S ribosomal protein L35, mitochondrial



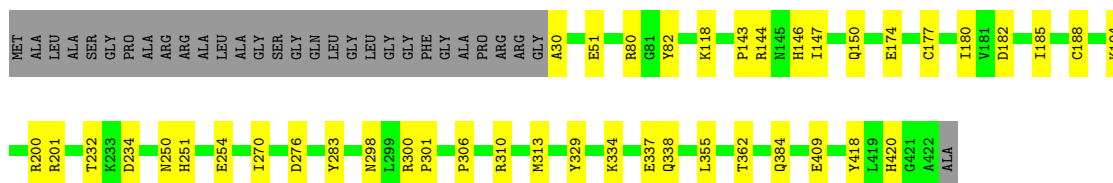
- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:  30% 7% 63%



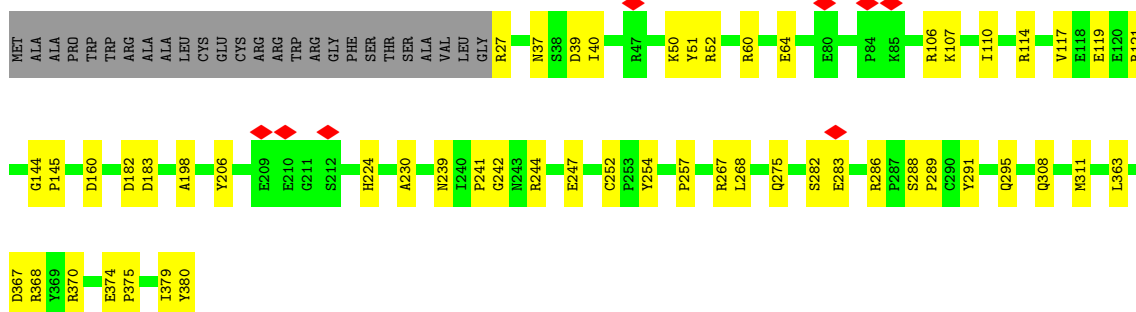
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:  83% 10% 7%



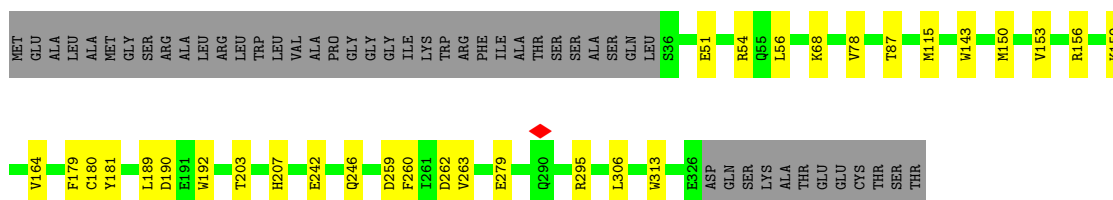
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:  79% 14% 7%



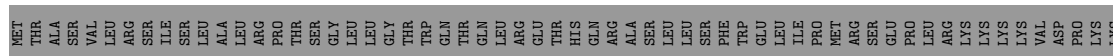
- Molecule 8: 39S ribosomal protein L39, mitochondrial

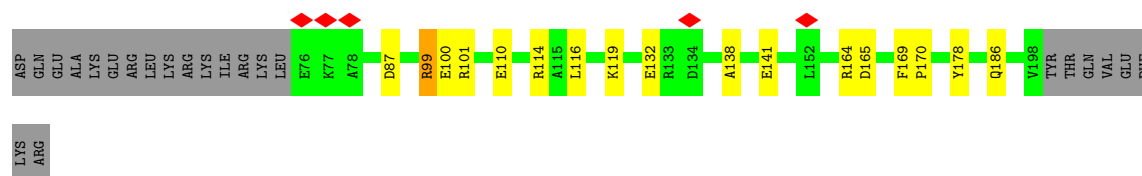
Chain 7:  77% 9% 14%



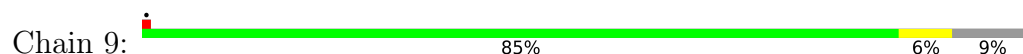
- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:  51% 8% 40%

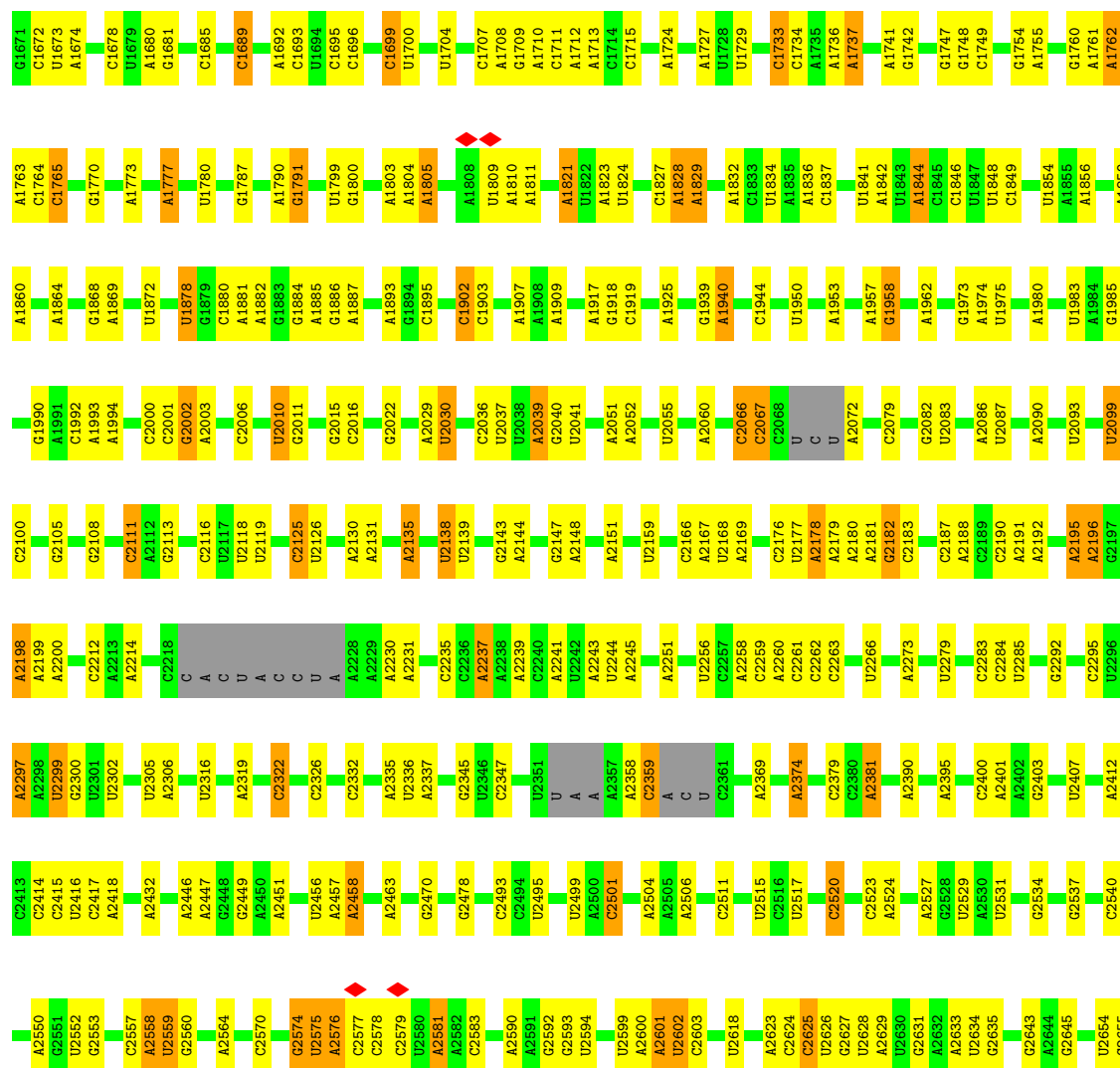


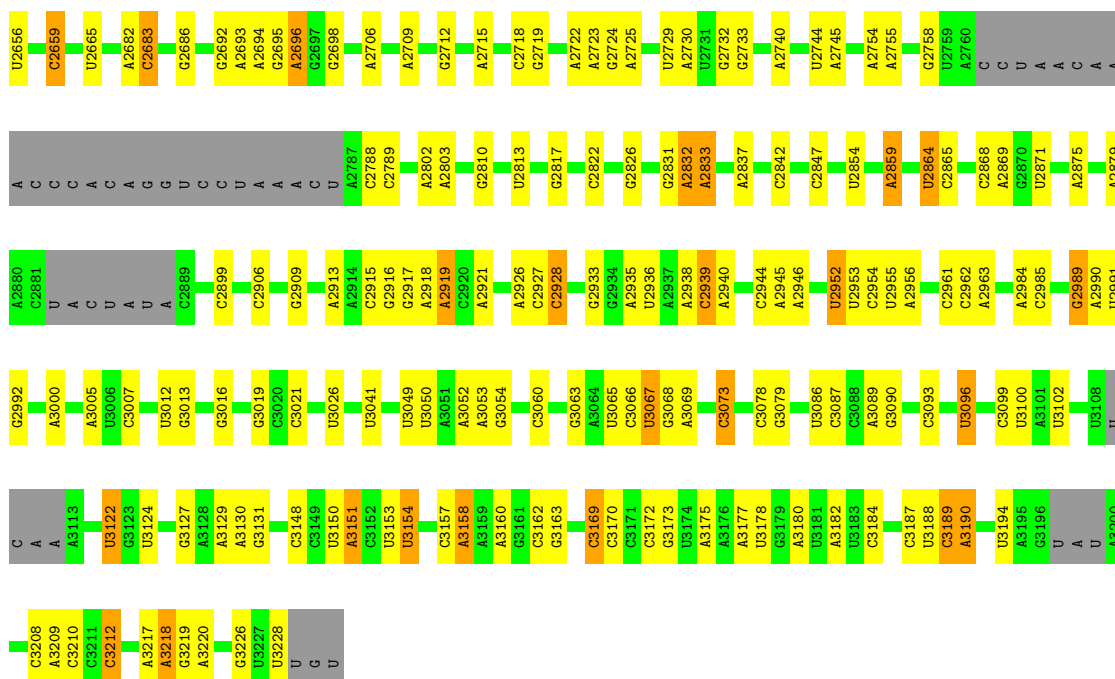


- Molecule 10: 39S ribosomal protein L41, mitochondrial

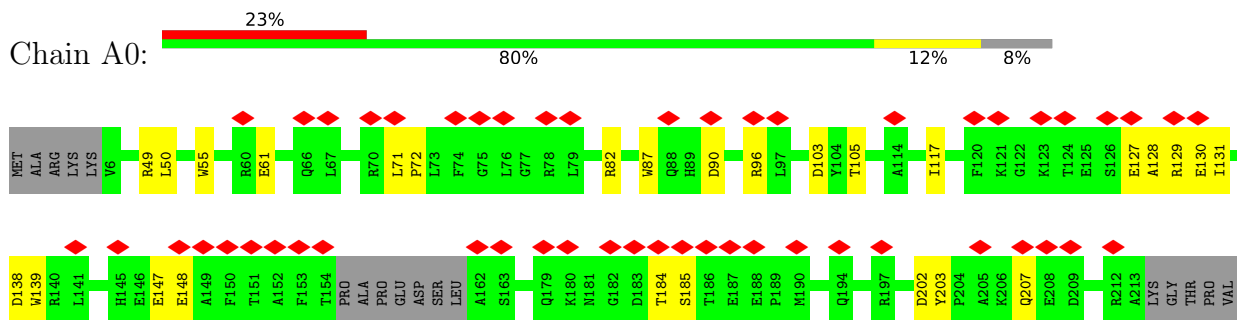


- Molecule 11: 16S mitochondrial rRNA

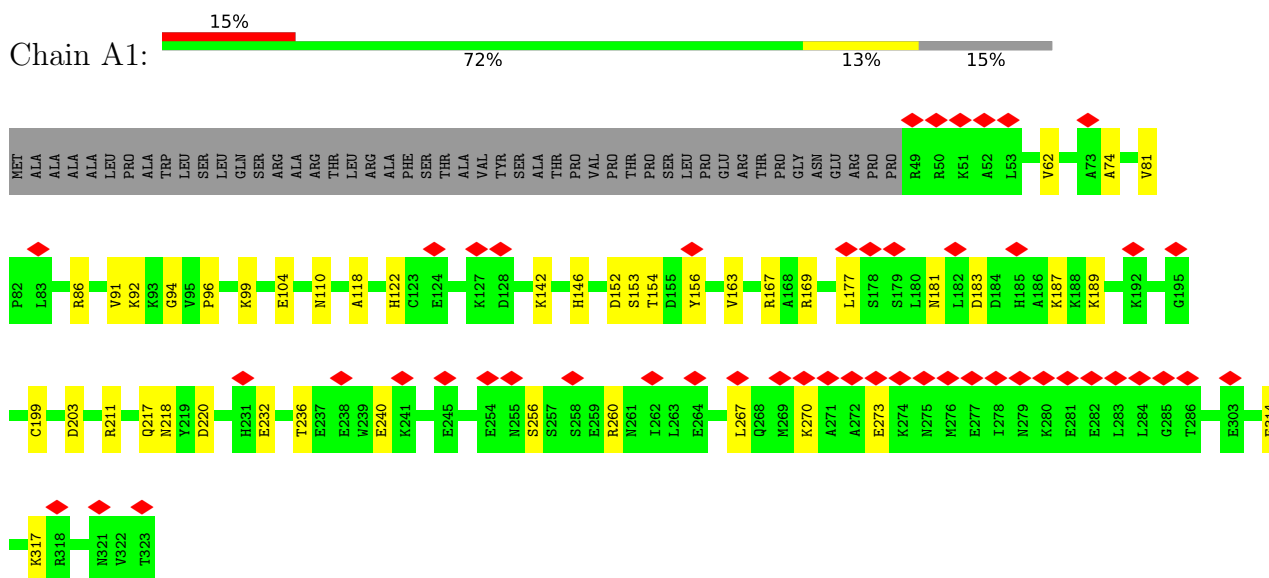




- Molecule 12: 28S ribosomal protein S34, mitochondrial

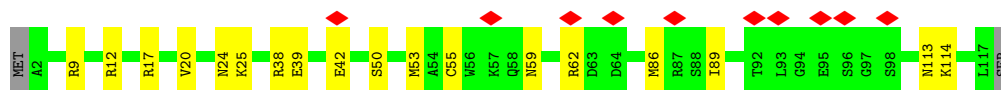


- Molecule 13: 28S ribosomal protein S35, mitochondrial



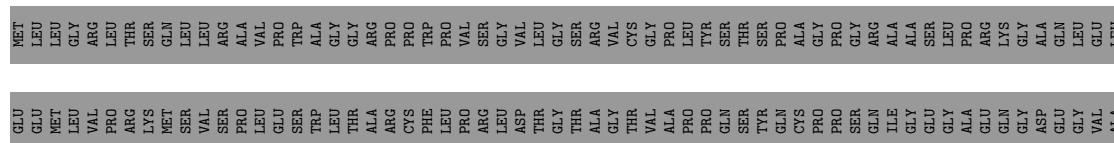
- Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2: 



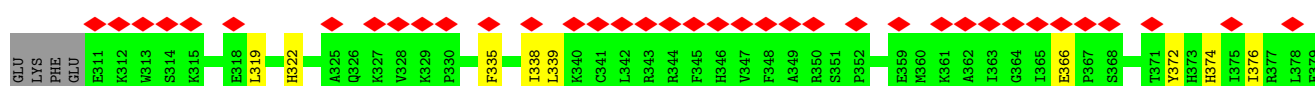
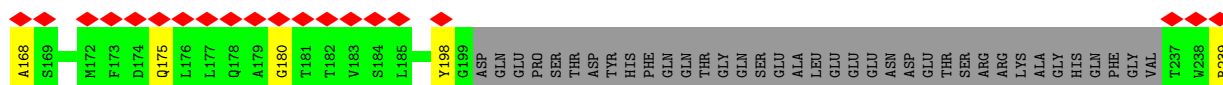
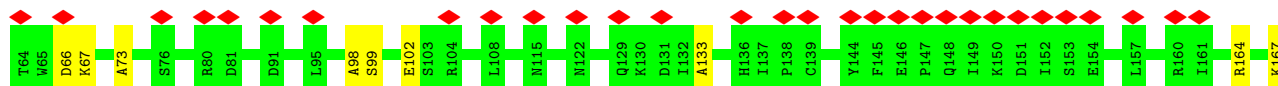
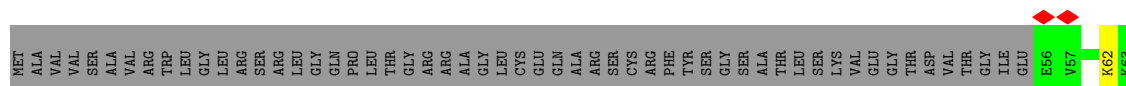
- Molecule 15: Aurora kinase A-interacting protein

Chain A3: 



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

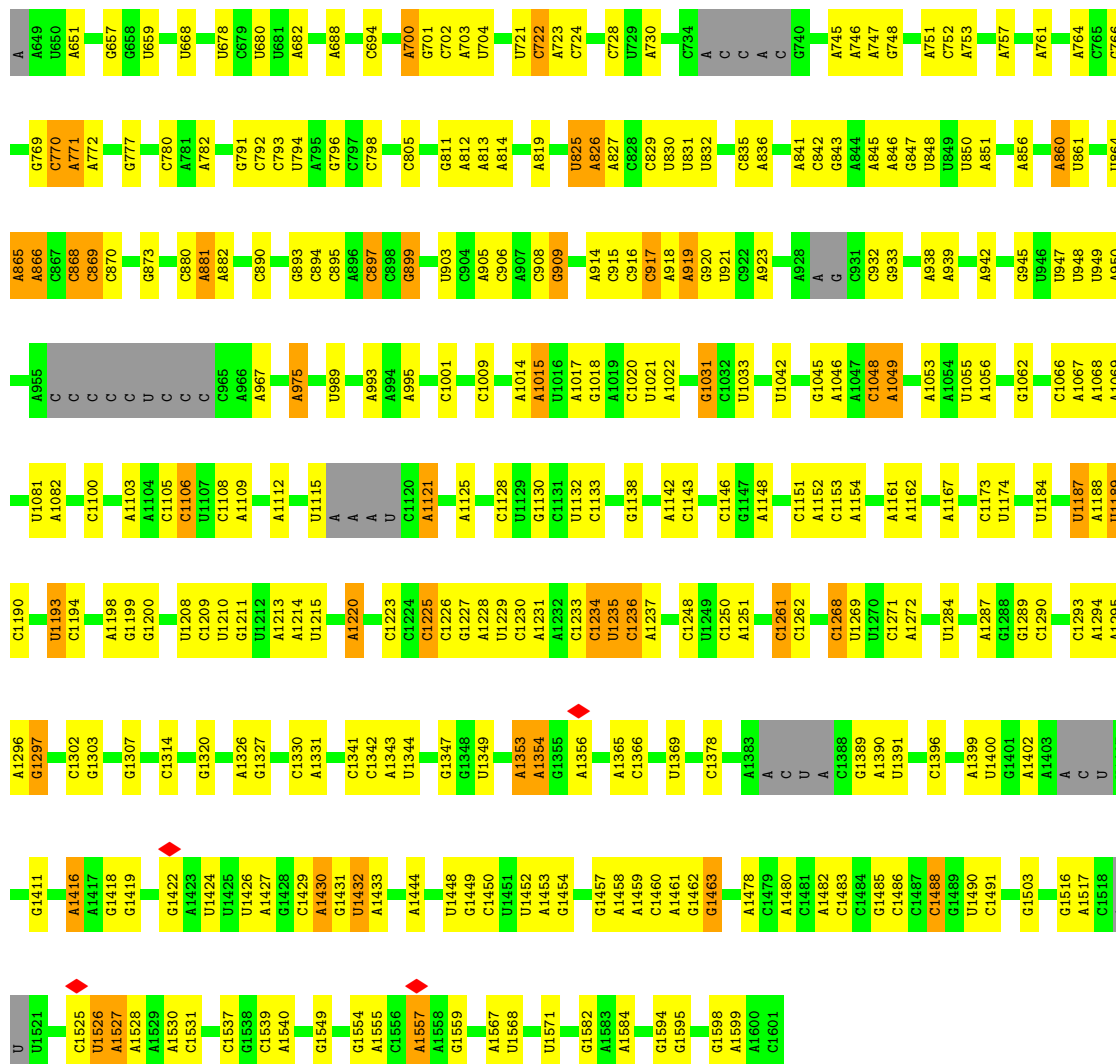
Chain A4: 





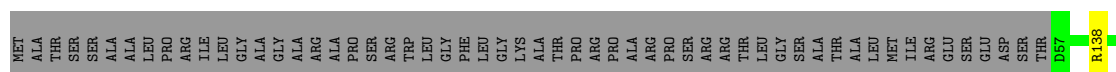
• Molecule 17: 12S mitochondrial rRNA

Chain AA: 64% 28% 5%



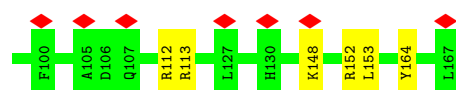
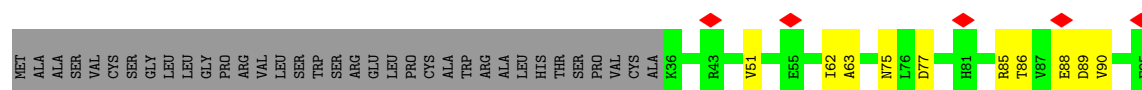
• Molecule 18: 28S ribosomal protein S2, mitochondrial

Chain AB: 69% 5% 26%

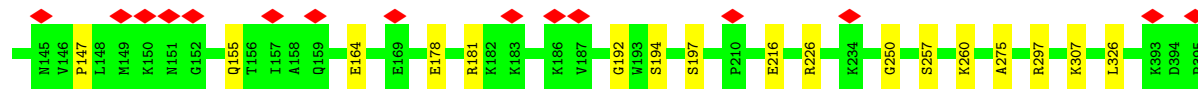
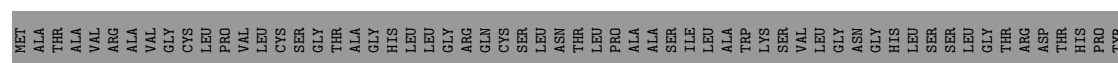
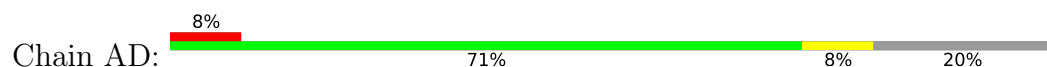




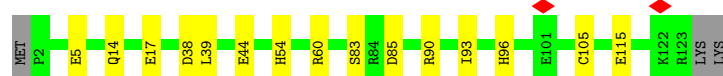
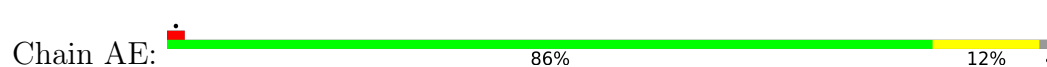
- Molecule 19: 28S ribosomal protein S24, mitochondrial



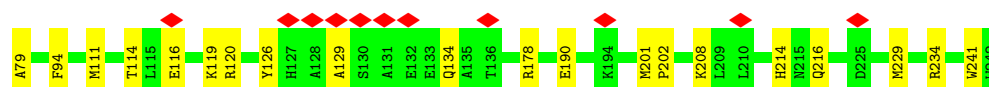
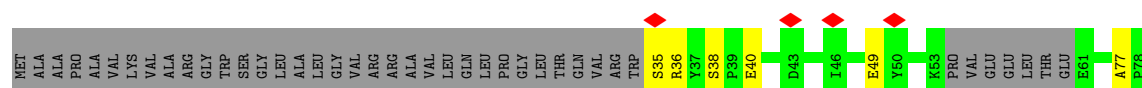
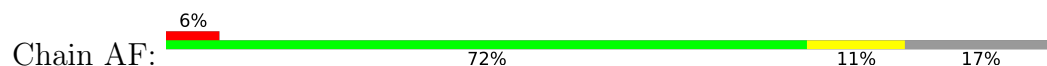
- Molecule 20: 28S ribosomal protein S5, mitochondrial



- Molecule 21: 28S ribosomal protein S6, mitochondrial



- Molecule 22: 28S ribosomal protein S7, mitochondrial

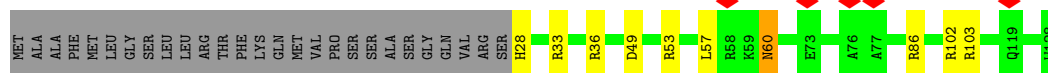


- Chain AG:



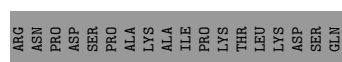
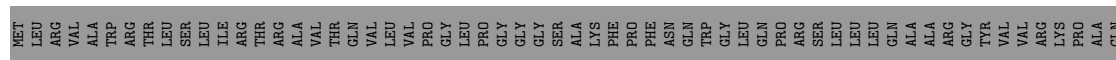
- Molecule 27: 28S ribosomal protein S14, mitochondrial

Chain AK: 



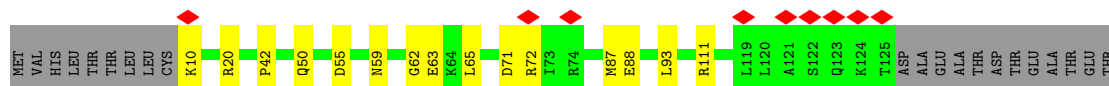
- Molecule 28: 28S ribosomal protein S15, mitochondrial

Chain AL: 



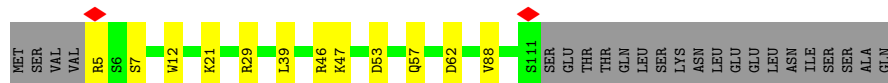
- Molecule 29: 28S ribosomal protein S16, mitochondrial

Chain AM: 



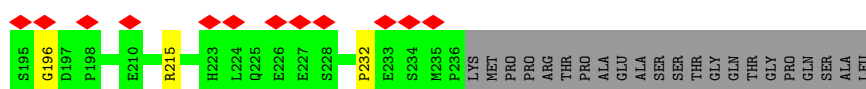
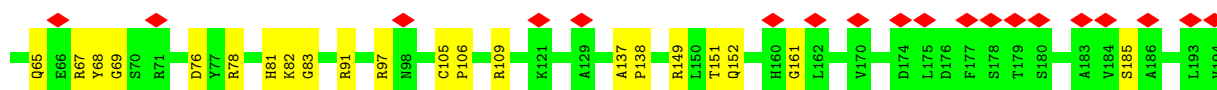
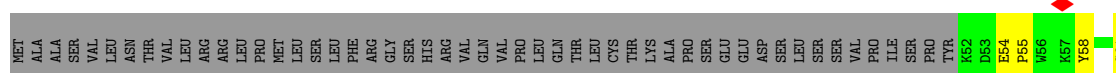
- Molecule 30: 28S ribosomal protein S17, mitochondrial

Chain AN: 

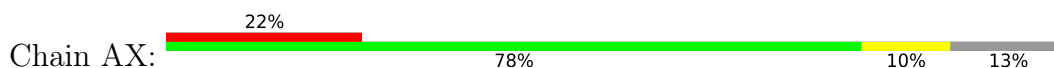


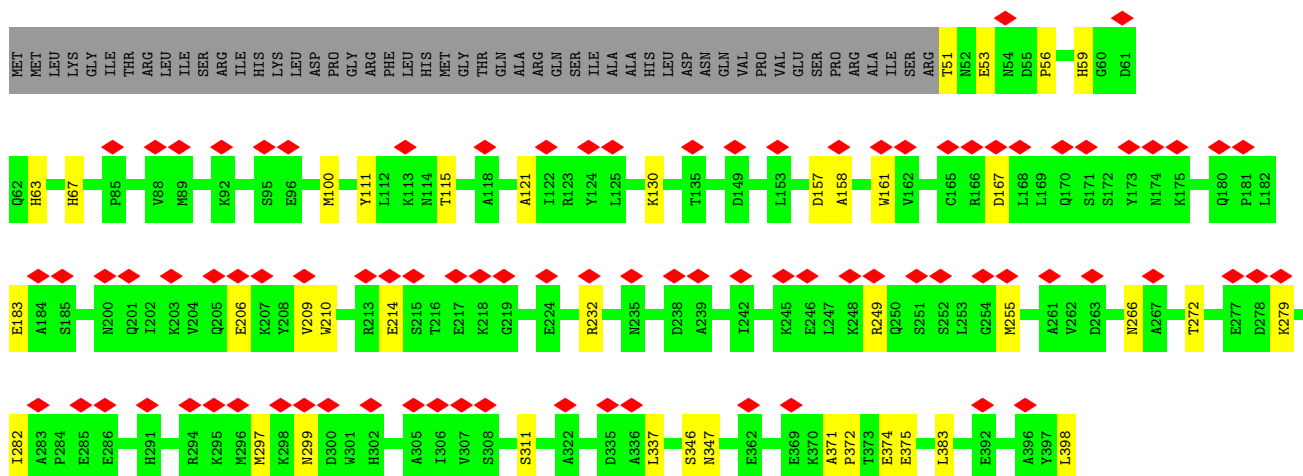
- Molecule 31: 28S ribosomal protein S18b, mitochondrial

Chain AO: 

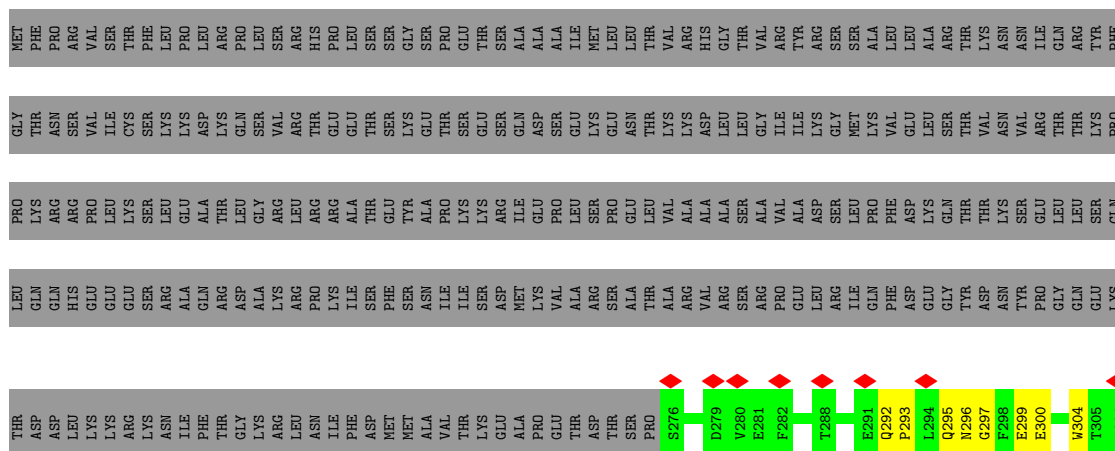


- Chain AT:  82% 12% 6%

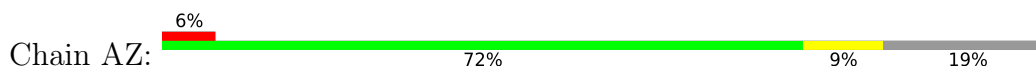




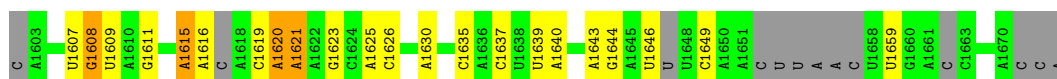
- Molecule 41: 28S ribosomal protein S31, mitochondrial

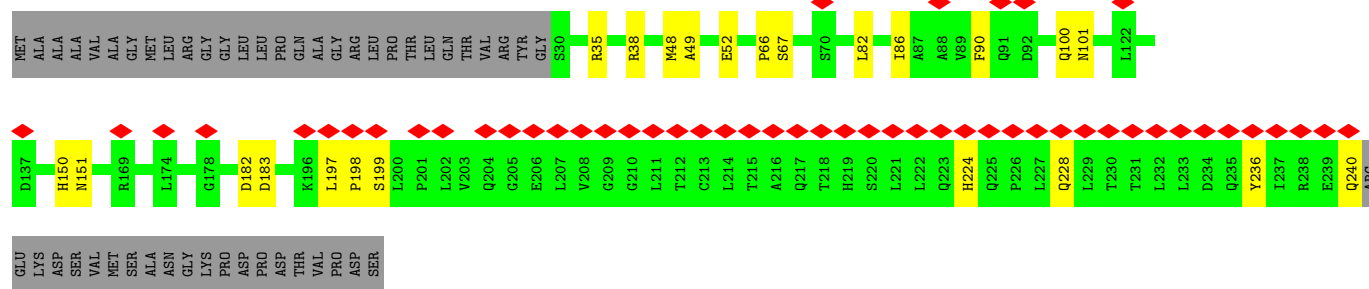
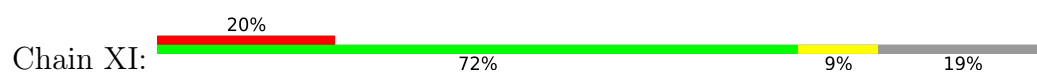


- Molecule 42: 28S ribosomal protein S33, mitochondrial

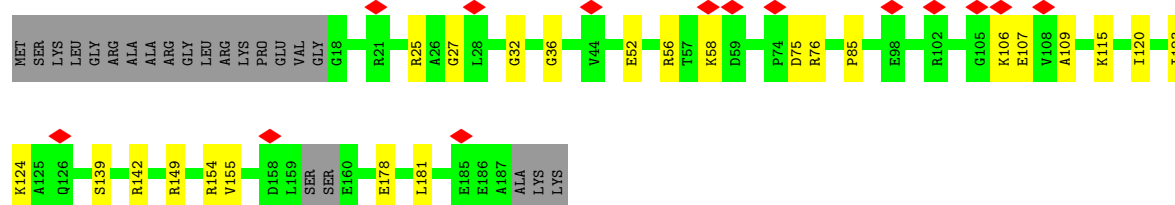
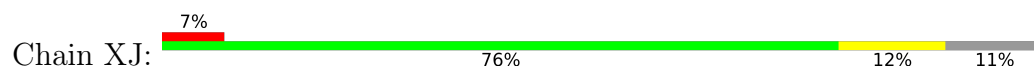


- Molecule 43: mitochondrial tRNAVal





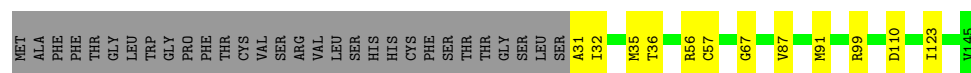
- Molecule 49: 39S ribosomal protein L11, mitochondrial



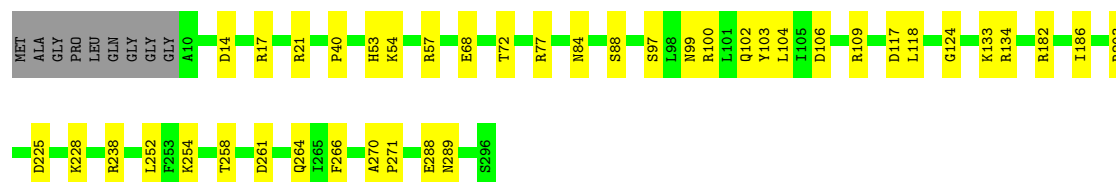
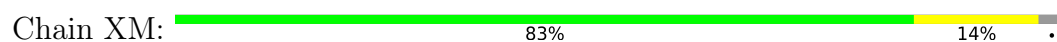
- Molecule 50: 39S ribosomal protein L13, mitochondrial



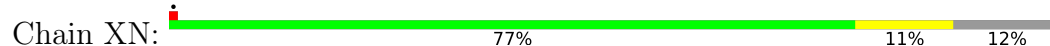
- Molecule 51: 39S ribosomal protein L14, mitochondrial

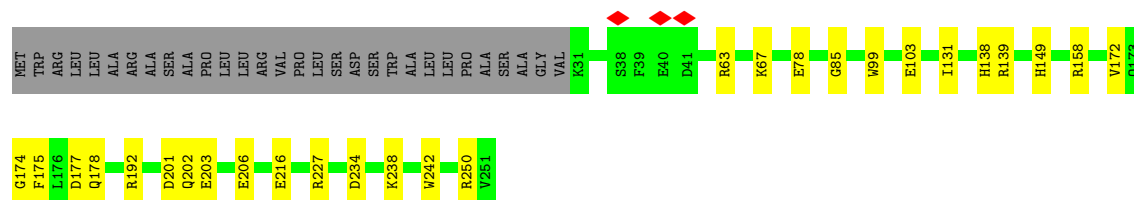


- Molecule 52: 39S ribosomal protein L15, mitochondrial



- Molecule 53: 39S ribosomal protein L16, mitochondrial





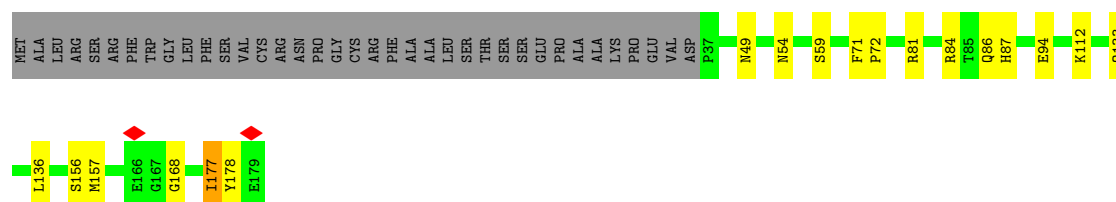
- Molecule 54: 39S ribosomal protein L17, mitochondrial

Chain XO: 75% 12% 13%



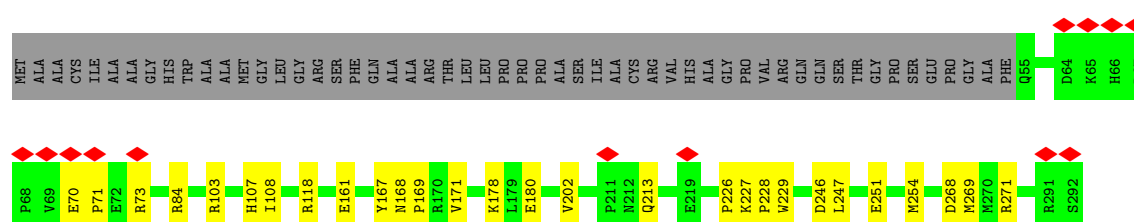
- Molecule 55: 39S ribosomal protein L18, mitochondrial

Chain XP: 69% 9% 21%



- Molecule 56: 39S ribosomal protein L19, mitochondrial

Chain XQ: 72% 10% 18%



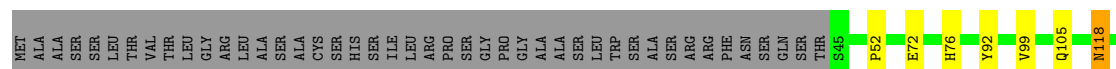
- Molecule 57: 39S ribosomal protein L20, mitochondrial

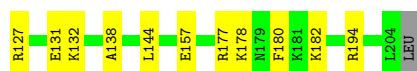
Chain XR: 78% 15% 6%



- Molecule 58: 39S ribosomal protein L21, mitochondrial

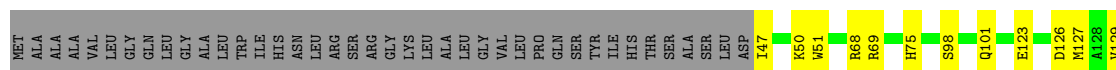
Chain XS: 69% 8% 22%





- Molecule 59: 39S ribosomal protein L22, mitochondrial

Chain XT: 73% 8% 19%



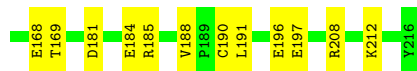
- Molecule 60: 39S ribosomal protein L23, mitochondrial

Chain XU: 83% 9% 8%



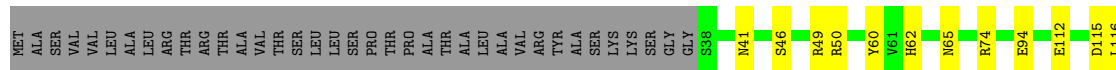
- Molecule 61: 39S ribosomal protein L24, mitochondrial

Chain XV: 78% 15% 6%



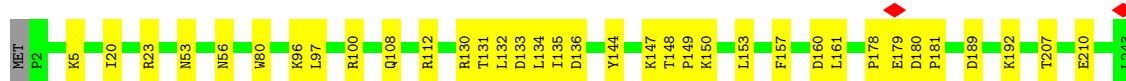
- Molecule 62: 39S ribosomal protein L27, mitochondrial

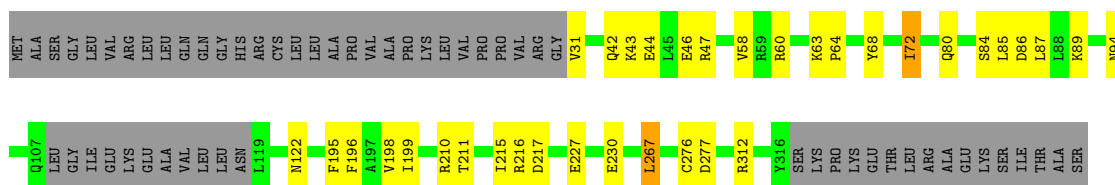
Chain XW: 64% 11% 25%



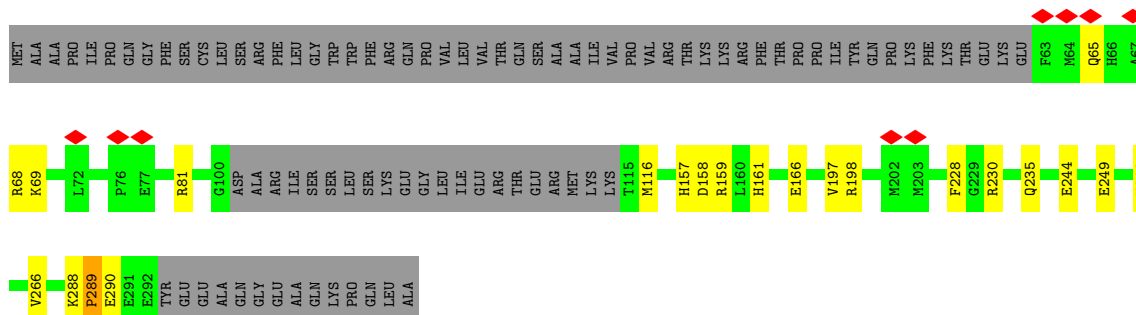
- Molecule 63: 39S ribosomal protein L28, mitochondrial

Chain XX: 81% 14% 5%

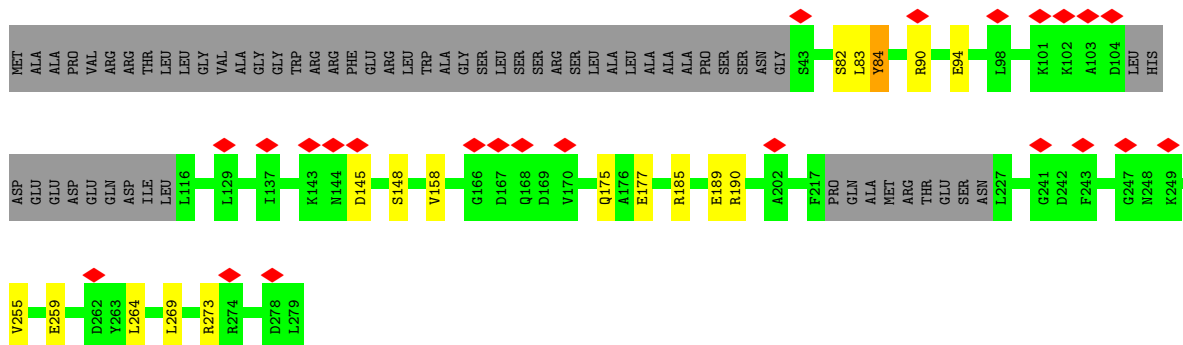




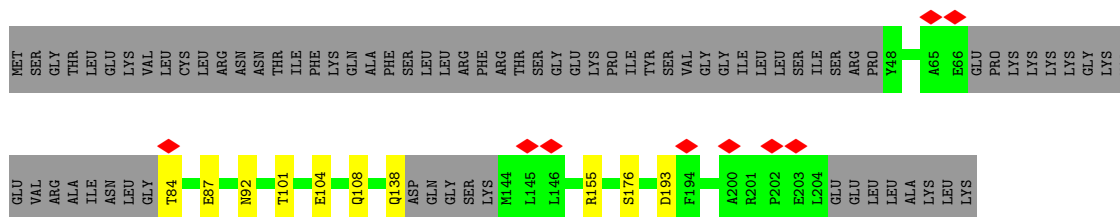
- Molecule 69: 39S ribosomal protein L45, mitochondrial



- Molecule 70: 39S ribosomal protein L46, mitochondrial

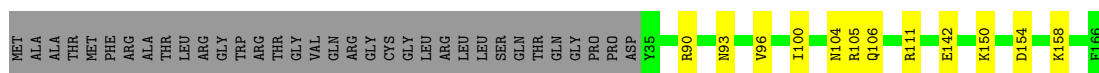


- Molecule 71: 39S ribosomal protein L48, mitochondrial

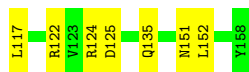
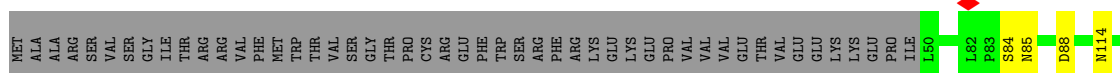


- Molecule 72: 39S ribosomal protein L49, mitochondrial

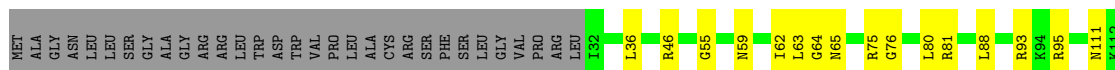




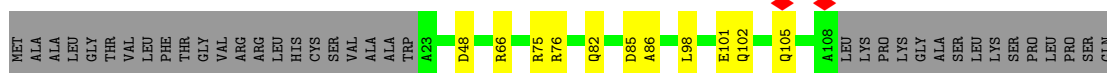
- Molecule 73: 39S ribosomal protein L50, mitochondrial



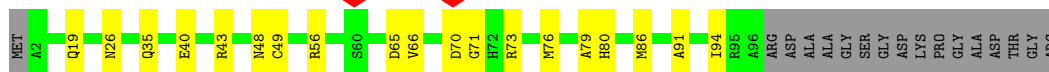
- Molecule 74: 39S ribosomal protein L51, mitochondrial



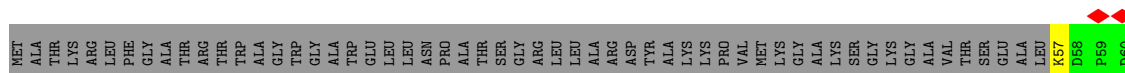
- Molecule 75: 39S ribosomal protein L52, mitochondrial



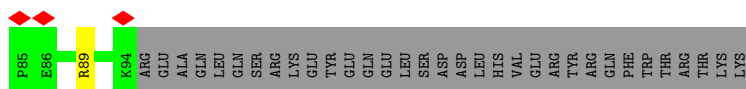
- Molecule 76: 39S ribosomal protein L53, mitochondrial



- Molecule 77: 39S ribosomal protein L54, mitochondrial



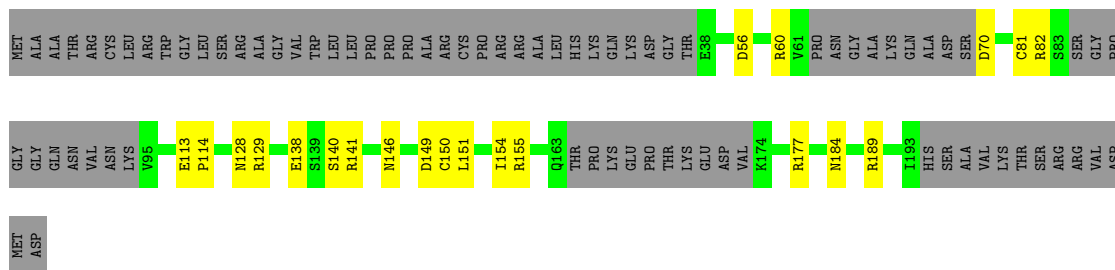
- Chain m: 

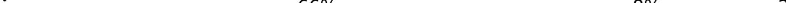


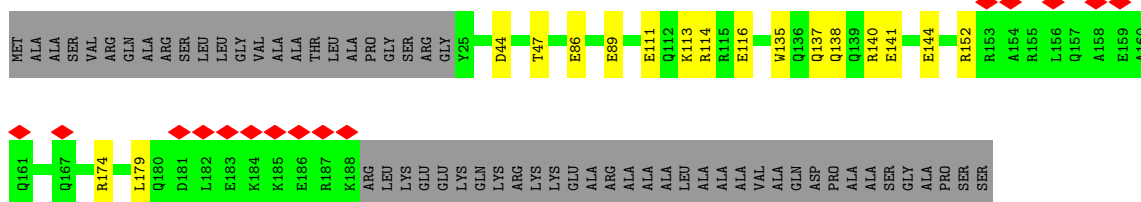
- Chain o: 79% 13% 8%



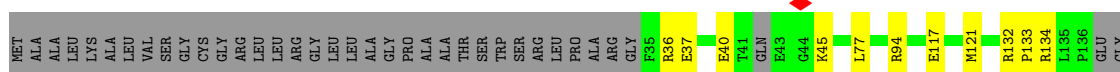
- Chain p: 51% 10% 38%



- Chain q: 



- Chain r: 69% 8% 22%



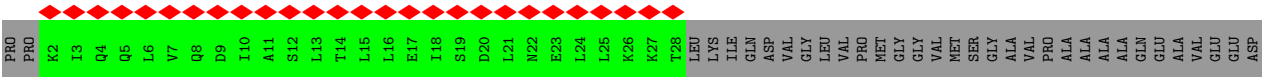
ILE
PRO
LEU
ILE
ALA
LYS
LYS
LYS
GLU
ARG
THR
HIS
LEU
PHE
THR
VAL
GLY
ARG
LEU
THR
LEU
ALA
LYS
PRO
VAL
ASP
LYS
LYS
LYS
LYS
LEU
ILE
LYS
LYS
LYS
TYR
ASN
HIS
GLY
LEU
ASN
LEU
VAL
GLN
GLY
ALA
LYS
LYS
LEU
VAL
GLU
SER
SER
PRO
GLY
HIS
LYS
ARG
GLN
CYS
VAL
ARG
GLU
ALA
LEU
LEU
LEU
PRO
GLY
ALA
GLY
ALA
ILE
LEU
LYS
LYS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

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

● Molecule 85: 39S ribosomal protein L12, mitochondrial



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



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

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

● Molecule 86: Quinupristin



MHT1
T2
DBB3
P4
F5
MHV6
O047
MHT8

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36165	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	0.277	Depositor
Minimum map value	-0.142	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: Y5P, MHT, ZN, P5P, MHW, GTP, MHU, MG, MHV, DOL, 004, DBB

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	0.21	0/895	0.33	0/1201
2	1	0.18	0/444	0.35	0/591
3	2	0.32	0/382	0.44	0/507
4	3	0.29	0/852	0.37	0/1136
5	4	0.21	0/349	0.36	0/461
6	5	0.17	0/3299	0.32	0/4495
7	6	0.16	0/3040	0.32	0/4134
8	7	0.15	0/2420	0.30	0/3270
9	8	1.59	1/1057 (0.1%)	0.39	2/1428 (0.1%)
10	9	0.18	0/1024	0.30	0/1379
11	XA	0.19	0/35637	0.27	0/55463
12	A0	0.12	0/1727	0.32	0/2338
13	A1	0.10	0/2276	0.27	0/3079
14	A2	0.14	0/939	0.32	0/1256
15	A3	0.18	0/621	0.34	0/820
16	A4	0.12	0/4559	0.32	0/6149
17	AA	0.11	0/21952	0.23	0/34164
18	AB	0.13	0/1819	0.28	0/2462
19	AC	0.11	0/1112	0.27	0/1505
20	AD	0.13	0/2768	0.32	0/3707
21	AE	0.13	0/989	0.31	0/1335
22	AF	0.11	0/1708	0.29	0/2291
23	AG	0.11	0/2559	0.28	0/3429
24	AH	0.12	0/1128	0.29	0/1529
25	AI	0.13	0/1031	0.29	0/1390
26	AJ	0.13	0/854	0.31	0/1148
27	AK	0.13	0/879	0.32	0/1182
28	AL	0.13	0/1406	0.30	0/1878
29	AM	0.12	0/941	0.31	0/1265
30	AN	0.12	0/864	0.30	0/1169
31	AO	0.11	0/1580	0.28	0/2150
32	AP	0.13	0/782	0.27	0/1050

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AQ	0.16	0/746	0.32	0/993
34	AR	0.69	1/2103 (0.0%)	0.58	6/2842 (0.2%)
35	AS	0.12	0/1127	0.28	0/1518
36	AT	0.11	0/1361	0.30	0/1829
37	AU	0.13	0/1482	0.29	0/1987
38	AV	0.10	0/2925	0.29	0/3948
39	AW	0.11	0/778	0.27	0/1048
40	AX	0.10	0/2886	0.29	0/3909
41	AY	0.11	0/985	0.31	0/1329
42	AZ	0.12	0/748	0.30	0/1000
43	XB	0.10	0/1400	0.20	0/2168
44	XD	0.22	0/1879	0.37	0/2527
45	XE	0.22	0/2465	0.31	0/3344
46	XF	0.27	0/2071	0.36	0/2817
47	XH	0.17	0/798	0.36	0/1073
48	XI	0.15	0/1727	0.33	0/2340
49	XJ	0.11	0/1309	0.28	0/1764
50	XK	0.25	0/1495	0.33	0/2029
51	XL	0.19	0/904	0.29	0/1218
52	XM	0.24	0/2359	0.36	0/3185
53	XN	0.22	0/1825	0.36	0/2458
54	XO	0.21	0/1269	0.38	0/1708
55	XP	0.20	0/1190	0.34	0/1611
56	XQ	0.17	0/2026	0.33	0/2734
57	XR	0.29	0/1174	0.38	0/1572
58	XS	0.26	0/1311	0.34	0/1778
59	XT	0.24	0/1402	0.35	0/1886
60	XU	0.21	0/1200	0.35	0/1623
61	XV	0.16	0/1693	0.34	0/2297
62	XW	0.23	0/893	0.34	0/1204
63	XX	0.36	2/2090 (0.1%)	0.49	3/2825 (0.1%)
64	XY	0.20	0/1571	0.34	0/2106
65	XZ	0.25	0/1003	0.36	0/1354
66	a	0.20	0/834	0.36	0/1133
67	b	0.23	0/1202	0.37	0/1626
68	c	0.19	0/2264	0.31	0/3059
69	d	0.14	0/1807	0.27	0/2450
70	e	0.77	6/1797 (0.3%)	0.29	0/2422
71	f	0.16	0/1103	0.31	0/1490
72	g	0.25	0/1134	0.39	0/1547
73	h	0.15	0/909	0.30	0/1238
74	i	0.28	0/849	0.42	0/1135
75	j	0.19	0/703	0.32	0/947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	k	0.12	0/743	0.30	0/1003
77	l	0.12	0/692	0.30	0/939
78	m	0.13	0/508	0.36	0/682
79	o	0.26	0/818	0.36	0/1097
80	p	0.14	0/1071	0.27	0/1433
81	q	0.15	0/1413	0.31	0/1906
82	r	0.19	0/1282	0.32	0/1734
84	s	0.20	0/3114	0.34	0/4225
85	t1	0.13	0/366	0.28	0/497
85	t2	0.08	0/238	0.22	0/319
85	t3	0.10	0/238	0.23	0/319
85	t4	0.09	0/229	0.23	0/308
85	t5	0.10	0/229	0.23	0/308
85	t6	0.12	0/213	0.28	0/286
86	A	0.65	0/13	0.82	0/15
All	All	0.24	10/175857 (0.0%)	0.31	11/249503 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
44	XD	0	1
48	XI	0	2
55	XP	0	1
71	f	0	1
86	A	2	3
All	All	2	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	99	ARG	CG-CD	51.33	3.06	1.52
34	AR	308	HIS	C-N	-30.34	1.00	1.34
70	e	84	TYR	CD2-CE2	16.29	1.87	1.38
70	e	84	TYR	CD1-CE1	15.58	1.85	1.38
70	e	84	TYR	CE1-CZ	12.32	1.67	1.38
70	e	84	TYR	CE2-CZ	11.91	1.66	1.38
63	XX	150	LYS	C-N	11.86	1.50	1.33
70	e	84	TYR	CG-CD1	11.35	1.63	1.39
70	e	84	TYR	CG-CD2	9.87	1.60	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	XX	149	PRO	N-CD	5.36	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AR	309	PRO	O-C-N	13.55	141.32	122.35
63	XX	150	LYS	CA-C-N	12.27	141.22	120.72
63	XX	150	LYS	C-N-CA	12.27	141.22	120.72
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	6.77	126.88	111.30
63	XX	149	PRO	CB-CA-C	6.71	119.74	110.95
34	AR	308	HIS	CA-C-N	-6.12	113.50	119.87
34	AR	308	HIS	C-N-CA	-6.12	113.50	119.87
34	AR	308	HIS	O-C-N	6.02	126.79	121.37
9	8	99	ARG	CG-CD-NE	5.45	123.99	112.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
86	A	2	THR	CB
86	A	4	PRO	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
86	A	3	DBB	Peptide
86	A	4	PRO	Peptide
86	A	5	MHU	Peptide
44	XD	206	TYR	Peptide
48	XI	197	LEU	Peptide
48	XI	90	PHE	Peptide
55	XP	177	ILE	Peptide
71	f	138	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	880	903	903	13	0
2	1	439	480	480	4	0
3	2	376	407	406	5	0
4	3	831	883	883	10	0
5	4	341	361	361	6	0
6	5	3204	3201	3201	33	0
7	6	2947	2839	2839	38	0
8	7	2365	2372	2372	17	0
9	8	1033	1036	1036	41	0
10	9	996	987	987	6	0
11	XA	31853	16172	16181	252	0
12	A0	1684	1685	1685	17	0
13	A1	2230	2261	2261	27	0
14	A2	925	964	964	15	0
15	A3	610	682	682	8	0
16	A4	4470	4485	4486	39	0
17	AA	19628	9964	9971	150	0
18	AB	1776	1769	1769	9	0
19	AC	1082	1088	1088	12	0
20	AD	2716	2785	2785	26	0
21	AE	972	1001	1001	10	0
22	AF	1668	1714	1716	21	0
23	AG	2505	2491	2490	29	0
24	AH	1105	1136	1136	13	0
25	AI	1011	1052	1052	8	0
26	AJ	838	887	887	9	0
27	AK	861	885	885	8	0
28	AL	1382	1472	1472	13	0
29	AM	920	951	951	14	0
30	AN	846	908	908	12	0
31	AO	1528	1489	1489	20	0
32	AP	765	796	796	6	0
33	AQ	734	749	749	6	0
34	AR	2060	2074	2074	33	0
35	AS	1100	1103	1103	10	0
36	AT	1330	1342	1342	14	0
37	AU	1461	1471	1471	13	0
38	AV	2867	2863	2862	24	0
39	AW	766	785	785	6	0
40	AX	2814	2805	2804	25	0
41	AY	956	912	911	11	0
42	AZ	731	734	734	6	0
43	XB	1255	635	640	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	XD	1842	1896	1896	21	0
45	XE	2396	2402	2402	18	0
46	XF	2013	2045	2044	28	0
47	XH	784	832	832	7	0
48	XI	1691	1783	1783	13	0
49	XJ	1291	1366	1364	17	0
50	XK	1451	1448	1448	9	0
51	XL	889	941	941	8	0
52	XM	2305	2377	2377	28	0
53	XN	1778	1808	1808	18	0
54	XO	1245	1283	1283	16	0
55	XP	1164	1162	1162	16	0
56	XQ	1978	2022	2022	17	0
57	XR	1153	1214	1214	23	0
58	XS	1284	1354	1354	18	0
59	XT	1368	1410	1410	15	0
60	XU	1171	1164	1164	10	0
61	XV	1648	1656	1654	25	0
62	XW	871	898	898	14	0
63	XX	2035	2054	2054	29	0
64	XY	1534	1575	1575	23	0
65	XZ	978	1030	1030	15	0
66	a	809	775	773	4	0
67	b	1178	1180	1180	8	0
68	c	2217	2220	2220	20	0
69	d	1758	1743	1742	17	0
70	e	1762	1767	1767	42	0
71	f	1083	1089	1089	7	0
72	g	1097	1086	1085	11	0
73	h	886	870	870	7	0
74	i	827	857	857	18	0
75	j	689	678	678	11	0
76	k	732	745	745	12	0
77	l	673	654	653	11	0
78	m	500	525	525	11	0
79	o	797	804	804	11	0
80	p	1058	1083	1083	16	0
81	q	1379	1359	1359	10	0
82	r	1247	1267	1267	14	0
83	r4	1485	0	835	41	0
84	s	3036	3023	3022	39	0
85	t1	354	379	374	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	t2	238	268	270	1	0
85	t3	238	268	270	2	0
85	t4	229	255	257	0	0
85	t5	229	255	257	0	0
85	t6	214	236	236	0	0
86	A	73	67	64	4	0
87	0	1	0	0	0	0
87	4	1	0	0	0	0
87	AB	1	0	0	0	0
87	AO	1	0	0	0	0
87	AP	1	0	0	0	0
87	AT	1	0	0	0	0
87	r	1	0	0	0	0
88	AA	46	0	0	0	0
88	XA	143	0	0	0	0
88	XD	1	0	0	0	0
88	XE	1	0	0	0	0
88	XI	1	0	0	0	0
88	XM	2	0	0	0	0
88	g	1	0	0	0	0
89	XA	48	50	50	2	0
90	AX	32	10	12	1	0
All	All	168800	142812	143657	1401	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 (1401) 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	1.85	1.64
70:e:84:TYR:CD2	70:e:84:TYR:CE2	1.87	1.58
9:8:99:ARG:CD	70:e:84:TYR:CD1	2.25	1.20
9:8:99:ARG:CG	70:e:84:TYR:CD2	2.27	1.17
9:8:99:ARG:CD	70:e:84:TYR:CD2	2.29	1.16
9:8:99:ARG:CG	70:e:84:TYR:CD1	2.28	1.15
9:8:99:ARG:CG	70:e:84:TYR:CE1	2.30	1.15
9:8:99:ARG:CD	70:e:84:TYR:CE1	2.28	1.15
9:8:99:ARG:CG	70:e:84:TYR:CE2	2.30	1.14
9:8:99:ARG:CD	70:e:84:TYR:CE2	2.29	1.13
9:8:99:ARG:CD	70:e:84:TYR:CG	2.32	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:99:ARG:CD	70:e:84:TYR:CZ	2.33	1.11
9:8:99:ARG:CG	70:e:84:TYR:CZ	2.35	1.10
9:8:99:ARG:CG	70:e:84:TYR:CG	2.33	1.09
63:XX:144:TYR:CE1	63:XX:148:THR:HG21	1.91	1.04
34:AR:305:HIS:HD2	34:AR:314:ALA:HB2	1.23	1.02
9:8:99:ARG:HD3	70:e:84:TYR:CD1	1.94	0.99
11:XA:1881:A:OP2	72:g:111:ARG:NH2	1.96	0.97
9:8:99:ARG:HD2	70:e:84:TYR:CZ	1.97	0.96
9:8:99:ARG:HG2	70:e:84:TYR:CD2	2.01	0.94
9:8:99:ARG:HG3	70:e:84:TYR:CZ	2.01	0.93
34:AR:305:HIS:HD2	34:AR:314:ALA:CB	1.81	0.93
58:XS:138:ALA:O	67:b:127:GLN:NE2	2.02	0.92
11:XA:1777:A:N6	11:XA:1780:U:OP2	2.02	0.91
55:XP:49:ASN:ND2	55:XP:54:ASN:OD1	2.03	0.91
11:XA:2144:A:OP1	57:XR:57:ARG:NH1	2.05	0.90
13:A1:154:THR:OG1	24:AH:171:GLU:OE2	1.89	0.89
68:c:42:GLN:NE2	74:i:36:LEU:O	2.05	0.89
70:e:264:LEU:O	70:e:273:ARG:NH2	2.04	0.89
6:5:300:ARG:NH2	11:XA:2390:A:OP1	2.06	0.88
11:XA:1837:C:OP1	67:b:4:ARG:NH2	2.07	0.88
11:XA:1680:A:OP1	64:XY:230:LYS:NZ	2.07	0.88
9:8:99:ARG:NE	70:e:84:TYR:CD2	2.42	0.88
25:AI:71:SER:O	25:AI:74:ARG:NH1	2.07	0.88
34:AR:305:HIS:CD2	34:AR:314:ALA:HB2	2.10	0.87
11:XA:2754:A:OP1	47:XH:91:LYS:NZ	2.07	0.87
11:XA:2108:G:N7	53:XN:67:LYS:NZ	2.22	0.86
84:s:152:GLN:NE2	84:s:179:GLN:OE1	2.08	0.86
11:XA:2517:U:OP1	44:XD:287:ARG:NH2	2.08	0.86
1:0:139:ARG:NH2	11:XA:2322:C:OP1	2.09	0.85
11:XA:2822:C:O2'	11:XA:2915:C:OP2	1.95	0.85
9:8:99:ARG:CB	70:e:84:TYR:CD1	2.59	0.85
1:0:95:ARG:NH1	11:XA:1821:A:OP2	2.10	0.85
17:AA:826:A:OP1	26:AJ:55:ARG:NH1	2.10	0.84
17:AA:1530:A:OP1	38:AV:64:LYS:NZ	2.11	0.84
37:AU:126:GLN:OE1	37:AU:129:ARG:NH2	2.10	0.84
9:8:87:ASP:O	78:m:45:ARG:NH1	2.10	0.84
22:AF:79:ALA:O	23:AG:312:GLN:NE2	2.11	0.83
44:XD:132:ASP:OD2	44:XD:135:ARG:NH1	2.10	0.83
11:XA:2111:C:OP1	48:XI:35:ARG:NH1	2.11	0.83
11:XA:2864:U:O5'	62:XW:50:ARG:NH1	2.10	0.83
11:XA:1689:C:OP2	63:XX:5:LYS:NZ	2.11	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:1958:G:OP2	59:XT:160:GLY:N	2.12	0.83
51:XL:31:ALA:N	51:XL:91:MET:SD	2.52	0.83
17:AA:728:C:OP1	30:AN:5:ARG:NH2	2.11	0.83
29:AM:55:ASP:OD2	36:AT:146:GLN:NE2	2.12	0.83
23:AG:198:ARG:N	23:AG:246:ARG:O	2.11	0.82
20:AD:127:ASN:O	42:AZ:72:ARG:NH1	2.11	0.82
11:XA:2166:C:O2	11:XA:2214:A:N6	2.12	0.82
25:AI:81:GLU:O	25:AI:148:ARG:NH1	2.12	0.82
68:c:80:GLN:O	68:c:210:ARG:NH2	2.12	0.82
17:AA:1396:C:O3'	78:m:89:ARG:NH1	2.11	0.82
12:A0:49:ARG:NH2	37:AU:41:ARG:O	2.11	0.82
11:XA:2537:G:O2'	11:XA:2634:U:OP2	1.97	0.82
17:AA:1483:C:N3	17:AA:1567:A:N1	2.28	0.81
46:XF:257:GLN:OE1	52:XM:21:ARG:NH1	2.13	0.81
9:8:99:ARG:HG2	70:e:84:TYR:CE2	2.14	0.81
15:A3:142:LYS:NZ	17:AA:1490:U:OP1	2.14	0.81
71:f:176:SER:O	78:m:35:SER:N	2.12	0.81
7:6:160:ASP:OD2	7:6:267:ARG:NH1	2.12	0.81
63:XX:144:TYR:CE1	63:XX:148:THR:CG2	2.63	0.81
9:8:164:ARG:NH1	71:f:87:GLU:O	2.14	0.80
13:A1:92:LYS:NZ	17:AA:1302:C:OP2	2.12	0.80
2:1:34:ARG:NH2	2:1:38:ARG:O	2.15	0.80
11:XA:2187:C:O3'	49:XJ:106:LYS:NZ	2.15	0.80
17:AA:701:G:N2	17:AA:841:A:O2'	2.14	0.80
10:9:137:ARG:NE	60:XU:21:ARG:O	2.14	0.80
32:AP:140:TYR:O	32:AP:141:ARG:NE	2.15	0.80
1:0:136:GLU:OE1	1:0:177:ARG:NH2	2.13	0.80
44:XD:124:GLU:OE2	44:XD:165:ASN:ND2	2.15	0.79
56:XQ:178:LYS:NZ	56:XQ:180:GLU:OE2	2.14	0.79
60:XU:11:ARG:NH2	61:XV:212:LYS:O	2.15	0.79
29:AM:93:LEU:O	34:AR:175:ARG:NH2	2.14	0.79
23:AG:200:LEU:O	23:AG:218:TYR:OH	2.01	0.79
17:AA:868:C:OP2	17:AA:870:C:N4	2.17	0.78
9:8:164:ARG:NH1	71:f:84:THR:O	2.16	0.78
17:AA:659:U:OP1	20:AD:226:ARG:NH2	2.17	0.78
69:d:288:LYS:O	69:d:290:GLU:N	2.16	0.78
11:XA:1773:A:OP2	68:c:31:VAL:N	2.17	0.78
14:A2:12:ARG:NH2	17:AA:1125:A:O4'	2.17	0.78
53:XN:201:ASP:OD1	53:XN:202:GLN:N	2.17	0.77
17:AA:947:U:OP1	28:AL:162:GLN:NE2	2.16	0.77
13:A1:74:ALA:O	13:A1:110:ASN:ND2	2.17	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A2:42:GLU:N	22:AF:241:TRP:O	2.18	0.77
29:AM:20:ARG:NH1	29:AM:42:PRO:O	2.17	0.77
56:XQ:70:GLU:OE1	56:XQ:213:GLN:NE2	2.17	0.77
81:q:111:GLU:OE2	81:q:114:ARG:NH1	2.17	0.77
18:AB:149:ARG:NH2	33:AQ:82:ASP:OD2	2.18	0.77
80:p:56:ASP:OD2	80:p:60:ARG:NH2	2.18	0.77
7:6:282:SER:O	7:6:283:GLU:N	2.18	0.77
9:8:110:GLU:OE2	9:8:114:ARG:NE	2.18	0.77
23:AG:357:THR:OG1	23:AG:360:GLU:OE1	2.03	0.77
7:6:380:TYR:O	52:XM:97:SER:OG	2.02	0.76
20:AD:178:GLU:OE2	20:AD:181:ARG:NH2	2.18	0.76
38:AV:192:LYS:NZ	38:AV:194:THR:O	2.18	0.76
46:XF:167:MET:SD	46:XF:279:ARG:NH1	2.57	0.76
1:0:181:ARG:NH1	1:0:186:THR:O	2.19	0.76
11:XA:1747:G:OP2	11:XA:1749:C:N4	2.18	0.76
48:XI:224:HIS:O	48:XI:228:GLN:N	2.18	0.76
8:7:242:GLU:OE2	8:7:246:GLN:NE2	2.19	0.76
14:A2:9:ARG:NH2	17:AA:1021:U:OP2	2.19	0.76
23:AG:276:ARG:NH1	23:AG:373:ASP:OD2	2.19	0.76
26:AJ:84:ARG:NH1	26:AJ:85:LEU:O	2.19	0.76
11:XA:1828:A:N6	11:XA:2683:C:O2	2.18	0.76
23:AG:310:ARG:NH1	40:AX:383:LEU:O	2.18	0.76
4:3:168:ARG:NH2	4:3:170:ASN:OD1	2.18	0.76
18:AB:197:HIS:NE2	18:AB:240:ASP:O	2.19	0.75
40:AX:111:TYR:O	40:AX:115:THR:OG1	2.04	0.75
47:XH:103:GLU:OE1	47:XH:104:ASN:ND2	2.20	0.75
17:AA:917:C:OP2	31:AO:91:ARG:NH2	2.19	0.75
57:XR:122:ARG:NH2	57:XR:126:GLU:OE2	2.19	0.75
61:XV:197:GLU:OE2	64:XY:95:ASN:ND2	2.19	0.75
3:2:56:SER:OG	11:XA:1980:A:OP1	2.04	0.75
38:AV:96:ARG:NH2	38:AV:101:CYS:O	2.18	0.75
11:XA:2529:U:OP2	44:XD:208:ARG:NH1	2.20	0.75
63:XX:144:TYR:CD1	63:XX:148:THR:HG21	2.20	0.75
10:9:22:THR:OG1	10:9:36:ARG:NH1	2.19	0.75
17:AA:860:A:N7	17:AA:919:A:O2'	2.19	0.75
17:AA:906:C:OP1	20:AD:117:ARG:NE	2.19	0.75
40:AX:53:GLU:N	40:AX:67:HIS:O	2.20	0.75
13:A1:181:ASN:ND2	13:A1:183:ASP:OD1	2.20	0.74
58:XS:194:ARG:NH2	67:b:13:SER:OG	2.19	0.74
63:XX:144:TYR:CD1	63:XX:148:THR:CG2	2.70	0.74
71:f:101:THR:OG1	78:m:67:ARG:NH1	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2237:A:OP1	82:r:168:ARG:NH1	2.19	0.74
41:AY:340:SER:OG	41:AY:377:ARG:NH2	2.20	0.74
8:7:190:ASP:O	8:7:295:ARG:NH1	2.20	0.74
34:AR:308:HIS:C	34:AR:310:ASP:H	1.93	0.74
7:6:27:ARG:N	11:XA:2832:A:N1	2.36	0.74
48:XI:48:MET:O	53:XN:250:ARG:NH1	2.21	0.74
19:AC:113:ARG:NH2	24:AH:166:GLU:OE2	2.20	0.74
9:8:99:ARG:HG3	70:e:84:TYR:CE1	2.17	0.74
16:A4:269:HIS:O	16:A4:270:ARG:NE	2.20	0.74
11:XA:2191:A:N6	11:XA:2198:A:OP2	2.21	0.74
31:AO:185:SER:O	34:AR:183:LYS:NZ	2.21	0.73
19:AC:88:GLU:OE2	19:AC:112:ARG:NH1	2.20	0.73
9:8:132:GLU:OE2	78:m:37:ARG:NH2	2.21	0.73
17:AA:1220:A:O2'	23:AG:395:LYS:O	2.06	0.73
12:A0:82:ARG:NH2	12:A0:138:ASP:O	2.21	0.73
46:XF:70:ARG:NH1	46:XF:194:GLU:OE2	2.22	0.73
46:XF:75:GLU:OE2	46:XF:210:ARG:NE	2.21	0.73
52:XM:238:ARG:NH1	80:p:70:ASP:OD1	2.21	0.73
7:6:308:GLN:NE2	7:6:311:MET:SD	2.60	0.73
15:A3:155:ARG:NH2	17:AA:1154:A:OP2	2.22	0.73
11:XA:1673:U:O2'	59:XT:149:ARG:NH2	2.22	0.73
22:AF:126:TYR:O	22:AF:134:GLN:NE2	2.22	0.72
7:6:114:ARG:NH1	43:XB:1643:A:OP1	2.21	0.72
40:AX:121:ALA:N	40:AX:299:ASN:OD1	2.22	0.72
49:XJ:154:ARG:NH1	49:XJ:155:VAL:O	2.23	0.72
2:1:23:GLU:N	2:1:23:GLU:OE1	2.22	0.72
11:XA:2599:U:OP2	11:XA:2625:C:N4	2.22	0.72
16:A4:479:GLU:HA	16:A4:482:ILE:HD12	1.71	0.71
61:XV:150:SER:O	61:XV:152:ARG:NH1	2.23	0.71
48:XI:100:GLN:NE2	48:XI:150:HIS:O	2.22	0.71
11:XA:1880:C:OP2	72:g:111:ARG:NH1	2.24	0.71
9:8:99:ARG:HB3	70:e:84:TYR:CD1	2.26	0.71
74:i:125:GLY:O	74:i:128:ARG:NH1	2.23	0.71
35:AS:52:ARG:NH1	35:AS:56:ALA:O	2.23	0.71
43:XB:1635:C:OP1	71:f:108:GLN:NE2	2.23	0.71
6:5:334:LYS:N	6:5:362:THR:OG1	2.24	0.71
83:r4:8:Y5P:O2'	83:r4:46:P5P:O2'	1.98	0.71
13:A1:169:ARG:O	13:A1:218:ASN:ND2	2.24	0.71
40:AX:206:GLU:OE1	40:AX:249:ARG:NH1	2.24	0.71
70:e:177:GLU:O	70:e:190:ARG:NH2	2.24	0.70
11:XA:2010:U:OP2	74:i:115:ARG:NH1	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:52:ARG:NH1	43:XB:1637:C:OP1	2.25	0.70
11:XA:2167:A:N6	11:XA:2212:C:OP2	2.24	0.70
17:AA:945:G:O2'	28:AL:154:ARG:NH2	2.24	0.70
63:XX:144:TYR:O	63:XX:148:THR:HG23	1.91	0.70
34:AR:305:HIS:CD2	34:AR:314:ALA:HA	2.26	0.70
76:k:26:ASN:ND2	76:k:79:ALA:O	2.24	0.70
11:XA:3220:A:OP1	45:XE:260:LYS:NZ	2.24	0.70
16:A4:470:GLN:OE1	16:A4:472:ASP:N	2.25	0.70
11:XA:2416:U:OP1	84:s:313:ARG:NH1	2.25	0.70
23:AG:379:ARG:NH2	24:AH:133:GLN:OE1	2.24	0.70
45:XE:69:ASP:OD1	45:XE:70:LYS:N	2.25	0.69
20:AD:216:GLU:N	20:AD:216:GLU:OE1	2.25	0.69
23:AG:312:GLN:OE1	23:AG:345:ARG:NH2	2.25	0.69
40:AX:56:PRO:O	40:AX:59:HIS:NE2	2.25	0.69
84:s:191:HIS:O	84:s:428:ARG:NH2	2.24	0.69
13:A1:256:SER:O	13:A1:260:ARG:NH1	2.25	0.69
17:AA:949:U:O3'	30:AN:29:ARG:NH1	2.25	0.69
20:AD:123:ARG:NH1	20:AD:124:LYS:O	2.26	0.69
59:XT:98:SER:OG	59:XT:101:GLN:OE1	2.10	0.69
17:AA:752:C:O2'	17:AA:793:C:N4	2.25	0.69
41:AY:333:PHE:O	41:AY:336:LYS:NZ	2.26	0.69
17:AA:825:U:N3	17:AA:827:A:OP1	2.25	0.69
11:XA:2231:A:OP1	79:o:9:ARG:NH1	2.25	0.69
21:AE:54:HIS:NE2	21:AE:83:SER:O	2.26	0.69
39:AW:132:GLU:O	39:AW:135:GLN:NE2	2.26	0.69
17:AA:780:C:N3	28:AL:197:ARG:NH2	2.41	0.69
49:XJ:25:ARG:NH2	77:l:57:LYS:O	2.26	0.69
9:8:101:ARG:NH1	70:e:82:SER:O	2.26	0.68
11:XA:1925:A:OP2	44:XD:101:LYS:NZ	2.26	0.68
22:AF:214:HIS:O	22:AF:216:GLN:NE2	2.27	0.68
75:j:101:GLU:OE1	75:j:105:GLN:NE2	2.26	0.68
3:2:82:ARG:NH2	11:XA:1791:G:OP2	2.24	0.68
41:AY:299:GLU:OE1	41:AY:299:GLU:N	2.26	0.68
1:0:84:ARG:NH2	11:XA:2306:A:O2'	2.27	0.68
17:AA:703:A:OP2	37:AU:43:ASN:ND2	2.27	0.68
61:XV:181:ASP:O	64:XY:93:LYS:NZ	2.27	0.68
7:6:183:ASP:OD2	80:p:189:ARG:NH1	2.26	0.68
5:4:84:ARG:NE	11:XA:3188:U:OP2	2.27	0.68
25:AI:192:ARG:NH1	33:AQ:44:TYR:OH	2.26	0.68
76:k:40:GLU:OE1	76:k:43:ARG:NH2	2.27	0.68
76:k:80:HIS:O	82:r:36:ARG:NH1	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:117:VAL:O	7:6:121:ARG:NH2	2.27	0.68
49:XJ:115:LYS:N	77:l:92:TYR:OH	2.27	0.68
61:XV:143:ARG:NH2	61:XV:144:VAL:O	2.26	0.68
71:f:92:ASN:ND2	71:f:193:ASP:OD2	2.26	0.68
17:AA:1429:C:OP1	23:AG:388:ARG:NH2	2.26	0.68
59:XT:126:ASP:OD1	59:XT:127:MET:N	2.27	0.68
59:XT:69:ARG:NH1	69:d:228:PHE:O	2.27	0.68
63:XX:160:ASP:OD1	63:XX:161:LEU:N	2.27	0.68
25:AI:79:LYS:N	25:AI:82:GLU:OE2	2.26	0.67
38:AV:132:LYS:O	38:AV:136:GLY:N	2.27	0.67
15:A3:187:GLU:O	28:AL:212:ARG:NH2	2.26	0.67
17:AA:1557:A:O2'	26:AJ:72:LYS:NZ	2.26	0.67
56:XQ:118:ARG:NH2	56:XQ:202:VAL:O	2.27	0.67
6:5:201:ARG:NH2	6:5:420:HIS:O	2.28	0.67
11:XA:2011:G:O6	74:i:113:ARG:NH1	2.25	0.67
34:AR:305:HIS:CD2	34:AR:314:ALA:CA	2.77	0.67
11:XA:1962:A:OP2	11:XA:2501:C:N4	2.27	0.67
11:XA:2499:U:OP2	11:XA:2504:A:N6	2.27	0.67
35:AS:75:TYR:OH	39:AW:91:GLN:O	2.13	0.67
62:XW:60:TYR:OH	62:XW:94:GLU:OE2	2.13	0.67
11:XA:2744:U:O2	11:XA:2745:A:N6	2.27	0.67
17:AA:668:U:O2'	31:AO:83:GLY:O	2.13	0.67
34:AR:308:HIS:C	34:AR:310:ASP:N	2.46	0.67
61:XV:20:ARG:NH1	61:XV:42:ARG:O	2.28	0.67
11:XA:3012:U:O4'	11:XA:3173:G:N2	2.28	0.66
11:XA:3063:G:O2'	11:XA:3066:C:OP2	2.13	0.66
57:XR:149:HIS:O	65:XZ:151:LEU:N	2.28	0.66
9:8:99:ARG:HD3	70:e:84:TYR:CE1	2.28	0.66
18:AB:162:CYS:O	18:AB:261:LYS:NZ	2.28	0.66
11:XA:2576:A:N6	17:AA:1491:C:O2'	2.28	0.66
27:AK:57:LEU:O	27:AK:60:ASN:ND2	2.28	0.66
62:XW:62:HIS:N	62:XW:65:ASN:OD1	2.27	0.66
64:XY:140:ASP:OD1	64:XY:141:ALA:N	2.28	0.66
13:A1:62:VAL:O	23:AG:90:ASN:ND2	2.29	0.66
19:AC:75:ASN:O	27:AK:103:ARG:NH2	2.28	0.66
21:AE:5:GLU:OE2	21:AE:96:HIS:ND1	2.29	0.66
61:XV:168:GLU:OE2	61:XV:169:THR:OG1	2.13	0.66
43:XB:1625:A:N7	55:XP:86:GLN:NE2	2.44	0.66
56:XQ:71:PRO:O	56:XQ:73:ARG:NH1	2.28	0.66
16:A4:478:TYR:CE2	16:A4:482:ILE:HD11	2.31	0.66
11:XA:3068:G:OP2	11:XA:3068:G:N2	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:1225:C:O2'	17:AA:1449:G:O2'	2.14	0.65
61:XV:66:GLU:N	61:XV:66:GLU:OE1	2.29	0.65
83:r4:30:P5P:H2'	83:r4:31:P5P:H8	1.78	0.65
21:AE:38:ASP:OD1	21:AE:39:LEU:N	2.29	0.65
53:XN:85:GLY:O	53:XN:192:ARG:NH2	2.28	0.65
34:AR:203:LYS:NZ	36:AT:144:GLU:OE2	2.28	0.65
9:8:99:ARG:CB	70:e:84:TYR:CG	2.79	0.65
17:AA:1236:C:OP2	27:AK:33:ARG:NH2	2.29	0.65
17:AA:1433:A:N3	17:AA:1458:A:N6	2.45	0.65
12:A0:147:GLU:N	12:A0:147:GLU:OE1	2.30	0.65
16:A4:198:TYR:O	16:A4:239:ARG:NH1	2.28	0.65
17:AA:1488:C:O2	17:AA:1584:A:O2'	2.15	0.65
19:AC:89:ASP:OD1	19:AC:90:VAL:N	2.29	0.65
61:XV:136:ARG:O	61:XV:143:ARG:NH2	2.30	0.65
75:j:101:GLU:O	75:j:105:GLN:NE2	2.30	0.65
6:5:276:ASP:OD2	84:s:158:ARG:NH1	2.30	0.65
43:XB:1621:A:OP1	55:XP:112:LYS:NZ	2.29	0.64
34:AR:305:HIS:CD2	34:AR:314:ALA:CB	2.72	0.64
23:AG:117:PHE:O	23:AG:122:ARG:NH1	2.30	0.64
46:XF:119:GLU:OE2	46:XF:156:ARG:NH2	2.29	0.64
9:8:99:ARG:HB3	70:e:84:TYR:CG	2.32	0.64
11:XA:1678:C:O4'	61:XV:42:ARG:NH2	2.30	0.64
11:XA:1699:C:OP1	64:XY:197:LYS:NZ	2.29	0.64
18:AB:138:ARG:NH1	35:AS:30:LEU:O	2.31	0.64
65:XZ:84:ASP:OD1	65:XZ:85:ILE:N	2.30	0.64
68:c:94:ASN:OD1	68:c:122:ASN:ND2	2.31	0.64
8:7:87:THR:OG1	8:7:115:MET:O	2.15	0.64
16:A4:478:TYR:CD2	16:A4:482:ILE:HD11	2.32	0.64
23:AG:204:GLU:N	23:AG:204:GLU:OE2	2.30	0.64
23:AG:308:GLN:NE2	23:AG:309:ASP:OD1	2.31	0.64
28:AL:149:ASP:OD2	28:AL:152:HIS:ND1	2.31	0.64
40:AX:266:ASN:ND2	40:AX:311:SER:O	2.31	0.64
58:XS:72:GLU:O	58:XS:76:HIS:ND1	2.27	0.64
7:6:239:ASN:OD1	7:6:275:GLN:NE2	2.30	0.64
53:XN:227:ARG:NH1	65:XZ:39:SER:OG	2.31	0.64
15:A3:165:LYS:NZ	17:AA:1148:A:OP2	2.31	0.63
36:AT:109:ASN:ND2	36:AT:111:GLU:OE2	2.31	0.63
1:0:79:ALA:N	11:XA:3099:C:O2	2.32	0.63
8:7:279:GLU:OE2	8:7:313:TRP:NE1	2.31	0.63
11:XA:3127:G:O2'	11:XA:3130:A:N6	2.31	0.63
17:AA:897:C:OP1	26:AJ:114:ARG:NH2	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AD:410:ASP:OD1	20:AD:411:VAL:N	2.32	0.63
7:6:368:ARG:NH2	11:XA:2859:A:OP2	2.31	0.63
17:AA:869:C:OP2	31:AO:97:ARG:NH2	2.32	0.63
11:XA:2600:A:O2'	11:XA:2601:A:O3'	2.16	0.63
33:AQ:55:GLU:OE2	33:AQ:59:ARG:NE	2.32	0.63
13:A1:314:GLU:OE1	13:A1:317:LYS:NZ	2.30	0.63
17:AA:1233:C:OP1	17:AA:1353:A:N6	2.32	0.63
63:XX:144:TYR:CZ	63:XX:148:THR:HG21	2.34	0.63
79:o:42:GLU:OE2	79:o:46:HIS:NE2	2.31	0.63
12:A0:130:GLU:OE2	12:A0:207:GLN:N	2.32	0.62
32:AP:65:CYS:SG	32:AP:68:CYS:N	2.72	0.62
23:AG:155:LYS:NZ	23:AG:217:ASP:OD2	2.32	0.62
61:XV:147:SER:OG	61:XV:152:ARG:N	2.30	0.62
11:XA:3019:G:N2	11:XA:3131:G:O2'	2.32	0.62
16:A4:455:ASN:O	16:A4:486:TYR:OH	2.17	0.62
11:XA:1884:G:N3	11:XA:1895:C:O2'	2.32	0.62
89:XA:5144:DOL:H343	89:XA:5144:DOL:H311	1.81	0.62
17:AA:1314:C:N3	22:AF:36:ARG:NH2	2.47	0.62
30:AN:12:TRP:NE1	36:AT:81:ASP:O	2.32	0.62
11:XA:1800:G:N1	11:XA:1803:A:OP2	2.32	0.62
36:AT:130:GLY:N	36:AT:135:CYS:SG	2.73	0.62
17:AA:1411:G:O3'	40:AX:279:LYS:NZ	2.32	0.62
17:AA:1053:A:N1	17:AA:1100:C:O2'	2.32	0.62
17:AA:1347:G:OP1	27:AK:36:ARG:NH1	2.33	0.62
29:AM:59:ASN:OD1	29:AM:62:GLY:N	2.33	0.62
84:s:103:ASP:OD1	84:s:104:ARG:N	2.33	0.62
11:XA:2457:A:O2'	54:XO:17:ARG:NH2	2.33	0.61
11:XA:2655:G:N2	11:XA:2659:C:O2'	2.33	0.61
51:XL:35:MET:N	51:XL:57:CYS:O	2.29	0.61
17:AA:1289:G:O2'	17:AA:1297:G:OP2	2.18	0.61
47:XH:108:ARG:NH1	47:XH:143:GLU:OE2	2.31	0.61
67:b:132:PRO:O	67:b:136:LYS:NZ	2.33	0.61
17:AA:1389:G:N1	17:AA:1416:A:OP2	2.34	0.61
23:AG:272:SER:OG	23:AG:347:ALA:O	2.18	0.61
75:j:85:ASP:OD1	75:j:86:ALA:N	2.33	0.61
17:AA:1483:C:N4	17:AA:1567:A:C2	2.68	0.61
11:XA:2195:A:O2'	11:XA:2196:A:O5'	2.17	0.61
11:XA:2712:G:N2	45:XE:257:MET:SD	2.74	0.61
11:XA:1733:C:O4'	74:i:95:ARG:NH2	2.33	0.61
11:XA:2813:U:N3	11:XA:2817:G:OP2	2.31	0.61
52:XM:109:ARG:NH1	52:XM:124:GLY:O	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:AX:214:GLU:OE2	40:AX:232:ARG:NH2	2.34	0.61
11:XA:2581:A:O2'	11:XA:2583:C:N4	2.34	0.60
17:AA:722:C:N3	17:AA:798:C:O2'	2.34	0.60
17:AA:850:U:O2'	37:AU:27:ARG:NH2	2.34	0.60
34:AR:305:HIS:HD2	34:AR:314:ALA:CA	2.12	0.60
4:3:116:ARG:NH2	4:3:159:ASP:OD1	2.34	0.60
4:3:179:LYS:O	7:6:370:ARG:NH2	2.34	0.60
17:AA:769:G:N2	17:AA:772:A:OP2	2.31	0.60
34:AR:202:ARG:NE	34:AR:233:ALA:O	2.33	0.60
9:8:100:GLU:N	9:8:100:GLU:OE1	2.32	0.60
11:XA:1953:A:O2'	11:XA:2463:A:OP1	2.18	0.60
12:A0:103:ASP:OD2	12:A0:105:THR:OG1	2.20	0.60
70:e:90:ARG:NH1	70:e:94:GLU:OE1	2.35	0.60
83:r4:13:Y5P:HC	83:r4:24:P5P:H2	1.82	0.60
13:A1:81:VAL:O	13:A1:99:LYS:NZ	2.33	0.60
22:AF:119:LYS:NZ	40:AX:398:LEU:O	2.35	0.60
68:c:86:ASP:OD1	68:c:87:LEU:N	2.34	0.60
50:XK:176:TYR:OH	82:r:94:ARG:NH2	2.33	0.60
60:XU:9:LEU:N	64:XY:183:GLN:OE1	2.35	0.60
63:XX:80:TRP:O	63:XX:131:THR:OG1	2.19	0.60
76:k:19:GLN:OE1	76:k:56:ARG:NH2	2.33	0.60
22:AF:77:ALA:N	23:AG:368:GLY:O	2.35	0.60
64:XY:137:ASP:OD1	64:XY:138:SER:N	2.34	0.60
17:AA:700:A:OP2	37:AU:27:ARG:NH1	2.35	0.60
17:AA:1048:C:O2'	17:AA:1049:A:OP1	2.19	0.60
38:AV:141:ASN:OD1	38:AV:142:PHE:N	2.35	0.60
84:s:148:ASP:OD1	84:s:149:CYS:N	2.34	0.60
7:6:198:ALA:O	7:6:254:TYR:OH	2.20	0.60
14:A2:17:ARG:NH2	17:AA:1022:A:OP2	2.33	0.60
17:AA:1483:C:C4	17:AA:1567:A:N1	2.69	0.60
82:r:37:GLU:OE1	82:r:37:GLU:N	2.34	0.60
17:AA:1231:A:O2'	17:AA:1236:C:N4	2.35	0.60
76:k:71:GLY:O	82:r:45:LYS:NZ	2.35	0.60
17:AA:678:U:N3	17:AA:920:G:O6	2.35	0.59
11:XA:1878:U:O2'	46:XF:92:ARG:NH2	2.36	0.59
16:A4:99:SER:N	16:A4:102:GLU:OE2	2.33	0.59
13:A1:177:LEU:O	13:A1:187:LYS:NZ	2.35	0.59
17:AA:702:C:O2'	17:AA:842:C:O2	2.20	0.59
17:AA:1444:A:OP2	27:AK:102:ARG:NH1	2.35	0.59
10:9:134:ASN:OD1	10:9:135:PHE:N	2.35	0.59
11:XA:2928:C:OP2	11:XA:3073:C:O2'	2.19	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AE:44:GLU:OE1	21:AE:60:ARG:NH2	2.36	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
57:XR:96:GLU:O	58:XS:105:GLN:NE2	2.32	0.59
22:AF:229:MET:HE1	83:r4:40:Y5P:HC	1.84	0.59
83:r4:76:P5P:OP2	83:r4:76:P5P:H3'	2.02	0.59
27:AK:28:HIS:NE2	42:AZ:60:GLU:OE2	2.35	0.59
44:XD:253:ASN:OD1	44:XD:254:LYS:N	2.36	0.59
23:AG:105:ASP:OD1	23:AG:106:ARG:N	2.36	0.59
11:XA:2643:G:O2'	11:XA:2645:G:OP2	2.19	0.58
17:AA:975:A:OP1	21:AE:90:ARG:NH1	2.36	0.58
53:XN:234:ASP:O	53:XN:238:LYS:HA	2.02	0.58
80:p:149:ASP:OD1	80:p:150:CYS:N	2.36	0.58
24:AH:74:LYS:N	24:AH:175:THR:O	2.36	0.58
17:AA:1200:G:N2	17:AA:1418:G:O2'	2.36	0.58
23:AG:129:GLU:N	23:AG:129:GLU:OE1	2.36	0.58
26:AJ:78:ARG:NH2	26:AJ:117:ASP:OD2	2.36	0.58
36:AT:95:ASN:OD1	36:AT:96:LYS:N	2.36	0.58
11:XA:2182:G:O2'	11:XA:2183:C:O4'	2.21	0.58
23:AG:217:ASP:OD1	23:AG:218:TYR:N	2.37	0.58
37:AU:110:GLN:O	37:AU:114:ARG:NE	2.34	0.58
83:r4:62:Y5P:H2'	83:r4:63:P5P:H8	1.84	0.58
11:XA:2295:C:O2'	11:XA:2297:A:OP1	2.22	0.58
11:XA:1902:C:O2	74:i:126:LYS:N	2.36	0.58
60:XU:14:GLY:O	61:XV:208:ARG:NE	2.37	0.58
84:s:178:ASP:OD2	84:s:203:ARG:NH1	2.37	0.58
60:XU:16:GLN:NE2	60:XU:17:LEU:O	2.36	0.58
11:XA:1672:C:O2'	59:XT:149:ARG:O	2.22	0.58
42:AZ:54:ASN:ND2	42:AZ:57:THR:OG1	2.36	0.58
65:XZ:99:VAL:O	75:j:76:ARG:NH2	2.37	0.58
52:XM:99:ASN:OD1	52:XM:100:ARG:N	2.37	0.57
1:0:163:GLU:OE1	1:0:181:ARG:NH2	2.38	0.57
17:AA:1066:C:O2'	25:AI:187:ARG:O	2.21	0.57
32:AP:49:ASP:OD2	39:AW:82:SER:N	2.37	0.57
61:XV:86:VAL:N	61:XV:115:LEU:O	2.37	0.57
7:6:286:ARG:NE	7:6:295:GLN:O	2.36	0.57
29:AM:71:ASP:OD1	29:AM:72:ARG:N	2.37	0.57
11:XA:3175:A:OP2	11:XA:3187:C:N4	2.35	0.57
37:AU:77:GLU:OE1	37:AU:80:ARG:NH2	2.38	0.57
12:A0:96:ARG:N	12:A0:117:ILE:O	2.36	0.57
11:XA:1805:A:OP2	61:XV:94:HIS:NE2	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:1844:A:OP2	57:XR:48:ARG:NH2	2.38	0.57
6:5:200:ARG:NH1	6:5:234:ASP:OD2	2.38	0.56
11:XA:2401:A:OP1	44:XD:262:ARG:NH1	2.37	0.56
13:A1:152:ASP:N	13:A1:152:ASP:OD1	2.37	0.56
22:AF:190:GLU:O	22:AF:208:LYS:NZ	2.38	0.56
6:5:118:LYS:NZ	6:5:254:GLU:OE1	2.38	0.56
31:AO:76:ASP:OD1	31:AO:109:ARG:NH2	2.37	0.56
49:XJ:149:ARG:NH2	77:l:101:LEU:O	2.38	0.56
74:i:76:GLY:O	74:i:81:ARG:NH2	2.37	0.56
14:A2:24:ASN:OD1	14:A2:25:LYS:N	2.39	0.56
40:AX:255:MET:SD	40:AX:255:MET:N	2.77	0.56
49:XJ:27:GLY:O	49:XJ:58:LYS:NZ	2.37	0.56
56:XQ:227:LYS:O	56:XQ:229:TRP:N	2.38	0.56
84:s:294:TYR:OH	84:s:353:ARG:NH2	2.38	0.56
63:XX:53:ASN:ND2	63:XX:56:ASN:OD1	2.38	0.56
13:A1:236:THR:OG1	13:A1:240:GLU:OE1	2.24	0.56
36:AT:103:ARG:NH1	36:AT:110:GLU:OE2	2.37	0.56
53:XN:138:HIS:ND1	53:XN:139:ARG:O	2.36	0.56
17:AA:1262:C:O3'	20:AD:100:LYS:NZ	2.39	0.56
17:AA:1454:G:OP2	23:AG:377:ARG:NH2	2.39	0.56
85:t1:4:GLN:OE1	85:t1:8:GLN:NE2	2.39	0.56
52:XM:117:ASP:OD1	52:XM:118:LEU:N	2.38	0.56
5:4:99:LYS:NZ	11:XA:3013:G:O3'	2.37	0.56
7:6:106:ARG:NH1	43:XB:1621:A:OP2	2.39	0.56
46:XF:94:ASP:OD1	46:XF:95:ILE:N	2.38	0.56
69:d:249:GLU:OE2	69:d:262:HIS:ND1	2.39	0.56
77:l:112:PRO:O	77:l:118:TRP:NE1	2.38	0.56
17:AA:873:G:O2'	17:AA:921:U:O2	2.24	0.56
20:AD:192:GLY:O	31:AO:78:ARG:NH2	2.39	0.56
38:AV:159:ASP:OD1	38:AV:160:ALA:N	2.37	0.56
64:XY:143:ASP:OD1	64:XY:144:LYS:N	2.39	0.56
11:XA:1990:G:OP1	44:XD:269:ARG:NH2	2.34	0.56
11:XA:2052:A:OP1	72:g:150:LYS:NZ	2.39	0.56
11:XA:1761:A:O2'	11:XA:1762:A:O5'	2.15	0.55
55:XP:81:ARG:NH1	55:XP:94:GLU:OE2	2.39	0.55
26:AJ:50:GLY:O	26:AJ:89:ARG:NH1	2.40	0.55
38:AV:108:THR:O	38:AV:111:THR:OG1	2.18	0.55
13:A1:163:VAL:O	41:AY:317:ASN:ND2	2.37	0.55
84:s:62:ARG:O	84:s:65:ARG:HG2	2.05	0.55
84:s:77:ASP:OD1	84:s:78:GLU:N	2.39	0.55
34:AR:135:ARG:NH2	34:AR:236:GLU:OE2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:XH:135:GLU:N	47:XH:135:GLU:OE2	2.40	0.55
31:AO:161:GLY:O	34:AR:223:ARG:NH2	2.40	0.55
16:A4:175:GLN:O	16:A4:180:GLY:N	2.40	0.55
78:m:52:TYR:N	78:m:68:TYR:O	2.36	0.55
6:5:174:GLU:OE1	6:5:298:ASN:ND2	2.40	0.55
7:6:241:PRO:O	7:6:244:ARG:NE	2.36	0.55
11:XA:1864:A:OP1	57:XR:17:ARG:NH1	2.40	0.55
16:A4:264:ARG:HE	16:A4:293:THR:HG22	1.72	0.55
81:q:44:ASP:O	81:q:47:THR:OG1	2.25	0.55
17:AA:798:C:OP1	29:AM:10:LYS:N	2.39	0.55
6:5:51:GLU:OE1	6:5:51:GLU:N	2.40	0.55
8:7:262:ASP:OD1	8:7:263:VAL:N	2.39	0.55
11:XA:2926:A:O2'	11:XA:3087:C:OP1	2.20	0.55
11:XA:2256:U:OP1	75:j:66:ARG:NH1	2.40	0.55
56:XQ:103:ARG:NH2	56:XQ:167:TYR:OH	2.39	0.55
6:5:337:GLU:N	6:5:337:GLU:OE1	2.40	0.54
11:XA:1957:A:O4'	59:XT:163:ARG:NH1	2.40	0.54
35:AS:82:GLN:NE2	35:AS:133:ARG:O	2.41	0.54
54:XO:129:CYS:SG	54:XO:130:LEU:N	2.80	0.54
56:XQ:268:ASP:OD1	56:XQ:269:MET:N	2.40	0.54
83:r4:30:P5P:C2'	83:r4:31:P5P:H8	2.38	0.54
43:XB:1630:A:OP1	78:m:42:ARG:NE	2.40	0.54
2:1:42:THR:O	81:q:135:TRP:NE1	2.35	0.54
4:3:124:ARG:NH2	11:XA:2868:C:OP1	2.40	0.54
7:6:37:ASN:ND2	62:XW:125:VAL:O	2.37	0.54
17:AA:1198:A:N6	17:AA:1199:G:O6	2.40	0.54
30:AN:53:ASP:OD2	30:AN:57:GLN:N	2.38	0.54
55:XP:59:SER:OG	80:p:177:ARG:NH1	2.40	0.54
21:AE:14:GLN:N	21:AE:17:GLU:OE2	2.36	0.54
85:t3:4:GLN:OE1	85:t3:4:GLN:N	2.40	0.54
11:XA:2693:A:OP1	79:o:15:ARG:NH2	2.35	0.54
11:XA:3178:U:O2'	82:r:134:ARG:NH1	2.41	0.54
20:AD:307:LYS:NZ	34:AR:103:TYR:OH	2.38	0.54
38:AV:250:ILE:O	38:AV:255:TYR:OH	2.25	0.54
56:XQ:84:ARG:NH1	56:XQ:271:ARG:O	2.38	0.54
84:s:108:TYR:O	84:s:212:ARG:NE	2.41	0.54
13:A1:156:TYR:O	13:A1:167:ARG:NH1	2.41	0.54
35:AS:7:GLU:N	35:AS:7:GLU:OE1	2.41	0.54
83:r4:13:Y5P:HC	83:r4:24:P5P:C2	2.38	0.54
72:g:104:ASN:OD1	72:g:105:ARG:N	2.41	0.54
6:5:300:ARG:N	6:5:301:PRO:HD2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:338:GLN:N	6:5:338:GLN:OE1	2.36	0.54
11:XA:2335:A:O4'	84:s:277:GLN:NE2	2.41	0.54
13:A1:91:VAL:O	13:A1:94:GLY:N	2.40	0.54
13:A1:118:ALA:O	13:A1:122:HIS:ND1	2.39	0.54
15:A3:179:LYS:NZ	17:AA:764:A:OP1	2.39	0.54
56:XQ:108:ILE:HD12	56:XQ:108:ILE:O	2.08	0.54
11:XA:2524:A:OP1	44:XD:67:LYS:NZ	2.36	0.54
17:AA:949:U:O2'	30:AN:29:ARG:NH1	2.40	0.54
20:AD:250:GLY:N	20:AD:326:LEU:O	2.40	0.54
68:c:227:GLU:OE2	68:c:230:GLU:N	2.40	0.54
14:A2:55:CYS:SG	14:A2:59:ASN:ND2	2.80	0.53
41:AY:300:GLU:OE2	41:AY:304:TRP:NE1	2.40	0.53
17:AA:1430:A:OP1	23:AG:388:ARG:NH2	2.33	0.53
29:AM:55:ASP:OD1	29:AM:65:LEU:N	2.40	0.53
6:5:144:ARG:O	6:5:194:LYS:NZ	2.39	0.53
7:6:252:CYS:SG	7:6:286:ARG:NH2	2.81	0.53
11:XA:2279:U:OP2	74:i:46:ARG:NH2	2.37	0.53
17:AA:1108:C:N4	17:AA:1125:A:N7	2.56	0.53
28:AL:169:ASN:OD1	28:AL:170:LEU:N	2.42	0.53
41:AY:292:GLN:OE1	41:AY:292:GLN:N	2.42	0.53
11:XA:1846:C:OP2	58:XS:177:ARG:N	2.38	0.53
51:XL:35:MET:SD	51:XL:56:ARG:NH1	2.81	0.53
14:A2:113:ASN:OD1	14:A2:114:LYS:N	2.41	0.53
22:AF:49:GLU:N	22:AF:49:GLU:OE2	2.39	0.53
89:XA:5144:DOL:H311	89:XA:5144:DOL:C34	2.39	0.53
83:r4:61:Y5P:H4A	83:r4:62:Y5P:H4	1.91	0.53
84:s:296:HIS:NE2	84:s:427:ASN:O	2.39	0.53
11:XA:3078:C:N4	11:XA:3079:G:O6	2.42	0.53
45:XE:247:ASP:OD1	45:XE:248:ILE:N	2.42	0.53
11:XA:1907:A:O2'	46:XF:130:GLN:OE1	2.21	0.53
13:A1:86:ARG:NH1	13:A1:96:PRO:O	2.42	0.53
24:AH:51:HIS:NE2	24:AH:53:ASP:O	2.41	0.53
33:AQ:27:ASN:OD1	33:AQ:28:ARG:N	2.42	0.53
69:d:158:ASP:OD1	69:d:159:ARG:N	2.41	0.53
17:AA:843:G:N1	17:AA:847:G:O6	2.42	0.53
35:AS:6:LEU:O	35:AS:15:ARG:NH1	2.42	0.53
63:XX:148:THR:OG1	63:XX:153:LEU:HD23	2.09	0.53
84:s:174:LEU:HB3	84:s:175:PRO:HD3	1.91	0.53
17:AA:748:G:N2	30:AN:7:SER:O	2.42	0.52
24:AH:89:ASP:OD1	24:AH:141:ARG:NH1	2.41	0.52
38:AV:123:ASP:OD1	38:AV:124:LYS:N	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:XF:142:ARG:HA	46:XF:149:GLY:HA2	1.91	0.52
11:XA:2458:A:O2'	45:XE:215:PHE:O	2.24	0.52
17:AA:1268:C:OP2	17:AA:1269:U:O2'	2.27	0.52
40:AX:161:TRP:NE1	40:AX:183:GLU:OE2	2.43	0.52
83:r4:1:P5P:H8	83:r4:1:P5P:P	2.50	0.52
83:r4:12:Y5P:O5'	83:r4:12:Y5P:H6	2.09	0.52
11:XA:3066:C:O2'	45:XE:233:GLN:OE1	2.23	0.52
17:AA:1233:C:O2'	27:AK:86:ARG:NH2	2.43	0.52
17:AA:1526:U:O2	17:AA:1526:U:O2'	2.27	0.52
21:AE:105:CYS:SG	32:AP:64:LYS:NZ	2.82	0.52
31:AO:196:GLY:O	34:AR:146:LYS:NZ	2.43	0.52
83:r4:55:Y5P:H6	83:r4:55:Y5P:O5'	2.10	0.52
12:A0:90:ASP:OD1	31:AO:215:ARG:NH1	2.43	0.52
17:AA:1272:A:N6	17:AA:1320:G:O2'	2.43	0.52
58:XS:132:LYS:NZ	75:j:48:ASP:OD1	2.42	0.52
68:c:58:VAL:O	68:c:63:LYS:NZ	2.43	0.52
43:XB:1640:A:OP2	55:XP:84:ARG:NH1	2.37	0.52
55:XP:94:GLU:N	55:XP:94:GLU:OE1	2.43	0.52
6:5:177:CYS:O	6:5:180:ILE:HG22	2.10	0.52
77:l:76:ASN:OD1	77:l:82:GLN:N	2.43	0.52
55:XP:168:GLY:O	80:p:184:ASN:ND2	2.42	0.52
6:5:329:TYR:OH	6:5:338:GLN:NE2	2.38	0.52
9:8:99:ARG:HD2	70:e:84:TYR:CE2	2.30	0.52
11:XA:1755:A:O2'	47:XH:64:LEU:O	2.24	0.52
11:XA:2600:A:O2'	11:XA:2602:U:O2	2.28	0.52
11:XA:2403:G:OP2	44:XD:105:ARG:NH2	2.38	0.51
12:A0:61:GLU:OE2	12:A0:139:TRP:N	2.44	0.51
17:AA:1429:C:O2	17:AA:1460:C:N4	2.42	0.51
24:AH:67:ASP:N	24:AH:67:ASP:OD1	2.43	0.51
38:AV:83:GLU:O	38:AV:87:HIS:ND1	2.42	0.51
43:XB:1644:G:O6	55:XP:87:HIS:NE2	2.39	0.51
45:XE:316:PHE:HB3	45:XE:317:PRO:HD3	1.93	0.51
11:XA:2552:U:C2	11:XA:2553:G:C8	2.98	0.51
11:XA:2909:G:C2	83:r4:76:P5P:H6	2.44	0.51
17:AA:819:A:O2'	17:AA:831:U:O2'	2.28	0.51
17:AA:1261:C:OP1	20:AD:109:GLY:N	2.38	0.51
34:AR:140:ASP:OD1	34:AR:141:VAL:N	2.42	0.51
63:XX:133:ASP:OD1	63:XX:134:LEU:N	2.43	0.51
83:r4:2:Y5P:H4A	83:r4:3:Y5P:H4	1.91	0.51
16:A4:478:TYR:O	16:A4:482:ILE:HG13	2.11	0.51
60:XU:138:GLN:N	60:XU:138:GLN:OE1	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:XV:184:GLU:O	64:XY:93:LYS:NZ	2.41	0.51
79:o:33:GLN:HA	79:o:36:ILE:HG12	1.92	0.51
11:XA:2182:G:N2	11:XA:2199:A:N3	2.58	0.51
16:A4:98:ALA:N	16:A4:102:GLU:OE2	2.44	0.51
17:AA:864:U:O4	17:AA:865:A:N6	2.44	0.51
23:AG:321:ASP:OD1	23:AG:322:ARG:NH1	2.40	0.51
52:XM:203:ARG:NH2	52:XM:261:ASP:O	2.44	0.51
73:h:114:ASN:HA	73:h:117:LEU:HD22	1.93	0.51
12:A0:50:LEU:O	12:A0:55:TRP:NE1	2.42	0.51
46:XF:191:ASP:OD1	46:XF:192:SER:N	2.44	0.51
17:AA:777:G:OP1	30:AN:21:LYS:NZ	2.41	0.51
54:XO:124:GLU:OE2	54:XO:128:ASN:ND2	2.44	0.51
82:r:117:GLU:O	82:r:121:MET:HG2	2.10	0.51
11:XA:2239:A:OP2	50:XK:75:LYS:NZ	2.42	0.51
43:XB:1626:C:N4	55:XP:86:GLN:OE1	2.42	0.51
6:5:283:TYR:OH	84:s:152:GLN:OE1	2.26	0.50
24:AH:126:ILE:HD12	24:AH:126:ILE:O	2.11	0.50
56:XQ:226:PRO:O	56:XQ:229:TRP:NE1	2.44	0.50
70:e:158:VAL:O	70:e:255:VAL:N	2.36	0.50
84:s:271:LEU:O	84:s:273:LEU:N	2.44	0.50
8:7:51:GLU:OE2	8:7:54:ARG:NH2	2.42	0.50
11:XA:2400:C:O2'	11:XA:2401:A:O5'	2.28	0.50
83:r4:40:Y5P:N3	83:r4:41:Y5P:H5	2.27	0.50
11:XA:1860:A:O2'	11:XA:2682:A:OP1	2.28	0.50
11:XA:2624:C:O2'	11:XA:2625:C:H5'	2.12	0.50
34:AR:254:ASP:OD1	34:AR:259:TYR:OH	2.30	0.50
40:AX:157:ASP:OD1	40:AX:158:ALA:N	2.45	0.50
6:5:201:ARG:NH1	6:5:418:TYR:O	2.43	0.50
18:AB:219:THR:O	18:AB:233:THR:OG1	2.29	0.50
42:AZ:31:MET:O	42:AZ:35:LYS:HD3	2.10	0.50
51:XL:99:ARG:NH1	56:XQ:161:GLU:OE1	2.42	0.50
83:r4:10:P5P:OP2	83:r4:45:Y5P:O2'	2.18	0.50
6:5:338:GLN:O	6:5:338:GLN:HG2	2.10	0.50
8:7:180:CYS:SG	8:7:181:TYR:N	2.84	0.50
11:XA:2381:A:N6	11:XA:2412:A:N1	2.60	0.50
54:XO:64:LYS:NZ	54:XO:97:TYR:O	2.38	0.50
74:i:88:LEU:HB2	74:i:117:LEU:CD1	2.42	0.50
80:p:81:CYS:SG	80:p:82:ARG:N	2.83	0.50
11:XA:1729:U:OP2	63:XX:100:ARG:NH1	2.44	0.50
14:A2:38:ARG:NH2	17:AA:1184:U:OP2	2.44	0.50
46:XF:292:ASP:OD1	46:XF:293:PHE:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2192:A:OP2	77:l:119:ARG:NH1	2.45	0.50
27:AK:49:ASP:OD2	27:AK:53:ARG:NH2	2.45	0.50
53:XN:99:TRP:NE1	53:XN:103:GLU:OE2	2.45	0.50
81:q:152:ARG:O	81:q:174:ARG:NH2	2.45	0.50
17:AA:1483:C:N3	17:AA:1567:A:C6	2.79	0.50
11:XA:2842:C:O4'	53:XN:63:ARG:NH1	2.45	0.49
16:A4:247:ILE:O	16:A4:254:LYS:NZ	2.39	0.49
17:AA:1483:C:O2	17:AA:1567:A:N6	2.43	0.49
47:XH:120:ARG:NH2	63:XX:136:ASP:OD2	2.41	0.49
62:XW:115:ASP:OD1	62:XW:116:LEU:N	2.45	0.49
6:5:185:ILE:HA	6:5:188:CYS:SG	2.52	0.49
9:8:99:ARG:HD2	70:e:84:TYR:CE1	2.29	0.49
45:XE:119:VAL:HG21	45:XE:284:TYR:HB3	1.93	0.49
49:XJ:85:PRO:O	49:XJ:124:LYS:NZ	2.45	0.49
69:d:197:VAL:O	69:d:198:ARG:NE	2.45	0.49
83:r4:9:P5P:H6	83:r4:24:P5P:H6	1.94	0.49
11:XA:2515:U:O2'	44:XD:282:ALA:O	2.30	0.49
15:A3:161:ARG:NH2	17:AA:1146:C:OP1	2.44	0.49
17:AA:915:C:C2	17:AA:916:C:C5	3.01	0.49
31:AO:149:ARG:O	31:AO:152:GLN:NE2	2.45	0.49
83:r4:28:P5P:N1	83:r4:44:P5P:H8	2.27	0.49
11:XA:2347:C:O3'	69:d:69:LYS:NZ	2.45	0.49
13:A1:267:LEU:O	13:A1:270:LYS:NZ	2.46	0.49
36:AT:9:ILE:O	36:AT:12:THR:OG1	2.29	0.49
7:6:375:PRO:O	80:p:141:ARG:NH2	2.44	0.49
13:A1:142:LYS:O	13:A1:146:HIS:ND1	2.42	0.49
22:AF:38:SER:OG	22:AF:40:GLU:OE1	2.29	0.49
46:XF:277:ASP:O	72:g:90:ARG:NH2	2.46	0.49
52:XM:264:GLN:NE2	52:XM:266:PHE:O	2.45	0.49
58:XS:127:ARG:NH2	58:XS:157:GLU:OE1	2.37	0.49
76:k:65:ASP:OD1	76:k:66:VAL:N	2.45	0.49
11:XA:1787:G:N2	11:XA:1790:A:OP2	2.34	0.49
11:XA:2139:U:O4	65:XZ:77:ARG:NH1	2.45	0.49
17:AA:989:U:OP1	25:AI:94:ASN:ND2	2.44	0.49
39:AW:109:GLU:O	39:AW:126:ARG:NH1	2.43	0.49
38:AV:131:ASN:ND2	38:AV:134:GLN:OE1	2.46	0.49
47:XH:117:SER:O	47:XH:121:ASN:ND2	2.46	0.49
48:XI:236:TYR:O	48:XI:240:GLN:NE2	2.46	0.49
10:9:126:LYS:NZ	61:XV:196:GLU:OE2	2.38	0.49
11:XA:1672:C:OP1	59:XT:50:LYS:N	2.45	0.49
17:AA:1106:C:O2'	17:AA:1108:C:OP2	2.29	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AR:107:THR:OG1	34:AR:108:GLN:OE1	2.30	0.49
57:XR:17:ARG:HA	57:XR:20:ARG:HG2	1.95	0.49
61:XV:185:ARG:NE	64:XY:92:ASN:OD1	2.42	0.49
11:XA:1742:G:O2'	11:XA:1754:G:O6	2.28	0.49
11:XA:2235:C:O2'	82:r:165:LYS:N	2.39	0.49
21:AE:115:GLU:N	21:AE:115:GLU:OE1	2.46	0.49
29:AM:50:GLN:NE2	36:AT:129:PHE:O	2.43	0.49
52:XM:72:THR:OG1	52:XM:77:ARG:NH2	2.46	0.49
63:XX:147:LYS:O	63:XX:147:LYS:HG2	2.13	0.49
11:XA:3066:C:H2'	11:XA:3067:U:H5'	1.95	0.48
20:AD:96:ASP:OD1	20:AD:97:GLU:N	2.46	0.48
23:AG:321:ASP:OD1	23:AG:321:ASP:C	2.56	0.48
30:AN:53:ASP:OD1	30:AN:57:GLN:NE2	2.46	0.48
46:XF:194:GLU:OE1	46:XF:194:GLU:N	2.46	0.48
82:r:176:VAL:N	82:r:194:LEU:O	2.42	0.48
6:5:182:ASP:O	6:5:185:ILE:HG13	2.13	0.48
21:AE:85:ASP:OD1	44:XD:171:ARG:NH1	2.45	0.48
46:XF:91:PRO:O	46:XF:176:VAL:HG21	2.13	0.48
57:XR:38:CYS:HB2	57:XR:41:LEU:HD21	1.95	0.48
61:XV:127:ASP:OD2	61:XV:152:ARG:NH2	2.46	0.48
11:XA:2826:G:OP2	62:XW:46:SER:OG	2.29	0.48
25:AI:94:ASN:OD1	25:AI:95:THR:N	2.46	0.48
85:t2:5:GLN:NE2	85:t2:9:ASP:OD2	2.46	0.48
11:XA:2016:C:OP1	11:XA:2039:A:O2'	2.25	0.48
11:XA:2754:A:N3	63:XX:108:GLN:NE2	2.57	0.48
23:AG:295:VAL:N	23:AG:298:ILE:O	2.40	0.48
61:XV:103:ASP:OD1	61:XV:104:TYR:N	2.46	0.48
76:k:70:ASP:OD1	76:k:71:GLY:N	2.46	0.48
48:XI:182:ASP:O	48:XI:183:ASP:OD1	2.31	0.48
7:6:39:ASP:OD1	7:6:40:ILE:N	2.47	0.48
11:XA:2082:G:OP2	79:o:66:ARG:NH2	2.47	0.48
17:AA:845:A:O2'	17:AA:846:A:O4'	2.26	0.48
48:XI:101:ASN:OD1	48:XI:151:ASN:N	2.46	0.48
69:d:116:MET:SD	69:d:116:MET:N	2.86	0.48
11:XA:1885:A:OP2	46:XF:168:LYS:NZ	2.47	0.48
11:XA:3066:C:C2'	11:XA:3067:U:H5'	2.43	0.48
17:AA:881:A:O2'	17:AA:882:A:O4'	2.21	0.48
34:AR:208:ILE:O	34:AR:214:ASN:ND2	2.42	0.48
46:XF:185:ASP:OD1	46:XF:185:ASP:C	2.57	0.48
17:AA:918:A:O2'	17:AA:919:A:O4'	2.31	0.48
17:AA:1287:A:OP2	20:AD:260:LYS:NZ	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AR:169:GLU:N	34:AR:169:GLU:OE1	2.47	0.48
11:XA:2623:A:O2'	17:AA:1549:G:O2'	2.29	0.48
17:AA:847:G:C2	17:AA:848:U:C5	3.02	0.48
39:AW:146:ASP:OD1	39:AW:148:GLU:N	2.46	0.48
40:AX:272:THR:OG1	40:AX:282:ILE:O	2.28	0.48
46:XF:228:GLN:HA	46:XF:231:VAL:HG12	1.96	0.48
12:A0:87:TRP:O	31:AO:215:ARG:NH2	2.47	0.48
17:AA:948:U:OP2	17:AA:1045:G:N1	2.41	0.48
38:AV:378:ASN:OD1	38:AV:381:GLN:NE2	2.41	0.48
52:XM:252:LEU:HD23	52:XM:252:LEU:H	1.78	0.48
57:XR:38:CYS:O	57:XR:42:ALA:HB2	2.14	0.48
60:XU:49:THR:O	60:XU:52:ASP:OD1	2.32	0.48
11:XA:2166:C:N4	11:XA:2212:C:OP2	2.47	0.47
11:XA:2842:C:OP2	62:XW:41:ASN:ND2	2.43	0.47
46:XF:249:ASN:ND2	74:i:55:GLY:O	2.47	0.47
52:XM:182:ARG:O	52:XM:186:ILE:HG12	2.14	0.47
7:6:60:ARG:NH2	7:6:64:GLU:OE2	2.46	0.47
7:6:206:TYR:OH	7:6:242:GLY:O	2.25	0.47
55:XP:71:PHE:HB3	55:XP:72:PRO:HD3	1.96	0.47
9:8:186:GLN:N	9:8:186:GLN:OE1	2.46	0.47
11:XA:2125:C:OP2	58:XS:178:LYS:NZ	2.44	0.47
11:XA:2909:G:N3	83:r4:76:P5P:H6	2.30	0.47
17:AA:1399:A:H2'	17:AA:1400:U:C6	2.50	0.47
41:AY:293:PRO:O	41:AY:295:GLN:NE2	2.42	0.47
11:XA:1765:C:OP2	74:i:75:ARG:NH2	2.47	0.47
11:XA:1957:A:OP2	86:A:8:MHT:H7A	2.14	0.47
11:XA:2938:A:OP1	11:XA:2984:A:N6	2.46	0.47
16:A4:62:LYS:O	24:AH:66:SER:N	2.47	0.47
17:AA:1432:U:H2'	17:AA:1433:A:O4'	2.14	0.47
45:XE:334:ASP:OD1	45:XE:335:GLU:N	2.47	0.47
62:XW:112:GLU:O	62:XW:115:ASP:OD1	2.32	0.47
64:XY:140:ASP:O	64:XY:143:ASP:OD1	2.33	0.47
5:4:68:ASN:HD21	11:XA:3026:U:H4'	1.78	0.47
17:AA:1067:A:H2'	17:AA:1068:A:O4'	2.13	0.47
20:AD:164:GLU:OE1	20:AD:164:GLU:N	2.44	0.47
31:AO:65:GLN:O	31:AO:69:GLY:N	2.47	0.47
52:XM:102:GLN:NE2	52:XM:106:ASP:OD2	2.48	0.47
53:XN:201:ASP:OD1	53:XN:201:ASP:C	2.57	0.47
70:e:269:LEU:O	70:e:273:ARG:HD3	2.14	0.47
11:XA:3096:U:C5	86:A:7:004:O	2.67	0.47
34:AR:254:ASP:OD2	34:AR:280:LYS:NZ	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:YN:172:VAL:HG13	53:YN:175:PHE:CZ	2.50	0.47
83:r4:9:P5P:OP2	83:r4:13:Y5P:H5	2.14	0.47
11:XA:2148:A:OP2	57:XR:65:ARG:NH1	2.46	0.47
16:A4:366:GLU:OE1	16:A4:366:GLU:N	2.42	0.47
49:XJ:52:GLU:OE2	49:XJ:56:ARG:NH2	2.42	0.47
64:XY:130:GLU:O	64:XY:133:ASP:OD1	2.33	0.47
68:c:84:SER:OG	68:c:86:ASP:OD1	2.31	0.47
80:p:151:LEU:O	80:p:154:ILE:HG13	2.14	0.47
83:r4:35:P5P:H2'	83:r4:36:P5P:H8	1.96	0.47
7:6:379:ILE:O	7:6:379:ILE:HD12	2.14	0.47
8:7:192:TRP:O	8:7:295:ARG:NH1	2.48	0.47
11:XA:2358:A:C2	11:XA:2359:C:H1'	2.49	0.47
11:XA:2826:G:OP1	62:XW:49:ARG:NH1	2.40	0.47
49:XJ:107:GLU:OE1	49:XJ:109:ALA:N	2.48	0.47
63:XX:132:LEU:O	63:XX:135:ILE:HG13	2.14	0.47
67:b:86:GLU:OE1	67:b:86:GLU:N	2.48	0.47
11:XA:1791:G:HO2'	11:XA:2006:C:HO2'	1.61	0.47
11:XA:1799:U:H2'	11:XA:1800:G:O4'	2.15	0.47
17:AA:701:G:O5'	37:AU:38:LYS:NZ	2.47	0.47
46:XF:109:ILE:HD11	46:XF:111:TYR:CZ	2.49	0.47
46:XF:238:LYS:O	46:XF:241:ASN:ND2	2.48	0.47
58:XS:76:HIS:CD2	66:a:50:ALA:HA	2.50	0.47
68:c:276:CYS:O	68:c:277:ASP:OD1	2.32	0.47
83:r4:9:P5P:O3'	83:r4:45:Y5P:H2'	2.15	0.47
84:s:324:PHE:CD1	84:s:361:ILE:CD1	2.98	0.47
85:t1:-1:TYR:HB3	85:t1:0:PRO:CD	2.45	0.47
1:0:96:ASN:ND2	11:XA:2709:A:O2'	2.41	0.47
3:2:58:ILE:HD13	10:9:30:PHE:CZ	2.49	0.47
11:XA:1939:G:O2'	11:XA:1973:G:H4'	2.14	0.47
11:XA:2051:A:N3	72:g:104:ASN:ND2	2.60	0.47
11:XA:2292:G:N1	57:XR:10:LEU:N	2.63	0.47
11:XA:2990:A:H4'	11:XA:2991:U:OP1	2.15	0.47
17:AA:1033:U:O2'	21:AE:93:ILE:O	2.33	0.47
19:AC:77:ASP:OD2	24:AH:140:TYR:OH	2.30	0.47
34:AR:247:HIS:O	34:AR:251:GLU:OE1	2.33	0.47
48:XI:38:ARG:O	53:YN:242:TRP:NE1	2.44	0.47
54:XO:94:ALA:HB3	54:XO:95:PRO:HD3	1.97	0.47
56:XQ:107:HIS:C	56:XQ:108:ILE:HG13	2.40	0.47
85:t3:5:GLN:NE2	85:t3:9:ASP:OD2	2.48	0.47
44:XD:251:ASP:OD1	44:XD:251:ASP:C	2.58	0.46
11:XA:2755:A:O2'	63:XX:112:ARG:NH2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:s:279:GLU:OE1	84:s:281:HIS:NE2	2.49	0.46
11:XA:2192:A:OP1	49:XJ:142:ARG:NE	2.45	0.46
20:AD:108:ALA:O	20:AD:114:ARG:NH1	2.49	0.46
29:AM:88:GLU:OE1	37:AU:63:TYR:OH	2.33	0.46
73:h:151:ASN:OD1	73:h:152:LEU:N	2.49	0.46
11:XA:2131:A:N1	82:r:168:ARG:NH1	2.63	0.46
11:XA:2624:C:C2'	11:XA:2625:C:H5'	2.45	0.46
58:XS:92:TYR:O	68:c:312:ARG:NE	2.49	0.46
63:XX:189:ASP:O	63:XX:192:LYS:NZ	2.45	0.46
73:h:88:ASP:OD1	73:h:124:ARG:NH2	2.48	0.46
8:7:143:TRP:HE3	8:7:179:PHE:HB3	1.81	0.46
11:XA:2130:A:C2	79:o:17:TRP:CH2	3.04	0.46
11:XA:2143:G:C6	11:XA:2258:A:C2	3.03	0.46
11:XA:2506:A:N6	11:XA:3093:C:O4'	2.46	0.46
11:XA:2574:G:O2'	11:XA:2575:U:P	2.74	0.46
38:AV:144:PHE:CZ	38:AV:167:VAL:HG21	2.50	0.46
60:XU:71:ARG:NH2	60:XU:73:GLN:OE1	2.37	0.46
64:XY:111:MET:O	64:XY:114:THR:OG1	2.27	0.46
79:o:34:ASN:O	79:o:37:ARG:HG2	2.16	0.46
9:8:165:ASP:OD1	9:8:165:ASP:N	2.49	0.46
10:9:120:GLU:N	10:9:120:GLU:OE1	2.48	0.46
11:XA:2457:A:N3	54:XO:17:ARG:NH2	2.63	0.46
14:A2:17:ARG:NH1	17:AA:1022:A:OP2	2.47	0.46
22:AF:129:ALA:O	22:AF:134:GLN:NE2	2.49	0.46
43:XB:1615:A:O2'	43:XB:1616:A:O4'	2.32	0.46
48:XI:101:ASN:O	76:k:35:GLN:NE2	2.48	0.46
52:XM:238:ARG:O	80:p:155:ARG:NH2	2.39	0.46
54:XO:41:ARG:NH2	54:XO:131:PRO:O	2.40	0.46
70:e:185:ARG:O	70:e:189:GLU:OE1	2.34	0.46
17:AA:1234:C:H2'	17:AA:1234:C:O2	2.15	0.46
30:AN:62:ASP:OD1	30:AN:88:VAL:N	2.45	0.46
45:XE:310:LEU:HG	45:XE:310:LEU:O	2.16	0.46
54:XO:149:LEU:HA	54:XO:152:LEU:CD2	2.45	0.46
83:r4:49:Y5P:OP2	83:r4:59:Y5P:O2'	2.31	0.46
7:6:182:ASP:OD1	7:6:183:ASP:N	2.49	0.46
13:A1:153:SER:OG	13:A1:154:THR:N	2.49	0.46
16:A4:643:GLU:O	16:A4:646:THR:OG1	2.34	0.46
52:XM:225:ASP:OD2	52:XM:228:LYS:NZ	2.47	0.46
74:i:64:GLY:O	74:i:65:ASN:OD1	2.34	0.46
84:s:358:GLN:NE2	84:s:424:PHE:O	2.44	0.46
11:XA:2029:A:O2'	11:XA:2030:U:OP1	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:826:A:N7	26:AJ:55:ARG:NE	2.64	0.46
17:AA:1462:G:C2	17:AA:1463:G:C5	3.04	0.46
40:AX:130:LYS:O	40:AX:130:LYS:HG3	2.16	0.46
11:XA:2192:A:H4'	49:XJ:139:SER:HB2	1.98	0.45
11:XA:2273:A:O2'	57:XR:16:ASP:OD2	2.29	0.45
11:XA:2601:A:H1'	11:XA:2602:U:OP1	2.16	0.45
20:AD:400:GLU:N	20:AD:400:GLU:OE1	2.48	0.45
28:AL:188:GLU:N	28:AL:188:GLU:OE2	2.50	0.45
42:AZ:66:ARG:NH1	42:AZ:77:ASP:OD1	2.39	0.45
55:XP:156:SER:OG	55:XP:157:MET:SD	2.73	0.45
65:XZ:131:GLU:HA	65:XZ:134:MET:HG2	1.97	0.45
71:f:104:GLU:OE2	71:f:155:ARG:NH2	2.49	0.45
8:7:306:LEU:O	8:7:306:LEU:HG	2.17	0.45
11:XA:2319:A:O3'	54:XO:42:ILE:HD11	2.16	0.45
11:XA:2520:C:OP2	44:XD:295:TYR:OH	2.25	0.45
16:A4:66:ASP:OD1	16:A4:67:LYS:N	2.49	0.45
17:AA:745:A:C4	17:AA:746:A:C8	3.04	0.45
42:AZ:38:SER:OG	42:AZ:39:GLU:OE2	2.34	0.45
62:XW:115:ASP:O	62:XW:119:ARG:NE	2.46	0.45
16:A4:164:ARG:H	16:A4:167:LYS:HE3	1.82	0.45
28:AL:87:ASP:OD1	28:AL:88:VAL:N	2.48	0.45
52:XM:100:ARG:O	52:XM:104:LEU:HG	2.16	0.45
57:XR:96:GLU:OE1	57:XR:96:GLU:N	2.49	0.45
63:XX:96:LYS:HG3	63:XX:97:LEU:HD22	1.99	0.45
69:d:235:GLN:OE1	69:d:235:GLN:N	2.49	0.45
11:XA:1737:A:N6	11:XA:1760:G:O2'	2.46	0.45
11:XA:2447:A:OP1	84:s:59:ARG:NE	2.44	0.45
11:XA:2802:A:H2'	11:XA:2803:A:O4'	2.17	0.45
11:XA:3151:A:N6	11:XA:3163:G:O2'	2.49	0.45
12:A0:202:ASP:OD1	12:A0:202:ASP:N	2.50	0.45
17:AA:812:A:O2'	17:AA:813:A:O4'	2.28	0.45
38:AV:47:HIS:N	38:AV:78:ASN:OD1	2.48	0.45
70:e:175:GLN:N	70:e:175:GLN:OE1	2.49	0.45
80:p:149:ASP:OD1	80:p:149:ASP:C	2.59	0.45
6:5:384:GLN:OE1	11:XA:2395:A:O2'	2.35	0.45
17:AA:1433:A:C4	17:AA:1458:A:N6	2.84	0.45
83:r4:10:P5P:OP1	83:r4:45:Y5P:H2	2.17	0.45
83:r4:28:P5P:H2'	83:r4:29:P5P:O4'	2.15	0.45
8:7:259:ASP:OD1	8:7:260:PHE:N	2.50	0.45
11:XA:2099:U:H2'	11:XA:2100:C:C6	2.51	0.45
11:XA:2130:A:C2	79:o:17:TRP:CZ3	3.05	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2682:A:H4'	57:XR:41:LEU:HD13	1.97	0.45
18:AB:153:TYR:O	18:AB:157:ASN:ND2	2.49	0.45
40:AX:346:SER:OG	40:AX:347:ASN:N	2.49	0.45
45:XE:142:MET:HG2	45:XE:181:ILE:O	2.17	0.45
45:XE:327:GLU:OE1	45:XE:327:GLU:N	2.49	0.45
54:XO:86:ILE:N	54:XO:87:PRO:CD	2.80	0.45
54:XO:113:ARG:O	54:XO:117:ARG:NH1	2.49	0.45
63:XX:207:THR:N	63:XX:210:GLU:OE2	2.38	0.45
84:s:145:VAL:O	84:s:148:ASP:OD1	2.35	0.45
11:XA:2190:C:OP2	77:l:120:ARG:NH2	2.46	0.45
12:A0:127:GLU:OE2	12:A0:128:ALA:N	2.50	0.45
48:XI:198:PRO:O	48:XI:199:SER:C	2.60	0.45
57:XR:66:THR:HA	57:XR:69:ILE:HG22	1.98	0.45
59:XT:68:ARG:HE	69:d:230:ARG:HD3	1.82	0.45
83:r4:49:Y5P:N3	83:r4:66:Y5P:H4	2.31	0.45
86:A:1:MHW:OG1	86:A:1:MHW:O	2.33	0.45
6:5:143:PRO:HA	6:5:146:HIS:ND1	2.31	0.45
11:XA:2593:G:O2'	11:XA:2631:G:O6	2.32	0.45
40:AX:51:THR:O	40:AX:67:HIS:N	2.48	0.45
49:XJ:149:ARG:NH2	77:l:102:GLY:O	2.50	0.45
56:XQ:246:ASP:OD1	56:XQ:247:LEU:N	2.49	0.45
57:XR:85:ALA:O	57:XR:89:ASN:OD1	2.35	0.45
60:XU:40:VAL:HG12	60:XU:41:GLN:N	2.32	0.45
74:i:59:ASN:O	74:i:63:LEU:HD23	2.16	0.45
3:2:82:ARG:HH11	3:2:87:ARG:HD2	1.82	0.45
11:XA:2625:C:OP2	11:XA:2625:C:H6	2.00	0.45
14:A2:9:ARG:O	14:A2:20:VAL:N	2.46	0.45
28:AL:142:HIS:NE2	28:AL:149:ASP:OD2	2.42	0.45
74:i:80:LEU:HD12	74:i:80:LEU:O	2.17	0.45
4:3:100:ARG:NH1	11:XA:1733:C:O2'	2.40	0.45
11:XA:3218:A:O3'	45:XE:263:ASN:ND2	2.51	0.45
17:AA:1121:A:OP2	20:AD:297:ARG:NH2	2.50	0.45
22:AF:201:MET:N	22:AF:202:PRO:HD2	2.32	0.45
29:AM:111:ARG:NH2	31:AO:232:PRO:O	2.50	0.45
52:XM:133:LYS:C	52:XM:134:ARG:HG2	2.42	0.45
61:XV:112:GLU:OE1	69:d:81:ARG:NH2	2.47	0.45
17:AA:723:A:OP1	17:AA:724:C:N4	2.42	0.44
17:AA:1526:U:O2'	17:AA:1527:A:O4'	2.27	0.44
22:AF:116:GLU:O	22:AF:120:ARG:HG2	2.17	0.44
29:AM:63:GLU:OE1	29:AM:63:GLU:N	2.48	0.44
46:XF:77:VAL:O	46:XF:77:VAL:HG13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:XX:160:ASP:OD1	63:XX:160:ASP:C	2.59	0.44
7:6:247:GLU:OE2	7:6:247:GLU:N	2.50	0.44
16:A4:482:ILE:CG2	16:A4:519:TYR:HE2	2.30	0.44
17:AA:1366:C:O2'	17:AA:1419:G:O4'	2.29	0.44
36:AT:117:GLU:OE1	36:AT:120:LYS:NZ	2.50	0.44
43:XB:1620:A:N3	43:XB:1620:A:H2'	2.32	0.44
44:XD:292:MET:SD	44:XD:292:MET:N	2.90	0.44
59:XT:51:TRP:NE1	59:XT:75:HIS:O	2.46	0.44
83:r4:30:P5P:H2'	83:r4:31:P5P:C8	2.46	0.44
6:5:232:THR:OG1	6:5:234:ASP:O	2.33	0.44
7:6:107:LYS:O	7:6:110:ILE:HG13	2.17	0.44
11:XA:1940:A:OP1	11:XA:2495:U:O2'	2.27	0.44
11:XA:2954:C:H2'	11:XA:2955:U:O4'	2.17	0.44
32:AP:127:PRO:HA	32:AP:130:LEU:HD23	2.00	0.44
38:AV:36:ASP:OD1	38:AV:37:SER:N	2.50	0.44
68:c:267:LEU:O	68:c:267:LEU:HD12	2.18	0.44
80:p:146:ASN:O	80:p:149:ASP:OD1	2.35	0.44
83:r4:23:P5P:N3	83:r4:23:P5P:H2'	2.32	0.44
38:AV:235:GLU:O	38:AV:239:GLY:N	2.47	0.44
50:XK:114:LYS:HD2	50:XK:114:LYS:N	2.33	0.44
52:XM:14:ASP:OD1	52:XM:17:ARG:NH2	2.50	0.44
84:s:63:ILE:HA	84:s:66:TRP:CD1	2.52	0.44
84:s:300:HIS:HB2	84:s:361:ILE:HG22	1.99	0.44
6:5:30:ALA:N	44:XD:201:GLY:O	2.50	0.44
11:XA:2066:C:O2'	11:XA:2067:C:OP1	2.36	0.44
12:A0:129:ARG:NH1	12:A0:203:TYR:OH	2.50	0.44
17:AA:770:C:O2'	17:AA:771:A:OP1	2.31	0.44
17:AA:1132:U:H2'	17:AA:1133:C:C6	2.52	0.44
38:AV:201:GLU:OE1	38:AV:233:LYS:NZ	2.51	0.44
63:XX:20:ILE:HA	63:XX:23:ARG:HE	1.83	0.44
11:XA:1828:A:H4'	11:XA:1829:A:C8	2.53	0.44
69:d:157:HIS:O	69:d:161:HIS:ND1	2.49	0.44
84:s:66:TRP:O	84:s:69:THR:OG1	2.30	0.44
7:6:288:SER:O	7:6:289:PRO:C	2.61	0.44
28:AL:127:ALA:O	28:AL:130:ILE:HG13	2.18	0.44
65:XZ:84:ASP:O	65:XZ:88:MET:SD	2.75	0.44
72:g:96:VAL:HG21	72:g:158:LYS:HG3	2.00	0.44
1:0:91:ARG:HG2	1:0:95:ARG:HD2	2.00	0.44
11:XA:1749:C:OP2	11:XA:2899:C:O2'	2.33	0.44
11:XA:2456:U:H2'	11:XA:2457:A:O4'	2.17	0.44
17:AA:1272:A:N1	17:AA:1303:G:O2'	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AC:89:ASP:OD1	19:AC:89:ASP:C	2.60	0.44
34:AR:135:ARG:HE	34:AR:186:TRP:CG	2.36	0.44
64:XY:134:LYS:O	64:XY:137:ASP:OD1	2.35	0.44
69:d:288:LYS:HG2	69:d:289:PRO:HD2	2.00	0.44
70:e:145:ASP:O	70:e:148:SER:OG	2.30	0.44
6:5:306:PRO:O	6:5:310:ARG:NE	2.45	0.44
11:XA:3169:C:O2'	11:XA:3170:C:O4'	2.30	0.44
17:AA:1516:G:C6	17:AA:1517:A:N6	2.86	0.44
22:AF:201:MET:N	22:AF:201:MET:SD	2.89	0.44
38:AV:79:ILE:CD1	38:AV:88:ALA:HB2	2.48	0.44
40:AX:297:MET:O	40:AX:297:MET:HG2	2.18	0.44
52:XM:88:SER:O	52:XM:134:ARG:NE	2.51	0.44
52:XM:270:ALA:HB1	52:XM:271:PRO:HD2	2.00	0.44
65:XZ:106:VAL:HG12	65:XZ:110:LEU:HD23	2.00	0.44
6:5:409:GLU:OE1	6:5:409:GLU:N	2.50	0.43
7:6:379:ILE:O	7:6:380:TYR:CG	2.71	0.43
11:XA:2944:C:H2'	11:XA:2945:A:O4'	2.18	0.43
17:AA:805:C:O4'	17:AA:805:C:O2	2.36	0.43
17:AA:1452:U:H2'	17:AA:1453:A:C8	2.53	0.43
18:AB:202:ILE:O	18:AB:202:ILE:HG22	2.16	0.43
28:AL:216:GLU:O	28:AL:219:LYS:HG3	2.18	0.43
40:AX:337:LEU:HG	40:AX:337:LEU:O	2.18	0.43
51:XL:32:ILE:O	51:XL:67:GLY:N	2.51	0.43
57:XR:41:LEU:HD23	57:XR:41:LEU:H	1.83	0.43
11:XA:2305:U:OP1	59:XT:149:ARG:NH1	2.51	0.43
17:AA:746:A:C4	17:AA:747:A:C8	3.05	0.43
63:XX:130:ARG:O	63:XX:133:ASP:OD1	2.36	0.43
64:XY:140:ASP:OD1	64:XY:140:ASP:C	2.60	0.43
68:c:85:LEU:O	68:c:89:LYS:HG2	2.19	0.43
70:e:83:LEU:N	78:m:48:TYR:O	2.42	0.43
70:e:264:LEU:CD1	70:e:269:LEU:HB3	2.48	0.43
83:r4:8:Y5P:H6	83:r4:8:Y5P:O5'	2.18	0.43
7:6:374:GLU:OE2	80:p:140:SER:OG	2.25	0.43
29:AM:55:ASP:OD1	29:AM:65:LEU:O	2.36	0.43
29:AM:59:ASN:OD1	29:AM:63:GLU:N	2.51	0.43
41:AY:365:SER:N	41:AY:368:GLN:OE1	2.44	0.43
54:XO:86:ILE:CG1	54:XO:87:PRO:HD3	2.49	0.43
58:XS:99:VAL:HG23	58:XS:132:LYS:O	2.18	0.43
68:c:216:ARG:O	68:c:217:ASP:C	2.61	0.43
83:r4:73:P5P:O3'	83:r4:75:Y5P:OP1	2.36	0.43
8:7:189:LEU:HD23	8:7:189:LEU:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2458:A:OP2	54:XO:9:ILE:N	2.51	0.43
11:XA:2875:A:H4'	55:XP:178:TYR:CZ	2.54	0.43
18:AB:142:ILE:N	18:AB:164:GLU:OE1	2.50	0.43
34:AR:168:ARG:NH1	34:AR:236:GLU:OE1	2.50	0.43
36:AT:81:ASP:OD1	36:AT:82:SER:N	2.52	0.43
83:r4:28:P5P:C5	83:r4:29:P5P:H8	2.48	0.43
84:s:407:ASP:O	84:s:408:ASN:OD1	2.36	0.43
9:8:178:TYR:N	78:m:63:THR:O	2.47	0.43
11:XA:2696:A:H1'	11:XA:2698:G:OP2	2.19	0.43
14:A2:59:ASN:OD1	14:A2:62:ARG:NH2	2.51	0.43
16:A4:256:GLU:O	16:A4:257:HIS:C	2.61	0.43
31:AO:67:ARG:NH2	31:AO:68:TYR:OH	2.52	0.43
31:AO:137:ALA:HB3	31:AO:138:PRO:HD3	2.00	0.43
52:XM:288:GLU:HG2	52:XM:289:ASN:N	2.33	0.43
55:XP:177:ILE:O	55:XP:178:TYR:C	2.61	0.43
57:XR:95:VAL:HG23	57:XR:95:VAL:O	2.18	0.43
68:c:196:PHE:HA	68:c:199:ILE:HG12	1.99	0.43
82:r:132:ARG:HD3	82:r:133:PRO:HD2	2.01	0.43
7:6:144:GLY:N	7:6:145:PRO:CD	2.82	0.43
11:XA:1846:C:P	58:XS:177:ARG:H	2.40	0.43
11:XA:1848:U:O4	58:XS:177:ARG:HD3	2.18	0.43
11:XA:2083:U:OP1	75:j:76:ARG:NH1	2.45	0.43
11:XA:2449:G:OP2	84:s:225:ARG:NH2	2.47	0.43
17:AA:895:C:N4	17:AA:899:G:O6	2.52	0.43
17:AA:1234:C:O2'	17:AA:1235:U:OP1	2.27	0.43
20:AD:407:ASP:O	20:AD:410:ASP:OD1	2.37	0.43
45:XE:277:ASN:HB3	45:XE:282:ILE:HG13	2.00	0.43
49:XJ:178:GLU:HA	49:XJ:181:LEU:CD2	2.48	0.43
59:XT:126:ASP:HA	59:XT:129:VAL:HG22	2.01	0.43
78:m:50:ARG:NH2	78:m:52:TYR:OH	2.48	0.43
84:s:90:LYS:NZ	84:s:280:ASN:OD1	2.39	0.43
11:XA:2302:U:H1'	46:XF:147:ARG:HD2	2.00	0.43
11:XA:2520:C:O2'	44:XD:205:GLN:OE1	2.33	0.43
11:XA:3158:A:O2'	54:XO:11:HIS:O	2.32	0.43
16:A4:634:ALA:HB3	16:A4:641:ILE:HG21	2.01	0.43
19:AC:51:VAL:O	19:AC:164:TYR:N	2.43	0.43
40:AX:209:VAL:HG22	40:AX:210:TRP:N	2.34	0.43
57:XR:35:LYS:O	57:XR:42:ALA:HB2	2.19	0.43
68:c:44:GLU:O	68:c:47:ARG:HG2	2.19	0.43
11:XA:1884:G:N7	46:XF:281:ARG:HD2	2.34	0.43
11:XA:1917:A:C8	11:XA:1983:U:C4	3.07	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:1015:A:O2'	33:AQ:38:ASP:OD2	2.37	0.43
39:AW:103:ARG:O	39:AW:115:ASP:N	2.51	0.43
41:AY:296:ASN:OD1	41:AY:297:GLY:N	2.51	0.43
61:XV:188:VAL:O	61:XV:190:CYS:N	2.52	0.43
72:g:154:ASP:OD1	72:g:154:ASP:N	2.51	0.43
5:4:75:ARG:HD2	5:4:98:HIS:CD2	2.54	0.43
5:4:84:ARG:C	5:4:85:ARG:HD2	2.43	0.43
17:AA:1457:G:OP2	23:AG:338:SER:OG	2.29	0.43
48:XI:66:PRO:O	48:XI:67:SER:OG	2.33	0.43
58:XS:118:ASN:HD22	58:XS:118:ASN:C	2.27	0.43
81:q:141:GLU:O	81:q:144:GLU:HG3	2.18	0.43
82:r:40:GLU:N	82:r:40:GLU:OE1	2.52	0.43
11:XA:1761:A:HO2'	11:XA:1762:A:P	2.40	0.43
11:XA:2138:U:O2'	11:XA:2151:A:N3	2.46	0.43
11:XA:2195:A:OP1	77:l:119:ARG:NE	2.45	0.43
17:AA:1193:U:O3'	22:AF:178:ARG:NH2	2.48	0.43
22:AF:35:SER:OG	22:AF:36:ARG:N	2.51	0.43
58:XS:131:GLU:OE1	58:XS:131:GLU:N	2.52	0.43
60:XU:28:LEU:N	64:XY:114:THR:HG22	2.34	0.43
64:XY:123:ARG:NE	69:d:68:ARG:O	2.32	0.43
69:d:65:GLN:HA	69:d:65:GLN:OE1	2.19	0.43
80:p:138:GLU:N	80:p:138:GLU:OE1	2.52	0.43
84:s:212:ARG:O	84:s:229:LEU:HB2	2.18	0.43
11:XA:2939:C:H2'	11:XA:2940:A:O4'	2.19	0.42
11:XA:3212:C:O2	11:XA:3212:C:O4'	2.36	0.42
34:AR:107:THR:HG1	34:AR:108:GLN:H	1.67	0.42
36:AT:89:ASP:OD2	37:AU:120:ARG:NH2	2.52	0.42
59:XT:123:GLU:O	59:XT:126:ASP:OD1	2.36	0.42
63:XX:180:ASP:N	63:XX:181:PRO:HD3	2.34	0.42
76:k:48:ASN:OD1	76:k:49:CYS:N	2.52	0.42
83:r4:2:Y5P:H2'	83:r4:3:Y5P:C6	2.49	0.42
4:3:94:LEU:HD11	4:3:107:VAL:HG11	2.01	0.42
7:6:367:ASP:OD1	7:6:367:ASP:C	2.63	0.42
8:7:150:MET:HA	8:7:153:VAL:HG12	2.01	0.42
9:8:99:ARG:NE	70:e:84:TYR:CG	2.78	0.42
11:XA:2623:A:C2	11:XA:2624:C:C4	3.07	0.42
11:XA:3226:G:H5''	45:XE:174:GLN:OE1	2.19	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
19:AC:86:THR:O	19:AC:89:ASP:OD1	2.37	0.42
20:AD:420:SER:OG	20:AD:423:SER:OG	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AD:422:TRP:HA	20:AD:425:LEU:HD21	2.00	0.42
23:AG:214:SER:O	23:AG:217:ASP:OD1	2.37	0.42
45:XE:100:ILE:HD11	45:XE:149:GLY:CA	2.49	0.42
58:XS:144:LEU:HB2	66:a:58:ILE:HB	2.01	0.42
6:5:270:ILE:HG22	6:5:270:ILE:O	2.19	0.42
8:7:68:LYS:HG2	8:7:78:VAL:HG12	2.01	0.42
11:XA:1834:U:C4	59:XT:206:ARG:HA	2.53	0.42
11:XA:1848:U:H2'	11:XA:1849:C:O4'	2.19	0.42
11:XA:2511:C:O2'	44:XD:257:ILE:O	2.33	0.42
11:XA:2939:C:O2'	11:XA:2940:A:H5'	2.19	0.42
16:A4:73:ALA:HB2	24:AH:61:PRO:HG2	2.01	0.42
38:AV:354:SER:O	38:AV:357:THR:OG1	2.34	0.42
40:AX:63:HIS:O	40:AX:63:HIS:ND1	2.51	0.42
65:XZ:134:MET:SD	75:j:75:ARG:NE	2.90	0.42
17:AA:894:C:N4	26:AJ:117:ASP:OD2	2.45	0.42
17:AA:1193:U:O2'	22:AF:178:ARG:NH1	2.53	0.42
31:AO:106:PRO:HA	31:AO:109:ARG:HG2	2.00	0.42
48:XI:49:ALA:HA	48:XI:52:GLU:OE2	2.18	0.42
53:XN:203:GLU:O	53:XN:206:GLU:HG3	2.20	0.42
61:XV:148:THR:O	61:XV:149:ARG:C	2.63	0.42
75:j:98:LEU:O	75:j:101:GLU:HG3	2.20	0.42
84:s:260:GLU:N	84:s:260:GLU:OE1	2.53	0.42
7:6:51:TYR:CZ	62:XW:122:LYS:HA	2.54	0.42
17:AA:782:A:O2'	30:AN:46:ARG:NH1	2.52	0.42
17:AA:1020:C:H4'	32:AP:94:ARG:NH1	2.34	0.42
46:XF:225:GLU:OE1	46:XF:225:GLU:N	2.43	0.42
49:XJ:120:ILE:HA	49:XJ:123:ILE:HG22	2.01	0.42
50:XK:2:SER:OG	50:XK:3:SER:N	2.51	0.42
7:6:50:LYS:HA	62:XW:121:PRO:HA	2.02	0.42
11:XA:2118:U:C2	11:XA:2119:U:C5	3.08	0.42
16:A4:638:SER:OG	16:A4:640:PRO:HD2	2.20	0.42
17:AA:657:G:O4'	17:AA:1480:A:O2'	2.32	0.42
34:AR:113:GLU:O	34:AR:116:ARG:HG3	2.18	0.42
41:AY:377:ARG:HA	41:AY:380:PHE:CE2	2.55	0.42
49:XJ:32:GLY:O	49:XJ:36:GLY:N	2.40	0.42
57:XR:69:ILE:CD1	57:XR:83:TYR:CD2	3.03	0.42
63:XX:178:PRO:C	63:XX:179:GLU:HG3	2.45	0.42
64:XY:230:LYS:O	64:XY:233:ILE:HG13	2.20	0.42
68:c:60:ARG:NH2	68:c:64:PRO:O	2.52	0.42
69:d:244:GLU:N	69:d:244:GLU:OE1	2.52	0.42
83:r4:31:P5P:N3	83:r4:31:P5P:H2'	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:116:LEU:HD23	1:0:116:LEU:H	1.85	0.42
11:XA:2002:G:O2'	11:XA:2927:C:N3	2.41	0.42
11:XA:2833:A:OP1	62:XW:74:ARG:NH1	2.42	0.42
16:A4:319:LEU:HA	16:A4:322:HIS:CD2	2.55	0.42
20:AD:410:ASP:OD1	20:AD:410:ASP:C	2.63	0.42
35:AS:15:ARG:O	35:AS:18:ASP:OD1	2.37	0.42
49:XJ:52:GLU:O	49:XJ:56:ARG:NE	2.53	0.42
53:XN:174:GLY:O	53:XN:177:ASP:OD1	2.38	0.42
69:d:166:GLU:OE1	69:d:166:GLU:N	2.51	0.42
73:h:122:ARG:NH1	73:h:125:ASP:OD1	2.53	0.42
77:l:106:THR:N	77:l:109:GLU:OE2	2.40	0.42
78:m:55:LEU:HD13	78:m:56:LEU:N	2.34	0.42
83:r4:71:P5P:O5'	83:r4:71:P5P:H8	2.20	0.42
1:0:158:VAL:HA	1:0:175:ILE:HG13	2.02	0.42
11:XA:2682:A:OP1	57:XR:34:ARG:NH2	2.53	0.42
22:AF:94:PHE:CD2	22:AF:111:MET:HE1	2.54	0.42
24:AH:126:ILE:O	24:AH:127:TYR:CG	2.73	0.42
30:AN:39:LEU:O	36:AT:11:ARG:NH1	2.53	0.42
50:XK:27:PRO:HG2	50:XK:30:LYS:HG2	2.00	0.42
53:XN:177:ASP:OD1	53:XN:178:GLN:N	2.53	0.42
61:XV:77:VAL:HG23	61:XV:89:GLY:N	2.34	0.42
84:s:171:VAL:HG13	84:s:172:ILE:HG13	2.00	0.42
5:4:90:VAL:O	5:4:99:LYS:HA	2.20	0.42
8:7:159:LYS:HA	66:a:92:ASP:HB2	2.00	0.42
11:XA:2040:G:H2'	11:XA:2041:U:O4'	2.19	0.42
11:XA:2041:U:OP1	52:XM:57:ARG:HG3	2.19	0.42
11:XA:2116:C:O2	11:XA:2837:A:H2	2.02	0.42
11:XA:2534:G:OP2	44:XD:268:LYS:NZ	2.52	0.42
15:A3:164:ARG:O	15:A3:167:ILE:HG13	2.20	0.42
16:A4:335:PHE:HA	16:A4:338:ILE:HG22	2.01	0.42
17:AA:682:A:N6	17:AA:865:A:H61	2.18	0.42
46:XF:184:GLN:O	46:XF:185:ASP:OD1	2.37	0.42
48:XI:82:LEU:O	48:XI:86:ILE:HG12	2.20	0.42
50:XK:107:ALA:O	50:XK:111:MET:SD	2.78	0.42
76:k:91:ALA:O	76:k:94:ILE:HG13	2.20	0.42
11:XA:3153:U:C2'	11:XA:3154:U:H5'	2.50	0.42
14:A2:50:SER:O	14:A2:53:MET:HG2	2.19	0.42
16:A4:640:PRO:O	16:A4:643:GLU:HG2	2.20	0.42
31:AO:81:HIS:ND1	31:AO:82:LYS:O	2.52	0.42
37:AU:52:GLU:OE1	37:AU:52:GLU:N	2.48	0.42
43:XB:1623:G:OP2	55:XP:87:HIS:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:XB:1639:U:O4	43:XB:1640:A:N6	2.53	0.42
46:XF:284:TYR:HB2	46:XF:285:PRO:HD2	2.01	0.42
53:XN:78:GLU:OE2	53:XN:158:ARG:NE	2.49	0.42
72:g:100:ILE:CD1	72:g:106:GLN:OE1	2.68	0.42
75:j:82:GLN:O	75:j:85:ASP:OD1	2.37	0.42
6:5:306:PRO:C	6:5:310:ARG:HE	2.28	0.41
8:7:203:THR:O	8:7:207:HIS:ND1	2.49	0.41
9:8:169:PHE:HB2	9:8:170:PRO:HD3	2.02	0.41
11:XA:2336:U:C2	11:XA:2337:A:C8	3.08	0.41
11:XA:2531:U:O4	44:XD:246:ARG:NH2	2.53	0.41
11:XA:2682:A:H2'	11:XA:2683:C:C5'	2.50	0.41
11:XA:2952:U:N3	11:XA:2953:U:C5	2.88	0.41
13:A1:104:GLU:OE1	13:A1:104:GLU:N	2.51	0.41
34:AR:67:LYS:N	34:AR:68:PRO:CD	2.83	0.41
58:XS:52:PRO:HD2	82:r:77:LEU:HD21	2.02	0.41
65:XZ:110:LEU:HB3	79:o:49:LEU:HD21	2.02	0.41
4:3:152:LYS:NZ	11:XA:2090:A:OP2	2.53	0.41
6:5:201:ARG:HG2	6:5:232:THR:HG22	2.02	0.41
6:5:313:MET:HE2	6:5:355:LEU:CD2	2.50	0.41
11:XA:3180:A:C4	11:XA:3190:A:C6	3.09	0.41
14:A2:86:MET:O	14:A2:89:ILE:HG13	2.20	0.41
17:AA:1235:U:H5''	17:AA:1236:C:OP2	2.19	0.41
34:AR:307:LEU:C	34:AR:309:PRO:HD3	2.44	0.41
37:AU:125:ARG:O	37:AU:128:GLU:HG3	2.20	0.41
37:AU:178:GLU:OE1	37:AU:178:GLU:N	2.47	0.41
38:AV:79:ILE:O	38:AV:115:GLN:NE2	2.53	0.41
49:XJ:75:ASP:O	49:XJ:76:ARG:HB3	2.20	0.41
52:XM:68:GLU:N	52:XM:68:GLU:OE1	2.53	0.41
76:k:76:MET:SD	76:k:86:MET:HB2	2.60	0.41
83:r4:49:Y5P:C4	83:r4:50:Y5P:H5	2.50	0.41
1:0:138:ARG:O	1:0:141:ILE:HG13	2.20	0.41
4:3:177:TYR:O	4:3:181:HIS:ND1	2.52	0.41
11:XA:2143:G:C5	11:XA:2258:A:C2	3.09	0.41
11:XA:2665:U:OP2	54:XO:17:ARG:HD2	2.20	0.41
11:XA:2692:G:N1	11:XA:2696:A:OP2	2.44	0.41
16:A4:455:ASN:HA	16:A4:486:TYR:CE1	2.55	0.41
20:AD:147:PRO:O	20:AD:155:GLN:NE2	2.53	0.41
51:XL:110:ASP:OD1	51:XL:110:ASP:N	2.52	0.41
52:XM:103:TYR:OH	72:g:93:ASN:ND2	2.46	0.41
53:XN:216:GLU:HB2	53:XN:238:LYS:HD2	2.02	0.41
56:XQ:251:GLU:HA	56:XQ:254:MET:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:XY:170:ARG:NH1	64:XY:174:GLY:O	2.54	0.41
68:c:68:TYR:O	68:c:72:ILE:HD12	2.20	0.41
83:r4:6:P5P:O5'	83:r4:6:P5P:H8	2.19	0.41
6:5:147:ILE:HD11	6:5:150:GLN:HA	2.02	0.41
11:XA:2550:A:C8	11:XA:2590:A:C4	3.08	0.41
11:XA:2558:A:C4'	11:XA:2559:U:OP2	2.69	0.41
11:XA:3050:U:C2	11:XA:3052:A:OP2	2.74	0.41
13:A1:217:GLN:O	13:A1:220:ASP:OD1	2.39	0.41
15:A3:174:ARG:HA	15:A3:177:TRP:CD2	2.56	0.41
17:AA:1187:U:OP2	17:AA:1189:U:N3	2.41	0.41
17:AA:1208:U:C4	17:AA:1209:C:C4	3.08	0.41
19:AC:62:ILE:HG23	19:AC:63:ALA:N	2.35	0.41
35:AS:18:ASP:OD1	35:AS:19:LEU:N	2.54	0.41
38:AV:353:LEU:O	38:AV:356:THR:OG1	2.38	0.41
43:XB:1607:U:O2'	43:XB:1608:G:H5'	2.21	0.41
50:XK:39:LEU:HD21	50:XK:125:LEU:HB2	2.03	0.41
50:XK:42:LEU:O	57:XR:74:ALA:HB2	2.19	0.41
56:XQ:168:ASN:OD1	56:XQ:169:PRO:HD2	2.20	0.41
76:k:65:ASP:OD2	76:k:73:ARG:NH2	2.53	0.41
77:l:125:ASN:O	77:l:128:ARG:HG3	2.20	0.41
79:o:36:ILE:HA	79:o:39:LEU:HG	2.02	0.41
81:q:86:GLU:O	81:q:89:GLU:HG3	2.21	0.41
83:r4:49:Y5P:C5	83:r4:50:Y5P:H5	2.50	0.41
11:XA:1696:C:OP2	64:XY:180:LYS:NZ	2.52	0.41
11:XA:2374:A:N6	84:s:272:PRO:O	2.45	0.41
13:A1:199:CYS:O	13:A1:203:ASP:N	2.52	0.41
16:A4:133:ALA:HB2	19:AC:148:LYS:HB2	2.03	0.41
17:AA:751:A:OP1	30:AN:47:LYS:NZ	2.53	0.41
23:AG:360:GLU:OE1	23:AG:360:GLU:N	2.53	0.41
28:AL:78:ASN:OD1	28:AL:79:VAL:N	2.53	0.41
46:XF:63:GLN:O	73:h:117:LEU:HD21	2.20	0.41
52:XM:203:ARG:NE	52:XM:264:GLN:O	2.54	0.41
52:XM:254:LYS:O	52:XM:258:THR:OG1	2.30	0.41
62:XW:115:ASP:OD1	62:XW:115:ASP:C	2.63	0.41
65:XZ:148:GLN:N	65:XZ:148:GLN:OE1	2.54	0.41
70:e:255:VAL:CG2	70:e:259:GLU:HG2	2.50	0.41
81:q:113:LYS:O	81:q:116:GLU:HG3	2.21	0.41
82:r:121:MET:HE3	82:r:151:LEU:HA	2.02	0.41
84:s:311:LEU:HD12	84:s:316:CYS:HB2	2.02	0.41
4:3:110:VAL:HG11	4:3:161:MET:SD	2.60	0.41
11:XA:1674:A:N7	59:XT:47:ILE:N	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:1737:A:O2'	74:i:93:ARG:NH1	2.50	0.41
11:XA:2629:A:N3	11:XA:3079:G:O2'	2.50	0.41
11:XA:2729:U:O4	11:XA:2730:A:N6	2.54	0.41
13:A1:189:LYS:NZ	13:A1:232:GLU:O	2.50	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:1014:A:O2'	17:AA:1031:G:O4'	2.31	0.41
17:AA:1554:G:H2'	17:AA:1555:A:O4'	2.20	0.41
18:AB:186:THR:HG23	18:AB:186:THR:O	2.20	0.41
29:AM:87:MET:SD	29:AM:88:GLU:N	2.94	0.41
40:AX:167:ASP:OD1	40:AX:167:ASP:O	2.39	0.41
50:XK:40:GLN:NE2	50:XK:113:PRO:HD3	2.36	0.41
57:XR:57:ARG:O	57:XR:61:LYS:HD3	2.21	0.41
64:XY:211:LEU:O	64:XY:214:GLU:HG2	2.21	0.41
65:XZ:75:THR:OG1	65:XZ:83:LYS:HG2	2.21	0.41
65:XZ:133:ASN:HB3	65:XZ:147:VAL:HG22	2.03	0.41
69:d:266:VAL:O	69:d:266:VAL:HG13	2.21	0.41
73:h:135:GLN:N	73:h:135:GLN:OE1	2.53	0.41
74:i:59:ASN:O	74:i:62:ILE:N	2.52	0.41
80:p:128:ASN:OD1	80:p:129:ARG:N	2.49	0.41
2:1:20:MET:HA	2:1:58:GLU:HA	2.03	0.41
6:5:80:ARG:NH2	6:5:82:TYR:OH	2.53	0.41
7:6:257:PRO:HB3	7:6:268:LEU:HD21	2.02	0.41
7:6:289:PRO:C	7:6:291:TYR:H	2.29	0.41
9:8:138:ALA:O	9:8:141:GLU:HG3	2.21	0.41
11:XA:1859:A:OP1	11:XA:2299:U:O2'	2.38	0.41
13:A1:91:VAL:HG12	13:A1:92:LYS:N	2.36	0.41
17:AA:995:A:P	25:AI:120:ALA:HB2	2.61	0.41
17:AA:1055:U:C2	17:AA:1056:A:C8	3.09	0.41
46:XF:49:ARG:HD2	46:XF:263:LEU:HD12	2.03	0.41
52:XM:53:HIS:CD2	52:XM:54:LYS:HD3	2.56	0.41
61:XV:190:CYS:O	61:XV:191:LEU:HB3	2.20	0.41
64:XY:165:PRO:HB2	64:XY:181:PHE:CD2	2.56	0.41
65:XZ:81:TRP:O	65:XZ:84:ASP:OD1	2.39	0.41
68:c:43:LYS:O	68:c:46:GLU:HG3	2.21	0.41
84:s:337:GLY:O	84:s:341:MET:HG2	2.21	0.41
7:6:224:HIS:CD2	7:6:230:ALA:HB3	2.55	0.41
11:XA:1841:U:H2'	11:XA:1842:A:O4'	2.21	0.41
11:XA:2072:A:N6	11:XA:2831:G:H2'	2.36	0.41
11:XA:2135:A:N3	11:XA:2135:A:H2'	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XA:2919:A:C6	63:XX:97:LEU:HD12	2.56	0.41
17:AA:908:C:N4	17:AA:909:G:O6	2.53	0.41
20:AD:257:SER:HB2	20:AD:275:ALA:HB2	2.03	0.41
55:XP:133:GLN:HA	55:XP:136:LEU:CD2	2.51	0.41
74:i:111:ASN:O	74:i:114:ILE:HG13	2.21	0.41
84:s:242:ARG:NH2	84:s:292:CYS:O	2.53	0.41
3:2:82:ARG:NH2	11:XA:1790:A:P	2.94	0.41
9:8:116:LEU:O	9:8:119:LYS:HG3	2.21	0.41
11:XA:2259:C:O2'	11:XA:2261:C:OP2	2.33	0.41
11:XA:2470:G:O2'	51:XL:36:THR:HG22	2.19	0.41
11:XA:2933:G:N2	11:XA:2936:U:O2	2.49	0.41
11:XA:3096:U:C6	86:A:7:004:O	2.74	0.41
11:XA:3148:C:OP1	45:XE:211:ILE:HG12	2.21	0.41
11:XA:3189:C:C2'	11:XA:3190:A:OP2	2.69	0.41
12:A0:147:GLU:HG2	12:A0:148:GLU:N	2.35	0.41
12:A0:184:THR:HG23	12:A0:185:SER:N	2.36	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:1152:A:C2	17:AA:1153:C:C6	3.08	0.41
17:AA:1161:A:C2	17:AA:1162:A:C8	3.09	0.41
17:AA:1210:U:H2'	17:AA:1211:G:C8	2.56	0.41
19:AC:152:ARG:NH1	19:AC:153:LEU:O	2.54	0.41
20:AD:127:ASN:OD1	20:AD:128:ARG:N	2.54	0.41
26:AJ:49:LEU:HD23	26:AJ:51:PRO:HD2	2.03	0.41
31:AO:58:TYR:O	31:AO:61:SER:OG	2.30	0.41
38:AV:47:HIS:O	38:AV:47:HIS:ND1	2.54	0.41
56:XQ:168:ASN:O	56:XQ:171:VAL:HG22	2.21	0.41
63:XX:157:PHE:O	63:XX:160:ASP:OD1	2.39	0.41
64:XY:137:ASP:O	64:XY:140:ASP:OD1	2.39	0.41
67:b:72:VAL:HG23	67:b:72:VAL:O	2.20	0.41
81:q:137:GLN:HA	81:q:140:ARG:CD	2.51	0.41
81:q:179:LEU:HD11	83:r4:47:Y5P:H2	2.03	0.41
83:r4:28:P5P:C4	83:r4:29:P5P:H8	2.51	0.41
7:6:119:GLU:OE1	7:6:119:GLU:N	2.45	0.41
11:XA:3122:U:O2	11:XA:3122:U:O4'	2.37	0.41
17:AA:1173:C:H2'	17:AA:1174:U:C6	2.56	0.41
65:XZ:106:VAL:O	65:XZ:110:LEU:HD23	2.20	0.41
67:b:112:VAL:HG23	67:b:112:VAL:O	2.21	0.41
74:i:88:LEU:HB2	74:i:117:LEU:HD13	2.03	0.41
1:0:126:CYS:O	1:0:129:LYS:HG2	2.21	0.40
6:5:250:ASN:OD1	6:5:251:HIS:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:156:ARG:HG2	8:7:156:ARG:O	2.20	0.40
11:XA:2335:A:C1'	84:s:277:GLN:HE21	2.34	0.40
14:A2:39:GLU:OE2	14:A2:39:GLU:N	2.45	0.40
17:AA:865:A:H2'	17:AA:866:A:N9	2.36	0.40
17:AA:1211:G:N1	17:AA:1354:A:C6	2.89	0.40
17:AA:1426:U:O4	17:AA:1427:A:N6	2.54	0.40
23:AG:299:ASP:OD1	23:AG:300:TYR:N	2.54	0.40
34:AR:308:HIS:N	34:AR:309:PRO:HD3	2.35	0.40
38:AV:338:HIS:ND1	38:AV:342:GLN:OE1	2.54	0.40
40:AX:371:ALA:N	40:AX:372:PRO:CD	2.85	0.40
44:XD:109:PHE:HB3	44:XD:204:ALA:HB3	2.03	0.40
45:XE:66:SER:O	45:XE:69:ASP:OD1	2.39	0.40
53:XN:131:ILE:HD11	53:XN:149:HIS:CE1	2.55	0.40
68:c:211:THR:HG22	68:c:215:ILE:HD13	2.03	0.40
84:s:350:ASP:OD1	84:s:351:VAL:N	2.53	0.40
4:3:180:TYR:CD2	7:6:363:LEU:HD21	2.56	0.40
6:5:201:ARG:NH2	6:5:418:TYR:O	2.54	0.40
11:XA:2990:A:OP2	11:XA:2990:A:H3'	2.22	0.40
12:A0:71:LEU:HB2	12:A0:72:PRO:HD2	2.03	0.40
14:A2:53:MET:SD	22:AF:234:ARG:HD2	2.61	0.40
17:AA:1017:A:OP2	17:AA:1018:G:O2'	2.33	0.40
17:AA:1485:G:C6	17:AA:1486:C:C5	3.09	0.40
20:AD:194:SER:O	20:AD:197:SER:OG	2.37	0.40
34:AR:72:ASP:OD1	34:AR:72:ASP:N	2.54	0.40
83:r4:3:Y5P:C2	83:r4:71:P5P:H2	2.51	0.40
11:XA:1868:G:H2'	52:XM:40:PRO:HG3	2.03	0.40
11:XA:2111:C:H1'	11:XA:2944:C:O2'	2.20	0.40
11:XA:2178:A:H2'	11:XA:2179:A:C5	2.56	0.40
11:XA:2989:G:H5''	11:XA:2990:A:H5''	2.04	0.40
17:AA:1112:A:N6	17:AA:1130:G:O6	2.55	0.40
17:AA:1431:G:N1	17:AA:1458:A:OP2	2.46	0.40
22:AF:114:THR:HG22	22:AF:202:PRO:HA	2.02	0.40
24:AH:123:SER:OG	24:AH:124:VAL:N	2.53	0.40
28:AL:166:MET:O	28:AL:169:ASN:OD1	2.39	0.40
35:AS:114:GLU:OE2	35:AS:114:GLU:N	2.49	0.40
52:XM:84:ASN:OD1	52:XM:84:ASN:N	2.54	0.40
56:XQ:227:LYS:N	56:XQ:228:PRO:CD	2.84	0.40
58:XS:180:PHE:CZ	58:XS:182:LYS:NZ	2.89	0.40
61:XV:60:ASP:OD1	61:XV:61:THR:N	2.54	0.40
66:a:96:LYS:O	66:a:97:THR:C	2.64	0.40
67:b:126:ILE:O	67:b:127:GLN:HB2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:c:195:PHE:O	68:c:198:VAL:HG12	2.20	0.40
11:XA:2093:U:O2	11:XA:2266:U:O2'	2.38	0.40
12:A0:131:ILE:C	12:A0:131:ILE:HD12	2.47	0.40
13:A1:211:ARG:NH2	41:AY:359:SER:OG	2.54	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:1115:U:C4	35:AS:53:TYR:HB2	2.56	0.40
17:AA:1449:G:C2	17:AA:1450:C:C6	3.09	0.40
17:AA:1483:C:C2	17:AA:1567:A:N6	2.88	0.40
19:AC:85:ARG:O	19:AC:88:GLU:HG3	2.21	0.40
31:AO:54:GLU:N	31:AO:55:PRO:CD	2.84	0.40
31:AO:105:CYS:HB2	31:AO:106:PRO:HD2	2.02	0.40
33:AQ:26:LEU:O	33:AQ:29:ILE:HG22	2.21	0.40
34:AR:260:ASP:OD1	34:AR:291:ARG:NH1	2.54	0.40
38:AV:195:ASP:OD1	38:AV:196:PHE:N	2.51	0.40
40:AX:100:MET:HB3	90:AX:500:GTP:HN1	1.87	0.40
70:e:84:TYR:H	70:e:84:TYR:HD1	1.68	0.40
81:q:138:GLN:HA	81:q:141:GLU:OE1	2.22	0.40
9:8:99:ARG:O	9:8:100:GLU:C	2.64	0.40
11:XA:2086:A:H2'	11:XA:2087:U:C6	2.56	0.40
11:XA:2326:C:OP2	84:s:55:SER:OG	2.30	0.40
11:XA:2379:C:O2	11:XA:2379:C:O4'	2.40	0.40
13:A1:273:GLU:OE2	13:A1:273:GLU:N	2.54	0.40
17:AA:747:A:C2	17:AA:748:G:N7	2.90	0.40
17:AA:914:A:H2'	17:AA:915:C:H6	1.86	0.40
36:AT:55:ILE:O	36:AT:59:ASN:OD1	2.40	0.40
40:AX:374:GLU:HG2	40:AX:375:GLU:N	2.35	0.40
51:XL:87:VAL:HG11	51:XL:123:ILE:HG22	2.04	0.40
54:XO:115:LEU:HD23	54:XO:115:LEU:H	1.86	0.40
63:XX:133:ASP:OD1	63:XX:133:ASP:C	2.64	0.40
72:g:142:GLU:HG3	79:o:88:ILE:HD12	2.04	0.40
73:h:84:SER:OG	73:h:85:ASN:N	2.54	0.40
75:j:101:GLU:OE2	75:j:102:GLN:NE2	2.55	0.40
80:p:113:GLU:N	80:p:114:PRO:HD2	2.37	0.40
83:r4:51:Y5P:H6	83:r4:51:Y5P:O5'	2.21	0.40
84:s:299:PHE:CD2	84:s:360:VAL:CG1	3.05	0.40
84:s:419:LEU:HA	84:s:422:VAL:HG22	2.03	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%)	101 (95%)	5 (5%)	0	100	100
2	1	51/65 (78%)	47 (92%)	4 (8%)	0	100	100
3	2	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
4	3	93/188 (50%)	93 (100%)	0	0	100	100
5	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
6	5	391/423 (92%)	365 (93%)	26 (7%)	0	100	100
7	6	348/380 (92%)	324 (93%)	24 (7%)	0	100	100
8	7	285/338 (84%)	265 (93%)	20 (7%)	0	100	100
9	8	121/206 (59%)	116 (96%)	5 (4%)	0	100	100
10	9	122/137 (89%)	117 (96%)	5 (4%)	0	100	100
12	A0	197/218 (90%)	186 (94%)	11 (6%)	0	100	100
13	A1	273/323 (84%)	254 (93%)	19 (7%)	0	100	100
14	A2	114/118 (97%)	109 (96%)	5 (4%)	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%)	212 (98%)	4 (2%)	0	100	100
19	AC	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
20	AD	341/430 (79%)	320 (94%)	21 (6%)	0	100	100
21	AE	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
22	AF	197/242 (81%)	191 (97%)	6 (3%)	0	100	100
23	AG	300/396 (76%)	287 (96%)	13 (4%)	0	100	100
24	AH	133/201 (66%)	124 (93%)	9 (7%)	0	100	100
25	AI	134/194 (69%)	128 (96%)	6 (4%)	0	100	100
26	AJ	106/138 (77%)	96 (91%)	10 (9%)	0	100	100
27	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	AL	162/257 (63%)	157 (97%)	5 (3%)	0	100	100
29	AM	114/137 (83%)	112 (98%)	2 (2%)	0	100	100
30	AN	105/130 (81%)	100 (95%)	5 (5%)	0	100	100
31	AO	183/258 (71%)	180 (98%)	3 (2%)	0	100	100
32	AP	93/142 (66%)	87 (94%)	6 (6%)	0	100	100
33	AQ	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
34	AR	248/360 (69%)	238 (96%)	10 (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%)	321 (94%)	20 (6%)	0	100	100
39	AW	95/187 (51%)	93 (98%)	2 (2%)	0	100	100
40	AX	346/398 (87%)	327 (94%)	19 (6%)	0	100	100
41	AY	111/395 (28%)	103 (93%)	8 (7%)	0	100	100
42	AZ	84/106 (79%)	83 (99%)	1 (1%)	0	100	100
44	XD	234/305 (77%)	223 (95%)	10 (4%)	1 (0%)	30	62
45	XE	302/348 (87%)	291 (96%)	11 (4%)	0	100	100
46	XF	248/311 (80%)	242 (98%)	6 (2%)	0	100	100
47	XH	93/267 (35%)	89 (96%)	4 (4%)	0	100	100
48	XI	209/261 (80%)	194 (93%)	15 (7%)	0	100	100
49	XJ	168/192 (88%)	153 (91%)	15 (9%)	0	100	100
50	XK	175/178 (98%)	166 (95%)	9 (5%)	0	100	100
51	XL	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
52	XM	285/296 (96%)	272 (95%)	13 (5%)	0	100	100
53	XN	219/251 (87%)	207 (94%)	12 (6%)	0	100	100
54	XO	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
55	XP	141/180 (78%)	136 (96%)	5 (4%)	0	100	100
56	XQ	236/292 (81%)	228 (97%)	8 (3%)	0	100	100
57	XR	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
58	XS	158/205 (77%)	154 (98%)	4 (2%)	0	100	100
59	XT	164/206 (80%)	161 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	XU	137/153 (90%)	129 (94%)	8 (6%)	0	100	100
61	XV	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
62	XW	109/148 (74%)	105 (96%)	4 (4%)	0	100	100
63	XX	241/256 (94%)	234 (97%)	7 (3%)	0	100	100
64	XY	176/250 (70%)	170 (97%)	6 (3%)	0	100	100
65	XZ	118/161 (73%)	114 (97%)	4 (3%)	0	100	100
66	a	93/142 (66%)	84 (90%)	9 (10%)	0	100	100
67	b	146/215 (68%)	137 (94%)	9 (6%)	0	100	100
68	c	271/332 (82%)	262 (97%)	9 (3%)	0	100	100
69	d	212/306 (69%)	201 (95%)	10 (5%)	1 (0%)	24	57
70	e	211/279 (76%)	208 (99%)	3 (1%)	0	100	100
71	f	131/212 (62%)	125 (95%)	6 (5%)	0	100	100
72	g	130/166 (78%)	123 (95%)	7 (5%)	0	100	100
73	h	107/158 (68%)	101 (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%)	74 (95%)	4 (5%)	0	100	100
78	m	58/128 (45%)	54 (93%)	4 (7%)	0	100	100
79	o	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
80	p	119/206 (58%)	117 (98%)	2 (2%)	0	100	100
81	q	162/222 (73%)	160 (99%)	2 (1%)	0	100	100
82	r	144/196 (74%)	139 (96%)	5 (4%)	0	100	100
84	s	366/439 (83%)	353 (96%)	13 (4%)	0	100	100
85	t1	45/198 (23%)	40 (89%)	5 (11%)	0	100	100
85	t2	28/198 (14%)	28 (100%)	0	0	100	100
85	t3	28/198 (14%)	27 (96%)	1 (4%)	0	100	100
85	t4	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
85	t5	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
85	t6	25/198 (13%)	25 (100%)	0	0	100	100
86	A	2/8 (25%)	0	1 (50%)	1 (50%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	13765/19166 (72%)	13136 (95%)	626 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
86	A	4	PRO
44	XD	207	ILE
69	d	289	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/164 (59%)	97 (100%)	0	100	100
2	1	50/60 (83%)	50 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	267/303 (88%)	265 (99%)	2 (1%)	76	78
9	8	113/190 (60%)	113 (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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
23	AG	264/342 (77%)	264 (100%)	0	100	100
24	AH	125/180 (69%)	124 (99%)	1 (1%)	73	77
25	AI	104/147 (71%)	104 (100%)	0	100	100
26	AJ	93/118 (79%)	92 (99%)	1 (1%)	65	74
27	AK	91/113 (80%)	90 (99%)	1 (1%)	65	74
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%)	165 (99%)	1 (1%)	78	79
32	AP	86/123 (70%)	86 (100%)	0	100	100
33	AQ	77/77 (100%)	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%)	216 (100%)	1 (0%)	81	80
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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%)	117 (99%)	1 (1%)	73	77
58	XS	145/180 (81%)	144 (99%)	1 (1%)	76	78
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%)	178 (99%)	1 (1%)	78	79
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%)	110 (99%)	1 (1%)	70	76
66	a	92/133 (69%)	92 (100%)	0	100	100
67	b	130/186 (70%)	130 (100%)	0	100	100
68	c	241/288 (84%)	239 (99%)	2 (1%)	73	77
69	d	196/274 (72%)	196 (100%)	0	100	100
70	e	188/236 (80%)	188 (100%)	0	100	100
71	f	121/188 (64%)	121 (100%)	0	100	100
72	g	122/148 (82%)	122 (100%)	0	100	100
73	h	103/148 (70%)	103 (100%)	0	100	100
74	i	86/110 (78%)	86 (100%)	0	100	100
75	j	68/97 (70%)	68 (100%)	0	100	100
76	k	80/90 (89%)	80 (100%)	0	100	100
77	l	74/116 (64%)	74 (100%)	0	100	100
78	m	54/113 (48%)	54 (100%)	0	100	100
79	o	80/87 (92%)	80 (100%)	0	100	100
80	p	117/181 (65%)	117 (100%)	0	100	100
81	q	141/178 (79%)	141 (100%)	0	100	100
82	r	138/169 (82%)	138 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	s	326/381 (86%)	326 (100%)	0	100	100
85	t1	41/158 (26%)	40 (98%)	1 (2%)	43	64
85	t2	29/158 (18%)	29 (100%)	0	100	100
85	t3	29/158 (18%)	29 (100%)	0	100	100
85	t4	28/158 (18%)	28 (100%)	0	100	100
85	t5	28/158 (18%)	28 (100%)	0	100	100
85	t6	26/158 (16%)	26 (100%)	0	100	100
86	A	2/2 (100%)	2 (100%)	0	100	100
All	All	12376/16507 (75%)	12362 (100%)	14 (0%)	87	87

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	7	56	LEU
8	7	164	VAL
24	AH	126	ILE
26	AJ	49	LEU
27	AK	60	ASN
31	AO	151	THR
46	XF	203	LEU
57	XR	10	LEU
58	XS	118	ASN
61	XV	148	THR
65	XZ	88	MET
68	c	72	ILE
68	c	267	LEU
85	t1	21[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	98	GLN
1	0	115	HIS
2	1	45	HIS
4	3	178	GLN
5	4	95	HIS
6	5	186	GLN
6	5	420	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	6	249	GLN
7	6	307	HIS
8	7	232	HIS
8	7	305	HIS
15	A3	140	HIS
16	A4	129	GLN
16	A4	590	GLN
18	AB	90	HIS
18	AB	126	GLN
18	AB	216	ASN
18	AB	228	ASN
20	AD	174	GLN
20	AD	341	ASN
21	AE	56	GLN
21	AE	58	HIS
21	AE	59	ASN
22	AF	122	GLN
23	AG	77	GLN
23	AG	288	HIS
24	AH	183	HIS
25	AI	146	HIS
25	AI	163	HIS
27	AK	55	ASN
27	AK	89	ASN
29	AM	61	HIS
31	AO	80	ASN
31	AO	98	ASN
31	AO	204	ASN
35	AS	91	ASN
36	AT	35	ASN
37	AU	139	GLN
37	AU	147	GLN
38	AV	388	GLN
38	AV	395	GLN
40	AX	67	HIS
40	AX	110	HIS
40	AX	114	ASN
40	AX	140	HIS
40	AX	291	HIS
40	AX	385	ASN
40	AX	394	HIS
41	AY	285	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	AZ	63	GLN
44	XD	158	GLN
44	XD	276	HIS
45	XE	72	GLN
45	XE	117	HIS
45	XE	137	ASN
46	XF	58	HIS
46	XF	74	GLN
46	XF	251	HIS
48	XI	36	HIS
50	XK	64	HIS
50	XK	94	GLN
50	XK	117	HIS
50	XK	126	HIS
52	XM	26	ASN
52	XM	219	ASN
53	XN	178	GLN
55	XP	114	HIS
56	XQ	158	GLN
57	XR	22	GLN
57	XR	94	GLN
57	XR	147	GLN
58	XS	100	HIS
59	XT	151	GLN
62	XW	51	GLN
63	XX	15	GLN
63	XX	215	GLN
64	XY	147	GLN
65	XZ	100	HIS
66	a	111	GLN
66	a	126	HIS
68	c	77	HIS
69	d	157	HIS
69	d	211	GLN
69	d	251	GLN
70	e	75	GLN
70	e	87	HIS
71	f	54	HIS
71	f	94	HIS
72	g	63	HIS
72	g	73	GLN
73	h	118	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
73	h	119	GLN
74	i	120	HIS
77	l	82	GLN
79	o	58	GLN
80	p	125	ASN
81	q	120	HIS
81	q	139	GLN
84	s	191	HIS
84	s	240	GLN
84	s	327	ASN
85	t5	22	ASN
85	t6	22	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	XA	1491/1561 (95%)	268 (17%)	9 (0%)
17	AA	916/954 (96%)	160 (17%)	4 (0%)
43	XB	54/72 (75%)	10 (18%)	0
83	r4	75/76 (98%)	30 (40%)	0
All	All	2536/2663 (95%)	468 (18%)	13 (0%)

All (468) 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

Continued on next page...

Continued from previous page...

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	1777	A
11	XA	1791	G
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	1824	U
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	1854	U
11	XA	1856	A
11	XA	1869	A
11	XA	1872	U
11	XA	1878	U
11	XA	1882	A
11	XA	1886	G
11	XA	1887	A
11	XA	1893	A
11	XA	1902	C
11	XA	1903	C
11	XA	1909	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	XA	1918	G
11	XA	1919	C
11	XA	1940	A
11	XA	1944	C
11	XA	1950	U
11	XA	1958	G
11	XA	1974	A
11	XA	1975	U
11	XA	1985	G
11	XA	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	2099	U
11	XA	2105	G
11	XA	2111	C
11	XA	2113	G
11	XA	2125	C
11	XA	2126	U
11	XA	2135	A
11	XA	2138	U
11	XA	2147	G
11	XA	2159	U
11	XA	2168	U
11	XA	2169	A
11	XA	2176	C
11	XA	2177	U
11	XA	2178	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	XA	2180	A
11	XA	2181	A
11	XA	2182	G
11	XA	2188	A
11	XA	2195	A
11	XA	2196	A
11	XA	2198	A
11	XA	2200	A
11	XA	2230	A
11	XA	2237	A
11	XA	2241	A
11	XA	2243	A
11	XA	2244	U
11	XA	2245	A
11	XA	2251	A
11	XA	2260	A
11	XA	2262	C
11	XA	2263	C
11	XA	2283	C
11	XA	2284	C
11	XA	2285	U
11	XA	2297	A
11	XA	2299	U
11	XA	2300	G
11	XA	2316	U
11	XA	2322	C
11	XA	2332	C
11	XA	2345	G
11	XA	2359	C
11	XA	2369	A
11	XA	2374	A
11	XA	2381	A
11	XA	2407	U
11	XA	2414	C
11	XA	2415	C
11	XA	2418	A
11	XA	2432	A
11	XA	2446	A
11	XA	2451	A
11	XA	2458	A
11	XA	2478	G
11	XA	2493	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	XA	2501	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	2560	G
11	XA	2564	A
11	XA	2570	C
11	XA	2575	U
11	XA	2576	A
11	XA	2577	C
11	XA	2578	C
11	XA	2579	C
11	XA	2581	A
11	XA	2592	G
11	XA	2594	U
11	XA	2601	A
11	XA	2602	U
11	XA	2603	C
11	XA	2618	U
11	XA	2625	C
11	XA	2626	U
11	XA	2627	G
11	XA	2628	U
11	XA	2633	A
11	XA	2635	G
11	XA	2654	U
11	XA	2656	U
11	XA	2659	C
11	XA	2683	C
11	XA	2686	G
11	XA	2694	A
11	XA	2695	G
11	XA	2696	A
11	XA	2706	A
11	XA	2715	A
11	XA	2718	C
11	XA	2719	G
11	XA	2722	A

Continued on next page...

Continued from previous page...

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	2758	G
11	XA	2788	C
11	XA	2789	C
11	XA	2810	G
11	XA	2832	A
11	XA	2833	A
11	XA	2847	C
11	XA	2854	U
11	XA	2859	A
11	XA	2864	U
11	XA	2865	C
11	XA	2869	A
11	XA	2871	U
11	XA	2879	A
11	XA	2906	C
11	XA	2913	A
11	XA	2916	G
11	XA	2917	G
11	XA	2918	A
11	XA	2919	A
11	XA	2921	A
11	XA	2928	C
11	XA	2935	A
11	XA	2939	C
11	XA	2946	A
11	XA	2952	U
11	XA	2956	A
11	XA	2962	C
11	XA	2963	A
11	XA	2985	C
11	XA	2989	G
11	XA	2992	G
11	XA	3000	A
11	XA	3005	A
11	XA	3007	C
11	XA	3016	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	XA	3021	C
11	XA	3041	U
11	XA	3049	U
11	XA	3053	A
11	XA	3054	G
11	XA	3060	C
11	XA	3065	U
11	XA	3067	U
11	XA	3069	A
11	XA	3073	C
11	XA	3086	U
11	XA	3089	A
11	XA	3090	G
11	XA	3096	U
11	XA	3100	U
11	XA	3102	U
11	XA	3122	U
11	XA	3124	U
11	XA	3129	A
11	XA	3150	U
11	XA	3151	A
11	XA	3154	U
11	XA	3157	C
11	XA	3158	A
11	XA	3160	A
11	XA	3162	C
11	XA	3169	C
11	XA	3172	C
11	XA	3177	A
11	XA	3182	A
11	XA	3184	C
11	XA	3189	C
11	XA	3190	A
11	XA	3194	U
11	XA	3208	C
11	XA	3209	A
11	XA	3210	C
11	XA	3212	C
11	XA	3217	A
11	XA	3218	A
11	XA	3219	G
11	XA	3228	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	AA	651	A
17	AA	680	U
17	AA	688	A
17	AA	694	C
17	AA	700	A
17	AA	704	U
17	AA	721	U
17	AA	722	C
17	AA	730	A
17	AA	753	A
17	AA	757	A
17	AA	761	A
17	AA	766	G
17	AA	771	A
17	AA	791	G
17	AA	792	C
17	AA	794	U
17	AA	796	G
17	AA	811	G
17	AA	814	A
17	AA	825	U
17	AA	826	A
17	AA	829	C
17	AA	830	U
17	AA	832	U
17	AA	835	C
17	AA	836	A
17	AA	851	A
17	AA	856	A
17	AA	860	A
17	AA	861	U
17	AA	865	A
17	AA	866	A
17	AA	868	C
17	AA	869	C
17	AA	880	C
17	AA	881	A
17	AA	890	C
17	AA	893	G
17	AA	897	C
17	AA	899	G
17	AA	903	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1001	C
17	AA	1009	C
17	AA	1015	A
17	AA	1031	G
17	AA	1042	U
17	AA	1046	A
17	AA	1049	A
17	AA	1062	G
17	AA	1069	A
17	AA	1081	U
17	AA	1082	A
17	AA	1103	A
17	AA	1105	C
17	AA	1106	C
17	AA	1109	A
17	AA	1121	A
17	AA	1128	C
17	AA	1138	G
17	AA	1142	A
17	AA	1143	C
17	AA	1151	C
17	AA	1167	A
17	AA	1187	U
17	AA	1188	A
17	AA	1189	U
17	AA	1190	C
17	AA	1193	U
17	AA	1194	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	AA	1213	A
17	AA	1214	A
17	AA	1215	U
17	AA	1220	A
17	AA	1223	C
17	AA	1225	C
17	AA	1226	C
17	AA	1227	G
17	AA	1228	A
17	AA	1229	U
17	AA	1230	C
17	AA	1235	U
17	AA	1236	C
17	AA	1237	A
17	AA	1248	C
17	AA	1250	C
17	AA	1251	A
17	AA	1261	C
17	AA	1268	C
17	AA	1271	C
17	AA	1284	U
17	AA	1290	C
17	AA	1293	C
17	AA	1294	A
17	AA	1295	A
17	AA	1296	A
17	AA	1297	G
17	AA	1307	G
17	AA	1326	A
17	AA	1327	G
17	AA	1330	C
17	AA	1331	A
17	AA	1341	C
17	AA	1342	C
17	AA	1343	A
17	AA	1344	U
17	AA	1349	U
17	AA	1353	A
17	AA	1354	A
17	AA	1356	A
17	AA	1365	A
17	AA	1369	U

Continued on next page...

Continued from previous page...

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	1424	U
17	AA	1430	A
17	AA	1432	U
17	AA	1448	U
17	AA	1459	A
17	AA	1461	A
17	AA	1463	G
17	AA	1478	A
17	AA	1482	A
17	AA	1488	C
17	AA	1503	G
17	AA	1525	C
17	AA	1526	U
17	AA	1527	A
17	AA	1528	A
17	AA	1531	C
17	AA	1537	C
17	AA	1539	C
17	AA	1540	A
17	AA	1557	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
43	XB	1619	C
43	XB	1620	A
43	XB	1621	A
43	XB	1646	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	XB	1649	C
43	XB	1659	U
83	r4	6	P5P
83	r4	9	P5P
83	r4	13	Y5P
83	r4	17	Y5P
83	r4	18	P5P
83	r4	19	P5P
83	r4	21	P5P
83	r4	22	P5P
83	r4	25	Y5P
83	r4	26	P5P
83	r4	27	P5P
83	r4	28	P5P
83	r4	29	P5P
83	r4	30	P5P
83	r4	32	Y5P
83	r4	33	Y5P
83	r4	34	P5P
83	r4	35	P5P
83	r4	41	Y5P
83	r4	45	Y5P
83	r4	47	Y5P
83	r4	49	Y5P
83	r4	56	Y5P
83	r4	59	Y5P
83	r4	64	P5P
83	r4	66	Y5P
83	r4	72	Y5P
83	r4	74	Y5P
83	r4	75	Y5P
83	r4	76	P5P

All (13) 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	2601	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1527	A

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

81 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
83	P5P	r4	5	83	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
83	Y5P	r4	67	83	14,19,20	7.39	3 (21%)	18,26,29	0.56	0
83	P5P	r4	23	83	20,23,24	1.28	3 (15%)	27,33,36	2.51	11 (40%)
83	Y5P	r4	3	83	14,19,20	7.39	3 (21%)	18,26,29	0.55	0
83	Y5P	r4	12	83	14,19,20	7.39	3 (21%)	18,26,29	0.55	0
83	Y5P	r4	41	83	14,19,20	7.40	3 (21%)	18,26,29	0.56	0
83	Y5P	r4	75	83	14,19,20	7.31	3 (21%)	18,26,29	0.58	0
83	Y5P	r4	51	83	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
83	P5P	r4	7	83	20,23,24	1.27	3 (15%)	27,33,36	2.47	11 (40%)
83	Y5P	r4	55	83	14,19,20	7.41	3 (21%)	18,26,29	0.57	0
83	Y5P	r4	49	83	14,19,20	7.34	3 (21%)	18,26,29	0.55	0
83	Y5P	r4	45	83	14,19,20	7.39	3 (21%)	18,26,29	0.55	0
83	P5P	r4	22	83	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)
83	Y5P	r4	72	83	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
83	P5P	r4	30	83	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
83	P5P	r4	10	83	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
83	P5P	r4	31	83	20,23,24	1.27	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
83	Y5P	r4	17	83	14,19,20	7.37	3 (21%)	18,26,29	0.54	0
83	P5P	r4	35	83	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
83	Y5P	r4	47	83	14,19,20	7.39	3 (21%)	18,26,29	0.59	0
83	Y5P	r4	16	83	14,19,20	7.42	3 (21%)	18,26,29	0.60	0
83	P5P	r4	26	83	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)
83	Y5P	r4	32	83	14,19,20	7.41	3 (21%)	18,26,29	0.56	0
83	P5P	r4	52	83	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
83	Y5P	r4	25	83	14,19,20	7.36	3 (21%)	18,26,29	0.55	0
83	P5P	r4	36	83	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
83	P5P	r4	64	83	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
83	Y5P	r4	48	83	14,19,20	7.41	3 (21%)	18,26,29	0.57	0
83	P5P	r4	34	83	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
83	P5P	r4	28	83	20,23,24	1.28	3 (15%)	27,33,36	2.51	11 (40%)
83	P5P	r4	71	83	20,23,24	1.28	3 (15%)	27,33,36	2.46	11 (40%)
83	Y5P	r4	20	83	14,19,20	7.40	3 (21%)	18,26,29	0.57	0
83	P5P	r4	19	83	20,23,24	1.27	3 (15%)	27,33,36	2.47	11 (40%)
83	P5P	r4	57	83	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
83	P5P	r4	69	83	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
83	P5P	r4	58	83	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
83	Y5P	r4	40	83	14,19,20	7.42	3 (21%)	18,26,29	0.57	0
83	Y5P	r4	2	83	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
83	Y5P	r4	50	83	14,19,20	7.42	3 (21%)	18,26,29	0.55	0
83	Y5P	r4	4	83	14,19,20	7.38	3 (21%)	18,26,29	0.56	0
83	Y5P	r4	43	83	14,19,20	7.40	3 (21%)	18,26,29	0.56	0
83	P5P	r4	44	83	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
86	DBB	A	3	86	4,5,6	0.58	0	1,5,7	0.28	0
83	P5P	r4	27	83	20,23,24	1.27	3 (15%)	27,33,36	2.46	11 (40%)
86	004	A	7	86	9,10,11	1.14	1 (11%)	9,12,14	1.60	2 (22%)
83	P5P	r4	29	83	20,23,24	1.27	3 (15%)	27,33,36	2.51	11 (40%)
86	MHU	A	5	86	14,15,16	0.44	0	18,19,21	1.25	3 (16%)
83	P5P	r4	24	83	20,23,24	1.28	3 (15%)	27,33,36	2.48	10 (37%)
83	P5P	r4	37	83	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
83	P5P	r4	6	83	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
83	P5P	r4	14	83	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
83	Y5P	r4	42	83	14,19,20	7.35	3 (21%)	18,26,29	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	P5P	r4	70	83	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)
83	P5P	r4	21	83	20,23,24	1.30	3 (15%)	27,33,36	2.47	11 (40%)
83	P5P	r4	63	83	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)
83	Y5P	r4	8	83	14,19,20	7.38	3 (21%)	18,26,29	0.55	0
83	P5P	r4	65	83	20,23,24	1.28	3 (15%)	27,33,36	2.48	10 (37%)
83	P5P	r4	53	83	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)
83	Y5P	r4	68	83	14,19,20	7.34	3 (21%)	18,26,29	0.57	0
83	P5P	r4	9	83	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
83	P5P	r4	1	83	20,23,24	1.30	3 (15%)	27,33,36	2.49	10 (37%)
83	Y5P	r4	11	83	14,19,20	7.36	3 (21%)	18,26,29	0.54	0
83	Y5P	r4	54	83	14,19,20	7.39	3 (21%)	18,26,29	0.54	0
83	Y5P	r4	33	83	14,19,20	7.38	3 (21%)	18,26,29	0.52	0
83	Y5P	r4	66	83	14,19,20	7.34	3 (21%)	18,26,29	0.56	0
83	Y5P	r4	61	83	14,19,20	7.40	3 (21%)	18,26,29	0.54	0
83	Y5P	r4	13	83	14,19,20	7.37	3 (21%)	18,26,29	0.54	0
83	P5P	r4	73	83	20,23,24	1.28	3 (15%)	27,33,36	2.53	11 (40%)
83	Y5P	r4	56	83	14,19,20	7.44	3 (21%)	18,26,29	0.56	0
83	Y5P	r4	39	83	14,19,20	7.36	3 (21%)	18,26,29	0.58	0
83	P5P	r4	38	83	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
83	Y5P	r4	74	83	14,19,20	7.36	3 (21%)	18,26,29	0.57	0
83	P5P	r4	76	11,83	20,23,24	1.37	3 (15%)	27,33,36	2.48	10 (37%)
83	P5P	r4	18	83	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
86	MHW	A	1	86	9,9,10	0.79	0	10,11,13	2.49	3 (30%)
83	Y5P	r4	62	83	14,19,20	7.37	3 (21%)	18,26,29	0.56	0
83	P5P	r4	15	83	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
83	Y5P	r4	60	83	14,19,20	7.38	3 (21%)	18,26,29	0.56	0
83	P5P	r4	46	83	20,23,24	1.28	3 (15%)	27,33,36	2.48	10 (37%)
83	Y5P	r4	59	83	14,19,20	7.40	3 (21%)	18,26,29	0.57	0
86	MHV	A	6	86	7,9,10	0.34	0	8,11,13	1.75	3 (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
83	P5P	r4	5	83	-	0/7/25/26	0/3/3/3
83	Y5P	r4	67	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	23	83	-	5/7/25/26	0/3/3/3
83	Y5P	r4	3	83	-	1/7/33/34	0/2/2/2
83	Y5P	r4	12	83	-	1/7/33/34	0/2/2/2
83	Y5P	r4	41	83	-	3/7/33/34	0/2/2/2
83	Y5P	r4	75	83	-	3/7/33/34	0/2/2/2
83	Y5P	r4	51	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	7	83	-	1/7/25/26	0/3/3/3
83	Y5P	r4	55	83	-	1/7/33/34	0/2/2/2
83	Y5P	r4	49	83	-	3/7/33/34	0/2/2/2
83	Y5P	r4	45	83	-	4/7/33/34	0/2/2/2
83	P5P	r4	22	83	-	3/7/25/26	0/3/3/3
83	Y5P	r4	72	83	-	3/7/33/34	0/2/2/2
83	P5P	r4	30	83	-	1/7/25/26	0/3/3/3
83	P5P	r4	10	83	-	3/7/25/26	0/3/3/3
83	P5P	r4	31	83	-	3/7/25/26	0/3/3/3
83	Y5P	r4	17	83	-	3/7/33/34	0/2/2/2
83	P5P	r4	35	83	-	0/7/25/26	0/3/3/3
83	Y5P	r4	47	83	-	4/7/33/34	0/2/2/2
83	Y5P	r4	16	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	26	83	-	2/7/25/26	0/3/3/3
83	Y5P	r4	32	83	-	3/7/33/34	0/2/2/2
83	P5P	r4	52	83	-	2/7/25/26	0/3/3/3
83	Y5P	r4	25	83	-	3/7/33/34	0/2/2/2
83	P5P	r4	36	83	-	0/7/25/26	0/3/3/3
83	P5P	r4	64	83	-	2/7/25/26	0/3/3/3
83	Y5P	r4	48	83	-	3/7/33/34	0/2/2/2
83	P5P	r4	34	83	-	2/7/25/26	0/3/3/3
83	P5P	r4	28	83	-	2/7/25/26	0/3/3/3
83	P5P	r4	71	83	-	0/7/25/26	0/3/3/3
83	Y5P	r4	20	83	-	2/7/33/34	0/2/2/2
83	P5P	r4	19	83	-	0/7/25/26	0/3/3/3
83	P5P	r4	57	83	-	0/7/25/26	0/3/3/3
83	P5P	r4	69	83	-	0/7/25/26	0/3/3/3
83	P5P	r4	58	83	-	0/7/25/26	0/3/3/3
83	Y5P	r4	40	83	-	1/7/33/34	0/2/2/2
83	Y5P	r4	2	83	-	1/7/33/34	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	Y5P	r4	50	83	-	2/7/33/34	0/2/2/2
83	Y5P	r4	4	83	-	1/7/33/34	0/2/2/2
83	Y5P	r4	43	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	44	83	-	0/7/25/26	0/3/3/3
86	DBB	A	3	86	-	0/3/4/6	-
83	P5P	r4	27	83	-	5/7/25/26	0/3/3/3
86	004	A	7	86	-	0/4/6/8	0/1/1/1
83	P5P	r4	29	83	-	4/7/25/26	0/3/3/3
86	MHU	A	5	86	-	5/9/12/14	0/1/1/1
83	P5P	r4	24	83	-	0/7/25/26	0/3/3/3
83	P5P	r4	37	83	-	0/7/25/26	0/3/3/3
83	P5P	r4	6	83	-	2/7/25/26	0/3/3/3
83	P5P	r4	14	83	-	0/7/25/26	0/3/3/3
83	Y5P	r4	42	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	70	83	-	0/7/25/26	0/3/3/3
83	P5P	r4	21	83	-	1/7/25/26	0/3/3/3
83	P5P	r4	63	83	-	0/7/25/26	0/3/3/3
83	Y5P	r4	8	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	65	83	-	0/7/25/26	0/3/3/3
83	P5P	r4	53	83	-	0/7/25/26	0/3/3/3
83	Y5P	r4	68	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	9	83	-	2/7/25/26	0/3/3/3
83	P5P	r4	1	83	-	3/7/25/26	0/3/3/3
83	Y5P	r4	11	83	-	1/7/33/34	0/2/2/2
83	Y5P	r4	54	83	-	1/7/33/34	0/2/2/2
83	Y5P	r4	33	83	-	2/7/33/34	0/2/2/2
83	Y5P	r4	66	83	-	3/7/33/34	0/2/2/2
83	Y5P	r4	61	83	-	1/7/33/34	0/2/2/2
83	Y5P	r4	13	83	-	3/7/33/34	0/2/2/2
83	P5P	r4	73	83	-	5/7/25/26	0/3/3/3
83	Y5P	r4	56	83	-	3/7/33/34	0/2/2/2
83	Y5P	r4	39	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	38	83	-	2/7/25/26	0/3/3/3
83	Y5P	r4	74	83	-	6/7/33/34	0/2/2/2
83	P5P	r4	76	11,83	-	3/7/25/26	0/3/3/3
83	P5P	r4	18	83	-	1/7/25/26	0/3/3/3
86	MHW	A	1	86	-	0/2/2/4	0/1/1/1
83	Y5P	r4	62	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	15	83	-	0/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	Y5P	r4	60	83	-	1/7/33/34	0/2/2/2
83	P5P	r4	46	83	-	2/7/25/26	0/3/3/3
83	Y5P	r4	59	83	-	1/7/33/34	0/2/2/2
86	MHV	A	6	86	-	0/1/12/14	0/1/1/1

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r4	56	Y5P	C2-N3	26.92	1.48	1.27
83	r4	40	Y5P	C2-N3	26.85	1.48	1.27
83	r4	50	Y5P	C2-N3	26.85	1.48	1.27
83	r4	16	Y5P	C2-N3	26.84	1.48	1.27
83	r4	48	Y5P	C2-N3	26.81	1.48	1.27
83	r4	32	Y5P	C2-N3	26.81	1.48	1.27
83	r4	55	Y5P	C2-N3	26.80	1.48	1.27
83	r4	59	Y5P	C2-N3	26.78	1.48	1.27
83	r4	20	Y5P	C2-N3	26.77	1.48	1.27
83	r4	61	Y5P	C2-N3	26.77	1.48	1.27
83	r4	43	Y5P	C2-N3	26.77	1.48	1.27
83	r4	41	Y5P	C2-N3	26.76	1.48	1.27
83	r4	12	Y5P	C2-N3	26.75	1.48	1.27
83	r4	45	Y5P	C2-N3	26.75	1.48	1.27
83	r4	67	Y5P	C2-N3	26.73	1.48	1.27
83	r4	54	Y5P	C2-N3	26.72	1.48	1.27
83	r4	3	Y5P	C2-N3	26.72	1.48	1.27
83	r4	47	Y5P	C2-N3	26.71	1.48	1.27
83	r4	60	Y5P	C2-N3	26.69	1.48	1.27
83	r4	4	Y5P	C2-N3	26.69	1.48	1.27
83	r4	33	Y5P	C2-N3	26.68	1.48	1.27
83	r4	8	Y5P	C2-N3	26.68	1.48	1.27
83	r4	17	Y5P	C2-N3	26.67	1.48	1.27
83	r4	2	Y5P	C2-N3	26.66	1.48	1.27
83	r4	62	Y5P	C2-N3	26.66	1.48	1.27
83	r4	13	Y5P	C2-N3	26.65	1.48	1.27
83	r4	51	Y5P	C2-N3	26.65	1.48	1.27
83	r4	25	Y5P	C2-N3	26.63	1.48	1.27
83	r4	11	Y5P	C2-N3	26.63	1.48	1.27
83	r4	74	Y5P	C2-N3	26.61	1.47	1.27
83	r4	39	Y5P	C2-N3	26.61	1.47	1.27
83	r4	72	Y5P	C2-N3	26.60	1.47	1.27
83	r4	42	Y5P	C2-N3	26.59	1.47	1.27
83	r4	68	Y5P	C2-N3	26.56	1.47	1.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r4	66	Y5P	C2-N3	26.55	1.47	1.27
83	r4	49	Y5P	C2-N3	26.54	1.47	1.27
83	r4	75	Y5P	C2-N3	26.41	1.47	1.27
83	r4	8	Y5P	C6-C5	6.21	1.52	1.33
83	r4	33	Y5P	C6-C5	6.21	1.52	1.33
83	r4	47	Y5P	C6-C5	6.21	1.52	1.33
83	r4	13	Y5P	C6-C5	6.21	1.52	1.33
83	r4	51	Y5P	C6-C5	6.21	1.52	1.33
83	r4	39	Y5P	C6-C5	6.21	1.52	1.33
83	r4	54	Y5P	C6-C5	6.21	1.52	1.33
83	r4	75	Y5P	C6-C5	6.21	1.52	1.33
83	r4	41	Y5P	C6-C5	6.21	1.52	1.33
83	r4	72	Y5P	C6-C5	6.21	1.52	1.33
83	r4	74	Y5P	C6-C5	6.20	1.52	1.33
83	r4	11	Y5P	C6-C5	6.20	1.52	1.33
83	r4	49	Y5P	C6-C5	6.20	1.52	1.33
83	r4	56	Y5P	C6-C5	6.19	1.52	1.33
83	r4	68	Y5P	C6-C5	6.19	1.52	1.33
83	r4	3	Y5P	C6-C5	6.19	1.52	1.33
83	r4	66	Y5P	C6-C5	6.19	1.52	1.33
83	r4	45	Y5P	C6-C5	6.19	1.52	1.33
83	r4	20	Y5P	C6-C5	6.19	1.52	1.33
83	r4	61	Y5P	C6-C5	6.18	1.52	1.33
83	r4	40	Y5P	C6-C5	6.18	1.52	1.33
83	r4	17	Y5P	C6-C5	6.18	1.52	1.33
83	r4	67	Y5P	C6-C5	6.18	1.52	1.33
83	r4	32	Y5P	C6-C5	6.18	1.52	1.33
83	r4	60	Y5P	C6-C5	6.17	1.52	1.33
83	r4	62	Y5P	C6-C5	6.17	1.52	1.33
83	r4	2	Y5P	C6-C5	6.17	1.52	1.33
83	r4	43	Y5P	C6-C5	6.17	1.52	1.33
83	r4	12	Y5P	C6-C5	6.17	1.52	1.33
83	r4	25	Y5P	C6-C5	6.17	1.52	1.33
83	r4	55	Y5P	C6-C5	6.17	1.52	1.33
83	r4	4	Y5P	C6-C5	6.17	1.52	1.33
83	r4	50	Y5P	C6-C5	6.17	1.52	1.33
83	r4	42	Y5P	C6-C5	6.17	1.52	1.33
83	r4	59	Y5P	C6-C5	6.16	1.52	1.33
83	r4	16	Y5P	C6-C5	6.15	1.52	1.33
83	r4	48	Y5P	C6-C5	6.15	1.52	1.33
83	r4	76	P5P	C5-C4	-3.54	1.34	1.40
83	r4	1	P5P	C5-C4	-3.34	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r4	35	P5P	C5-C4	-3.27	1.35	1.40
83	r4	24	P5P	C5-C4	-3.26	1.35	1.40
83	r4	5	P5P	C5-C4	-3.25	1.35	1.40
83	r4	73	P5P	C5-C4	-3.25	1.35	1.40
83	r4	69	P5P	C5-C4	-3.25	1.35	1.40
83	r4	70	P5P	C5-C4	-3.25	1.35	1.40
83	r4	21	P5P	C5-C4	-3.25	1.35	1.40
83	r4	27	P5P	C5-C4	-3.24	1.35	1.40
83	r4	52	P5P	C5-C4	-3.23	1.35	1.40
83	r4	37	P5P	C5-C4	-3.23	1.35	1.40
83	r4	38	P5P	C5-C4	-3.23	1.35	1.40
83	r4	65	P5P	C5-C4	-3.23	1.35	1.40
83	r4	44	P5P	C5-C4	-3.23	1.35	1.40
83	r4	30	P5P	C5-C4	-3.23	1.35	1.40
83	r4	31	P5P	C5-C4	-3.22	1.35	1.40
83	r4	57	P5P	C5-C4	-3.22	1.35	1.40
83	r4	29	P5P	C5-C4	-3.22	1.35	1.40
83	r4	7	P5P	C5-C4	-3.22	1.35	1.40
83	r4	28	P5P	C5-C4	-3.22	1.35	1.40
83	r4	6	P5P	C5-C4	-3.21	1.35	1.40
83	r4	22	P5P	C5-C4	-3.21	1.35	1.40
83	r4	18	P5P	C5-C4	-3.21	1.35	1.40
83	r4	23	P5P	C5-C4	-3.21	1.35	1.40
83	r4	9	P5P	C5-C4	-3.20	1.35	1.40
83	r4	71	P5P	C5-C4	-3.20	1.35	1.40
83	r4	36	P5P	C5-C4	-3.20	1.35	1.40
83	r4	19	P5P	C5-C4	-3.20	1.35	1.40
83	r4	26	P5P	C5-C4	-3.20	1.35	1.40
83	r4	46	P5P	C5-C4	-3.20	1.35	1.40
83	r4	53	P5P	C5-C4	-3.19	1.35	1.40
83	r4	34	P5P	C5-C4	-3.19	1.35	1.40
83	r4	63	P5P	C5-C4	-3.19	1.35	1.40
86	A	7	004	CB-CA	-3.19	1.49	1.52
83	r4	64	P5P	C5-C4	-3.19	1.35	1.40
83	r4	58	P5P	C5-C4	-3.17	1.35	1.40
83	r4	14	P5P	C5-C4	-3.17	1.35	1.40
83	r4	15	P5P	C5-C4	-3.16	1.35	1.40
83	r4	10	P5P	C5-C4	-3.14	1.35	1.40
83	r4	60	Y5P	C6-N1	2.77	1.44	1.37
83	r4	3	Y5P	C6-N1	2.77	1.44	1.37
83	r4	43	Y5P	C6-N1	2.77	1.44	1.37
83	r4	41	Y5P	C6-N1	2.77	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r4	45	Y5P	C6-N1	2.76	1.44	1.37
83	r4	47	Y5P	C6-N1	2.76	1.44	1.37
83	r4	2	Y5P	C6-N1	2.76	1.44	1.37
83	r4	61	Y5P	C6-N1	2.76	1.44	1.37
83	r4	42	Y5P	C6-N1	2.76	1.43	1.37
83	r4	59	Y5P	C6-N1	2.76	1.43	1.37
83	r4	17	Y5P	C6-N1	2.76	1.43	1.37
83	r4	67	Y5P	C6-N1	2.76	1.43	1.37
83	r4	20	Y5P	C6-N1	2.75	1.43	1.37
83	r4	16	Y5P	C6-N1	2.75	1.43	1.37
83	r4	56	Y5P	C6-N1	2.75	1.43	1.37
83	r4	55	Y5P	C6-N1	2.75	1.43	1.37
83	r4	40	Y5P	C6-N1	2.75	1.43	1.37
83	r4	62	Y5P	C6-N1	2.75	1.43	1.37
83	r4	74	Y5P	C6-N1	2.75	1.43	1.37
83	r4	25	Y5P	C6-N1	2.75	1.43	1.37
83	r4	72	Y5P	C6-N1	2.75	1.43	1.37
83	r4	11	Y5P	C6-N1	2.75	1.43	1.37
83	r4	4	Y5P	C6-N1	2.74	1.43	1.37
83	r4	12	Y5P	C6-N1	2.74	1.43	1.37
83	r4	13	Y5P	C6-N1	2.74	1.43	1.37
83	r4	48	Y5P	C6-N1	2.74	1.43	1.37
83	r4	54	Y5P	C6-N1	2.74	1.43	1.37
83	r4	33	Y5P	C6-N1	2.74	1.43	1.37
83	r4	8	Y5P	C6-N1	2.74	1.43	1.37
83	r4	68	Y5P	C6-N1	2.74	1.43	1.37
83	r4	51	Y5P	C6-N1	2.73	1.43	1.37
83	r4	39	Y5P	C6-N1	2.73	1.43	1.37
83	r4	50	Y5P	C6-N1	2.73	1.43	1.37
83	r4	66	Y5P	C6-N1	2.73	1.43	1.37
83	r4	32	Y5P	C6-N1	2.72	1.43	1.37
83	r4	73	P5P	C5-N7	-2.72	1.34	1.39
83	r4	49	Y5P	C6-N1	2.71	1.43	1.37
83	r4	10	P5P	C5-N7	-2.71	1.34	1.39
83	r4	76	P5P	C5-N7	-2.71	1.34	1.39
83	r4	23	P5P	C5-N7	-2.70	1.34	1.39
83	r4	36	P5P	C5-N7	-2.70	1.34	1.39
83	r4	14	P5P	C5-N7	-2.69	1.34	1.39
83	r4	57	P5P	C5-N7	-2.69	1.34	1.39
83	r4	21	P5P	C5-N7	-2.68	1.34	1.39
83	r4	75	Y5P	C6-N1	2.68	1.43	1.37
83	r4	22	P5P	C5-N7	-2.68	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r4	5	P5P	C5-N7	-2.68	1.34	1.39
83	r4	71	P5P	C5-N7	-2.67	1.34	1.39
83	r4	28	P5P	C5-N7	-2.67	1.34	1.39
83	r4	58	P5P	C5-N7	-2.67	1.34	1.39
83	r4	38	P5P	C5-N7	-2.66	1.34	1.39
83	r4	7	P5P	C5-N7	-2.66	1.34	1.39
83	r4	69	P5P	C5-N7	-2.66	1.34	1.39
83	r4	52	P5P	C5-N7	-2.66	1.34	1.39
83	r4	30	P5P	C5-N7	-2.66	1.34	1.39
83	r4	63	P5P	C5-N7	-2.65	1.34	1.39
83	r4	35	P5P	C5-N7	-2.65	1.34	1.39
83	r4	34	P5P	C5-N7	-2.64	1.34	1.39
83	r4	9	P5P	C5-N7	-2.64	1.34	1.39
83	r4	26	P5P	C5-N7	-2.64	1.34	1.39
83	r4	44	P5P	C5-N7	-2.64	1.34	1.39
83	r4	65	P5P	C5-N7	-2.64	1.34	1.39
83	r4	15	P5P	C5-N7	-2.64	1.34	1.39
83	r4	31	P5P	C5-N7	-2.64	1.34	1.39
83	r4	64	P5P	C5-N7	-2.64	1.34	1.39
83	r4	29	P5P	C5-N7	-2.63	1.34	1.39
83	r4	6	P5P	C5-N7	-2.62	1.34	1.39
83	r4	27	P5P	C5-N7	-2.62	1.34	1.39
83	r4	53	P5P	C5-N7	-2.62	1.34	1.39
83	r4	1	P5P	C5-N7	-2.62	1.34	1.39
83	r4	37	P5P	C5-N7	-2.62	1.34	1.39
83	r4	46	P5P	C5-N7	-2.62	1.34	1.39
83	r4	70	P5P	C5-N7	-2.62	1.34	1.39
83	r4	18	P5P	C5-N7	-2.61	1.34	1.39
83	r4	19	P5P	C5-N7	-2.60	1.34	1.39
83	r4	24	P5P	C5-N7	-2.59	1.35	1.39
83	r4	37	P5P	C4-N9	-2.32	1.32	1.37
83	r4	76	P5P	C4-N9	-2.32	1.32	1.37
83	r4	1	P5P	C4-N9	-2.32	1.32	1.37
83	r4	30	P5P	C4-N9	-2.31	1.32	1.37
83	r4	65	P5P	C4-N9	-2.29	1.32	1.37
83	r4	24	P5P	C4-N9	-2.29	1.32	1.37
83	r4	35	P5P	C4-N9	-2.28	1.32	1.37
83	r4	36	P5P	C4-N9	-2.28	1.33	1.37
83	r4	70	P5P	C4-N9	-2.28	1.33	1.37
83	r4	31	P5P	C4-N9	-2.27	1.33	1.37
83	r4	71	P5P	C4-N9	-2.27	1.33	1.37
83	r4	58	P5P	C4-N9	-2.27	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r4	53	P5P	C4-N9	-2.26	1.33	1.37
83	r4	21	P5P	C4-N9	-2.26	1.33	1.37
83	r4	64	P5P	C4-N9	-2.26	1.33	1.37
83	r4	26	P5P	C4-N9	-2.26	1.33	1.37
83	r4	46	P5P	C4-N9	-2.26	1.33	1.37
83	r4	9	P5P	C4-N9	-2.26	1.33	1.37
83	r4	28	P5P	C4-N9	-2.25	1.33	1.37
83	r4	27	P5P	C4-N9	-2.25	1.33	1.37
83	r4	38	P5P	C4-N9	-2.25	1.33	1.37
83	r4	69	P5P	C4-N9	-2.25	1.33	1.37
83	r4	18	P5P	C4-N9	-2.25	1.33	1.37
83	r4	34	P5P	C4-N9	-2.25	1.33	1.37
83	r4	5	P5P	C4-N9	-2.24	1.33	1.37
83	r4	14	P5P	C4-N9	-2.24	1.33	1.37
83	r4	19	P5P	C4-N9	-2.24	1.33	1.37
83	r4	6	P5P	C4-N9	-2.24	1.33	1.37
83	r4	44	P5P	C4-N9	-2.23	1.33	1.37
83	r4	15	P5P	C4-N9	-2.23	1.33	1.37
83	r4	7	P5P	C4-N9	-2.22	1.33	1.37
83	r4	23	P5P	C4-N9	-2.22	1.33	1.37
83	r4	57	P5P	C4-N9	-2.22	1.33	1.37
83	r4	52	P5P	C4-N9	-2.21	1.33	1.37
83	r4	63	P5P	C4-N9	-2.21	1.33	1.37
83	r4	29	P5P	C4-N9	-2.18	1.33	1.37
83	r4	22	P5P	C4-N9	-2.17	1.33	1.37
83	r4	73	P5P	C4-N9	-2.15	1.33	1.37
83	r4	10	P5P	C4-N9	-2.14	1.33	1.37

All (435) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	A	1	MHW	O-C-CA	-6.19	116.60	124.37
83	r4	76	P5P	N9-C8-N7	-5.47	106.18	113.94
83	r4	1	P5P	N9-C8-N7	-5.36	106.33	113.94
83	r4	35	P5P	N9-C8-N7	-5.33	106.38	113.94
83	r4	65	P5P	N9-C8-N7	-5.32	106.38	113.94
83	r4	70	P5P	N9-C8-N7	-5.30	106.42	113.94
83	r4	46	P5P	N9-C8-N7	-5.30	106.42	113.94
83	r4	58	P5P	N9-C8-N7	-5.29	106.42	113.94
83	r4	30	P5P	N9-C8-N7	-5.29	106.43	113.94
83	r4	28	P5P	N9-C8-N7	-5.28	106.45	113.94
83	r4	57	P5P	N9-C8-N7	-5.28	106.45	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	38	P5P	N9-C8-N7	-5.28	106.45	113.94
83	r4	69	P5P	N9-C8-N7	-5.26	106.47	113.94
83	r4	34	P5P	N9-C8-N7	-5.26	106.47	113.94
83	r4	24	P5P	N9-C8-N7	-5.25	106.48	113.94
83	r4	64	P5P	N9-C8-N7	-5.25	106.49	113.94
83	r4	9	P5P	N9-C8-N7	-5.25	106.49	113.94
83	r4	14	P5P	N9-C8-N7	-5.25	106.49	113.94
83	r4	21	P5P	N9-C8-N7	-5.24	106.50	113.94
83	r4	52	P5P	N9-C8-N7	-5.24	106.50	113.94
83	r4	27	P5P	N9-C8-N7	-5.24	106.51	113.94
83	r4	37	P5P	N9-C8-N7	-5.24	106.51	113.94
83	r4	53	P5P	N9-C8-N7	-5.23	106.51	113.94
83	r4	18	P5P	N9-C8-N7	-5.22	106.53	113.94
83	r4	15	P5P	N9-C8-N7	-5.22	106.53	113.94
83	r4	63	P5P	N9-C8-N7	-5.22	106.53	113.94
83	r4	19	P5P	N9-C8-N7	-5.22	106.53	113.94
83	r4	36	P5P	N9-C8-N7	-5.22	106.53	113.94
83	r4	26	P5P	N9-C8-N7	-5.21	106.55	113.94
83	r4	5	P5P	N9-C8-N7	-5.21	106.55	113.94
83	r4	73	P5P	N9-C8-N7	-5.21	106.55	113.94
83	r4	44	P5P	N9-C8-N7	-5.20	106.56	113.94
83	r4	6	P5P	N9-C8-N7	-5.20	106.56	113.94
83	r4	7	P5P	N9-C8-N7	-5.19	106.57	113.94
83	r4	71	P5P	N9-C8-N7	-5.19	106.57	113.94
83	r4	31	P5P	N9-C8-N7	-5.16	106.62	113.94
83	r4	73	P5P	C5-C4-N3	-5.15	120.11	127.18
83	r4	23	P5P	N9-C8-N7	-5.14	106.64	113.94
83	r4	29	P5P	N9-C8-N7	-5.13	106.66	113.94
83	r4	10	P5P	N9-C8-N7	-5.11	106.69	113.94
83	r4	22	P5P	N9-C8-N7	-5.10	106.70	113.94
83	r4	29	P5P	C5-C4-N3	-5.07	120.22	127.18
83	r4	22	P5P	C5-C4-N3	-5.06	120.23	127.18
83	r4	23	P5P	C5-C4-N3	-5.05	120.25	127.18
83	r4	28	P5P	C5-C4-N3	-5.03	120.27	127.18
83	r4	15	P5P	C5-C4-N3	-5.01	120.30	127.18
83	r4	10	P5P	C5-C4-N3	-5.01	120.30	127.18
83	r4	18	P5P	C5-C4-N3	-5.01	120.30	127.18
83	r4	44	P5P	C5-C4-N3	-5.00	120.31	127.18
83	r4	36	P5P	C5-C4-N3	-4.99	120.32	127.18
83	r4	76	P5P	C5-C4-N3	-4.99	120.33	127.18
83	r4	57	P5P	C5-C4-N3	-4.99	120.33	127.18
83	r4	7	P5P	C5-C4-N3	-4.99	120.33	127.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	9	P5P	C5-C4-N3	-4.98	120.34	127.18
83	r4	19	P5P	C5-C4-N3	-4.97	120.35	127.18
83	r4	58	P5P	C5-C4-N3	-4.96	120.36	127.18
83	r4	14	P5P	C5-C4-N3	-4.96	120.36	127.18
83	r4	53	P5P	C5-C4-N3	-4.96	120.36	127.18
83	r4	63	P5P	C5-C4-N3	-4.96	120.38	127.18
83	r4	6	P5P	C5-C4-N3	-4.95	120.38	127.18
83	r4	46	P5P	C5-C4-N3	-4.95	120.39	127.18
83	r4	35	P5P	C5-C4-N3	-4.95	120.39	127.18
83	r4	69	P5P	C5-C4-N3	-4.95	120.39	127.18
83	r4	34	P5P	C5-C4-N3	-4.94	120.39	127.18
83	r4	64	P5P	C5-C4-N3	-4.94	120.39	127.18
83	r4	52	P5P	C5-C4-N3	-4.94	120.40	127.18
83	r4	5	P5P	C5-C4-N3	-4.93	120.42	127.18
83	r4	26	P5P	C5-C4-N3	-4.93	120.42	127.18
83	r4	37	P5P	C5-C4-N3	-4.93	120.42	127.18
83	r4	27	P5P	C5-C4-N3	-4.92	120.42	127.18
83	r4	70	P5P	C5-C4-N3	-4.92	120.42	127.18
83	r4	31	P5P	C5-C4-N3	-4.91	120.43	127.18
83	r4	71	P5P	C5-C4-N3	-4.91	120.43	127.18
83	r4	24	P5P	C5-C4-N3	-4.91	120.44	127.18
83	r4	38	P5P	C5-C4-N3	-4.91	120.44	127.18
83	r4	21	P5P	C5-C4-N3	-4.88	120.48	127.18
83	r4	1	P5P	C5-C4-N3	-4.86	120.50	127.18
83	r4	30	P5P	C5-C4-N3	-4.84	120.53	127.18
83	r4	65	P5P	C5-C4-N3	-4.83	120.55	127.18
83	r4	73	P5P	N1-C2-N3	-4.39	119.86	127.33
83	r4	1	P5P	N1-C2-N3	-4.37	119.91	127.33
83	r4	24	P5P	N1-C2-N3	-4.35	119.94	127.33
83	r4	29	P5P	N1-C2-N3	-4.33	119.98	127.33
83	r4	21	P5P	N1-C2-N3	-4.31	120.00	127.33
83	r4	53	P5P	N1-C2-N3	-4.31	120.01	127.33
83	r4	76	P5P	N1-C2-N3	-4.31	120.01	127.33
83	r4	63	P5P	N1-C2-N3	-4.30	120.02	127.33
83	r4	6	P5P	N1-C2-N3	-4.30	120.02	127.33
83	r4	70	P5P	N1-C2-N3	-4.30	120.03	127.33
83	r4	34	P5P	N1-C2-N3	-4.29	120.04	127.33
83	r4	5	P5P	N1-C2-N3	-4.29	120.04	127.33
83	r4	26	P5P	N1-C2-N3	-4.28	120.05	127.33
83	r4	65	P5P	N1-C2-N3	-4.28	120.05	127.33
83	r4	69	P5P	N1-C2-N3	-4.28	120.05	127.33
83	r4	7	P5P	N1-C2-N3	-4.28	120.06	127.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	31	P5P	N1-C2-N3	-4.28	120.06	127.33
83	r4	9	P5P	N1-C2-N3	-4.28	120.06	127.33
83	r4	30	P5P	N1-C2-N3	-4.27	120.07	127.33
83	r4	38	P5P	N1-C2-N3	-4.27	120.07	127.33
83	r4	18	P5P	N1-C2-N3	-4.27	120.07	127.33
83	r4	46	P5P	N1-C2-N3	-4.27	120.08	127.33
83	r4	57	P5P	N1-C2-N3	-4.27	120.08	127.33
83	r4	64	P5P	N1-C2-N3	-4.26	120.08	127.33
83	r4	36	P5P	N1-C2-N3	-4.26	120.09	127.33
83	r4	35	P5P	N1-C2-N3	-4.26	120.10	127.33
83	r4	52	P5P	N1-C2-N3	-4.26	120.10	127.33
83	r4	58	P5P	N1-C2-N3	-4.26	120.10	127.33
83	r4	22	P5P	N1-C2-N3	-4.25	120.10	127.33
83	r4	23	P5P	C1'-N9-C8	-4.25	117.66	127.09
83	r4	23	P5P	N1-C2-N3	-4.25	120.11	127.33
83	r4	28	P5P	N1-C2-N3	-4.25	120.11	127.33
83	r4	14	P5P	N1-C2-N3	-4.25	120.12	127.33
83	r4	44	P5P	N1-C2-N3	-4.25	120.12	127.33
83	r4	27	P5P	N1-C2-N3	-4.24	120.12	127.33
83	r4	19	P5P	N1-C2-N3	-4.24	120.12	127.33
83	r4	15	P5P	N1-C2-N3	-4.24	120.12	127.33
83	r4	37	P5P	N1-C2-N3	-4.23	120.15	127.33
83	r4	10	P5P	N1-C2-N3	-4.20	120.20	127.33
83	r4	76	P5P	C4-N9-C8	4.19	110.14	105.74
83	r4	71	P5P	N1-C2-N3	-4.18	120.23	127.33
83	r4	29	P5P	C1'-N9-C8	-4.17	117.85	127.09
83	r4	1	P5P	C4-N9-C8	4.16	110.10	105.74
83	r4	73	P5P	C1'-N9-C8	-4.15	117.89	127.09
83	r4	65	P5P	C4-N9-C8	4.14	110.08	105.74
83	r4	35	P5P	C4-N9-C8	4.12	110.06	105.74
83	r4	30	P5P	C4-N9-C8	4.11	110.06	105.74
83	r4	70	P5P	C4-N9-C8	4.11	110.05	105.74
83	r4	46	P5P	C4-N9-C8	4.10	110.04	105.74
83	r4	22	P5P	C1'-N9-C8	-4.09	118.02	127.09
83	r4	34	P5P	C4-N9-C8	4.07	110.01	105.74
83	r4	38	P5P	C4-N9-C8	4.06	110.01	105.74
83	r4	10	P5P	C1'-N9-C8	-4.06	118.07	127.09
83	r4	52	P5P	C4-N9-C8	4.06	110.00	105.74
83	r4	24	P5P	C4-N9-C8	4.06	110.00	105.74
83	r4	69	P5P	C4-N9-C8	4.06	110.00	105.74
83	r4	21	P5P	C4-N9-C8	4.05	109.99	105.74
83	r4	26	P5P	C4-N9-C8	4.05	109.99	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	28	P5P	C4-N9-C8	4.04	109.98	105.74
83	r4	58	P5P	C4-N9-C8	4.04	109.98	105.74
83	r4	37	P5P	C4-N9-C8	4.04	109.97	105.74
83	r4	6	P5P	C4-N9-C8	4.03	109.97	105.74
83	r4	53	P5P	C4-N9-C8	4.03	109.97	105.74
83	r4	14	P5P	C4-N9-C8	4.02	109.96	105.74
83	r4	64	P5P	C4-N9-C8	4.02	109.96	105.74
83	r4	19	P5P	C4-N9-C8	4.01	109.95	105.74
83	r4	31	P5P	C1'-N9-C8	-4.01	118.19	127.09
83	r4	5	P5P	C4-N9-C8	4.01	109.95	105.74
83	r4	36	P5P	C4-N9-C8	4.01	109.95	105.74
83	r4	26	P5P	C1'-N9-C8	-4.01	118.19	127.09
83	r4	9	P5P	C4-N9-C8	4.01	109.95	105.74
83	r4	15	P5P	C4-N9-C8	4.01	109.95	105.74
83	r4	57	P5P	C4-N9-C8	4.01	109.94	105.74
83	r4	31	P5P	C4-N9-C8	3.99	109.93	105.74
83	r4	18	P5P	C4-N9-C8	3.99	109.93	105.74
83	r4	27	P5P	C4-N9-C8	3.99	109.93	105.74
83	r4	28	P5P	C1'-N9-C8	-3.99	118.25	127.09
83	r4	71	P5P	C4-N9-C8	3.98	109.92	105.74
83	r4	63	P5P	C4-N9-C8	3.98	109.92	105.74
83	r4	36	P5P	C1'-N9-C8	-3.97	118.28	127.09
83	r4	44	P5P	C4-N9-C8	3.97	109.91	105.74
83	r4	6	P5P	C1'-N9-C8	-3.96	118.30	127.09
83	r4	23	P5P	C4-N9-C8	3.96	109.89	105.74
83	r4	44	P5P	C1'-N9-C8	-3.96	118.32	127.09
83	r4	52	P5P	C1'-N9-C8	-3.95	118.32	127.09
83	r4	71	P5P	C1'-N9-C8	-3.95	118.33	127.09
83	r4	64	P5P	C1'-N9-C8	-3.94	118.35	127.09
83	r4	69	P5P	C1'-N9-C8	-3.94	118.35	127.09
83	r4	73	P5P	C4-N9-C8	3.94	109.87	105.74
83	r4	9	P5P	C1'-N9-C8	-3.94	118.36	127.09
83	r4	5	P5P	C1'-N9-C8	-3.94	118.36	127.09
83	r4	63	P5P	C1'-N9-C8	-3.92	118.40	127.09
83	r4	7	P5P	C4-N9-C8	3.92	109.85	105.74
83	r4	30	P5P	C1'-N9-C8	-3.92	118.40	127.09
83	r4	1	P5P	C6-N1-C2	3.91	120.42	115.80
83	r4	29	P5P	C4-N9-C8	3.88	109.82	105.74
83	r4	24	P5P	C6-N1-C2	3.88	120.39	115.80
83	r4	37	P5P	C1'-N9-C8	-3.88	118.48	127.09
83	r4	15	P5P	C1'-N9-C8	-3.88	118.49	127.09
83	r4	53	P5P	C1'-N9-C8	-3.87	118.51	127.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	18	P5P	C1'-N9-C8	-3.86	118.52	127.09
83	r4	14	P5P	C1'-N9-C8	-3.86	118.53	127.09
83	r4	10	P5P	C4-N9-C8	3.86	109.79	105.74
83	r4	35	P5P	C1'-N9-C8	-3.86	118.54	127.09
83	r4	22	P5P	C4-N9-C8	3.85	109.78	105.74
83	r4	31	P5P	C6-N1-C2	3.84	120.34	115.80
83	r4	7	P5P	C1'-N9-C8	-3.83	118.59	127.09
83	r4	21	P5P	C1'-N9-C8	-3.83	118.60	127.09
83	r4	58	P5P	C1'-N9-C8	-3.83	118.60	127.09
83	r4	65	P5P	C6-N1-C2	3.83	120.32	115.80
83	r4	70	P5P	C1'-N9-C8	-3.83	118.60	127.09
83	r4	53	P5P	C6-N1-C2	3.82	120.31	115.80
83	r4	38	P5P	C1'-N9-C8	-3.81	118.64	127.09
83	r4	5	P5P	C6-N1-C2	3.81	120.30	115.80
83	r4	21	P5P	C6-N1-C2	3.81	120.30	115.80
83	r4	34	P5P	C1'-N9-C8	-3.80	118.65	127.09
83	r4	57	P5P	C1'-N9-C8	-3.80	118.65	127.09
83	r4	19	P5P	C1'-N9-C8	-3.80	118.65	127.09
83	r4	26	P5P	C6-N1-C2	3.80	120.28	115.80
83	r4	46	P5P	C1'-N9-C8	-3.79	118.68	127.09
83	r4	30	P5P	C6-N1-C2	3.78	120.27	115.80
83	r4	70	P5P	C6-N1-C2	3.78	120.26	115.80
83	r4	29	P5P	C6-N1-C2	3.78	120.26	115.80
83	r4	52	P5P	C6-N1-C2	3.78	120.26	115.80
83	r4	65	P5P	C1'-N9-C8	-3.78	118.72	127.09
83	r4	6	P5P	C6-N1-C2	3.77	120.26	115.80
83	r4	69	P5P	C6-N1-C2	3.77	120.25	115.80
83	r4	27	P5P	C1'-N9-C8	-3.77	118.73	127.09
83	r4	63	P5P	C6-N1-C2	3.77	120.25	115.80
83	r4	1	P5P	C1'-N9-C8	-3.76	118.74	127.09
83	r4	9	P5P	C6-N1-C2	3.76	120.24	115.80
83	r4	19	P5P	C6-N1-C2	3.76	120.24	115.80
83	r4	64	P5P	C6-N1-C2	3.76	120.24	115.80
83	r4	18	P5P	C6-N1-C2	3.75	120.23	115.80
83	r4	73	P5P	C6-N1-C2	3.74	120.22	115.80
83	r4	24	P5P	C1'-N9-C8	-3.74	118.79	127.09
83	r4	58	P5P	C6-N1-C2	3.74	120.21	115.80
83	r4	7	P5P	C6-N1-C2	3.74	120.21	115.80
83	r4	38	P5P	C6-N1-C2	3.74	120.21	115.80
83	r4	37	P5P	C6-N1-C2	3.74	120.21	115.80
83	r4	34	P5P	C6-N1-C2	3.74	120.21	115.80
83	r4	27	P5P	C6-N1-C2	3.73	120.21	115.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	36	P5P	C6-N1-C2	3.73	120.20	115.80
83	r4	28	P5P	C6-N1-C2	3.72	120.19	115.80
83	r4	46	P5P	C6-N1-C2	3.72	120.19	115.80
83	r4	57	P5P	C6-N1-C2	3.71	120.19	115.80
83	r4	14	P5P	C6-N1-C2	3.71	120.18	115.80
83	r4	23	P5P	C6-N1-C2	3.71	120.17	115.80
83	r4	22	P5P	C6-N1-C2	3.70	120.17	115.80
83	r4	35	P5P	C6-N1-C2	3.69	120.16	115.80
83	r4	71	P5P	C6-N1-C2	3.69	120.16	115.80
83	r4	44	P5P	C6-N1-C2	3.68	120.15	115.80
83	r4	15	P5P	C6-N1-C2	3.68	120.14	115.80
83	r4	10	P5P	C6-N1-C2	3.68	120.14	115.80
83	r4	73	P5P	N3-C4-N9	3.53	133.18	127.17
83	r4	76	P5P	C6-N1-C2	3.52	119.95	115.80
83	r4	76	P5P	C1'-N9-C8	-3.50	119.33	127.09
83	r4	23	P5P	N3-C4-N9	3.45	133.04	127.17
83	r4	29	P5P	N3-C4-N9	3.43	133.01	127.17
83	r4	76	P5P	C5-N7-C8	3.43	108.61	104.40
83	r4	22	P5P	N3-C4-N9	3.43	133.00	127.17
83	r4	10	P5P	N3-C4-N9	3.40	132.95	127.17
83	r4	28	P5P	N3-C4-N9	3.40	132.94	127.17
83	r4	28	P5P	C5-N7-C8	3.39	108.56	104.40
83	r4	57	P5P	C5-N7-C8	3.39	108.56	104.40
83	r4	15	P5P	N3-C4-N9	3.38	132.92	127.17
83	r4	58	P5P	C5-N7-C8	3.38	108.55	104.40
83	r4	73	P5P	C2-N3-C4	3.38	120.09	111.83
83	r4	44	P5P	N3-C4-N9	3.37	132.91	127.17
83	r4	6	P5P	N3-C4-N9	3.37	132.90	127.17
83	r4	36	P5P	N3-C4-N9	3.37	132.89	127.17
83	r4	26	P5P	N3-C4-N9	3.36	132.89	127.17
83	r4	52	P5P	N3-C4-N9	3.36	132.89	127.17
83	r4	69	P5P	N3-C4-N9	3.36	132.88	127.17
83	r4	5	P5P	N3-C4-N9	3.36	132.88	127.17
83	r4	14	P5P	N3-C4-N9	3.35	132.87	127.17
83	r4	63	P5P	N3-C4-N9	3.35	132.87	127.17
83	r4	18	P5P	N3-C4-N9	3.35	132.86	127.17
83	r4	1	P5P	C5-N7-C8	3.35	108.51	104.40
83	r4	14	P5P	C5-N7-C8	3.35	108.51	104.40
83	r4	46	P5P	C5-N7-C8	3.34	108.51	104.40
83	r4	9	P5P	N3-C4-N9	3.34	132.85	127.17
83	r4	35	P5P	C5-N7-C8	3.34	108.50	104.40
83	r4	53	P5P	N3-C4-N9	3.34	132.85	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	34	P5P	N3-C4-N9	3.34	132.85	127.17
83	r4	35	P5P	N3-C4-N9	3.34	132.85	127.17
83	r4	57	P5P	N3-C4-N9	3.34	132.85	127.17
83	r4	9	P5P	C5-N7-C8	3.34	108.50	104.40
83	r4	38	P5P	C5-N7-C8	3.34	108.50	104.40
83	r4	19	P5P	N3-C4-N9	3.34	132.85	127.17
83	r4	46	P5P	N3-C4-N9	3.34	132.85	127.17
83	r4	7	P5P	N3-C4-N9	3.34	132.84	127.17
83	r4	31	P5P	N3-C4-N9	3.34	132.84	127.17
83	r4	65	P5P	C5-N7-C8	3.34	108.50	104.40
83	r4	58	P5P	N3-C4-N9	3.33	132.84	127.17
83	r4	38	P5P	N3-C4-N9	3.33	132.83	127.17
83	r4	64	P5P	C5-N7-C8	3.33	108.48	104.40
86	A	7	004	CG2-CB-CA	-3.32	115.48	120.64
83	r4	71	P5P	N3-C4-N9	3.32	132.81	127.17
83	r4	73	P5P	C5-N7-C8	3.32	108.47	104.40
83	r4	64	P5P	N3-C4-N9	3.32	132.81	127.17
83	r4	34	P5P	C5-N7-C8	3.32	108.47	104.40
83	r4	76	P5P	N3-C4-N9	3.31	132.81	127.17
83	r4	15	P5P	C5-N7-C8	3.31	108.47	104.40
83	r4	70	P5P	N3-C4-N9	3.31	132.80	127.17
83	r4	27	P5P	C5-N7-C8	3.31	108.46	104.40
83	r4	63	P5P	C5-N7-C8	3.31	108.46	104.40
83	r4	70	P5P	C5-N7-C8	3.30	108.45	104.40
83	r4	76	P5P	C2-N3-C4	3.30	119.89	111.83
83	r4	30	P5P	N3-C4-N9	3.30	132.78	127.17
83	r4	21	P5P	N3-C4-N9	3.30	132.78	127.17
83	r4	44	P5P	C5-N7-C8	3.30	108.45	104.40
83	r4	69	P5P	C5-N7-C8	3.30	108.45	104.40
83	r4	37	P5P	N3-C4-N9	3.29	132.77	127.17
83	r4	52	P5P	C5-N7-C8	3.29	108.44	104.40
83	r4	27	P5P	N3-C4-N9	3.29	132.76	127.17
83	r4	24	P5P	C5-N7-C8	3.29	108.44	104.40
83	r4	29	P5P	C2-N3-C4	3.29	119.86	111.83
83	r4	19	P5P	C5-N7-C8	3.29	108.43	104.40
83	r4	18	P5P	C5-N7-C8	3.28	108.43	104.40
83	r4	24	P5P	N3-C4-N9	3.28	132.75	127.17
83	r4	21	P5P	C5-N7-C8	3.28	108.43	104.40
83	r4	53	P5P	C5-N7-C8	3.28	108.42	104.40
83	r4	30	P5P	C5-N7-C8	3.27	108.42	104.40
83	r4	22	P5P	C2-N3-C4	3.27	119.82	111.83
83	r4	7	P5P	C5-N7-C8	3.27	108.42	104.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	37	P5P	C5-N7-C8	3.27	108.41	104.40
83	r4	65	P5P	N3-C4-N9	3.27	132.73	127.17
83	r4	36	P5P	C5-N7-C8	3.27	108.41	104.40
83	r4	71	P5P	C5-N7-C8	3.27	108.41	104.40
83	r4	1	P5P	N3-C4-N9	3.26	132.72	127.17
83	r4	15	P5P	C2-N3-C4	3.26	119.80	111.83
83	r4	7	P5P	C2-N3-C4	3.26	119.80	111.83
83	r4	34	P5P	C2-N3-C4	3.26	119.80	111.83
83	r4	23	P5P	C2-N3-C4	3.26	119.79	111.83
83	r4	53	P5P	C2-N3-C4	3.26	119.78	111.83
83	r4	57	P5P	C2-N3-C4	3.26	119.78	111.83
83	r4	63	P5P	C2-N3-C4	3.26	119.78	111.83
83	r4	18	P5P	C2-N3-C4	3.25	119.78	111.83
83	r4	36	P5P	C2-N3-C4	3.25	119.77	111.83
83	r4	26	P5P	C5-N7-C8	3.25	108.39	104.40
83	r4	38	P5P	C2-N3-C4	3.25	119.76	111.83
83	r4	6	P5P	C2-N3-C4	3.25	119.76	111.83
83	r4	44	P5P	C2-N3-C4	3.25	119.76	111.83
83	r4	9	P5P	C2-N3-C4	3.24	119.76	111.83
83	r4	5	P5P	C5-N7-C8	3.24	108.38	104.40
83	r4	24	P5P	C2-N3-C4	3.24	119.75	111.83
83	r4	14	P5P	C2-N3-C4	3.24	119.75	111.83
83	r4	46	P5P	C2-N3-C4	3.24	119.75	111.83
83	r4	70	P5P	C2-N3-C4	3.24	119.75	111.83
83	r4	6	P5P	C5-N7-C8	3.24	108.38	104.40
83	r4	28	P5P	C2-N3-C4	3.24	119.75	111.83
86	A	1	MHW	CB-CA-C	-3.24	117.68	120.09
83	r4	10	P5P	C5-N7-C8	3.24	108.38	104.40
83	r4	58	P5P	C2-N3-C4	3.24	119.74	111.83
83	r4	35	P5P	C2-N3-C4	3.24	119.74	111.83
83	r4	1	P5P	C2-N3-C4	3.24	119.74	111.83
83	r4	5	P5P	C2-N3-C4	3.23	119.73	111.83
83	r4	10	P5P	C2-N3-C4	3.23	119.72	111.83
83	r4	69	P5P	C2-N3-C4	3.23	119.72	111.83
83	r4	19	P5P	C2-N3-C4	3.23	119.72	111.83
83	r4	31	P5P	C5-N7-C8	3.23	108.36	104.40
83	r4	23	P5P	C5-N7-C8	3.23	108.36	104.40
83	r4	64	P5P	C2-N3-C4	3.23	119.71	111.83
83	r4	29	P5P	C5-N7-C8	3.22	108.36	104.40
83	r4	26	P5P	C2-N3-C4	3.22	119.70	111.83
83	r4	27	P5P	C2-N3-C4	3.22	119.69	111.83
83	r4	21	P5P	C2-N3-C4	3.22	119.69	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	31	P5P	C2-N3-C4	3.22	119.69	111.83
83	r4	30	P5P	C2-N3-C4	3.22	119.68	111.83
83	r4	52	P5P	C2-N3-C4	3.21	119.68	111.83
83	r4	37	P5P	C2-N3-C4	3.21	119.67	111.83
83	r4	22	P5P	C5-N7-C8	3.20	108.33	104.40
86	A	7	004	CG1-CB-CA	3.20	125.62	120.64
83	r4	65	P5P	C2-N3-C4	3.20	119.65	111.83
83	r4	28	P5P	C6-C5-C4	3.20	119.73	116.24
83	r4	71	P5P	C2-N3-C4	3.18	119.59	111.83
83	r4	23	P5P	C6-C5-C4	3.18	119.71	116.24
83	r4	22	P5P	C6-C5-C4	3.16	119.70	116.24
83	r4	10	P5P	C6-C5-C4	3.16	119.69	116.24
83	r4	29	P5P	C6-C5-C4	3.15	119.68	116.24
83	r4	71	P5P	C6-C5-C4	3.14	119.67	116.24
83	r4	37	P5P	C6-C5-C4	3.13	119.66	116.24
83	r4	44	P5P	C6-C5-C4	3.12	119.65	116.24
83	r4	36	P5P	C6-C5-C4	3.12	119.65	116.24
83	r4	52	P5P	C6-C5-C4	3.12	119.65	116.24
83	r4	18	P5P	C6-C5-C4	3.11	119.64	116.24
83	r4	9	P5P	C6-C5-C4	3.10	119.63	116.24
83	r4	19	P5P	C6-C5-C4	3.10	119.63	116.24
83	r4	26	P5P	C6-C5-C4	3.09	119.62	116.24
83	r4	53	P5P	C6-C5-C4	3.08	119.61	116.24
83	r4	57	P5P	C6-C5-C4	3.08	119.61	116.24
83	r4	15	P5P	C6-C5-C4	3.08	119.61	116.24
83	r4	64	P5P	C6-C5-C4	3.08	119.61	116.24
83	r4	69	P5P	C6-C5-C4	3.08	119.61	116.24
83	r4	6	P5P	C6-C5-C4	3.07	119.60	116.24
83	r4	73	P5P	C6-C5-C4	3.07	119.59	116.24
83	r4	5	P5P	C6-C5-C4	3.06	119.58	116.24
83	r4	27	P5P	C6-C5-C4	3.06	119.58	116.24
83	r4	7	P5P	C6-C5-C4	3.05	119.58	116.24
83	r4	46	P5P	C6-C5-C4	3.05	119.58	116.24
83	r4	24	P5P	C6-C5-C4	3.05	119.58	116.24
83	r4	58	P5P	C6-C5-C4	3.05	119.58	116.24
83	r4	63	P5P	C6-C5-C4	3.04	119.57	116.24
83	r4	31	P5P	C6-C5-C4	3.04	119.56	116.24
83	r4	35	P5P	C6-C5-C4	3.04	119.56	116.24
83	r4	70	P5P	C6-C5-C4	3.03	119.55	116.24
83	r4	1	P5P	C6-C5-C4	3.02	119.55	116.24
83	r4	14	P5P	C6-C5-C4	3.02	119.54	116.24
83	r4	21	P5P	C6-C5-C4	3.02	119.54	116.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	30	P5P	C6-C5-C4	2.99	119.51	116.24
83	r4	34	P5P	C6-C5-C4	2.98	119.50	116.24
83	r4	38	P5P	C6-C5-C4	2.98	119.50	116.24
83	r4	65	P5P	C6-C5-C4	2.98	119.50	116.24
83	r4	76	P5P	C6-C5-C4	2.89	119.40	116.24
86	A	5	MHU	O-C-CA	-2.79	117.60	124.77
86	A	1	MHW	CE-N-CA	2.66	121.26	116.83
86	A	6	MHV	CD2-CG-CB	2.62	119.86	115.89
83	r4	23	P5P	C4-N9-C1'	2.49	132.45	126.63
86	A	5	MHU	CM-N-CA	2.44	121.00	113.70
83	r4	29	P5P	C4-N9-C1'	2.44	132.34	126.63
86	A	6	MHV	CB-CA-N	-2.42	107.50	112.50
83	r4	73	P5P	C4-N9-C1'	2.40	132.24	126.63
83	r4	22	P5P	C4-N9-C1'	2.38	132.19	126.63
83	r4	10	P5P	C4-N9-C1'	2.36	132.14	126.63
83	r4	31	P5P	C4-N9-C1'	2.24	131.88	126.63
83	r4	26	P5P	C4-N9-C1'	2.22	131.82	126.63
83	r4	44	P5P	C4-N9-C1'	2.20	131.77	126.63
83	r4	36	P5P	C4-N9-C1'	2.20	131.77	126.63
83	r4	28	P5P	C4-N9-C1'	2.20	131.77	126.63
83	r4	71	P5P	C4-N9-C1'	2.19	131.75	126.63
83	r4	6	P5P	C4-N9-C1'	2.18	131.73	126.63
83	r4	9	P5P	C4-N9-C1'	2.16	131.69	126.63
83	r4	64	P5P	C4-N9-C1'	2.16	131.69	126.63
83	r4	5	P5P	C4-N9-C1'	2.16	131.69	126.63
83	r4	63	P5P	C4-N9-C1'	2.16	131.69	126.63
83	r4	52	P5P	C4-N9-C1'	2.16	131.68	126.63
83	r4	69	P5P	C4-N9-C1'	2.14	131.65	126.63
83	r4	15	P5P	C4-N9-C1'	2.11	131.56	126.63
83	r4	7	P5P	C4-N9-C1'	2.10	131.55	126.63
83	r4	18	P5P	C4-N9-C1'	2.10	131.55	126.63
86	A	5	MHU	CB-CA-N	-2.10	107.38	110.48
83	r4	37	P5P	C4-N9-C1'	2.10	131.54	126.63
83	r4	30	P5P	C4-N9-C1'	2.10	131.54	126.63
83	r4	53	P5P	C4-N9-C1'	2.09	131.52	126.63
83	r4	14	P5P	C4-N9-C1'	2.08	131.50	126.63
86	A	6	MHV	CE-N-CA	2.07	116.43	111.75
83	r4	58	P5P	C4-N9-C1'	2.05	131.42	126.63
83	r4	21	P5P	C4-N9-C1'	2.04	131.41	126.63
83	r4	57	P5P	C4-N9-C1'	2.04	131.41	126.63
83	r4	35	P5P	C4-N9-C1'	2.04	131.40	126.63
83	r4	19	P5P	C4-N9-C1'	2.04	131.39	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r4	38	P5P	C4-N9-C1'	2.02	131.35	126.63
83	r4	70	P5P	C4-N9-C1'	2.01	131.34	126.63
83	r4	34	P5P	C4-N9-C1'	2.01	131.34	126.63
83	r4	27	P5P	C4-N9-C1'	2.01	131.34	126.63

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	r4	8	Y5P	O4'-C1'-N1-C2
83	r4	9	P5P	O4'-C4'-C5'-O5'
83	r4	12	Y5P	O4'-C1'-N1-C2
83	r4	13	Y5P	C3'-C4'-C5'-O5'
83	r4	16	Y5P	O4'-C1'-N1-C2
83	r4	21	P5P	C4'-C5'-O5'-P
83	r4	22	P5P	O4'-C4'-C5'-O5'
83	r4	26	P5P	O4'-C4'-C5'-O5'
83	r4	29	P5P	O4'-C4'-C5'-O5'
83	r4	32	Y5P	O4'-C4'-C5'-O5'
83	r4	40	Y5P	O4'-C1'-N1-C2
83	r4	47	Y5P	O4'-C4'-C5'-O5'
83	r4	51	Y5P	O4'-C1'-N1-C2
83	r4	54	Y5P	O4'-C1'-N1-C2
83	r4	55	Y5P	O4'-C1'-N1-C2
83	r4	56	Y5P	O4'-C4'-C5'-O5'
83	r4	62	Y5P	O4'-C1'-N1-C2
83	r4	64	P5P	O4'-C4'-C5'-O5'
83	r4	66	Y5P	O4'-C4'-C5'-O5'
83	r4	66	Y5P	C3'-C4'-C5'-O5'
83	r4	73	P5P	C2'-C1'-N9-C4
83	r4	73	P5P	C2'-C1'-N9-C8
83	r4	74	Y5P	C2'-C1'-N1-C6
86	A	5	MHU	O-C-CA-CB
83	r4	2	Y5P	O4'-C1'-N1-C2
83	r4	3	Y5P	O4'-C1'-N1-C2
83	r4	4	Y5P	O4'-C1'-N1-C2
83	r4	11	Y5P	O4'-C1'-N1-C2
83	r4	13	Y5P	O4'-C1'-N1-C2
83	r4	17	Y5P	O4'-C1'-N1-C2
83	r4	20	Y5P	O4'-C1'-N1-C2
83	r4	25	Y5P	O4'-C1'-N1-C2
83	r4	32	Y5P	O4'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
83	r4	39	Y5P	O4'-C1'-N1-C2
83	r4	41	Y5P	O4'-C1'-N1-C2
83	r4	42	Y5P	O4'-C1'-N1-C2
83	r4	43	Y5P	O4'-C1'-N1-C2
83	r4	48	Y5P	O4'-C1'-N1-C2
83	r4	49	Y5P	O4'-C1'-N1-C2
83	r4	50	Y5P	O4'-C1'-N1-C2
83	r4	56	Y5P	O4'-C1'-N1-C2
83	r4	59	Y5P	O4'-C1'-N1-C2
83	r4	60	Y5P	O4'-C1'-N1-C2
83	r4	61	Y5P	O4'-C1'-N1-C2
83	r4	66	Y5P	O4'-C1'-N1-C2
83	r4	67	Y5P	O4'-C1'-N1-C2
83	r4	68	Y5P	O4'-C1'-N1-C2
83	r4	72	Y5P	O4'-C1'-N1-C2
83	r4	75	Y5P	O4'-C1'-N1-C2
83	r4	74	Y5P	C2'-C1'-N1-C2
86	A	5	MHU	CE1-CZ-NZ-CZ2
83	r4	6	P5P	O4'-C4'-C5'-O5'
83	r4	13	Y5P	O4'-C4'-C5'-O5'
83	r4	22	P5P	C3'-C4'-C5'-O5'
83	r4	26	P5P	C3'-C4'-C5'-O5'
83	r4	29	P5P	C3'-C4'-C5'-O5'
83	r4	41	Y5P	O4'-C4'-C5'-O5'
83	r4	41	Y5P	C3'-C4'-C5'-O5'
83	r4	48	Y5P	C3'-C4'-C5'-O5'
83	r4	64	P5P	C3'-C4'-C5'-O5'
83	r4	75	Y5P	O4'-C4'-C5'-O5'
86	A	5	MHU	CE2-CZ-NZ-CZ1
86	A	5	MHU	CE1-CZ-NZ-CZ1
86	A	5	MHU	CE2-CZ-NZ-CZ2
83	r4	1	P5P	O4'-C4'-C5'-O5'
83	r4	25	Y5P	C3'-C4'-C5'-O5'
83	r4	28	P5P	O4'-C4'-C5'-O5'
83	r4	38	P5P	O4'-C4'-C5'-O5'
83	r4	45	Y5P	O4'-C4'-C5'-O5'
83	r4	47	Y5P	C3'-C4'-C5'-O5'
83	r4	49	Y5P	C3'-C4'-C5'-O5'
83	r4	52	P5P	C3'-C4'-C5'-O5'
83	r4	52	P5P	O4'-C4'-C5'-O5'
83	r4	72	Y5P	C3'-C4'-C5'-O5'
83	r4	73	P5P	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
83	r4	73	P5P	O4'-C4'-C5'-O5'
83	r4	29	P5P	C2'-C1'-N9-C4
83	r4	45	Y5P	O4'-C1'-N1-C2
83	r4	46	P5P	C2'-C1'-N9-C8
83	r4	9	P5P	C3'-C4'-C5'-O5'
83	r4	56	Y5P	C3'-C4'-C5'-O5'
83	r4	74	Y5P	O4'-C4'-C5'-O5'
83	r4	17	Y5P	O4'-C4'-C5'-O5'
83	r4	28	P5P	C3'-C4'-C5'-O5'
83	r4	32	Y5P	C3'-C4'-C5'-O5'
83	r4	49	Y5P	O4'-C4'-C5'-O5'
83	r4	29	P5P	C2'-C1'-N9-C8
83	r4	46	P5P	C2'-C1'-N9-C4
83	r4	6	P5P	C3'-C4'-C5'-O5'
83	r4	48	Y5P	O4'-C4'-C5'-O5'
83	r4	72	Y5P	O4'-C4'-C5'-O5'
83	r4	75	Y5P	C3'-C4'-C5'-O5'
83	r4	73	P5P	C4'-C5'-O5'-P
83	r4	25	Y5P	O4'-C4'-C5'-O5'
83	r4	23	P5P	C2'-C1'-N9-C4
83	r4	33	Y5P	O4'-C1'-N1-C2
83	r4	20	Y5P	C4'-C5'-O5'-P
83	r4	22	P5P	C4'-C5'-O5'-P
83	r4	23	P5P	C4'-C5'-O5'-P
83	r4	47	Y5P	O4'-C1'-N1-C2
83	r4	45	Y5P	C3'-C4'-C5'-O5'
83	r4	23	P5P	C2'-C1'-N9-C8
83	r4	38	P5P	C3'-C4'-C5'-O5'
83	r4	27	P5P	C2'-C1'-N9-C8
83	r4	23	P5P	C3'-C4'-C5'-O5'
83	r4	31	P5P	C2'-C1'-N9-C4
83	r4	74	Y5P	O4'-C1'-N1-C6
83	r4	1	P5P	C3'-C4'-C5'-O5'
83	r4	74	Y5P	C3'-C4'-C5'-O5'
83	r4	76	P5P	C2'-C1'-N9-C8
83	r4	27	P5P	C3'-C4'-C5'-O5'
83	r4	1	P5P	C4'-C5'-O5'-P
83	r4	31	P5P	C2'-C1'-N9-C8
83	r4	30	P5P	C4'-C5'-O5'-P
83	r4	45	Y5P	C4'-C5'-O5'-P
83	r4	47	Y5P	C4'-C5'-O5'-P
83	r4	27	P5P	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
83	r4	76	P5P	C2'-C1'-N9-C4
83	r4	10	P5P	C2'-C1'-N9-C8
83	r4	33	Y5P	C4'-C5'-O5'-P
83	r4	23	P5P	O4'-C4'-C5'-O5'
83	r4	18	P5P	C4'-C5'-O5'-P
83	r4	10	P5P	C2'-C1'-N9-C4
83	r4	7	P5P	O4'-C4'-C5'-O5'
83	r4	27	P5P	O4'-C4'-C5'-O5'
83	r4	76	P5P	C4'-C5'-O5'-P
83	r4	17	Y5P	C3'-C4'-C5'-O5'
83	r4	50	Y5P	C2'-C1'-N1-C6
83	r4	34	P5P	C4'-C5'-O5'-P
83	r4	74	Y5P	C4'-C5'-O5'-P
83	r4	27	P5P	O4'-C1'-N9-C8
83	r4	10	P5P	C4'-C5'-O5'-P
83	r4	31	P5P	O4'-C4'-C5'-O5'
83	r4	34	P5P	O4'-C4'-C5'-O5'

There are no ring outliers.

38 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	r4	23	P5P	1	0
83	r4	3	Y5P	3	0
83	r4	12	Y5P	1	0
83	r4	41	Y5P	1	0
83	r4	75	Y5P	1	0
83	r4	51	Y5P	1	0
83	r4	55	Y5P	1	0
83	r4	49	Y5P	4	0
83	r4	45	Y5P	3	0
83	r4	30	P5P	3	0
83	r4	10	P5P	2	0
83	r4	31	P5P	4	0
83	r4	35	P5P	1	0
83	r4	47	Y5P	1	0
83	r4	36	P5P	1	0
83	r4	28	P5P	4	0
83	r4	71	P5P	2	0
83	r4	40	Y5P	2	0
83	r4	2	Y5P	2	0
83	r4	50	Y5P	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	r4	44	P5P	1	0
86	A	7	004	2	0
83	r4	29	P5P	3	0
83	r4	24	P5P	3	0
83	r4	6	P5P	1	0
83	r4	63	P5P	1	0
83	r4	8	Y5P	2	0
83	r4	9	P5P	3	0
83	r4	1	P5P	1	0
83	r4	66	Y5P	1	0
83	r4	61	Y5P	1	0
83	r4	13	Y5P	3	0
83	r4	73	P5P	1	0
83	r4	76	P5P	3	0
86	A	1	MHW	1	0
83	r4	62	Y5P	2	0
83	r4	46	P5P	1	0
83	r4	59	Y5P	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 204 ligands modelled in this entry, 202 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
89	DOL	XA	5144	-	47,50,50	3.85	18 (38%)	57,70,70	3.05	13 (22%)
90	GTP	AX	500	-	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	DOL	XA	5144	-	-	21/64/77/77	0/2/3/3
90	GTP	AX	500	-	-	7/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	XA	5144	DOL	C28-C29	10.48	1.55	1.32
89	XA	5144	DOL	C6-N5	9.97	1.49	1.34
89	XA	5144	DOL	C22-C23	8.81	1.56	1.32
89	XA	5144	DOL	C10-N9	8.73	1.38	1.29
89	XA	5144	DOL	C19-C20	8.62	1.57	1.34
89	XA	5144	DOL	C26-N25	6.77	1.48	1.34
89	XA	5144	DOL	C13-C10	5.64	1.57	1.50
89	XA	5144	DOL	C22-C20	5.59	1.57	1.46
89	XA	5144	DOL	O36-C37	5.23	1.46	1.34
89	XA	5144	DOL	C8-C6	4.02	1.55	1.49
89	XA	5144	DOL	C16-C14	3.91	1.56	1.51
89	XA	5144	DOL	C12-C8	3.68	1.38	1.34
89	XA	5144	DOL	C28-C26	3.50	1.55	1.48
89	XA	5144	DOL	O18-C17	-2.94	1.38	1.43
89	XA	5144	DOL	O27-C26	-2.89	1.18	1.24
89	XA	5144	DOL	C3-C2	-2.65	1.50	1.54
89	XA	5144	DOL	O36-C32	-2.43	1.41	1.44
90	AX	500	GTP	C2-N3	2.23	1.38	1.33
89	XA	5144	DOL	C24-C23	2.16	1.57	1.49

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	XA	5144	DOL	O40-S39-O41	-15.69	100.33	118.13
89	XA	5144	DOL	O11-C10-C13	8.92	125.95	117.70
89	XA	5144	DOL	C24-N25-C26	-6.41	111.78	122.17
89	XA	5144	DOL	O11-C10-N9	-5.23	108.43	114.09
90	AX	500	GTP	C5-C4-N3	-5.11	120.25	128.39
90	AX	500	GTP	C2-N3-C4	4.58	120.19	112.30
89	XA	5144	DOL	O40-S39-C2	4.56	112.90	108.50
89	XA	5144	DOL	C23-C22-C20	-3.60	120.44	125.89
89	XA	5144	DOL	C32-O36-C37	-3.48	111.98	117.76
89	XA	5144	DOL	C4-N5-C1	-3.40	108.52	112.51
90	AX	500	GTP	N9-C4-N3	3.32	132.59	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	AX	500	GTP	C2-N1-C6	-3.07	119.53	125.11
89	XA	5144	DOL	C30-C29-C28	-2.66	119.26	126.30
90	AX	500	GTP	N9-C8-N7	-2.65	108.48	113.40
90	AX	500	GTP	C8-N7-C5	2.56	108.82	104.26
90	AX	500	GTP	C5-C6-N1	2.54	119.72	113.25
89	XA	5144	DOL	C21-C20-C22	2.54	121.97	118.09
89	XA	5144	DOL	C17-C16-C14	-2.50	108.64	113.90
89	XA	5144	DOL	C3-C4-N5	2.43	105.89	103.22
90	AX	500	GTP	O6-C6-C5	-2.40	120.19	126.53
89	XA	5144	DOL	O41-S39-C2	2.29	110.71	108.50

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	XA	5144	DOL	C3-C2-S39-O41
89	XA	5144	DOL	C3-C2-S39-C42
89	XA	5144	DOL	C1-C2-S39-O41
89	XA	5144	DOL	C1-C2-S39-O40
89	XA	5144	DOL	C1-C2-S39-C42
89	XA	5144	DOL	C43-C42-S39-C2
89	XA	5144	DOL	C43-C42-S39-O41
89	XA	5144	DOL	C31-C30-C32-C33
90	AX	500	GTP	PB-O3B-PG-O3G
90	AX	500	GTP	C5'-O5'-PA-O3A
90	AX	500	GTP	C5'-O5'-PA-O2A
89	XA	5144	DOL	C21-C20-C22-C23
89	XA	5144	DOL	C28-C29-C30-C31
89	XA	5144	DOL	C19-C20-C22-C23
90	AX	500	GTP	O4'-C4'-C5'-O5'
89	XA	5144	DOL	O11-C10-C13-C14
90	AX	500	GTP	C3'-C4'-C5'-O5'
89	XA	5144	DOL	C31-C30-C32-O36
89	XA	5144	DOL	C16-C17-C19-C20
89	XA	5144	DOL	O18-C17-C19-C20
89	XA	5144	DOL	S39-C42-C43-N44
89	XA	5144	DOL	N9-C10-C13-C14
89	XA	5144	DOL	C28-C29-C30-C32
90	AX	500	GTP	PB-O3B-PG-O1G
90	AX	500	GTP	PB-O3B-PG-O2G
89	XA	5144	DOL	C22-C23-C24-N25
89	XA	5144	DOL	C43-C42-S39-O40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
89	XA	5144	DOL	C29-C30-C32-O36

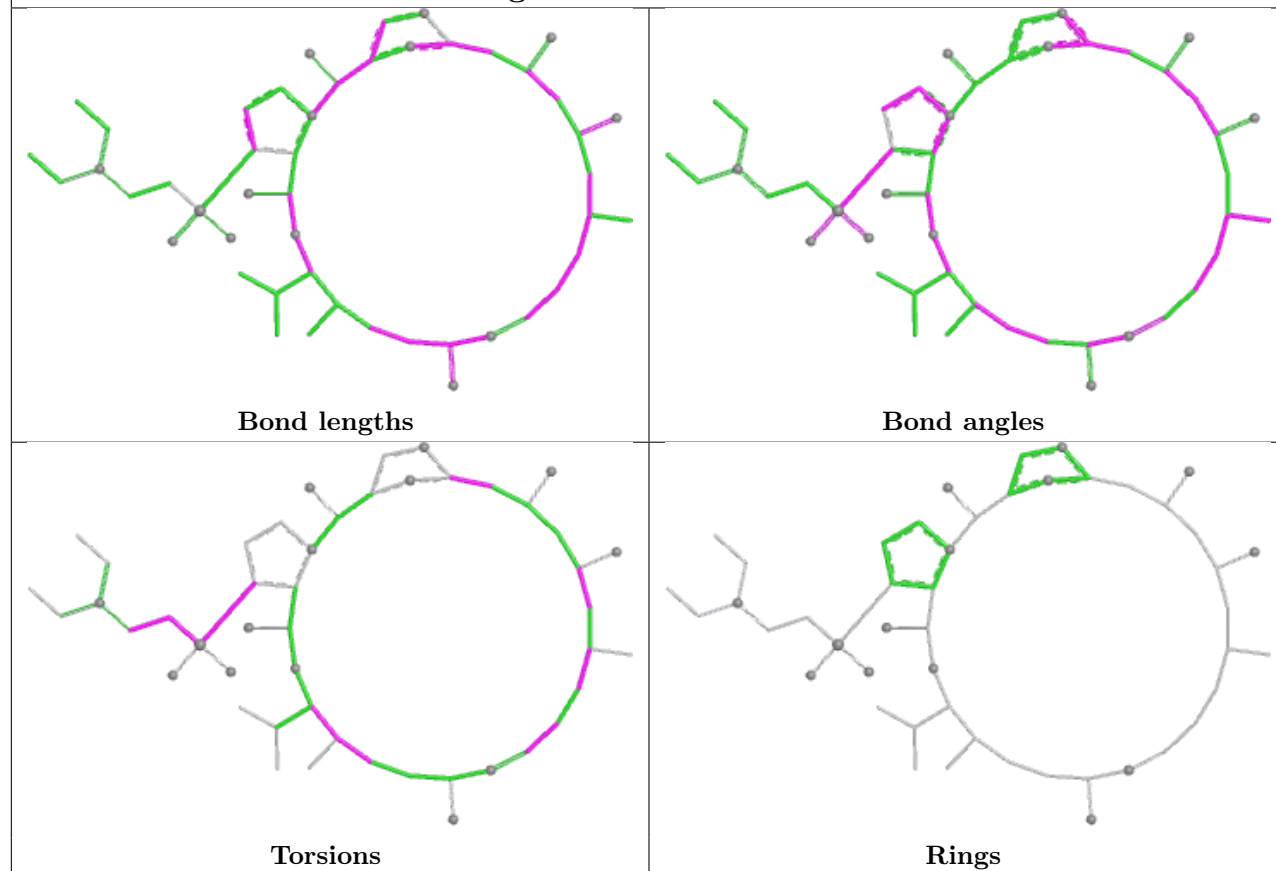
There are no ring outliers.

2 monomers are involved in 3 short contacts:

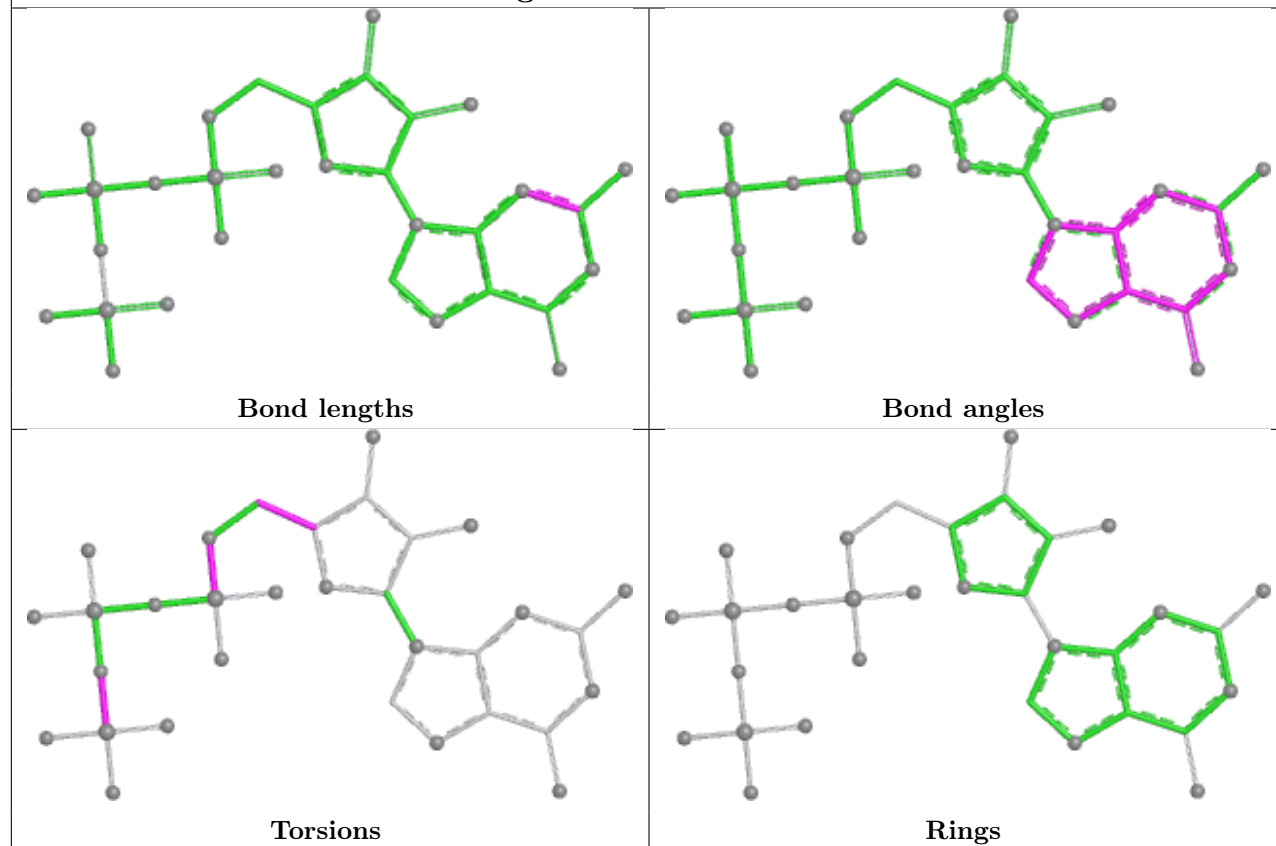
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	XA	5144	DOL	2	0
90	AX	500	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 DOL XA 5144



Ligand GTP AX 500



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
16	A4	2
8	7	2
7	6	2
82	r	1
38	AV	1
34	AR	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A4	537:ARG	C	538:ASP	N	6.17
1	7	285:ASN	C	286:LEU	N	5.95
1	r	134:ARG	C	135:LEU	N	5.40
1	AV	269:SER	C	270:PRO	N	4.56
1	6	282:SER	C	283:GLU	N	3.29
1	6	79:GLY	C	80:GLU	N	3.07
1	7	185:LEU	C	186:ASP	N	3.07
1	A4	143:GLU	C	144:TYR	N	3.07
1	AR	308:HIS	C	309:PRO	N	1.00

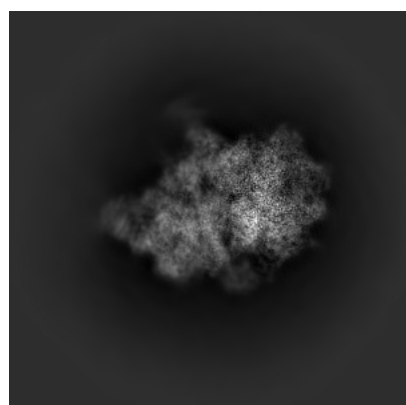
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11393. These allow visual inspection of the internal detail of the map and identification of artifacts.

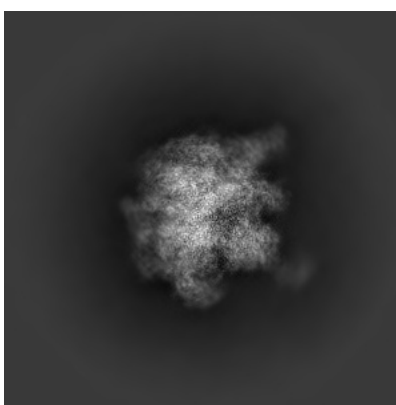
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

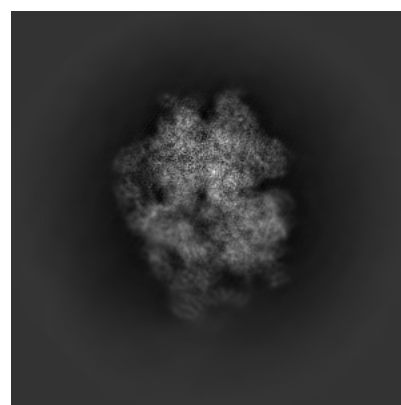
6.1.1 Primary map



X



Y

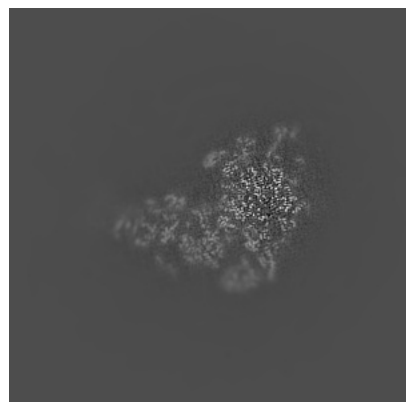


Z

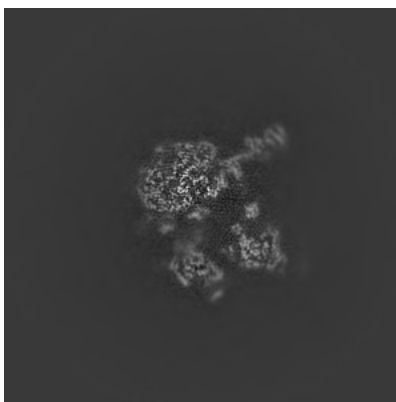
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

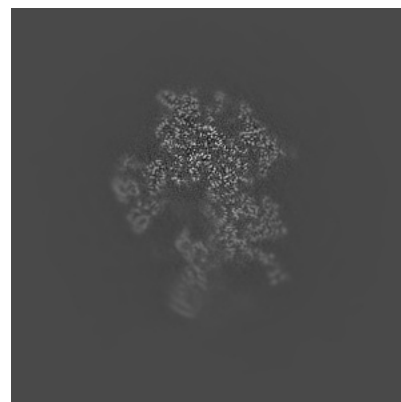
6.2.1 Primary map



X Index: 260



Y Index: 260

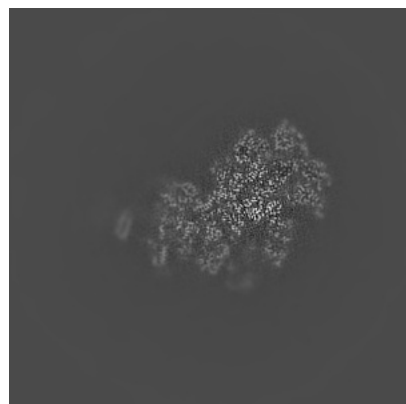


Z Index: 260

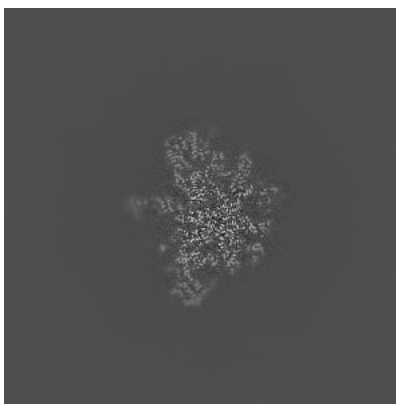
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

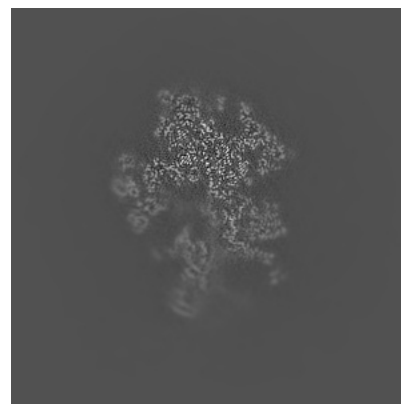
6.3.1 Primary map



X Index: 277



Y Index: 321

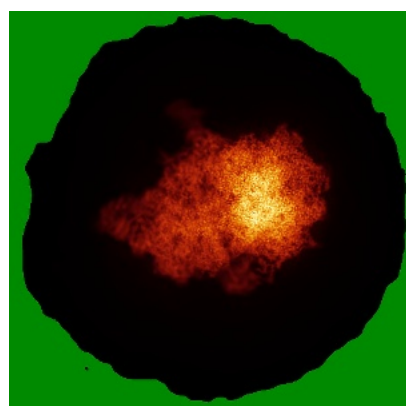


Z Index: 257

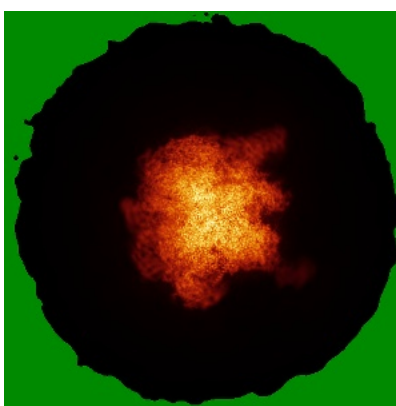
The images above show the largest variance slices of the map in three orthogonal directions.

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

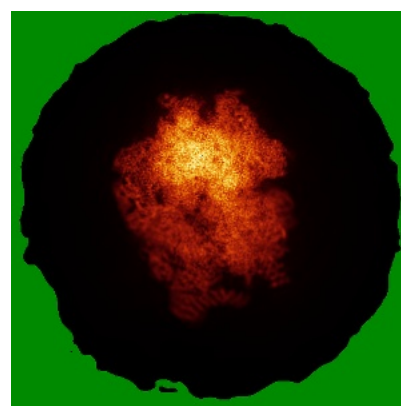
6.4.1 Primary map



X



Y

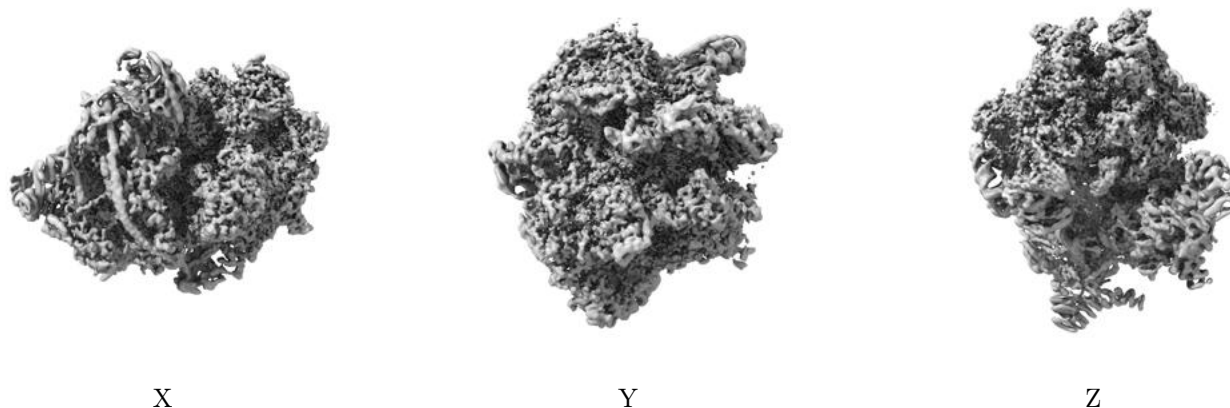


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

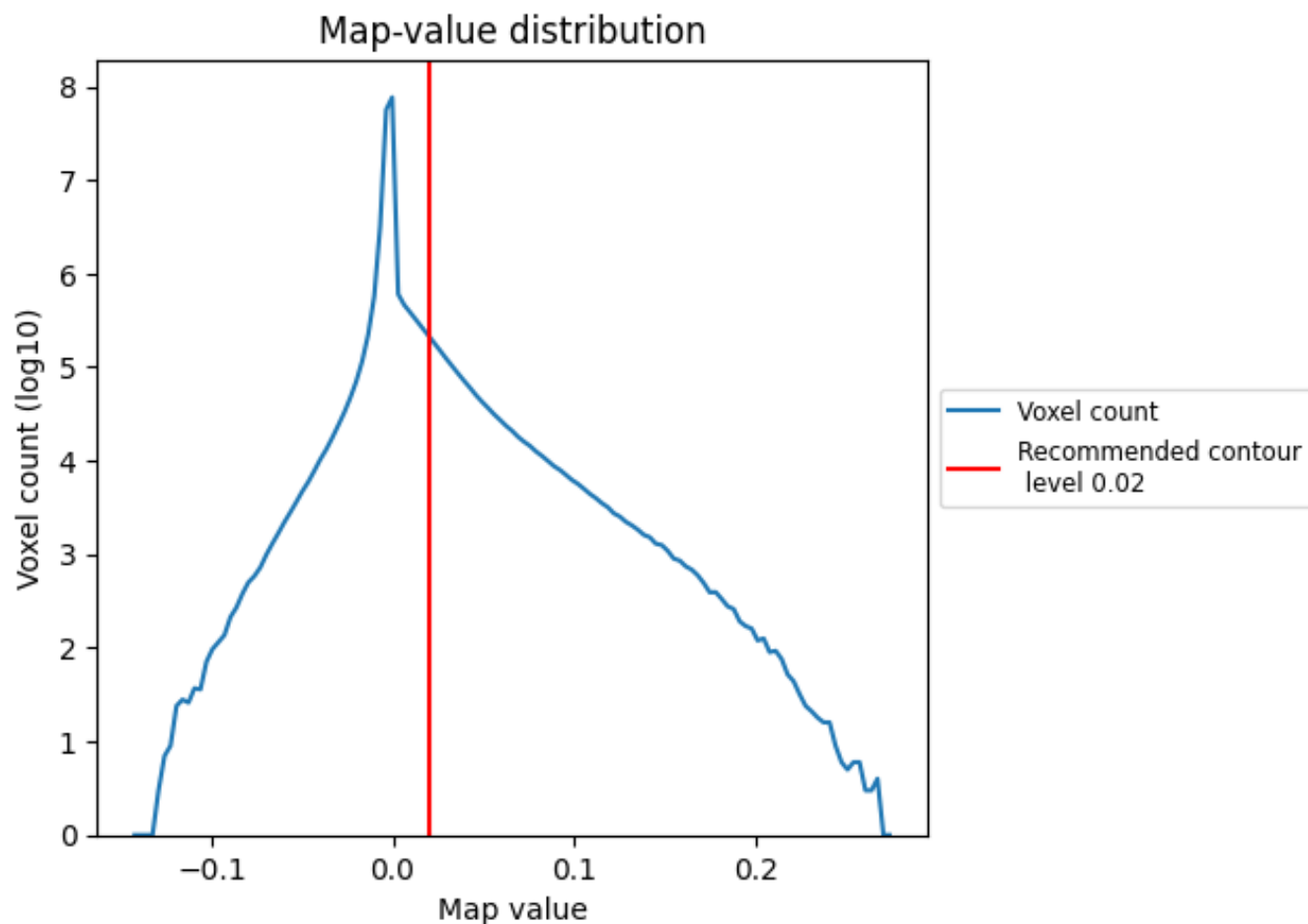
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

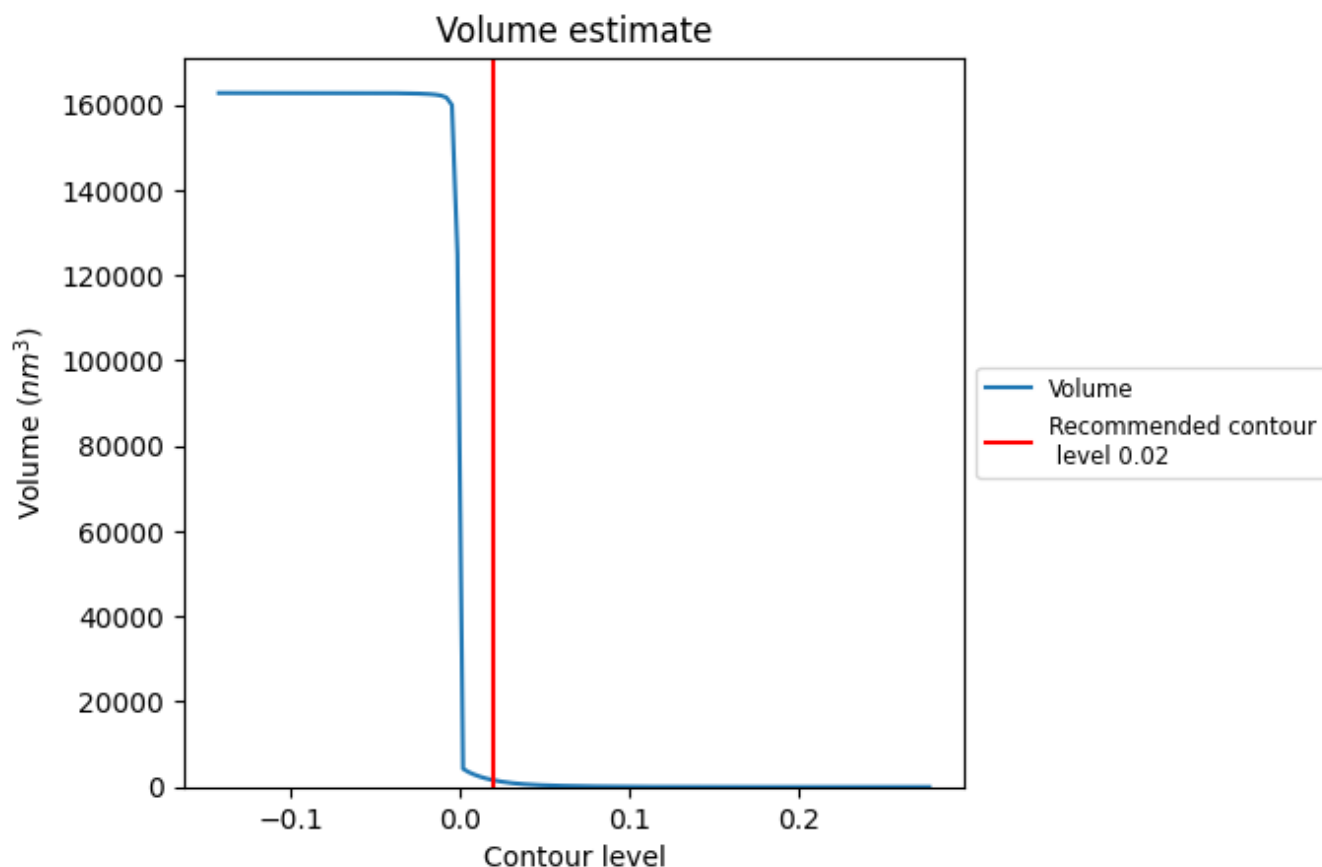
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

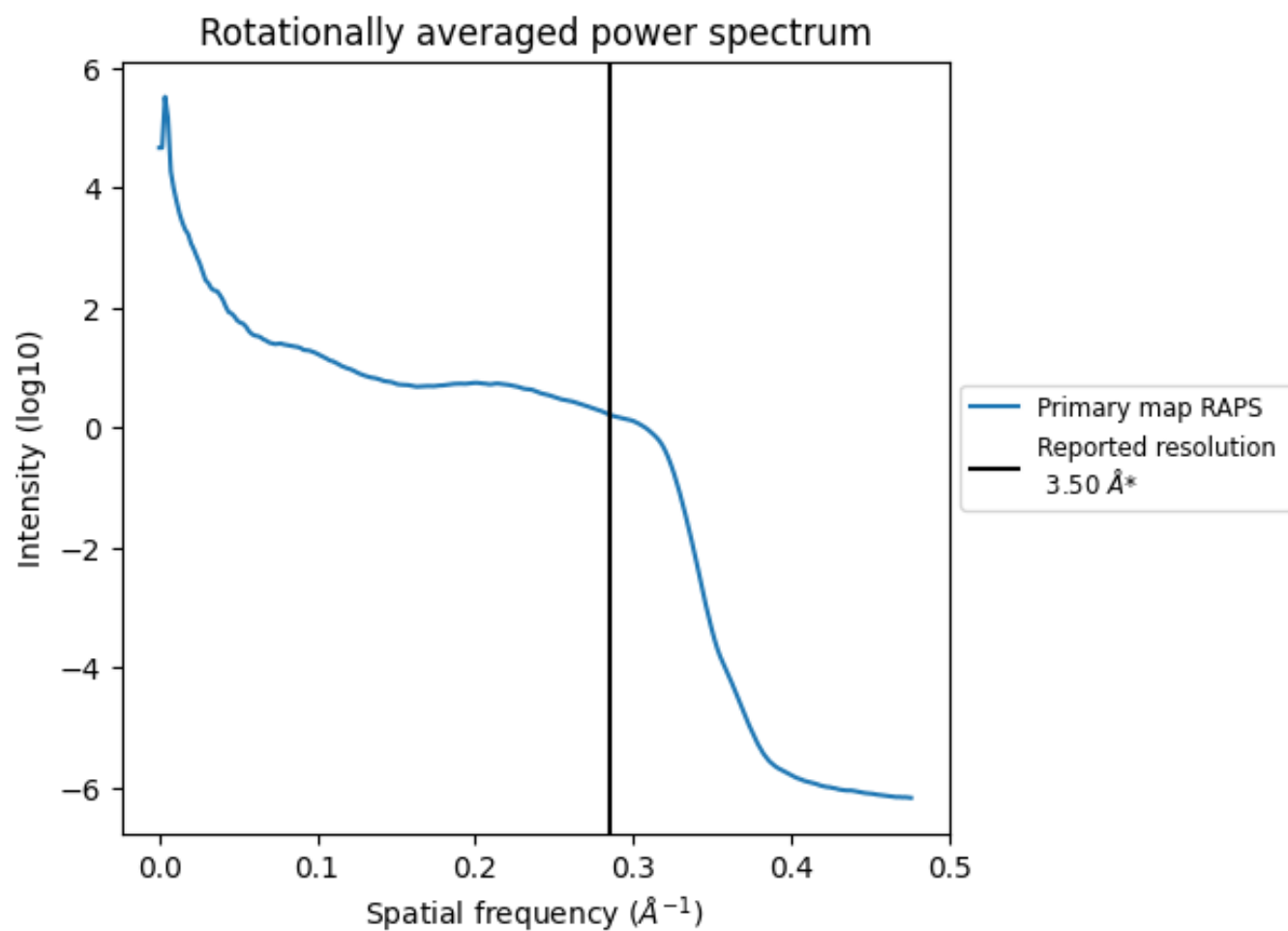
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1583 nm³; this corresponds to an approximate mass of 1430 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 0.286 Å⁻¹

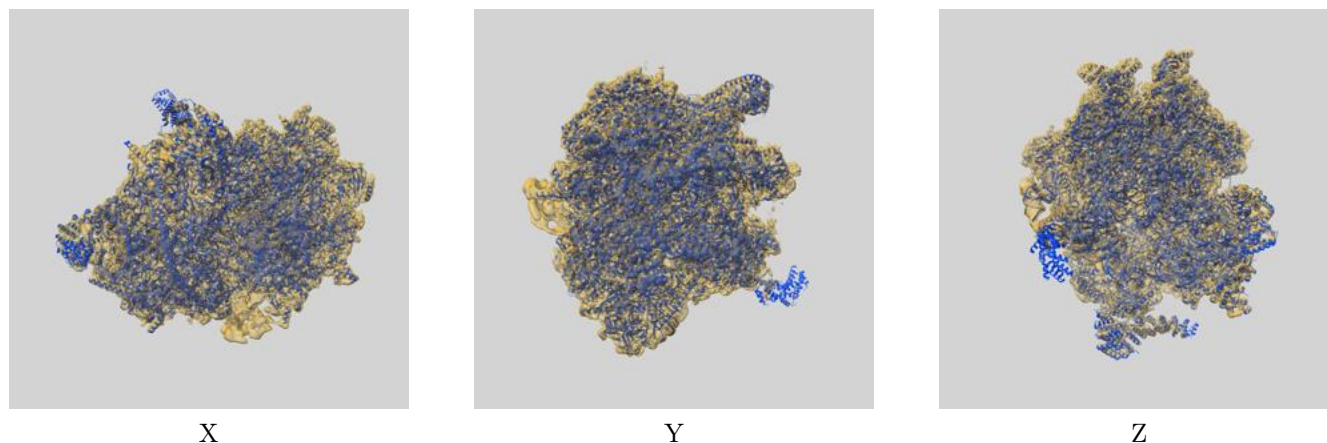
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

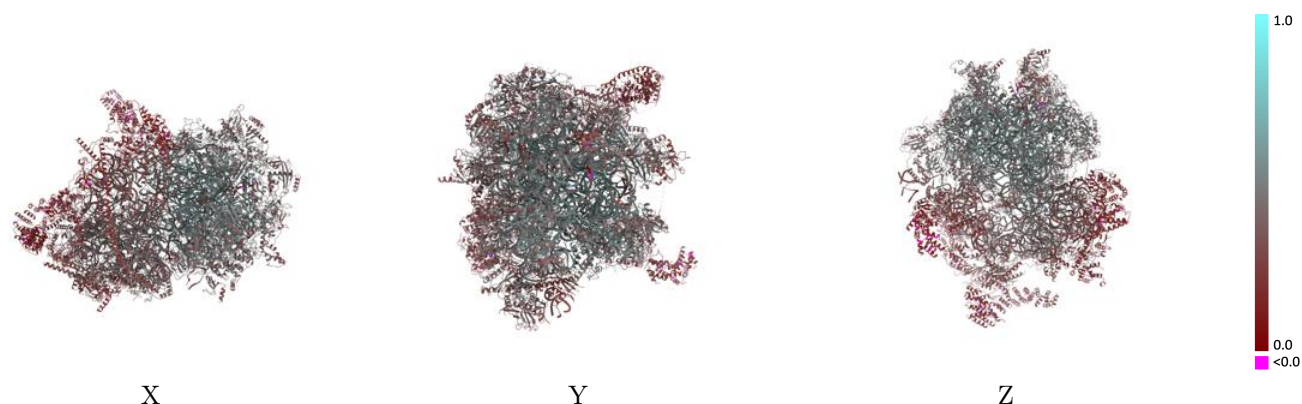
This section contains information regarding the fit between EMDB map EMD-11393 and PDB model 6ZSC. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



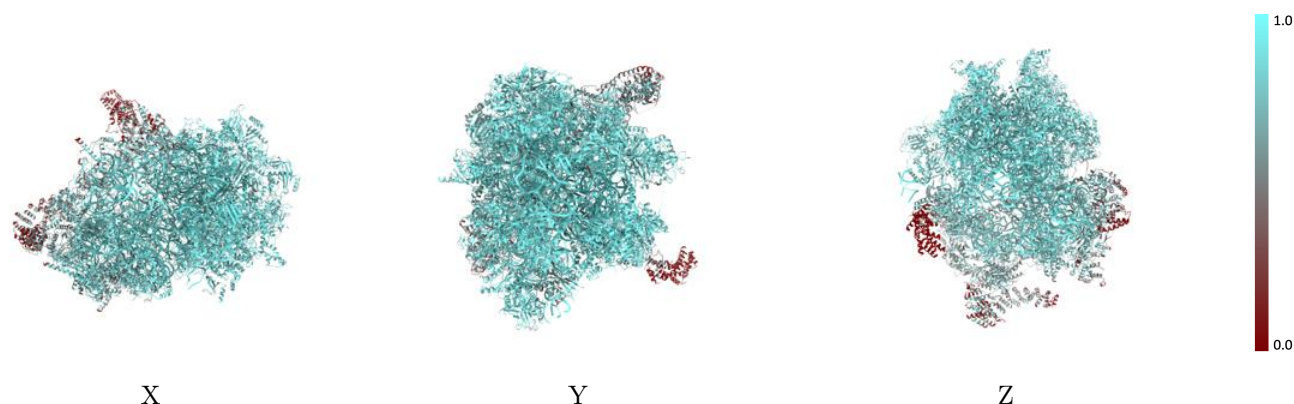
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



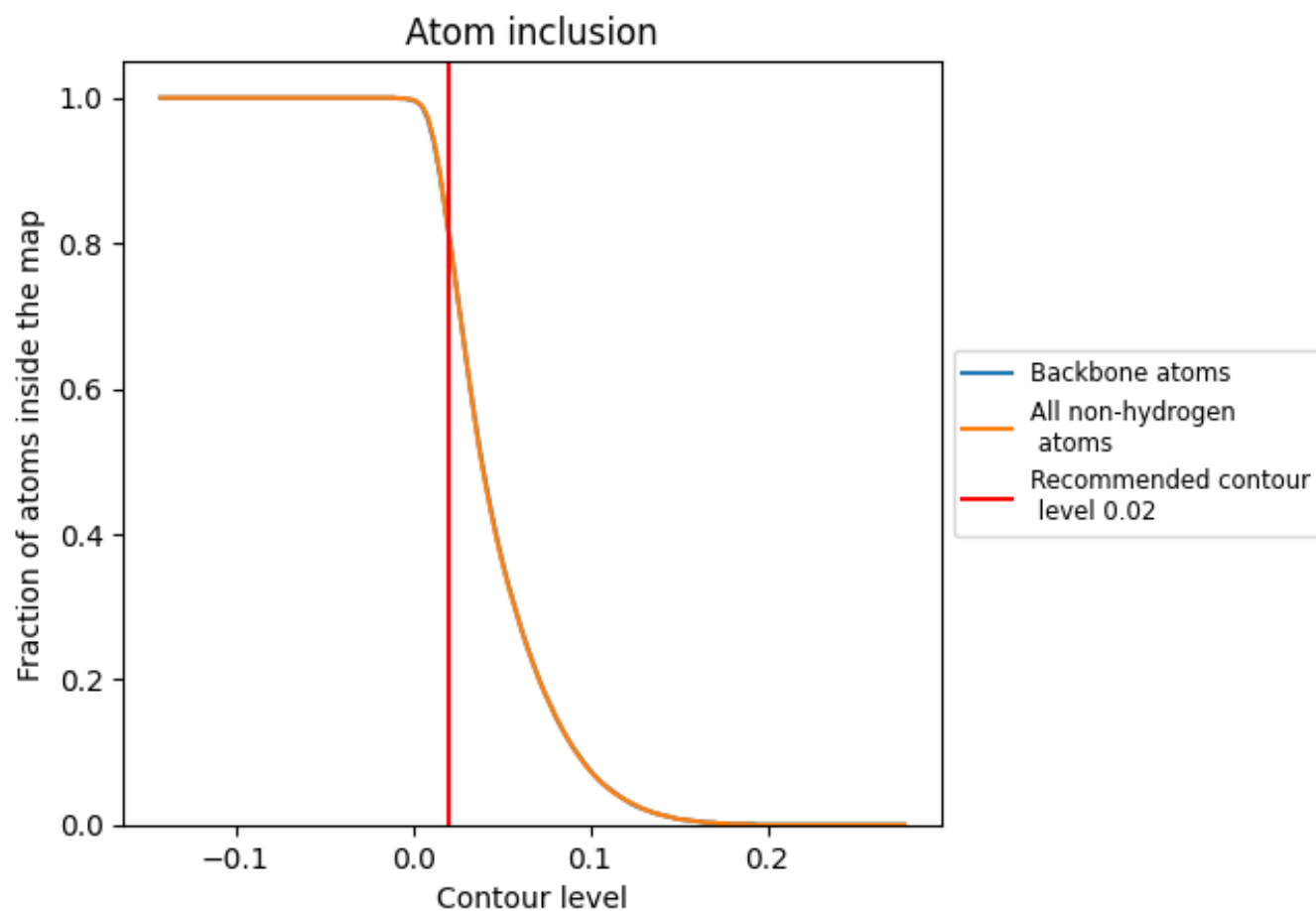
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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	 0.8190	 0.3980
0	 0.8690	 0.4500
1	 0.8850	 0.4590
2	 0.9530	 0.5370
3	 0.9220	 0.5320
4	 0.9200	 0.5050
5	 0.8700	 0.4380
6	 0.8390	 0.3900
7	 0.8320	 0.3940
8	 0.7120	 0.2730
9	 0.8600	 0.4400
A	 0.8900	 0.5010
A0	 0.5900	 0.2240
A1	 0.5860	 0.2260
A2	 0.7500	 0.3430
A3	 0.8560	 0.4470
A4	 0.4150	 0.1720
AA	 0.9430	 0.3940
AB	 0.7950	 0.3560
AC	 0.6980	 0.3270
AD	 0.7080	 0.3490
AE	 0.7870	 0.4010
AF	 0.7190	 0.3150
AG	 0.6920	 0.2920
AH	 0.6270	 0.2840
AI	 0.8120	 0.4020
AJ	 0.7620	 0.3700
AK	 0.7170	 0.2820
AL	 0.7920	 0.3750
AM	 0.6790	 0.2700
AN	 0.7760	 0.3790
AO	 0.6820	 0.2840
AP	 0.8300	 0.4040
AQ	 0.8140	 0.3980
AR	 0.5980	 0.2240



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AS	 0.6920	 0.3120
AT	 0.7580	 0.3350
AU	 0.7090	 0.2660
AV	 0.4730	 0.1820
AW	 0.7340	 0.3520
AX	 0.5680	 0.2000
AY	 0.5390	 0.2090
AZ	 0.6730	 0.2380
XA	 0.9700	 0.5190
XB	 0.9670	 0.3440
XD	 0.9030	 0.4920
XE	 0.8940	 0.4800
XF	 0.9030	 0.4990
XH	 0.8310	 0.4060
XI	 0.6240	 0.2950
XJ	 0.6880	 0.2340
XK	 0.9070	 0.4960
XL	 0.8870	 0.4710
XM	 0.8920	 0.4730
XN	 0.8720	 0.4700
XO	 0.8840	 0.4710
XP	 0.8670	 0.4250
XQ	 0.8110	 0.4320
XR	 0.8970	 0.4980
XS	 0.8950	 0.4880
XT	 0.8970	 0.5010
XU	 0.8890	 0.4670
XV	 0.8430	 0.4120
XW	 0.9150	 0.5120
XX	 0.8610	 0.4370
XY	 0.8780	 0.4640
XZ	 0.9130	 0.5090
a	 0.8500	 0.4450
b	 0.8960	 0.4920
c	 0.8700	 0.4350
d	 0.7960	 0.3780
e	 0.6830	 0.2170
f	 0.7600	 0.3320
g	 0.9000	 0.4710
h	 0.8410	 0.3980
i	 0.8960	 0.5130
j	 0.8650	 0.4540

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.7790	 0.3260
l	 0.7630	 0.2850
m	 0.7420	 0.2640
o	 0.9080	 0.4960
p	 0.8430	 0.3940
q	 0.7300	 0.3140
r	 0.8940	 0.4610
r4	 0.7480	 0.2000
s	 0.8820	 0.4600
t1	 0.2210	 0.2020
t2	 0.2230	 0.1900
t3	 0.0000	 0.1670
t4	 0.0000	 0.1500
t5	 0.0000	 0.1290
t6	 0.0000	 0.1090